Variational Bayes for high-dimensional linear regression with sparse priors

Kolyan Ray* and Botond Szabó†

King’s College London and Leiden University

Abstract

We study a mean-field variational Bayes (VB) approximation to Bayesian model selection priors, which include the popular spike-and-slab prior, in the sparse high-dimensional linear regression model. Under suitable conditions on the design matrix, the mean-field VB approximation is shown to converge to the sparse truth at the optimal rate for \( \ell_2 \)-recovery and to give optimal prediction of the response vector. The empirical performance of our algorithm is studied, showing that it works comparably well as other state-of-the-art Bayesian variable selection methods. We also numerically demonstrate that the widely used coordinate-ascent variational inference (CAVI) algorithm can be highly sensitive to the updating order of the parameters leading to potentially poor performance. To counteract this we propose a novel prioritized updating scheme that uses a data-driven updating order and performs better in simulations.

AMS 2000 subject classifications: Primary 62G20; secondary 62G05, 65K10.

Keywords and phrases: Bayesian inference, variational inference, sparsity, adaptation.

1 Introduction

Inference under sparsity constraints has found many applications in statistics and machine learning \[28, 32\]. Perhaps the most widely applied such model is sparse linear regression, where we observe

\[
Y = X\theta + Z,
\]

where \( Y \in \mathbb{R}^n \), \( X \) is a given, deterministic \( n \times p \) design matrix, \( \theta \in \mathbb{R}^p \) is the parameter of interest and \( Z \sim N_n(0, I_n) \) is additive Gaussian noise. We are interested in the sparse high-dimensional setting, where \( n \leq p \) and typically \( n \ll p \) and many of the coefficients \( \theta_i \) are (close to) zero.

From a Bayesian perspective, perhaps the most natural way to impose sparsity is through a model selection prior, which assigns probabilistic weights to each potential model, i.e. each subset of \( \{1, \ldots, p\} \) corresponding to selecting the non-zero coordinates of \( \theta \in \mathbb{R}^p \). This is one of the most widely used approaches within the Bayesian community \[17, 18, 28, 37\] and includes the popular spike-and-slab prior, which is often considered the gold standard in sparse...
Bayesian linear regression. Its high popularity in practical applications motivated researchers to investigate its theoretical behaviour, who showed that the corresponding posterior can optimally recover the underlying true signal of interest \cite{13, 15, 24}, under some additional (intuitive) assumptions give reliable uncertainty quantification \cite{14} and provide a reliable multiple hypothesis testing procedure \cite{12}.

However, while such priors perform excellently both empirically and theoretically, the discrete model selection component of the prior can make computation hugely challenging. For $\theta \in \mathbb{R}^p$, inference using the spike-and-slab prior on the $p$ input variables involves a combinatorial search over all $2^p$ models, a hugely expensive task for even moderate $p$. Fast algorithms for exact posterior computation are typically restricted to the diagonal design case ($X = I$), see \cite{15, 35}, and do not seem to generalize to other design matrices. Such computational problems led researchers to consider instead shrinkage type priors, such as the horseshoe prior and other scale mixtures of Gaussian kernels \cite{2, 10, 11, 32}. While (perhaps) computationally more feasible, such priors lose the desirable property of assigning exactly zero weights to posterior coefficients. Having potentially zero weights provides access to posterior probabilities of particular submodels and inclusion probabilities of particular features, amongst other things. Such a property is therefore highly valuable from both a modelling and interpretability perspective.

A popular alternative computational technique is the use of variational Bayes (VB) to approximate a difficult to compute posterior distribution. This recasts posterior approximation as an optimization problem, in which one minimizes the VB objective function, consisting of the Kullback-Leibler divergence between a family of tractable distributions called the variational family and the posterior. Though the resulting approximation does not provide exact Bayesian inference, picking a computationally convenient variational class can dramatically increase scalability, see for example \cite{4, 20}. A particularly popular variational family consists of distributions under which the model parameters are independent, so called \textit{mean-field variational Bayes}. For a nice recent review of VB, see \cite{3}.

In this work, we consider a mean field family consisting of distributions independently assigning each coordinate of $\theta$ an independent mixture of a Gaussian and Dirac mass at zero, thereby mirroring the form of the spike-and-slab prior (but crucially not the form of the posterior). Such a computational relaxation is significant, reducing the full $2^p$ model dimension to a much more tractable dimension $p$. This procedure is moreover \textit{adaptive} in that it does not depend on the typically unknown sparsity level. This is important from an implementation perspective, since this avoids delicate issues about hard to select tuning parameters. We study this procedure under the ‘frequentist’ assumption that the data $Y$ has in reality been generated according to a given sparse parameter $\theta_0$. We show that under standard conditions on the design matrix, such a mean-field VB approximation of model selection priors performs optimally regarding both model selection and estimation of a sparse $\theta$ in $\ell_2$ and prediction loss. This provides a theoretical justification for this attractive approximation algorithm in a sparsity context.

While similar VB approaches have been applied in the methodological literature \cite{25, 33, 8, 22, 29}, our contribution also possesses a crucial methodological difference. These existing works typically use Gaussian slabs for the prior, which allows analytic evaluation of certain formulas in the variational algorithm leading to fast optimization. However, Gaussian slabs are inappropriate for recovering the true signal $\theta_0$ since the true underlying posterior performs excessive shrinkage causing poor performance \cite{15}. One cannot typically expect a VB approximation based on a poorly performing underlying posterior to perform well for
recovery. We instead consider Laplace slabs for the prior, which result in optimal recovery when using the true posterior [15, 13]. We are thus using a similar variational family to estimate a different posterior distribution compared to previous works.

We also provide the methodological details for applying the widely-used coordinate-ascent variational inference (CAVI) algorithm [3] with Laplace slabs and investigate our method numerically on both simulated and real world ozone interaction data. As predicted by the theory, our method performs well in a number of settings and typically outperforms VB approaches with prior Gaussian slabs. In fact, we find that our approach generally performs at least as well as other state-of-the-art Bayesian variable selection methods. Our simulations also show that the CAVI algorithm can be highly sensitive to the updating order of the parameters. Since the VB objective function is non-convex and typically has multiple local minima, a poorly chosen updating order can trap the algorithm near a highly-suboptimal local minimum causing poor performance.

To counteract this we propose a novel prioritized update scheme where we base the CAVI parameter update order on the estimated size of the coefficients via a preliminary estimator. Our simulations indicate that such a data-driven updating order performs better than using either a naive or random update order and provides more robustness against being trapped at a suboptimal local minimum. This idea is applicable beyond the present setting and may be useful for other CAVI approaches.

Let us briefly describe how our theoretical contribution relates to existing work. Whilst VB has found increasing usage in practice, its theoretical understanding is still in the early stages. In low dimensional settings, some Bernstein-von Mises type results have been derived [27, 36], while in high-dimensional and nonparametric settings, first results have only recently appeared [39, 40, 30]. There has also been theoretical work on studying variational approximations to fractional posteriors, which down-weight the likelihood [1, 38], with the latter paper also containing some extensions to the full VB case. The papers [40, 30, 38] provide general proof methods which employ the classical prior mass and testing approach of Bayesian nonparametrics [19]. However, since it is known that posterior convergence rates for model selection priors cannot easily be established using this approach [15, 13], their results do not apply to our setting.

The paper is organized as follows. In Section 2 we give details of the prior and the required conditions on the design matrix. We present our main results in Section 3, details of the algorithm implementation in Section 4, the numerical study in Section 5 and conclusions in Section 6. In Section 7 we present some more general, but less accessible, theoretical results. Proofs are deferred to Sections 8 with some additional methodological details in Section 9.

**Notation:** Let $P_\theta$ be the probability distribution of the observation $Y$ arising in model (1) and let $E_\theta$ denote the corresponding expectation. For two probability distributions $P, Q$, $\text{KL}(P\|Q) = \int \log \frac{dP}{dQ} dP$ denotes the Kullback-Leibler divergence. For $x \in \mathbb{R}^d$, we write $\|x\|_2 = (\sum_{i=1}^d |x_i|^2)^{1/2}$ for the Euclidean norm.

For a vector $\theta \in \mathbb{R}^p$ and a subset $S \subseteq \{1, \ldots, p\}$ of indices, set $\theta_S$ to be the vector $(\theta_i)_{i \in S}$ in $\mathbb{R}^{|S|}$, where $|S|$ denotes the cardinality of $S$. Further let $S_\theta = \{i : \theta_i \neq 0\}$ be the set of non-zero coefficients of $\theta$. We will often write $s_0 = |S_{\theta_0}|$ where $\theta_0$ is the true vector.

For $X_i$ the $i^{th}$ column of $X$, set

$$\|X\| := \max_{1 \leq i \leq p} \|X_i\|_2 = \max_{1 \leq i \leq p} (X^T X)_{ii}^{1/2}. \tag{2}$$
2 Model selection priors and design matrices

2.1 Model selection priors

We first present the desirable but computationally challenging model selection priors that underlie our VB approximation. Consider a prior for $\theta \in \mathbb{R}^p$ that first selects a dimension $s$ from a prior $\pi_p$ on $\{0, \ldots, p\}$, then uniformly selects a random subset $S \subset \{1, \ldots, p\}$ of cardinality $|S| = s$ and lastly a set of non-zero values $\theta_S = \{\theta_i : i \in S\}$ from a prior density $g_S$ on $\mathbb{R}^S$. Since it is known that the ‘slab’ distribution should have exponential tails or heavier to achieve good recovery [15, 13], we restrict to the case where $g_S = \prod_{i \in S} \text{Lap}(\lambda)$ is a product of centered Laplace densities with parameter $\lambda > 0$ on $\mathbb{R}^s$. This yields the hierarchical prior:

\[
s \sim \pi_p(s) \\
S|s = s \sim \text{Unif}_{p,s} \\
\theta_i \overset{\text{iid}}{\sim} \begin{cases} \text{Lap}(\lambda), & i \in S, \\
\delta_0, & i \notin S,
\end{cases}
\]  

where $\text{Unif}_{p,s}$ selects $S$ from the $\binom{p}{s}$ possible subsets of $\{0, \ldots, p\}$ of size $s$ with equal probability and $\delta_0$ denotes the Dirac mass at zero. The prior (3) can alternatively be expressed as

\[
(S, \theta) \mapsto \pi_p(|S|) \frac{1}{\binom{p}{s}} \delta_0(\theta_{S^c}) \prod_{i \in S} \frac{\lambda}{2} e^{-\lambda|\theta_i|},
\]

where $\delta_0(\theta_{S^c})$ refers to $\theta_{S^c} = (\theta_i : i \in S^c)$ being zero. Since we wish the prior to perform model selection via the prior $\pi_p$ on the dimension $s$ rather than via shrinkage of the Laplace distribution, the choice of prior $\pi_p$ is crucial. The aim is to select a distribution which sufficiently downweights large models while simultaneously placing enough mass to the true model. Following [13], we select an exponentially decreasing prior: we assume that there are constants $A_1, A_2, A_3, A_4 > 0$ with

\[
A_1 p^{-A_3} \pi_p(s - 1) \leq \pi_p(s) \leq A_2 p^{-A_4} \pi_p(s - 1), \quad s = 1, \ldots, p.
\]

Assumption (4) is satisfied by a variety of priors, including those of the form $\pi_p(s) \propto a^{-s} p^{-bs}$ for constants $a, b > 0$ (‘complexity priors’ [15]) and binomial priors. The spike-and-slab prior with Laplace slabs, where we model $\theta_i \sim \text{iid} \text{Lap}(\lambda) + (1 - r)\delta_0$, also falls within this framework by taking $\pi_p$ to be $\text{Bin}(p, r)$. The value $r$ is the prior inclusion probability of the coordinate $i$ and controls the model selection. Taking a hyperprior $r \sim \text{Beta}(1, p^u)$ for $u > 1$ also satisfies (4) ([15], Example 2.2), allows mixing over the sparsity level $r$ and gives a prior that does not depend on unknown hyper-parameters.

It remains only to specify the regularization parameter $\lambda$ in the slab distribution in (3). This parameter is allowed to vary with $p$ within the range

\[
\frac{\|X\|}{p} \leq \lambda = o(\|X\|/\sqrt{\log p}),
\]

where the norm $\|X\|$ is the maximal column norm defined in (2). Large values of $\lambda$ may shrink many coordinates $\theta_i$ in the slab towards zero, which is undesirable in our Bayesian setup since we wish to induce sparsity via $\pi_p$ instead. Indeed, since the slab component identifies the non-zero coordinates it is unnatural to further shrink these values. It is natural to take fixed
values of $\lambda$ or $\lambda \to 0$, both of which are typically allowed by (5) depending on the specific design matrix and regression setting. Specific values of $\|X\|$ for some examples of design matrices are given in Section 2.2 below.

The theoretical frequentist behaviour of the full (computationally difficult) posterior arising from prior (3) has been studied in [15, 13], who show it converges to the truth at the optimal rate in many situations. We build on their work to show that these results also extend to the much more scalable variational approximation.

If the model has unknown variance $\sigma^2$, we instead observe $Y = X\theta + \sigma Z$. Since then $\frac{Y}{\sigma} = \left(\frac{X}{\sigma}\right)\theta + \frac{Z}{\sigma}$, one may first rescale the data using an estimate $\hat{\sigma}$ of $\sigma$ and as before endow $\theta$ with the prior (3), thereby obtaining an empirical Bayes approach. If $\hat{\sigma}$ is consistent for $\sigma$, we asymptotically recover the case $\sigma = 1$ given by model (1) with design matrix $(X/\sigma)$. We therefore restrict the theory to this case, rescaling the design matrix as just described if needed. We investigate this empirical Bayes approach numerically in Section 5.4, showing that our method continues to perform well in the more realistic scenario where the noise level is unknown. One can alternatively use a hierarchical Bayesian approach by endowing $\sigma$ with a hyper-prior, common choices including the inverse Gamma distribution, $c/\sigma^2$ or the improper prior $1/\sigma$.

### 2.2 Design matrix and sparsity assumptions

It is well-known that the parameter $\theta$ in the model (1) is not estimable without further conditions on the regression matrix $X$. For the high-dimensional case $p > n$, which is of most interest to us, $\theta$ is not even identifiable without additional assumptions. We thus assume that there is some “true” sparse $\theta_0$ generating the observation (1) with at most $s_n$ non-zero coefficients:

$$\theta_0 \in \ell_0[s_n] := \{ \theta : \#(j : \theta_j \neq 0) \leq s_n \}, \text{ for some } s_n = o(n).$$

In the sparse setting, it suffices for estimation to have ‘local invertibility’ of the Gram matrix $X^TX$. This can be quantified via the ‘mutual coherence’ of the design matrix, which is the maximal correlation between its columns and determines the rate at which the sparsity level $s_n$ can grow.

**Definition 1** (Mutual coherence). The *mutual coherence number* is

$$mc(X) = \max_{1 \leq i \neq j \leq p} \frac{|\langle X_i, X_j \rangle|}{\|X_i\|_2 \|X_j\|_2}.$$  \hspace{1cm} (6)

A small mutual coherence number implies the absence of too much correlation between the different predictors in the design matrix. We shall assume that the maximal sparsity level satisfies $s_n = o(1/mc(X))$, in which case we show below that the mean-field spike-and-slab VB algorithm recovers the truth at the optimal rate. Conditions of this type, which were introduced by [16], have been used by many authors to establish recovery in strong norms, for example supremum norm rates for the LASSO and Dantzig estimator [26] and the true model selection posterior [13]. Since our proof involves bounding the distance between the true posterior and the variational approximation in Kullback-Leibler sense, which is a particularly strong norm, such a condition is natural.

As a final condition, we require that the Euclidean norms of the columns are comparable, that is $\min_{1 \leq i \neq j \leq p} \|X_i\|_2/\|X_j\|_2 = \min_{1 \leq i \leq p} \|X_i\|_2/\|X\|$ is bounded away from zero. This
can easily be achieved by renormalizing the columns of $X$. Summarizing these conditions, we assume
\[ |S_{\theta_0}| \leq s_n, \quad s_n = o(1/\text{mc}(X)), \quad \min_{1 \leq i \neq j \leq p} \frac{\|X_i\|_2}{\|X_j\|_2} \geq \eta > 0, \quad (7) \]
where $|S_{\theta_0}|$ denotes the number of non-zero coordinates of $\theta_0$ and $\eta > 0$. One can slightly weaken these conditions at the expense of considerable technicality and several additional, albeit weaker, conditions on the design matrix. For clarity of exposition we have deferred such a full statement to Section 7, preferring to give slightly less general, but more interpretable, formulations of our results under assumption (7) in Section 3.

These conditions are illustrated via the following well-studied examples.

1. (Sequence model). We observe a vector $Y = (Y_1, \ldots, Y_n)$ of independent random variables with $Y_i \sim N(\theta_i, 1)$. This corresponds to model (1) with $n = p$ and $X = I_p$ the identity matrix, so that $\|X\| = \|X_i\|_2 = 1$ for all $i$ and $\text{mc}(X) = 0$. In this situation, condition (7) is satisfied for all sparsity levels $s_n \leq p$.

2. (Sequence model, multiple observations). We observe $n$ independent $N(\theta_i, \sigma_n^2)$ random variables with $\sigma_n \to 0$. Defining $Y_i$ as $\sigma_n^{-1}$ times the original observations, this falls within the framework of model (1) with $X = \sigma_n^{-1}I_p$, so that $\|X\| = \|X_i\|_2 = \sigma_n^{-1}$ for all $i$ and again $\text{mc}(X) = 0$. Thus condition (7) is satisfied for all sparsity levels $s_n \leq p$.

3. (Regression with orthogonal design). If $X$ is an orthogonal design matrix such that $\langle X_i, X_j \rangle = 0$ for $i \neq j$, the regression problem can be transformed into a sequence space model.

4. (Response model). Suppose the entries of the original regression matrix are i.i.d. random variables $W_{ij}$. We may then normalize the entries of the design matrix by defining $X_{ij} = W_{ij}/\|W_j\|_2$, so that the column lengths satisfy $\|X\| = \|X_i\|_2 = 1$ for all $i$. If $|W_{ij}| \leq C$ for a constant $C > 0$ and $\log p = o(n)$, or $E_{e_{i0}|W_{ij}|^\alpha} < \infty$ for some $\alpha$, $t_0 > 0$ and $\log p = o(n^{1/(4+\alpha)})$, then Theorems 1 and 2 of [8] show that $\sqrt{n/\log \text{mc}(W)} \to 2$ as $n \to \infty$. Since $\text{mc}(W) = \text{mc}(X)$, this shows that for any $\varepsilon > 0$, $P(\text{mc}(X) > (2 + \varepsilon)\sqrt{(\log p)/n}) \to 0$. Thus with probability approaching one, (7) is satisfied for sparsity levels $s_n = o(\sqrt{n/\log p})$.

A classic example is $W_{ij} \overset{iid}{\sim} N(0, 1)$. In this case, the above bound on the mutual coherence holds as long as $\log p = o(n^{1/3})$.

5. By rescaling the columns of $X$ as in the response model, one can set the $p \times p$ matrix $C := X^T X/n$ to take value one for all diagonal entries. Then $\|X\| = \|X_i\|_2 = \sqrt{n}$ for all $i$ and the elements $C_{ij}$, $i \neq j$, are the correlations between columns. If $C_{ij} = r$ for a constant $0 < r < (1 + cm)^{-1}$ and all $i \neq j$, or $|C_{ij}| \leq c/(2m - 1)$ for every $i \neq j$, then [41] show that models up to dimension $m$ satisfy the ‘strong irrepresentability condition’ and are hence estimable. In particular, $\text{mc}(X) = \max_{i \neq j} C_{ij} = O(1/m)$ and hence (7) is satisfied for sparsity levels $s_n = o(m)$.

We thus see that (7), and in particular the mutual coherence condition, is satisfied in a variety of relevant examples.
3 Main results

The posterior $\Pi(\cdot|Y)$ arising from the prior $\Pi$ and data $Y$ assigns weights to all the $2^p$ possible models, typically without further structure except in special instances of the design matrix $X$ (e.g. $n = p$ and $X = I_n$). Since the posterior is difficult to compute for even moderate $p$, we take a VB approximation using the mean-field variational family

$$P_{MF} = \left\{ P_{\mu,\sigma,\gamma} = \bigotimes_{i=1}^{p} \gamma_i N(\mu_i, \sigma_i^2) + (1 - \gamma_i)\delta_0 : \mu_i \in \mathbb{R}, \sigma_i \in \mathbb{R}^+, \gamma_i \in [0,1] \right\} \quad (8)$$

with corresponding VB estimate

$$\tilde{\Pi} = \arg\min_{P_{\mu,\sigma,\gamma} \in P_{MF}} KL(P_{\mu,\sigma,\gamma}||\Pi(\cdot|Y)), \quad (9)$$

the minimizer of the Kullback-Leibler (KL) divergence with respect to the posterior. We thus approximate the posterior with a spike-and-slab distribution with Gaussian slabs under which every coordinate is independent. Note that while the prior may take the form $\Pi$, the posterior will in general not. The key feature here is that we replace the $2^p$ model weights with the $p$ VB inclusion probabilities ($\gamma_i$), thereby dramatically shrinking the posterior dimension.

The VB approximation (9) forces (substantial) additional independence into the resulting distribution, breaking dependencies between the variables. For instance, pairwise information that two coefficients $\theta_i$ and $\theta_j$ are likely to be selected simultaneously or not at all is lost. That there is a loss of information on some aspects of the posterior is unsurprising, since there is clearly a price to pay for a dimension reduction of this magnitude. What is perhaps more surprising is that such a drastic dimension reduction still provides optimal recovery of the unknown $\theta_0$.

Computing the VB estimate (9) is an optimization problem that can be tackled using the coordinate-ascent variational inference (CAVI) algorithm (see Section 4). We recall that the variational family $\Pi$ has been studied from a methodological perspective in the literature, but typically for priors with Gaussian slabs $[25, 9, 22]$. While particularly efficient computationally, using Gaussian slabs causes the underlying posterior to convergence to the true $\theta_0$ at a highly sub-optimal rate $[15]$ due to excessive shrinkage occurring from both the model selection and Gaussian slabs. As expected, such poor behaviour crosses over to the resulting VB approximation as we demonstrate numerically in Section 5 below.

In the papers $[15, 13]$, it was shown that heavier tailed (at least exponential) slabs result in optimal recovery when using the posterior itself. While we use Gaussian slabs in our variational family, it is crucial that the true prior has slab distributions with at least exponential tails (e.g. Laplace). The reason a Gaussian approximation works well here is that the likelihood induces Gaussian tails in the posterior. We emphasize that we use the same variational family to estimate a different posterior distribution compared to the previous works $[25, 9, 22]$.

The following is the main result of this paper, which establishes convergence of the VB approximation (9) to the truth in both $\ell_2$ loss and prediction error $\|X(\theta - \theta_0)\|_2$. We consider the asymptotic regime $n \to \infty$ and hence also $p = p(n) \to \infty$.

**Theorem 1.** Suppose the model selection prior $\Pi$ satisfies (4) and (5). Suppose further that $s_n$ satisfies $\lambda_n \sqrt{\log p} / \|X\| \to 0$ and the design matrices satisfy $\min_{1 \leq i \neq j \leq p} \|X_i\|_2 / \|X_j\|_2 \geq \eta$ for some $\eta > 0$. Then for any $\nu_n \to 0$, the variational Bayes posterior $\tilde{\Pi}$ satisfies, with
\[ S_0 = S_{\theta_0}, \]

\[ \sup_{\theta_0 \mid |S_0| \leq s_n \atop |S_0| \leq v_{nmc}(X)^{-1}} E_{\theta_0} \bar{\Pi} \left( \theta : \| \theta - \theta_0 \|_2 \geq M_n \sqrt{|S_0| \log p/\|X\|} \right) \to 0, \]

\[ \sup_{\theta_0 \mid |S_0| \leq s_n \atop |S_0| \leq v_{nmc}(X)^{-1}} E_{\theta_0} \bar{\Pi} \left( \theta : \| X(\theta - \theta_0) \|_2 \geq M_n \sqrt{|S_0| \log p} \right) \to 0, \]

for any sequence \( M_n \) tending to infinity (arbitrarily slowly).

Recall that we are working under the frequentist model where there is a “true” \( \theta_0 \) generating data \( Y \) of the form (1). Since the above rates equal the minimax estimation rates over \( |S_0|\)-sparse vectors, Theorem 1 states that the VB posterior puts most of its mass in a neighbourhood of optimal size around the truth with high \( P_{\theta_0} \)-probability, both in terms of \( \ell_2 \) and prediction loss. Thus for estimating \( \theta_0 \), the VB approximation behaves optimally from a theoretical frequentist perspective. This backs up the empirical evidence that VB can provide excellent scalable estimation.

Since the prior and variational family do not depend on the unknown sparsity level \( |S_0| \) and the VB estimate contracts around the truth at the minimax rate, the procedure is adaptive. That is, the procedure can recover an \( |S_0|\)-sparse truth nearly as well as if we knew the exact level of sparsity of the unknown \( \theta_0 \). This avoids difficult issues about selecting tuning parameters, which often have a significant impact on the performance of statistical procedures.

Note that Theorem 1 does not imply that the VB posterior \( \bar{\Pi} \) converges to the true posterior \( \Pi(\cdot \mid Y) \). Indeed, this is neither a typical situation nor a necessary property since the VB estimate should be substantially simpler than the true posterior to be useful. Theorem 1 follows from the more general Theorem 5 found in Section 7 below. For discussion on the sparsity assumptions, see Section 2.2 above.

An important motivation for using model selection priors is their ability to perform variable selection. The following result shows that the variational approximation puts most of its mass on models of size at most a multiple of the true dimension, thereby bounding the number of false positives.

**Theorem 2.** Under the conditions of Theorem 1,

\[ \sup_{\theta_0 \mid |S_0| \leq s_n \atop |S_0| \leq v_{nmc}(X)^{-1}} E_{\theta_0} \bar{\Pi} \left( \theta : |S_0| \geq M_n |S_0| \right) \to 0, \]

for any \( M_n \to \infty \) (arbitrarily slowly).

Note that under the conditions of Theorems 1 and 2 it is not possible to consistently estimate the true support \( S_{\theta_0} \) of \( \theta_0 \) since one cannot separate small and exactly zero signals.

While the mean-field family \( P_{MF} \) in (8) is our main object of interest, we can obtain similar results for two other closely related variational families. Consider the family of distributions consisting of products of a single multivariate normal distribution with a Dirac measure:

\[ Q = \{ N_S(\mu_S, \Sigma_S) \otimes \delta_{S^c} : S \subseteq \{1, 2, \ldots, p\}, \mu_S \in \mathbb{R}^{|S|}, \Sigma_S \in \mathbb{R}^{|S| \times |S|} \text{ a positive definite covariance matrix} \}, \]

where \( \delta_{S^c} \) denotes the Dirac measure on the coordinates \( S^c \). This family is more rigid on the model selection level than \( P_{MF} \), selecting a distribution with a single fixed support set \( S \). On
this set, however, the family permits a richer representation for the non-zero coefficients, in particular allowing non-zero covariances. Denote the KL projection of the posterior onto the variational family $Q$ by $\hat{Q}$:

$$\hat{Q} = \arg\min_{Q \in Q} \text{KL}(Q \| \Pi(\cdot|Y)).$$

(11)

Next consider the mean field subclass of $Q$:

$$Q_{MF} = \{N_S(\mu_S, D_S) \otimes \delta_{S^c} : S \subseteq \{1, 2, \ldots, p\}, \mu_S \in \mathbb{R}^{|S|}, \, D_S \in \mathbb{R}^{|S| \times |S|} \text{ a positive definite diagonal matrix}\}. \tag{12}$$

This family again allows distributions with only a single fixed support set $S$, but further forces independence of the non-zero coefficients. This class is contained in $P_{MF}$ by considering distributions $P_{\mu, \sigma, \gamma}$ with the inclusion probabilities restricted to $\gamma_i \in \{0, 1\}$. Denote by $\tilde{Q}$ the corresponding variational approximation:

$$\tilde{Q} = \arg\min_{Q \in Q_{MF}} \text{KL}(Q \| \Pi(\cdot|Y)).$$

(13)

**Theorem 3.** Suppose the model selection prior (3) satisfies (4) and (5). Suppose further that $s_n$ satisfies $\lambda s_n \sqrt{\log p/\|X\|} \to 0$ and the design matrices satisfy $\min_{1 \leq i \neq j \leq p} \|X_i\|_2^2/\|X_j\|_2 \geq \eta$ for some $\eta > 0$. Then for any $v_n \to 0$, the variational Bayes posterior (11) satisfies, with $S_0 = S_{\theta_0}$,

$$\sup_{\theta_0 : |S_0| \leq s_n} \mathbb{E}_{\theta_0} \hat{Q} \left( \|\theta - \theta_0\|_2 \geq M_n \sqrt{|S_0| \log p/\|X\|} \right) \to 0,$n

$$\sup_{\theta_0 : |S_0| \leq s_n} \mathbb{E}_{\theta_0} \hat{Q} \left( \|X(\theta - \theta_0)\|_2 \geq M_n \sqrt{|S_0| \log p} \right) \to 0,$n

for any sequence $M_n$ tending to infinity (arbitrarily slowly). Moreover, the same holds true for $\tilde{Q}$ defined in (13).

From a theoretical point of view, either of the families $Q$ or $Q_{MF}$ provide optimal asymptotic estimation of $\theta_0$ in both $\ell_2$ and prediction loss. However, selecting a single support set $S$ in the approximating distribution is a strong restriction that is typically less desirable. A similar result holds regarding the dimension of the support set.

**Theorem 4.** Under the conditions of Theorem 3,

$$\sup_{\theta_0 : |S_0| \leq s_n} \mathbb{E}_{\theta_0} \hat{Q} \left( |S_0| \geq M_n |S_0| \right) \to 0,$n

for any $M_n \to \infty$ (arbitrarily slowly). Moreover, the same holds true for $\tilde{Q}$ defined in (13).

Since the variational families (10) and (12) contain only distributions with a single support set $S$, the last statement says that the resulting VB posteriors will select such a set of size at most a multiple times $|S_0|$ with high $P_{\theta_0}$-probability. The VB estimates based on these two variational families perform model selection in a hard-thresholding manner, reporting only
whether a variable is selected or not. On the other hand, the more flexible family (8) can quantify the individual variable selection via the reported non-trivial inclusion probabilities $0 \leq \gamma_i \leq 1$ and in this regard provides a richer approximation of the target posterior. Information on pairwise variable inclusion is obviously lost given the mean-field nature of the approximation. Nevertheless, it is interesting to note that all these families still permit good estimation of $\theta_0$.

4 Variational Bayes algorithm

In this section we provide an updated version of the coordinate-ascent variational inference (CAVI) algorithm (see for instance [3]) to compute the mean-field variational Bayes estimate based on the spike-and-slab prior with Laplace slab. We consider the natural variational family $P_{MF}$ given in (8). Since in the literature [25, 9, 22] the VB approximation is typically considered for Gaussian rather than Laplace slabs, and can therefore take advantage of some explicit analytic formulas, our algorithm requires modification.

We reformulate the spike-and-slab prior by introducing binary latent variables $z_i$, $i = 1, ..., p$,

$$w \sim \text{Beta}(a_0, b_0),$$

$$z_i | w \overset{iid}{\sim} \text{Bernoulli}(w),$$

$$\theta_i | z_i \overset{iid}{\sim} z_i \text{Lap}(\lambda) + (1 - z_i) \delta_0.$$ (14)

The prior inclusion probability equals $\Pi(z_i = 1) = \int w d\pi(w) = a_0/(a_0 + b_0)$, the expectation of a beta random variable. Following the CAVI algorithm, we sequentially update the parameters $\gamma_i, \sigma_i, \mu_i$, $i = 1, ..., p$, of the variational class by minimizing the Kullback-Leibler divergence between the variational class with the rest of the parameters kept fixed and the posterior. We iterate this algorithm until convergence, which we measure by the change in entropy.

Remark 1. In the recent paper [22] for Gaussian slabs, the authors propose to deviate from the standard CAVI method (see for instance [25, 9] for a more standard component-wise CAVI implementation) and propose a batch-wise update of the parameters. This approach is, however, not really feasible in our setting due to the lack of analytic formulas when using Laplace slabs.

Nevertheless, we show in our simulation study in Section 5 that our approach outperforms (in certain situations) both the component-wise and batch-wise variational algorithms applied for Gaussian slabs.

We next give the component-wise variational updates in the algorithm. Recall that in the mean-field variational class (8) the probability measure $P_{\mu, \sigma, \gamma}$ factorizes across the parameters. Fix the latent variable $z_i = 1$ and all the variational factors except $\mu_i$ or $\sigma_i$ (i.e. using vector notation, $\mu_{-i}, \sigma, \gamma$ or $\mu, \sigma_{-i}, \gamma$ are all fixed). Fixing $z_i = 1$, the minimizer of the conditional KL divergence between $P_{MF}$ and the posterior given $\mu_{-i}, \sigma, \gamma$ or $\mu, \sigma_{-i}, \gamma$ is the same as the minimizer of

$$f_i(\mu_i | \sigma, \mu_{-i}, \gamma, z_i = 1) = \mu_i \sum_{k \neq i} (X^T X)_{ik} \gamma_k \mu_k + \frac{1}{2} (X^T X)_{ii} \mu_i^2 - (Y^T X)_{i} \mu_i + \lambda \sigma_i \sqrt{2/\pi} e^{-\mu_i^2/(2\sigma_i^2)}$$

$$+ \lambda \mu_i (1 - 2\Phi(-\mu_i/\sigma_i)),$$

$$g_i(\sigma_i | \sigma_{-i}, \mu, \gamma, z_i = 1) = \frac{1}{2} (X^T X)_{ii} \sigma_i^2 + \lambda \mu_i \sigma_i \sqrt{2/\pi} e^{-\mu_i^2/(2\sigma_i^2)} + \lambda \mu_i (1 - \Phi(\mu_i/\sigma_i)) - \log \sigma_i,$$ (15)
respectively (see Section 9.1 for the proof of the above assertion), where \( \Phi \) denotes the cdf of the standard normal distribution. The minimizers of these functions do not have simple closed form expressions and hence we apply an optimization method to obtain them. In our R implementation, we use the built-in optimize() function for finding the minimizers of \( f_i \) and \( g_i \).

One can similarly obtain the KL divergence between the variational class and the posterior as a function of \( \gamma_i \), conditional on the other parameters. By differentiating this function, the minimizer \( \gamma_i \) satisfies

\[
\log \frac{\gamma_i}{1 - \gamma_i} = \log \frac{a_0}{b_0} + \log \frac{\sqrt{\pi} \sigma_i \lambda}{\sqrt{2}} + (Y^T X)_{\mu_i} - \mu_i \sum_{k \neq i} (X^T X)_{ik} \gamma_k \mu_k - \frac{1}{2} (X^T X)_{ii} (\sigma_i^2 + \mu_i^2) - \lambda \sigma_i \sqrt{2/\pi e^{-\mu_i^2/(2 \sigma_i^2)}} - \lambda \mu_i (1 - 2 \Phi(-\mu_i/\sigma_i)) + \frac{1}{2} =: \Gamma_i(\mu, \sigma, \gamma_{-i}).
\]

The proof of the above assertion is also given in Section 9.1.

In the CAVI algorithm, we update the parameters \( \mu_i, \gamma_i \) and \( \sigma_i, i = 1, ..., p \), coordinate-wise using the above functions and iterate this procedure until convergence of the parameters. Following [22], we terminate the procedure once the coordinate-wise maximal change in binary entropy of the posterior inclusion probabilities falls below a prespecified small threshold \( \varepsilon \) (e.g. \( \varepsilon = 10^{-5} \)), i.e. stop when \( \max_{i=1,...,p} |H(\gamma_i) - H(\gamma_i')| \leq \varepsilon \), where \( H(p) = -p \log p - (1-p) \log (1-p) \), \( p \in (0,1) \), and \( \gamma_i, \gamma_i' \) are the \( i \)th coordinate of the starting and updated parameters \( \gamma, \gamma' \), respectively.

Recall that the VB objective function is (generally) non-convex and so the CAVI algorithm can be sensitive to initialization [3]. It turns out the order of the component-wise updates is also crucial to the algorithm’s performance. In fact using the naive approach of updating the coordinates in lexicographical order \( i = 1, ..., p \) is typically suboptimal (at least in our setup). We demonstrate in the next section on various simulated data sets that unless the relevant non-zero coefficients are located at the beginning of the signal, the procedure stops at a highly suboptimal local minimum and gives misleading, inconsistent answers. In this case CAVI will return a solution that is far from the desired VB estimator it is trying to compute. It is clearly undesirable that the algorithm’s performance depends on the arbitrary ordering of the parameter coordinates. A natural correction is to randomize the order of the coordinate-wise updates and use different initializations, choosing the local minimum which provides the smallest overall KL-divergence with the posterior. We show, however, that due to the large number of local minima and their substantially different behaviour, this approach also performs highly suboptimally (although somewhat better than the lexicographic approach).

We instead propose a novel prioritized update scheme. In a first preprocessing step, we compute an initial estimator \( \hat{\mu}^{(0)} \) of the mean vector \( \mu \) of the variational class. We then place the coefficients in decreasing order with respect to the absolute value of their estimate and update the parameters coordinate-wise in the corresponding order, i.e. denoting by \( \alpha = (a_1, ..., a_p) \) the permutation of the indices \( (1, 2, ..., p) \) such that \( |\hat{\mu}_{a_i}^{(0)}| \geq |\hat{\mu}_{a_j}^{(0)}| \) for every \( 1 \leq i < j \leq p \), we update the coordinates in the order \( \mu_{a_i}, \sigma_{a_i}, \lambda_{a_i}, i = 1, ..., p \).

The intuition behind this method is that when the CAVI algorithm starts by updating indices whose signal coefficients are small or zero in the target VB posterior, it may incorrectly assign signal strength to such indices to better fit the data (this can especially be the case if the initialization value of the signal coefficient is not very close to its value in the target
VB posterior). Consequently, the estimates of the relevant non-zero signal components may be overly small since part of the signal strength has already been falsely assigned to signal coefficients that should in fact be small under the VB posterior. This can trap the algorithm near a highly suboptimal local minimum from which it cannot escape, see the corresponding simulation study in Section 5.

To prevent this, we wish to first update those coefficients which are large in the target VB posterior. Since these are unknown, the idea here is to identify them using a preliminary estimator: if the target VB posterior does a good job of estimating the signal, these large coefficients should (roughly) match those that are large in the true underlying signal, which can be identified using a reasonable estimator.

The algorithm is given in Algorithm 1 where the function $\text{order}(|\mu|)$ returns the indices of $|\mu|$ in descending order.

Algorithm 1 Variational Bayes for Laplace-slab

1: Initialization:
2: $\Delta_H := 1$
3: $\mu := \hat{\mu}^{(0)}$ (for some preliminary estimator $\hat{\mu}^{(0)}$)
4: $\sigma := (1, \ldots, 1)$, $\gamma = (a_0, a_0 + b_0, \ldots, a_0 + b_0)$
5: $a := \text{order}(|\mu|)$
6: while $\Delta_H \geq \varepsilon$ do

7: $\gamma_{\text{old}} := \gamma$
8: for $j = 1$ to $p$ do

9: $i := a_j$
10: $\mu_i := \text{argmax}_{\mu_i} f_i(\mu_i|\mu_{-i}, \sigma, \gamma, z_i = 1)$
11: $\sigma_i := \text{argmax}_{\sigma_i} g_i(\sigma_i|\mu, \sigma_{-i}, \gamma, z_i = 1)$
12: $\gamma_i = \log(\lambda - \mu_i - \frac{1}{2} \frac{\lambda^2}{\sigma_i^2}) + \frac{1}{2}

Remark 2. Instead of the prior (14) one can also consider the prior

$w_i \sim \text{Beta}(a_0, b_0)$,
$z_i|w_i \sim \text{Bernoulli}(w_i)$,
$\theta_i|z_i \sim z_i \text{Lap}(\lambda) + (1 - z_i)\delta_0$,

where the probabilities $w_i$ vary with $i$. This results in exactly the same variational algorithm since we are using a mean-field approximation. If one instead takes deterministic weights $w_i$, the above algorithm can be easily adapted by using the same update steps for $\mu_i$ and $\sigma_i$, while updating $\gamma_i$ as the solution to

$$\log \frac{\gamma_i}{1 - \gamma_i} = \log \frac{w_i}{1 - w_i} + \log \sqrt{\pi} \sigma_i \lambda + \frac{\sqrt{2} \lambda}{\sqrt{2}} + (Y^T X)_{ij} \gamma_{ij} \mu_{ij} - \sum_{j \neq i} (X^T X)_{ij} \gamma_{ij} \mu_{ij} - \frac{\mu_i^2 + \gamma_i}{2} (X^T X)_{ii}$$

$$- \lambda \sigma_i \sqrt{2/\pi} e^{-\mu_i^2/(2\sigma_i^2)} - \lambda \mu_i (1 - 2\Phi(-\mu_i/\gamma_i)) + \frac{1}{2}.$$
5  Numerical study

In this section we empirically investigate the performance of our variational Bayes method with Laplace slabs compared to various Bayesian (based) model selection methods on both simulated and real world data.

5.1  Simulation study I: comparing the performance of VB algorithms

Consider firstly the many normal means model

\[ Y_i = \theta_i + Z_i, \quad i = 1, \ldots, n, \]

where \( Z_i \sim \text{iid } N(0, 1) \), which corresponds to model (1) with \( n = p \) and identity design matrix \( X = I_n \). We compare our VB method with Laplace slabs (Algorithm 1 above) to the VB method with Gaussian slabs which is the standard approach in the literature, see for instance [25, 9, 22]. We consider both the suggested component-wise and batch-wise VB approaches, see Algorithms 2 and 3 in the supplement, respectively.

We take \( n = 200, 500, 2000, 5000, 20000 \) and \( s = n/5 \), set the nonzero signal coefficients to \( 2 \log n \) and the prior hyper-parameters to \( \lambda = 1, a_0 = 1, b_0 = p \) (the latter sets \( \Pi(\gamma_i = 1) = 1/(p + 1) \)). In our initialization for the Laplace VB we take \( \mu = (X^T X + I)^{-1} X^T Y \) to be the ridge regression estimator, \( \sigma_i = 1 \) and \( \gamma_i = 1/(p + 1) \) for all \( i = 1, \ldots, p \). In the Gaussian VB algorithms, we consider standard Gaussian slabs in the prior and use the same parameter initializations as in the Laplace case, i.e. we take \( \mu = (X^T X + I)^{-1} X^T Y \) to be the ridge regression estimator, \( \sigma_i = 1 \) and \( \gamma_i = 1/(p + 1) \) for all \( i = 1, \ldots, p \). We ran the simulation 10 times in each case and report the median \( \ell_2 \)-errors for the posterior means and median computational times in Tables 1 and 2, respectively. (The mean error and mean computational time are very skewed towards large values for the batch-wise VB algorithm, so we decided to use the medians as summary statistics).

Table 1 shows that the empirical \( \ell_2 \)-error of the posterior mean is considerably smaller when using Laplace slabs compared with Gaussian slabs due to large bias of the posterior mean in the latter case. This matches what is predicted by the theory given the suboptimality of Gaussian slabs [15] and our results in Section 3 on the optimality of Laplace slabs. The similar errors when using the component-wise and batch-wise approaches for Gaussian slabs suggest that these algorithms converge to similar VB estimators in this case (though not always, see below) and the problem here is indeed due to the ‘correct’ underlying VB estimator rather than convergence to a suboptimal local minimum.

Due to the explicit formula for the minimizer of the KL-divergence when using Gaussian slabs, the corresponding component-wise algorithm is considerably faster than our method for small sample sizes with comparable computational speed for large sample sizes. The faster speed of the Laplace method for large sample sizes is due to the prioritized updating scheme, which reduced the number of iterations needed compared to the standard implementation we employed for the Gaussian method. The batch-wise variational update is much slower than the other two methods; in fact we had to terminate the code for \( n = 20000 \), since the algorithm did not finish a single simulation cycle after running for a whole day.

In Figure 1, we plot the posterior means resulting from the variational methods for Laplace slabs (blue) and Gaussian slabs with component-wise (red) and batch-wise (light blue) updates together with the true underlying signal (green) and observations (gray). One observes that all methods shrink the irrelevant coordinates to zero and perform consistent model selection.
Table 1: $\ell_2$-Estimation error of the VB algorithms

| Method          | n  | 200  | 500  | 2000 | 5000 | 20000 |
|-----------------|----|------|------|------|------|-------|
| VB - Laplace    |    | 9.38 | 14.32| 28.47| 44.65| 90.33 |
| VB - Gauss (component-wise) | | 33.77 | 62.37| 152.63| 269.66| 627.5 |
| VB - Gauss (batch-wise)        | | 33.78 | 62.38| 152.64| 269.66| -     |

Table 2: Run time of the VB algorithms

| Method          | n  | 200  | 500  | 2000 | 5000 | 20000 |
|-----------------|----|------|------|------|------|-------|
| VB - Laplace    |    | 0.185s| 0.733s| 17.23s| 192.89s| 9938s |
| VB - Gauss (component-wise) | | 0.034 s | 0.181 s | 8.56 s | 150.38 s | 15047 s |
| VB - Gauss (batch-wise)        | | 0.19s | 0.994s| 43.31s| 934.5s| -     |

However, the VB methods with Gaussian slabs substantially underestimate the non-zero signals leading to poor recovery of the true signal compared to the optimal performance of the VB method with Laplace slabs. Note that the component-wise and batch-wise points very closely match and so may not be visible.

We next consider an i.i.d. Gaussian design matrix with entries $X_{ij} \sim N(0, \tau^2)$ and equally sized non-zero signal components $\theta_i = A$. We consider various combinations of $n, p, s, \tau$ and $A$, and choose different locations for the non-zero signal coefficients. These are plotted in Figure 2 using the same colour code as above. In (i) we take $n = 200$, $p = 800$, $s = 40$, $\tau = 1$, $A = 2 \log n$ and place the non-zero coefficients at the beginning of the signal. One can see that the two component-wise algorithms outperform the batch-wise VB method. We then consider various perturbations of these parameters. By increasing the sample size to $n = 800$ in (ii) (note that we have a square design matrix in this case), the performance of every method increases and all provide similarly good results. We next change the locations of the non-zero signal coefficients by moving them (iii) to the middle, (iv) to the end and (v) splitting them between the beginning and end of the signal. In all three scenarios the VB method for Laplace slabs substantially outperforms the VB methods for Gaussian slabs. The superior performance compared to the component-wise VB for Gaussian slabs is due to the prioritized updating scheme we employ (see the next section for further study of this updating scheme). In (vi) we increase the number of non-zero coefficients to $s = 80$ keeping the rest of the parameters unchanged. In this scenario, both component-wise algorithms perform comparably well while the batch-wise method is again suboptimal. For larger signal strengths, such as $A = n$ in (vii), using Laplace slabs performs substantially better. Finally, we change the scale of the design matrix by taking $\tau = 0.1$ in (viii), resulting in a smaller column norm $\|X\|$ of the design matrix. In this case Laplace slabs again result in substantially better VB estimators than the other methods due to the smaller signal to noise ratio (which leads to similar phenomena as in the many normal means model, studied above, where the signal to noise ratio is 1). We also note that the fastest algorithm is in all cases the component-wise VB method with Gaussian slabs, then our proposed VB method with Laplace slabs and the slowest is typically the batch-wise algorithm, which requires handling large matrices and hence is computationally inefficient.
Figure 1: Gaussian sequence model with true signal (green) and observed data (gray). The posterior means of the VB methods for Laplace slabs (blue) and Gaussian slabs using component-wise (red) and batch-wise (light blue) updates are plotted for $n = 200, 500, 2000$ and 5000 with $s = 40, 100, 400$ and 1000, respectively, and non-zero signal size $\theta_i = 2 \log n$. 
Figure 2: Linear regression with Gaussian design $X_{ij} \sim \text{iid } N(0, \tau^2)$. We plot the underlying signal with non-zero components $\theta_i = A$ (green) and the posterior means of the VB methods with Laplace slabs (blue) and Gaussian slabs with component wise (red) and batch-wise (light blue) updates. From left to right and top to bottom, we take $(n, p, s, \tau, A)$ equal to: (i) $(200, 800, 40, 1, 2\log n)$ (with non-zero coefficients in the beginning), (ii) $(800, 800, 40, 1, 2\log n)$ (in the beginning), (iii) $(200, 800, 40, 1, 2\log n)$ (in the middle), (iv) $(200, 800, 40, 1, 2\log n)$ (in the end), (v) $(200, 800, 40, 1, n)$ (in the beginning and end), (vi) $(200, 800, 80, 1, 2\log n)$ (in the beginning), (vii) $(200, 800, 40, 1, n)$ (in the beginning), (viii) $(200, 800, 40, 0.1, 2\log n)$ (in the beginning).
5.2 Simulation study II: investigating the prioritized updating scheme

We demonstrate here the relevance of our prioritized update scheme in the CAVI algorithm by comparing the performance of lexicographic, randomized and the prioritized updating methods. We take \( n = 200, p = 400, s = 40, \theta_i = 5 \log n \) and consider four scenarios for the locations of the non-zero signal components. In Figure 3 we place all non-zero coordinates (i) at the beginning of the signal, (ii) at the end of the signal, (iii) in the middle of the signal and (iv) randomly distributed.

One observes that apart from the first scenario, where the important signal coefficients are all located at the beginning of the signal, the prioritized method substantially outperforms both the randomized and the lexicographical updating schemes (recall that all three methods are trying to compute the same VB estimate). The random updating order also slightly improves upon the lexicographical order, except for the first scenario. As well as being sensitive to initialization \( [3] \), it seems the CAVI algorithm can also be very sensitive to the updating order of the parameters. Indeed we see here that without the prioritized ordering, the algorithm often terminates at highly-suboptimal local minima of the VB objective function. Since the VB objective is non-convex, naive (or random) update orderings may cause the CAVI algorithm to return a solution that is far from the true minimizer of the KL divergence that it is trying to compute. Performing updates in a prioritized order can add some robustness against this, see Section 4 for some heuristics behind this idea.

5.3 Simulation study III: comparing the performance of Bayesian variable selection methods

We next compare the performance of our VB method with various Bayesian (based) variable selection algorithms for sparse linear regression using simulated data. We consider the varbvs R-package (variational Bayes algorithm for spike-and-slab priors with Gaussian slabs using an importance sampling outer circle for estimating the posterior inclusion probabilities and the noise variance, proposed by \[ 9 \]), the EMVS R-package (spike-and-slab lasso algorithm, proposed by \[ 31 \]) and the spikeslab R-package (computing the K-fold cross-validated mean squared prediction error for the generalized elastic net from spike-and-slab regression, proposed by \[ 23 \]). We ran these procedures on test data sets similar to those in the preceding subsections, plotting in Figure 4 the true signal (green) and posterior means for our VB algorithm (blue), varbvs (red), EMVS (light blue) and spikeslab (purple). We ran each algorithm 50 times and report the mean \( \ell_2 \) distance between the true signal and posterior mean in Table 3.

For all the algorithms we took the ridge regression estimator \( (X^TX + I)^{-1}X^TY \) as the initial value for \( \theta \). In the varbvs method we worked with the initialization \( tol = 10^{-4}, \ maxiter = 10000, \ sigma = 1 \); in the EMVS method we took \( v_0 = 0.1, v_1 = 1000 \) (these quantities were used in one of the examples provided in the package), \( \sigma_{init} = 1, a = 1, b = p \) and \( \epsilon = 10^{-5} \); while in the cv.spikeslab function we worked with the configuration \( bigp.smalln = TRUE, \ parallel = 4 \).

We consider first \( n = 200, p = 800, s = 40 \) with the non-zero signal components set to \( \theta_i = 2 \log n \) and located at the beginning of the signal. The entries of the design matrix are taken to be iid standard normal random variables. Based on Figure 4(I) and Table 3 we see that varbvs has the best performance with our VB approach using Laplace slabs a close second best. We next consider various perturbations of the above parameters.

In (II) we again take \( n = p = 800, s = 40 \), and non-zero signal components \( \theta_i = 2 \log n \) located at the beginning of the signal, but instead consider the identity design matrix \( X = I \).
Figure 3: Linear regression with Gaussian design $X_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1)$. We plot the underlying signal (green) and posterior means of the VB method with Laplace slabs computed using the CAVI algorithm with parameter updates ordered in a prioritized way (blue), lexicographically (red) and randomly (light blue). We took $n = 200$, $p = 400$, $s = 40$, $\theta_i = 5 \log n$. From left to right and top to bottom we have: the non-zero coordinates are at the beginning, end, middle and random locations of the signal.
Note that in this case the VB method with Laplace slabs has the best performance. The poor performance of the varbvs method is not surprising since this method is not appropriate for sparse design matrices as explained in the corresponding manual. We next consider the same parameters as in (I), but move the non-zero signal coefficients (III) to the end and (IV) to the middle of the signal (here we have also set half of the coefficients to be negative). Our method greatly outperforms varbvs (due to the prioritized updating scheme) and provides also better results than EMVS (which is the second best method in this setting). In (V) we take Gaussian design with iid $\mathcal{N}(0,0.1^2)$ entries, thereby reducing the signal-to-noise ratio. Our method outperforms the rest of the algorithms (with varbvs second best). Lastly in (VI) we take $n = 200$, $p = 800$, $s = 40$, and non-zero signal components $\theta_i = n$ located at the beginning of the signal. In this case varbvs performs best with our approach second best. We summarize our findings by pointing out that the VB method with Laplace slabs was amongst the top two algorithms in all the test cases and two thirds of the time provided the single best estimator of the underlying sparse signal. We note that the $\ell_2$ error varied substantially between runs depending on the realisation of the random design matrix. We also comment that VB Laplace, varbvs and especially EMVS were highly sensitive to their initialization; it may well be possible to improve performance by selecting a better starting point.

### 5.4 Simulation study IV: unknown variance

We now extend our algorithm to the more realistic situation of unknown noise variance. As mentioned in Section 2, dividing both sides of the linear regression model by an empirical estimator $\hat{\sigma}$ for the noise standard deviation $\sigma$ gives

$$\tilde{Y} = \tilde{X}\theta + \tilde{Z},$$

where $\tilde{Y} = Y/\hat{\sigma}$, $\tilde{X} = X/\hat{\sigma}$ and $\tilde{Z} = (\sigma/\hat{\sigma})Z$, $Z \sim \mathcal{N}(0,I_n)$. Endowing $\theta$ with the spike-and-slab prior and if the estimator $\hat{\sigma}$ is consistent for $\sigma$, we asymptotically recover the $\sigma = 1$ case studied above. We then proceed as before with our VB estimator. For estimating $\sigma$ we have used the R package “selectiveInference”.

We compare our method with the ones investigated in the previous section, using the same initializations, except now taking $\sigma$ to be unknown. Similarly to above, we take $(n,p,s,\tau,A,\sigma)$ equal to: (i) $(100,400,20,1,\log n,5)$ (with non-zero coefficients at the beginning), (ii) $(200,800,40,1,2\log n,0.2)$ (in the middle), (iii) $(200,800,40,0.2,4\log n,5)$ (at the end), (iv) $(200,1600,40,1,4\log n,0.2)$ (at the beginning). The results are summarized in Table 4 where we report the mean $\ell_2$ distance between the posterior mean and the true parameter from 50 independent runs, and depicted in Figure 5. One can see that in all cases our methods performs best, in some cases substantially so.

### Table 3: Estimation errors of various Bayesian model selection methods

| Method \ case | I   | II  | III | IV  | V   | VI  |
|--------------|-----|-----|-----|-----|-----|-----|
| VB - Laplace | 25.8| 9.06| 25.74| 32.09| 6.76| 871 |
| varbvs       | 23.1| 28.24| 90.72| 84.62| 16.91| 510.8|
| EMVS         | 35.8| 34.14| 34.1| 42.16| 58.33| 1098.0|
| spikeslab    | 67.0| 23.9| 67.0| 67.9| 51.47| 1265.0|

Note that in this case the VB method with Laplace slabs has the best performance.

5.4 Simulation study IV: unknown variance

We now extend our algorithm to the more realistic situation of unknown noise variance. As mentioned in Section 2, dividing both sides of the linear regression model by an empirical estimator $\hat{\sigma}$ for the noise standard deviation $\sigma$ gives

$$\tilde{Y} = \tilde{X}\theta + \tilde{Z},$$

where $\tilde{Y} = Y/\hat{\sigma}$, $\tilde{X} = X/\hat{\sigma}$ and $\tilde{Z} = (\sigma/\hat{\sigma})Z$, $Z \sim \mathcal{N}(0,I_n)$. Endowing $\theta$ with the spike-and-slab prior and if the estimator $\hat{\sigma}$ is consistent for $\sigma$, we asymptotically recover the $\sigma = 1$ case studied above. We then proceed as before with our VB estimator. For estimating $\sigma$ we have used the R package “selectiveInference”.

We compare our method with the ones investigated in the previous section, using the same initializations, except now taking $\sigma$ to be unknown. Similarly to above, we take $(n,p,s,\tau,A,\sigma)$ equal to: (i) $(100,400,20,1,\log n,5)$ (with non-zero coefficients at the beginning), (ii) $(200,800,40,1,2\log n,0.2)$ (in the middle), (iii) $(200,800,40,0.2,4\log n,5)$ (at the end), (iv) $(200,1600,40,1,4\log n,0.2)$ (at the beginning). The results are summarized in Table 4 where we report the mean $\ell_2$ distance between the posterior mean and the true parameter from 50 independent runs, and depicted in Figure 5. One can see that in all cases our methods performs best, in some cases substantially so.
Figure 4: Comparing the performance of various Bayesian model selection methods for linear regression with design matrix $X$. We plot the underlying signal with non-zero components $\theta_i = A$ (green) and the posterior means arising from the VB method with Laplace slabs (blue), varbvs (red), EMVS (light blue) and spikeslab (purple) methods. From left to right and top to bottom we take $(n, p, s, A)$ and $X$ equal to: (I) $(200, 800, 40, 2 \log n)$ and $X_{ij} \overset{iid}{\sim} N(0, 1)$ (non-zero coefficients in the beginning); (II) $(800, 800, 40, 2 \log n)$ and $X = I$ (non-zero coefficients in the beginning); (III) $(200, 800, 40, 2 \log n)$ and $X_{ij} \overset{iid}{\sim} N(0, 1)$ (non-zero coefficients at the end); (IV) $(200, 800, 40, 2 \log n)$ and $X_{ij} \overset{iid}{\sim} N(0, 1)$ (non-zero coefficients in the middle); (V) $(200, 800, 40, 2 \log n)$ and $X_{ij} \overset{iid}{\sim} N(0, 0.1^2)$ (non-zero coefficients in the beginning); (VI) $(200, 800, 80, n)$ and $X_{ij} \overset{iid}{\sim} N(0, 1)$ (non-zero coefficients in the beginning).
Table 4: Estimation error of various Bayesian model selection methods

| Method \ case | I    | II   | III  | IV   |
|-------------|------|------|------|------|
| VB - Laplace| 10.03| 14.15| 68.59| 76.77|
| varbvs      | 12.87| 35.40| 84.71| 120.0|
| EMVS        | 13.82| 44.73| 88.23| 124.47|
| spikeslab   | 20.53| 67.85| 133.75| 134.04|

Figure 5: Comparing the performance of various Bayesian model selection methods for linear regression with design matrix $X$, where $X_{ij} \sim N(0, \tau^2)$, when the noise variance $\sigma^2$ is unknown. We plot the underlying signal with non-zero components $\theta_i = A$ (green) and the posterior means arising from the VB method with Laplace slabs (blue), varbvs (red), EMVS (light blue) and spikeslab (purple) methods. From left to right and top to bottom we take $(n, p, s, \tau, A, \sigma)$: (i) $(100, 400, 20, 1, \log n, 5)$ (non-zero coefficients at the beginning), (ii) $(200, 800, 40, 1, 2\log n, 0.2)$ (in the middle), (iii) $(200, 800, 40, 0.2, 4\log n, 5)$ (at the end), (iv) $(200, 1600, 40, 1, 4\log n, 0.2)$ (at the beginning).
5.5 Ozone interaction data

We lastly apply our method to real world ozone interaction data considered in [6], which is for instance available in the spikeslab package. The data consists of \( n = 203 \) readings of maximal daily ozone measured in the Los Angeles basin and \( p = 134 \) variables modelling the pairwise interaction of 9 meteorological and 3 time variables. We consider the cleaned up version of the data which removes missing observations.

For convenience, we firstly normalized the design matrix by dividing each column by its Euclidean norm. We then apply the four methods investigated above (i.e. our Laplace VB approach, varbvs, EMVS and spikeslab) with unknown noise variance \( \sigma^2 \). The resulting inclusion probabilities of each variable are shown in Figure 6, where we see that each method results in a substantially different outcome. Collecting the selected variables whose marginal posterior inclusion probability exceeds 0.5, we again obtain fairly different results. The selected variables for the Laplace VB approach are \((x_{40}, x_{47}, x_{48}, x_{50}, x_{53}, x_{118}, x_{123})\), for the EMVS method \((x_2, x_{81}, x_{83}, x_{85}, x_{86}, x_{88}, x_{93}, x_{94}, x_{100}, x_{102}, x_{108}, x_{112}, x_{114}, x_{115}, x_{118}, x_{120}, x_{122}, x_{123}, x_{126}, x_{127}, x_{129}, x_{132})\), for the varbvs method \((x_2, x_{53}, x_{118}, x_{127})\) and for the spikeslab method \((x_2, x_{45}, x_{47}, x_{48}, x_{50}, x_{53}, x_{64}, x_{102}, x_{115}, x_{118}, x_{120}, x_{127})\). We remark that the spikeslab algorithm was quite unstable since running the method multiple times on the same data set gave different outcomes. We have therefore omitted this procedure from the plots. One can see that although there is some overlap between the models selected by the different methods, the results are quite different. As there is no underlying truth to compare our results to, we cannot ascertain which methods performed well. However, in view of the good performance of the VB Laplace method demonstrated in the previous simulations, we think that the resulting model provides a good alternative which is worthwhile analyzing further from a practical point of view.
6 Conclusion

We studied the theoretical contraction rates of a natural sparsity-inducing mean-field variational Bayes approximation to posteriors arising from widely used, but computationally challenging, model selection priors in high-dimensional sparse linear regression. We showed that under a mutual coherence condition on the design matrix, such an approximation converges to a sparse truth at the optimal (minimax) rate in both $\ell_2$ and prediction loss, and performs suitable model selection. This provides a theoretical justification for this approximation algorithm in a sparsity context.

We investigated the empirical performance of our algorithm via simulated and real-world data and showed that it generally performs at least as well as other state-of-the-art Bayesian variable selection methods including existing VB approaches. We also demonstrated how the widely used coordinate-ascent variational inference (CAVI) algorithm can be highly sensitive to the updating order of the parameters. We therefore proposed a novel prioritized updating scheme that uses a data-driven updating order and performed better in simulations. This idea may be applicable for CAVI approaches in other settings.

7 General results

The conditions for Theorems 1-4 can be slightly weakened at the expense of several additional conditions on the design matrix. In this section we present these more technical results which directly imply Theorems 1-4.

We recall from Section 2.2 that in the sparse setting, ‘local invertibility’ of the Gram matrix $X^T X$ is sufficient for estimation, which was quantified via the mutual coherence number $\mu$. The notion of invertibility can be made more precise using the following definitions, which are based on the sparse high-dimensional literature (e.g. [6]), and have been adapted to the Bayesian setting in [13]. We provide only a brief description, referring the interested reader to Section 2.2 of [13] for further discussion.

**Definition 2 (Compatibility).** A model $S \subseteq \{1, \ldots, p\}$ has compatibility number

$$\phi(S) = \inf \left\{ \frac{\|X\theta\|_2^{1/2}|S|^{1/2}}{\|X||\theta_S\|_1} : \|\theta_{S^c}\|_1 \leq 7\|\theta_S\|_1, \theta_S \neq 0 \right\}.$$  

A model is considered ‘compatible’ if $\phi(S) > 0$, in which case $\|X\theta\|_2^{1/2} \geq \phi(S)\|X\|\|\theta_S\|_1$ for all $\theta$ in the above set. The number 7 is not important and is taken in Definition 2.1 of [13] to provide a specific numerical value; since we use several results from [13], we employ the same convention. Note that $\phi(S)$ equals $\phi_{\text{comp}}(7, S)/\|X\|$ in the notation of [6], p. 157. The compatibility number does not directly require sparsity, but reduces the problem to approximate sparsity by considering only vectors $\theta$ whose coordinates are small outside $S$.

Conversely, the following two definitions deal only with sparse vectors.

**Definition 3 (Uniform compatibility for sparse vectors).** The compatibility number for vectors of dimension $s$ is

$$\overline{\phi}(s) = \inf \left\{ \frac{\|X\theta\|_2|S\theta|^{1/2}}{\|X\|\|\theta\|_1} : 0 \neq |S\theta| \leq s \right\}.$$
Definition 4 (Smallest scaled sparse singular value). The smallest scaled sparse singular value of dimension $s$ is

$$\tilde{\phi}(s) := \inf \left\{ \frac{\|X\theta\|_2}{\|\theta\|_2} : 0 \neq |S_\theta| \leq s \right\}.$$  

In the notation of [7], these are equal to the minima over $|S| \leq s$ of the numbers $\Lambda_{\text{min},1}(\Sigma_{1,1}(S))/\|X\|$ and $\Lambda_{\text{min}}(\Sigma_{1,1}(S))/\|X\|$, respectively. We shall require that these numbers are bounded away from zero for $s$ a multiple of the true model size. Note that if $\|X\| = 1$, then $\tilde{\phi}(s)$ is simply the smallest scaled singular value of a submatrix of $X$ of dimension $s$.

Note that Definitions [2][4] are Definitions 2.1-2.3 of [13]. Such compatibility conditions are standard for sparse recovery problems, see Sections 6.13 and 7.15 of [7] for further discussion. These notions can be related with each other and the mutual coherence number (6) via the following result.

Lemma 1 (Lemma 1 of [13]). $\phi(S)^2 \geq \tilde{\phi}(1)^2 - 15|S|mc(X)$, $\tilde{\phi}(s)^2 \geq \bar{\phi}(s)^2 \geq \tilde{\phi}(1)^2 - smc(X)$.

By evaluating the infimum in Definition [3] at the unit vectors, one obtains $\tilde{\phi}(1) = \tilde{\phi}(1) = \min_{i} \|X_i\|_2/\|X\| = \min_{i \neq j} \|X_{i,j}\|_2/\|X\|_2$, which is bounded away from zero if the columns of $X$ have comparable Euclidean norms. In this case, Lemma [1] implies that the compatibility numbers and sparse singular values are bounded away from zero for models of size $O(1/mc(X))$. The mutual coherence condition is thus in some sense the strongest of these notions.

The contraction rate further depends on the compatibility constants in the following way. For $M > 0$, set

$$\bar{\psi}_M(S) = \tilde{\phi} \left( 2 + \frac{4M}{A_4} (1 + \frac{8}{\phi(S)^2 \|X\| \log p}) \right) |S|,$$

$$\tilde{\psi}_M(S) = \bar{\psi} \left( 2 + \frac{4M}{A_4} \left( 1 + \frac{8}{\phi(S)^2 \|X\| \sqrt{\log p}} \right) \right) |S|.$$  

(17)

By [5], $\lambda = o(\|X\|/\sqrt{\log p})$ and hence these constants are asymptotically bounded from below by $\tilde{\phi}(2 + 4M/A_4)|S|$ and $\phi(2 + 4M/A_4)|S|$ if $\phi(S)$ is bounded away from zero.

The following establishes contraction of the variational approximations in both $\ell_2$ and prediction loss.

Theorem 5. Suppose the model selection prior [3] satisfies [4] and [5], and $s_n$ satisfies $\lambda s_n \sqrt{\log p}/\|X\| \to 0$. For any $c_0 > 0$, any $d_0 \leq c_0^2 (1 + 2/A_4)^{-1}/8$ and any $\rho_n \to \infty$ (arbitrarily slowly), the variational Bayes posterior $\bar{\Pi}$ given in (9) satisfies, with $S_0 = S_{\theta_0}$,

$$\sup_{\theta_0, \phi(S_0) \geq c_0, \psi_{\rho_n}(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq d_0 mc(X)^{-1}} E_{\theta_0, \bar{\Pi}} \left( \theta : \|\theta - \theta_0\|_2 \geq M\sqrt{\rho_n |S_0| \log p}/\|X\| \right) \to 0,$$

$$\sup_{\theta_0, \phi(S_0) \geq c_0, \psi_{\rho_n}(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq d_0 mc(X)^{-1}} E_{\theta_0, \bar{\Pi}} \left( \theta : \|X(\theta - \theta_0)\|_2 \geq M\sqrt{\rho_n |S_0| \log p} \right) \to 0,$$

where $M > 0$ depends only on $c_0$. Moreover, the same holds true for the variational Bayes posteriors $\check{Q}$ and $\check{Q}$ based on the mean-field variational families [10] and [12], respectively.
This result gives a more explicit dependence on various compatibility constants that are common in the literature. Theorem 5 is only slightly more general than Theorems 1 and 3, essentially replacing the condition $|S_0| = o(mc(X)^{-1})$ with $|S_0| = O(mc(X)^{-1})$. Since the above is what we actually prove, we include the full statement for completeness. We also have an analogue for model selection, which implies Theorems 2 and 4.

**Theorem 6.** Suppose the model selection prior (3) satisfies (4) and (5), and $s_n$ satisfies $\lambda s_n \sqrt{\log p}/\|X\| \to 0$. For any $c_0 > 0$ and any $d_0 \leq c_0(1 + 2/A_4)^{-1}/8$,

$$\sup_{\theta_0: \phi(S_0) \geq c_0, \psi(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq d_0 mc(X)^{-1}} E_{\theta_0} \bar{\Pi}(\theta : |S_0| > M_n |S_0|) \to 0,$$

where $M_n \to \infty$ (arbitrarily slowly). Moreover, the same holds true for the variational Bayes posteriors $Q$ and $\tilde{Q}$ based on the mean-field variational families (10) and (12), respectively.

The proofs of Theorems 5 and 6 are deferred to Section 8. In particular, these results immediately imply Theorems 1, 4.

**Proof of Theorems 7 and 8.** We only need to show that the conditions in Theorems 1 and 3, which are identical, imply that the conditions in the supremum of Theorem 5 are satisfied for any $\rho_n \to \infty$ arbitrarily slowly, whence the result follows from the latter theorem.

Since $v_n \to 0$, it holds that $|S_0| \leq d_0 mc(X)^{-1}$ for any $d_0 > 0$ and $n$ large enough. Recall that $\bar{\psi}(1) = \min_{|X|} ||X||/||X|| \geq \eta > 0$ by assumption so that by Lemma 1, $\phi(S_0)^2 \geq \eta^2 - 15s_n \geq \eta^2/4$ for $n$ large enough. Again using Lemma 1, the definition (17) and that $\lambda = o(||X||/(s_n \sqrt{\log p}))$, for any $\rho_n > 0$ and $n$ large enough,

$$\bar{\psi}_{\rho_n}(S_0)^2 \geq \bar{\psi}(1)^2 - \left(2 + \frac{4\rho_n}{A_4} \left(1 + \frac{8}{\phi(S_0)^2 ||X|| \sqrt{\log p}}\right)\right) |S_0| mc(X)$$

$$\geq \eta^2 - \left(2 + \frac{4\rho_n}{A_4} \left(1 + \frac{32}{\eta^2 s_n \log p}\right)\right) v_n \geq \eta^2 - C\rho_n v_n.$$

Since $v_n \to 0$, taking $\rho_n \to \infty$ such that $\rho_n v_n \to 0$ gives that the right-hand side is lower bounded by $\eta^2 - o(1)$. We therefore have that for $n$ large enough,

$$\{ \theta_0 : |S_0| \leq s_n, |S_0| \leq v_n mc(X)^{-1} \}$$

$$\subset \{ \theta_0 : \phi(S_0) \geq \eta/2, \bar{\psi}_{\rho_n}(S_0) \geq \eta/2, |S_0| \leq s_n, |S_0| \leq d_0 mc(X)^{-1} \},$$

which is the supremum in Theorem 5. That theorem thus gives $\ell_2$ and prediction loss posterior contraction rates $M \sqrt{\rho_n |S_0| \log p}/||X||$ and $M \sqrt{\rho_n |S_0| \log p}$ for some $M > 0$, respectively. Since $\rho_n \to \infty$ can be taken to diverge arbitrarily slowly, this completes the proof.

**Proof of Theorems 2 and 4.** The proofs follow from Theorem 6 in a similar way to the proof of Theorems 1 and 3 above.

## 8 Proofs

### 8.1 Proof of Theorems 5 and 6

The proofs of Theorems 5 and 6 rely on the next result, which allows one to exploit exponential probability bounds for the posterior to control the corresponding probability under the
variational approximation. This result is similar in spirit to Theorem 2.1 of [40], which employs the classical prior mass and testing approach of Bayesian nonparametrics [19]. However, since it is known that posterior convergence rates for model selection priors cannot easily be established using this approach [15, 13], their result does not apply to our setting.

**Theorem 7.** Let \( \Theta_n \) be a subset of the parameter space, \( A \) be an event and \( Q \) be a distribution for \( \theta \). If there exist \( C > 0 \) and \( \delta_n > 0 \) such that

\[
E_{\theta_0} \Pi(\theta \in \Theta_n|Y)1_{A} \leq Ce^{-\delta_n},
\]

then

\[
E_{\theta_0} Q(\theta \in \Theta_n)1_{A} \leq \frac{2}{\delta_n} \left[ E_{\theta_0} KL(Q||\Pi(\cdot|Y))1_{A} + Ce^{-\delta_n/2} \right].
\]

**Proof.** Recall the duality formula for the Kullback-Leibler divergence ([5], Corollary 4.15)

\[
KL(Q||P) = \sup_f \left[ \int f dQ - \log \int e^f dP \right],
\]

where the supremum is taken over all measurable \( f \) such that \( \int e^f dP < \infty \). In particular, this yields

\[
\int f(\theta)dQ(\theta) \leq KL(Q||\Pi(\cdot|Y)) + \log \int e^{f(\theta)}d\Pi(\theta|Y).
\]

Applying this inequality with \( f(\theta) = \frac{1}{2} \delta_n 1_{\Theta_n}(\theta) \) and using that \( \log(1 + x) \leq x \) for \( x \geq 0 \),

\[
\frac{1}{2} \delta_n Q(\theta \in \Theta)1_{A} \leq KL(Q||\Pi(\cdot|Y))1_{A} + \log \left( 1 + \Pi(\theta \in \Theta_n|Y)e^{\delta_n/2} \right)1_{A}
\]

\[
\leq KL(Q||\Pi(\cdot|Y))1_{A} + e^{\delta_n/2}\Pi(\theta \in \Theta_n|Y)1_{A}.
\]

Taking \( E_{\theta_0} \)-expectations on both sides and using (18) gives the result. \( \square \)

To prove Theorem 5, it therefore suffices to show that on a suitable event, one can 1) control the Kullback-Leibler divergence between the variational approximation and the true posterior and 2) establish the appropriate posterior tail inequality (18). Define the events

\[
T_0 = \{ \|X^T(Y - X\theta_0)\|_\infty \leq 2\|X\|/\sqrt{\log p} \},
\]

and

\[
T_1 = T_0 \cap \left\{ \Pi(\theta : |S_0| \leq \left( 1 + \frac{12}{A_4} (1 + \frac{8}{\phi(S_0)^2 \|X\|/\sqrt{\log p}}) \right) |S_0| |Y| \geq 1 - \zeta_n \right\}
\]

\[
\cap \left\{ \Pi(\theta : S_0 \supseteq \{ i : |\theta_{0,i} | \geq K \sqrt{\log p}/\|X\| |Y| \} \geq 1 - \zeta_n \right\},
\]

where \( \zeta_n \to 0 \) and \( K > 0 \) is a sufficiently large constant. The middle event in \( T_1 \) says that with probability approaching 1, the posterior selects parameters with support of size at most \( L_0 s_0 \) for some \( L_0 > 1 \) depending on the compatibility number \( \phi(S_0) \) (note that our choice of \( \lambda \) in Theorem 5 ensures \( \lambda/(\|X\|/\sqrt{\log p}) = o(1) \)). The last event says that the posterior selects parameters whose support contains all indices for which the true signal is sufficiently large.
(i) The event $\mathcal{T}_0$ defined in (19) satisfies
\[ \inf_{\theta_0 \in \mathbb{R}^p} P_{\theta_0}(\mathcal{T}_0) \geq 1 - 2/p. \]
(ii) Suppose the prior $\pi_p$ satisfies (4) and (5), and $s_n$ satisfies $\lambda s_n \sqrt{\log p}/\|X\| \to 0$. Then for any $c_0 > 0$ and any $d_0 \leq c_0^2 (1 + 2/A_4)^{-1}/8$, the event $\mathcal{T}_1$ defined in (20) satisfies
\[ \inf_{\theta_0 : \phi(S_0) \geq c_0, \psi(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq d_0 c_0 \|X\|^{-1}} P_{\theta_0}(\mathcal{T}_1) \to 1 \]
for some $K > 0$ large enough and $\zeta_n \to 0$ slowly enough.

Proof. (i) Under $P_{\theta_0}$, $X^T(Y - X\theta_0) = X^T Z \sim N_p(0, X^T X)$. Since $(X^T Z)_i \sim N(0, (X^T X)_{ii})$ and $(X^T X)_{ii} \leq \|X\|^2$ for all $1 \leq i \leq p$, a union bound and the standard Gaussian tail inequality give
\[ P_{\theta_0}(\mathcal{T}_0^c) = P(\|X^T Z\|_\infty \geq 2\|X\| \sqrt{\log p}) \leq \sum_{i=1}^p P(\|N(0, 1)\| \geq 2 \sqrt{\log p}) \leq p \frac{2}{\sqrt{2\pi}} e^{-2 \log p}. \]

(ii) Note that to have $s_n \geq 1$ and $\lambda s_n \sqrt{\log p}/\|X\| \to 0$, we require $\lambda = o(\|X\|/\sqrt{\log p})$. We may thus apply Lemma 7 below with $M = 3$, so that writing $L_0 = 1 + \frac{12}{A_4} \left(1 + \frac{8}{\phi(S_0)^2 \|X\| \sqrt{\log p}}\right)$ and $L_1 = 1 + 8 \lambda/\|X\| \sqrt{\log p} \phi(S_0)^2$, for all $\theta_0 \in \mathbb{R}^p$,
\[ E_{\theta_0} \Pi(\theta : |S_\theta| > L_0 s_n |Y|) \frac{1}{T_0} \leq C(A_2, A_4) e^{-L_1 s_n \log p}. \]

By Markov's inequality, for any $\zeta > 0$,
\[ P_{\theta_0} \left( \{ \Pi(\theta : |S_\theta| > L_0 s_n |Y|) > \zeta \} \cap \mathcal{T}_0 \right) \leq \zeta^{-1} E_{\theta_0} \Pi(\theta : |S_\theta| > L_0 s_n |Y|) \frac{1}{T_0} \to 0 \]
uniformly over all $\theta_0$ with $\phi(S_0) \geq c_0 > 0$. The above convergence moreover extends to any sequence $\zeta_n \to 0$ sufficiently slowly, as required.

By Theorem 5 of [13], for every $c_0 > 0$, any $d_0 \leq c_0^2 (1 + 2/A_4)^{-1}/8$ and any $s_n$ with $\lambda s_n \sqrt{\log p}/\|X\| \to 0$, there exists a sufficiently large constant $K > 0$ such that
\[ \inf_{\theta_0 : \phi(S_0) \geq c_0, \psi(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq d_0 c_0 \|X\|^{-1}} E_{\theta_0} \Pi \left( \theta : S_\theta \supset \left\{ i : |\theta_{0,i}| \geq K \sqrt{\log p}/\|X\| \right\} \right) \frac{1}{Y} \to 1. \]

[In particular, they take the infimum over $\tilde{\psi}(S_0) \geq c_0$, where $\tilde{\psi}$ is defined in (2.5) of [13], instead of our $\psi_3(S_0) \geq c_0$, where $\psi_3$ comes from (17). One can check that $\psi(S_0) \geq \tilde{\psi}_3(S_0)$, so that the infimum in Theorem 5 of [13] is actually taken over a strictly larger set and so implies the last display.] Arguing exactly as above, the $P_{\theta_0}$-probability that the posterior probability in the last display is at least $1 - \zeta_n$ tends to one for $\zeta_n \to 0$ slowly enough. \qed

Proof of Theorem 3. Let $\mathcal{T}_1$ denote the event in (20), which by Lemma 2(ii) satisfies $P_{\theta_0}(\mathcal{T}_1) \to 1$ uniformly over all $\theta_0$ in the theorem hypothesis. Setting $\Theta_n = \{ \theta : \|\theta - \theta_0\|_2 \geq M \sqrt{\rho_n s_n \log p}/\|X\| \}$ for some $M > 0$, $E_{\theta_0} \Pi(\Theta_n) \leq E_{\theta_0} \Pi(\Theta_n) 1_{\mathcal{T}_1} + o(1)$. We now apply Theorem 7 with this choice of $\Theta_n$ on the event $\mathcal{T}_1$. Using the second part of Lemma 8 below with $L + 2 = p_n$ gives
\[ \sup_{\theta_0 : \phi(S_0) \geq c_0, \psi_n(S_0) \geq c_0} E_{\theta_0} \Pi \left( \theta : \|\theta - \theta_0\|_2 \geq M \sqrt{\rho_n s_n \log p}/\|X\| \right) 1_{\mathcal{T}_1} \leq C e^{-c_p n \log p}. \]
for $n$ large enough, where $M, c > 0$ are constants depending only on $c_0, A_4$ and $C > 0$ depends only on $A_2, A_4$. Since $T_1 \subset T_0$ by $(20)$, condition $(18)$ is satisfied on $T_1$ with $\delta_n = c \rho_n s_0 \log p$. By Lemma 6 below, KL($\hat{\Pi}||\Pi(\cdot|Y)$) $\leq M' \rho_n s_0 \log p$ uniformly over all $\theta_0$ in the theorem hypothesis, where $M' > 0$ depends only on $c_0, A_4$. Applying Theorem 7 therefore gives

$$
\sup_{\theta_0: \phi(S_0) \geq c_0, \hat{\psi}_n(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq \delta_0 mc(X)^{-1}} E_{\theta_0} \hat{\Pi}(\Theta_n) 1_{T_1} \leq \frac{2M'}{c \rho_n} + \frac{2Ce^{-c \rho_n s_0 \log p/2}}{c \rho_n s_0 \log p} \to 0
$$

since $\rho_n \to \infty$. The result for prediction loss follows exactly as above by considering $\Theta_n = \{\theta : \|X(\theta - \theta_0)\|_2 \geq M \sqrt{\rho_n s_0 \log p}\}$ and using the first part of Lemma 8 to establish $(18)$. The results for the variational Bayes posteriors $\hat{Q}$ and $\tilde{Q}$ based on the mean-field variational families $(10)$ and $(12)$ follow identically upon using Lemmas 3 and 5 instead of Lemma 6 to control the Kullback-Leibler divergence.

**Proof of Theorem 6**. The proof follows similarly to that of Theorem 3 by applying Theorem 7 with $\Theta_n = \{\theta : \|\theta - \theta_0\|_2 \geq M_n|\theta_0|\}$, again taking the event $A = T_1$ and using Lemma 7 instead of Lemma 5 to verify $(18)$. 

### 8.2 Kullback-Leibler divergences between variational classes and the posterior

To apply Theorem 7 we show that on the event $T_1$ in $(20)$ we can bound the (minimized) Kullback-Leibler divergences between the posterior and the approximating variational classes. This is the major technical difficulty in establishing our result. We first consider the family $Q$ of distributions $(10)$, which consists of products of non-diagonal multivariate normal distributions with Dirac delta distributions for a single fixed support set $S$.

For a given model $S \subseteq \{1, \ldots, p\}$, let $X_S$ denote the $n \times |S|$-submatrix of the full regression matrix $X$, where we keep only the columns $X_i, i \in S$. Let $\hat{\theta}_S = (X_S^T X_S)^{-1} X_S^T Y$ be the least squares estimator in the restricted model $Y = X_S \theta_S + Z$. If the restricted model were correctly specified, then $\hat{\theta}_S$ would have distribution $N_S(\theta_0, S, (X_S^T S)^{-1})$ under $P_{\theta_0}$. We approximate the posterior with a $N_S(\hat{\theta}_S, (X_S^T S)^{-1}) \otimes \delta_{S^c}$ distribution, where $S$ is a suitable approximating set to which the posterior assigns sufficient probability.

**Lemma 3**. Under the conditions of Lemma 2(ii), the variational posterior $\hat{Q}$ arising from the family $(10)$ satisfies

$$
\sup_{\theta_0: \phi(S_0) \geq c_0, \hat{\psi}_n(S_0) \geq c_0, |S_0| \leq s_n, |S_0| \leq \delta_0 mc(X)^{-1}} \frac{\text{KL}(\hat{Q}||\Pi(\cdot|Y))}{1 + \frac{12}{A_4}(1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\| \sqrt{\log p}})} \leq \frac{1}{s_0 \log p} \to 1 + o(1).
$$

**Proof.** We construct our posterior approximation on the event $T_1$ in $(20)$. For notational convenience write $L_0 = 1 + \frac{12}{A_4}(1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\| \sqrt{\log p}})$, the constant in the second event in $T_1$. Note also that to have $s_n \geq 1$ and $\lambda s_n \sqrt{\log p}/\|X\| \to 0$, we require $\lambda = o(\|X\|/\sqrt{\log p})$. The posterior takes the form

$$
\Pi(\cdot|Y) = \sum_{S \subseteq \{1, \ldots, p\}} q_S \Pi_S(\cdot|Y) \otimes \delta_{S^c},
$$

where $q_S = \frac{1}{L_0}$.
where the weights $\hat{q} = (\hat{q}_S : S \subseteq \{1, \ldots, p\})$ lie in the $2^p$-dimensional simplex and $\Pi_S(\cdot|Y)$ is the posterior for $\theta_S \in \mathbb{R}^{|S|}$ in the restricted model $Y = X_S\theta_S + Z$. This implies that on $\mathcal{T}_1$,

$$
\sum_{S:|S| \leq L_0s_0} \hat{q}_S \geq 1 - 2\zeta_n \geq 1/2
$$

for $n$ large enough since $\zeta_n \to 0$. Furthermore, since

$$
\left\{ S \subseteq \{1, \ldots, p\} : |S| \leq L_0s_0 \right\} = \sum_{s=0}^{L_0s_0} \binom{p}{s} \leq \sum_{s=0}^{L_0s_0} \frac{p^s}{s!} \leq e^{pL_0s_0},
$$

for any $n$ large enough and on $\mathcal{T}_1$ there exists a set $\hat{S}$ with $|\hat{S}| \leq L_0s_0$, $\hat{S} \supseteq \{ i : |\theta_0,i| \geq K\sqrt{\log p/\|X\|} \}$ and such that $\hat{q}_\hat{S} \geq (2e)^{-1}p^{-L_0s_0}$.

Since an $N_S(\mu_S, \Sigma_S) \otimes \delta_{S^c}$ distribution is only absolutely continuous with respect to the $\hat{q}\Pi_S(\cdot|Y) \otimes \delta_{S^c}$ term of the posterior,

$$
\inf_{Q \in \mathcal{Q}} KL(Q(\cdot|Y)) = \inf_{S:|S| \leq L_0s_0} E_{\theta \sim N_S(\mu_S, \Sigma_S) \otimes \delta_{S^c}} \log \frac{dN_S(\mu_S, \Sigma_S) \otimes \delta_{S^c}}{d\hat{q}\Pi_S(\cdot|Y) \otimes \delta_{S^c}} \leq \log \frac{1}{\hat{q}_\hat{S}} + \inf_{\mu_S, \Sigma_S} KL(N_S(\mu_S, \Sigma_S)\| \Pi_S(\cdot|Y)),
$$

where the last Kullback-Leibler divergence is over the $|\hat{S}|$-dimensional distributions. On $\mathcal{T}_1$ and for $n$ large enough, $\log(1/\hat{q}_\hat{S}) \leq \log(2ep^{L_0s_0}) = \log(2e) + L_0s_0 \log p$. It thus remains to show that the second term in (21) is $o(s_0 \log p)$.

Let $E_{\mu_S, \Sigma_S}$ denote the expectation under the law $\theta_S \sim N_S(\mu_S, \Sigma_S)$. Setting

$$
\mu_S = (X_S^T X_S)^{-1} X_S^T Y \quad \text{and} \quad \Sigma_S = (X_S^T X_S)^{-1},
$$

one can check that the resulting normal distribution has density function proportional to $e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2}$, $\theta_S \in \mathbb{R}^{|S|}$. Therefore,

$$
KL(N_S(\mu_S, \Sigma_S)\| \Pi_S(\cdot|Y)) = E_{\mu_S, \Sigma_S} \log \frac{D_{\Pi}}{D_N} e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2 - \lambda\|\theta_S\|_1} = E_{\mu_S, \Sigma_S} \lambda(\|\theta_S\|_1 - \|\theta_0,\hat{S}\|_1) + \log(D_{\Pi}/D_N),
$$

with $D_{\Pi} = \int_{\mathbb{R}^{|\hat{S}|}} e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2 - \lambda\|\theta_S\|_1} d\theta_S$ and $D_N = \int_{\mathbb{R}^{|\hat{S}|}} e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2 - \lambda\|\theta_S\|_1} d\theta_S$ the normalizing constants.

We firstly upper bound $\log(D_{\Pi}/D_N)$. Define

$$
B_S = \{ \theta_S \in \mathbb{R}^{|S|} : \|\theta_S - \theta_{0,S}\|_2 \leq \tilde{M} \sqrt{s_0 \log p/\|X\|} \}
$$

for some $\tilde{M} > 0$. Since $\mathcal{T}_1 \subset \mathcal{T}_0$, Lemma [4] yields that

$$
\Pi_S(B_S^c|Y)_{\mathcal{T}_1} = \frac{\int_{B_S^c} e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2 - \lambda\|\theta_S\|_1} d\theta_S}{\int_{\mathbb{R}^{|S|}} e^{-\frac{1}{2}\|Y - X_S\theta_S\|_2^2 - \lambda\|\theta_S\|_1} d\theta_S} 1_{\mathcal{T}_1} \to 0
$$

almost surely for

$$
\tilde{M} = \frac{1}{\phi(L_0s_0)} \left( 5Kd_0^{1/2} + L_0^{1/2} \left( 5 + \frac{32}{\phi(L_0s_0)} \right) \right),
$$

where $d_0 = \frac{2K}{\phi(L_0s_0)}$.
where we have used $s_0mc(X) \leq d_0$. In particular, $\int_{B_S} e^{-\frac{1}{2}\|Y-X_S\theta_S\|^2 - \lambda\|\theta_S\|_1} d\theta_S = D_\Pi(1-o(1))$ on $T_1$. Therefore on $T_1$,

$$
\log \frac{D_\Pi}{D_N} \leq \log \frac{\int_{B_S} e^{-\frac{1}{2}\|Y-X_S\theta_S\|^2 - \lambda\|\theta_S\|_1} d\theta_S(1 + o(1))}{\int_{B_S} e^{-\frac{1}{2}\|Y-X_S\theta_S\|^2 - \lambda\|\theta_S\|_1} d\theta_S}
$$

$$
\leq \sup_{\theta_S \in B_S} \log e^{\lambda\|\theta_S\|_1 - \lambda\|\theta_S\|_1} + \log(1 + o(1))
$$

$$
\leq \sup_{\theta_S \in B_S} \lambda\|\theta_S - \theta_S\|_1 + o(1)
$$

$$
\leq \sup_{\theta_S \in B_S} \lambda\|	ilde{S}\|^{1/2}\|\theta_S - \theta_S\|_2 + o(1)
$$

$$
\leq \lambda\tilde{M}L_0^{1/2}s_0\sqrt{\log p}/\|X\| + o(1),
$$

where in the fourth inequality we have applied Cauchy-Schwarz.

We now turn to the first term in (23). On $T_1$, using the triangle inequality and Cauchy-Schwarz,

$$
\lambda E_{\mu,\Sigma}(\|\theta\| - \|\theta_{\tilde{S}}\|_1) \leq \lambda\|\mu - \theta_S\|_1 + \lambda E_{\mu,\Sigma}(\|\theta\|_1)
$$

$$
\leq \lambda\|	ilde{S}\|^{1/2}(\|\mu - \theta_S\|_2 + \text{Tr}(\Sigma_{\tilde{S}})^{1/2})
$$

(24)

since $E_{\mu,\Sigma}(\|\theta\|_2^2) = \text{Tr}(\Sigma_{\tilde{S}})$. Let $\Lambda_{\text{min}}(A)$ and $\Lambda_{\text{max}}(A)$ denote the smallest and largest eigenvalues, respectively, of a symmetric, positive definite matrix $A$. Using the variational characterization of maximal/minimal eigenvalues (21), p. 234, for any $S \subseteq \{1, \ldots, p\}$,

$$
\Lambda_{\text{min}}(X_S^T X_S) = \min_{v \in \mathbb{R}^{|S|}: v \neq 0} \frac{v^T X_S^T X_S v}{\|v\|^2_2} = \min_{u \in \mathbb{R}^{|S|}: u \neq 0, u_{S^c} = 0} \frac{\|X u\|^2_2}{\|u\|^2_2} \geq \|X\|^2 \phi(|S|)^2.
$$

(25)

Therefore,

$$
\text{Tr}(\Sigma_{\tilde{S}}) \leq \|\tilde{S}\|\Lambda_{\text{max}}((X_S^T X_S)^{-1}) \leq \frac{L_0s_0}{\Lambda_{\text{min}}(X_S^T X_S)} \leq \frac{L_0s_0}{\|X\|^2 \phi(L_0s_0)^2}.
$$

Under $P_{\theta_0}$, using (1) and (22) the bias term can be decomposed as

$$
\|\mu_S - \theta_S\|_2 \leq \|\tilde{S}\|\Lambda_{\text{max}}((X_S^T X_S)^{-1}) X_S^T X_{\tilde{S}}^{0,\tilde{S}} \theta_{0,\tilde{S}}\|_2 + \|\tilde{S}\|\Lambda_{\text{max}}((X_S^T X_S)^{-1}) X_{\tilde{S}}^T Z_2 = I + II.
$$

Noting that the $\ell_2$-operator norm of $(X_S^T X_S)^{-1}$ is bounded by $1/\|X\|^2 \phi(|\tilde{S}|)^2$ by (25), we
have that on $\mathcal{T}_1$, using the definition of $\tilde{S}$,

$$I^2 \leq \frac{1}{\|X\|^4\tilde{\phi}(|\tilde{S}|)^4}\|X_S^TX_{\tilde{S}}\theta_{0,\tilde{S}}\|^2$$

$$= \frac{1}{\|X\|^4\tilde{\phi}(|\tilde{S}|)^4}\sum_{i \in \tilde{S}} \left(\sum_{k=1}^n\sum_{j \in \tilde{S}} X_{ki}X_{kj}\theta_{0,j}\right)^2$$

$$= \frac{1}{\|X\|^4\tilde{\phi}(|\tilde{S}|)^4}\sum_{i \in \tilde{S}} \left(\sum_{j \in \tilde{S} \cap S_0} \langle X_i, X_j \rangle \theta_{0,j}\right)^2$$

$$\leq \frac{mc(X)^2}{\tilde{\phi}(|\tilde{S}|)^4}\sum_{i \in \tilde{S}} \left(\sum_{j \in \tilde{S} \cap S_0} |\theta_{0,j}|\right)^2$$

$$\leq \frac{mc(X)^2|\tilde{S}|s_0^2K^2\log p}{\|X\|^2\tilde{\phi}(|\tilde{S}|)^4}.$$  

Using the same bound on the $\ell_2$-operator norm and $[1]$, on the event $\mathcal{T}_1 \subset \mathcal{T}_0$ it holds that

$$II \leq \frac{\|X_S^TZ\|^2}{\|X\|^2\tilde{\phi}(|\tilde{S}|)^2} \leq \frac{1}{\|X\|^2\tilde{\phi}(|\tilde{S}|)^2}\left(\sum_{i \in \tilde{S}} \langle X^T(Y - X\theta)\rangle_i^2\right)^{1/2} \leq \frac{2|\tilde{S}|^{1/2}\sqrt{\log p}}{\|X\|\tilde{\phi}(|\tilde{S}|)^2}.$$  

Combining all of the above bounds and using that $|\tilde{S}| \leq L_0s_0$, on the event $\mathcal{T}_1$,

$$\lambda E_{\mu_0,\Sigma_0}(\|\theta_{\tilde{S}}\|_1 - \|\theta_{0,\tilde{S}}\|_1) \leq \frac{\lambda L_0s_0}{\|X\|\tilde{\phi}(L_0s_0)} \left(1 + \frac{2 + Ks_0mc(X)}{\tilde{\phi}(L_0s_0)} \sqrt{\log p}\right).$$

Together with [23], the bound $\log(D_\Pi/D_N) \leq \lambda\tilde{\lambda}L_0^{1/2}s_0\sqrt{\log p}/\|X\|$ derived above and $s_0mc(X) \leq d_0$, this yields

$$\text{KL}(N_{\tilde{S}}(\mu_{\tilde{S}}, \Sigma_{\tilde{S}}) \| \Pi_{\tilde{S}}(\cdot|Y))_{1_{\mathcal{T}_1}} \leq \frac{\lambda_0^{1/2}s_0\sqrt{\log p}}{\|X\|}\left(\tilde{M} + \frac{L_0^{1/2}}{\tilde{\phi}(L_0s_0)\sqrt{\log p}} + \frac{L_0^{1/2}(2 + Kd_0)}{\tilde{\phi}(L_0s_0)} \right).$$

Since $\tilde{\phi}(L_0s_0) = \tilde{\psi}_3(S_0)$ by $[17]$ and $\lambda = o(\|X\|/\sqrt{\log p})$, the last display is $o(s_0 \log p)$ uniformly over the supremum in the lemma hypothesis. The dominant term in the upper bound for [21] is thus $\log(1/\hat{q}_{\tilde{S}}) \leq L_0s_0 \log p + o(1)$ derived above, which completes the proof.

\begin{lemma}
Let $S \subseteq \{1, \ldots, p\}$ and denote by $\Pi_{S}(\cdot|Y)$ the posterior distribution for $\theta_S \in \mathbb{R}^{|S|}$ in the restricted model $Y = X_S\theta_S + Z$. Then for any $L_0, K > 0$,

$$\sup_{\theta_0 \in \mathbb{R}^p} \max_{S: |S| \leq L_0s_0} \Pi_{S}(\theta_S \in \mathbb{R}^{|S|} : \|\theta_S - \theta_{0,S}\|_2 \geq R_0|Y)_{1_{\mathcal{T}_0}} \to 0$$

almost surely, where $\mathcal{T}_0$ is the event $[19]$ and

$$R_0 = \frac{1}{\|X\|\tilde{\phi}(L_0s_0)} \left(5Kmc(X)^{1/2}s_0^{1/2} + L_0^{1/2}\left(5 + \frac{32}{\tilde{\phi}(L_0s_0)}\right)\right) \sqrt{S_0\log p}.$$
Proof. Write \( s_0 = |S_{\theta_0}| \). Let \( \tilde{\theta}_S \) denote the extension of a vector \( \theta_S \in \mathbb{R}^{|S|} \) to \( \mathbb{R}^p \) with \( \tilde{\theta}_{S,i} = \theta_{S,i} \) for \( i \in S \) and \( \tilde{\theta}_{S,i} = 0 \) for \( i \notin S \). Essentially following the proof of Theorem 3 of [13], one obtains
\[
\max_{S: |S| \leq L_0 s_0} \Pi_S \left( \theta_S \in \mathbb{R}^{|S|}: \|X(\tilde{\theta}_S - \theta_0)\|_2 \geq 4 \|X(\tilde{\theta}_{S,0} - \theta_0)\|_2 + \left( 5 + \frac{32}{\phi(L_0 s_0)} \right) \sqrt{L_0 s_0 \log p} Y \right) 1_{\tau_0} \to 0
\]
almost surely, uniformly over \( \theta_0 \in \mathbb{R}^p \). For any \( S \supseteq \{ i: |\theta_{0,i}| \geq K \sqrt{\log p / \|X\|} \} \),
\[
\|X(\tilde{\theta}_S - \theta_0)\|_2^2 = \sum_{i=1}^n \left( \sum_{j \in S^c \cap S_0} X_{ij} \theta_{0,j} \right)^2
\]
\[
= \sum_{j \in S^c \cap S_0} \sum_{k \in S^c \cap S_0} (X_{j,k}) \theta_{0,j} \theta_{0,k} \leq K^2 \mathrm{mc}(X) s_0^2 \log p.
\]
Since \( \|X(\tilde{\theta}_S - \theta_0)\|_2 \geq \|X(\tilde{\theta}_{S,0} - \theta_0)\|_2 - \|X(\tilde{\theta}_{0,0} - \theta_0)\|_2 \), we obtain
\[
\max_{S: |S| \leq L_0 s_0, S \supseteq \{ i: |\theta_{0,i}| \geq K \sqrt{\log p / \|X\|} \}} \Pi_S \left( \theta_S \in \mathbb{R}^{|S|}: \|X(\tilde{\theta}_S - \tilde{\theta}_{S,0})\|_2 \geq \|X\| \tilde{\phi}(L_0 s_0) R_0 |Y| \right) 1_{\tau_0} \to 0.
\]
The result then follows since \( \|X(\tilde{\theta}_S - \tilde{\theta}_{S,0})\|_2 \geq \tilde{\phi}(|S|) \|X\| \|\theta_S - \theta_{S,0}\|_2 \geq \tilde{\phi}(L_0 s_0) \|X\| \|\theta_S - \theta_{S,0}\|_2 \).

We next consider the mean-field subclass \( \mathcal{Q}_{MF} \) of \( \mathcal{Q} \) given by (12). This again selects a single fixed support \( S \) but further requires the fitted normal distribution to have diagonal covariance matrix. We consider a diagonal version of \( N_S(\theta_S, (X_S^T X_S)^{-1}) \otimes \delta_{\tilde{S}} \) considered in Lemma 3.

**Lemma 5.** Under the conditions of Lemma 3(ii), the variational posterior \( \tilde{Q} \) arising from the family (12) satisfies
\[
\sup_{\theta_0, \tilde{\phi}(S_0) \geq 0, \psi(S_0) \geq 0, \|S_0\| \leq \tilde{S} \leq \tilde{S}, \|S_0\| \leq 0} \left( 1 + \frac{12}{\lambda_1} \left( 1 + \frac{8}{\phi(S_0)^2 \|X\| \sqrt{\log p}} \right) \right) s_0 \log p 1_{\tau_1} \leq 1 + o(1).
\]

**Proof.** We showed in the proof of Lemma 3 that on the event \( \tau_1 \) given in (20), there exists a set \( \tilde{S} \) with \( |\tilde{S}| \leq L_0 s_0 \), \( \tilde{S} \supseteq \{ i: |\theta_{0,i}| \geq K \sqrt{\log p / \|X\|} \} \) and such that \( \tilde{q}_\tilde{S} \geq (2e)^{-1} p L_0 s_0 \), where \( L_0 \) and \( K \) are uniform over the supremum in the present lemma and \( \tilde{q}_\tilde{S} \) is the posterior probability of the model \( S \subseteq \{ 1, \ldots, p \} \). Arguing as in (21),
\[
\inf_{Q \in \mathcal{Q}_{MF}} \mathrm{KL}(Q \| \Pi(\cdot | Y)) \leq \log \frac{1}{\tilde{q}_\tilde{S}} + \inf_{\mu_\tilde{S}, D_\tilde{S}} \mathrm{KL}(N_{\tilde{S}}(\mu_\tilde{S}, D_\tilde{S}) \| \Pi_{\tilde{S}}(\cdot | Y)),
\]
where the last Kullback-Leibler divergence is over the \( |\tilde{S}| \)-dimensional distributions and \( D_\tilde{S} \) ranges over diagonal positive definite matrices. On \( \tau_1 \) and for \( n \) large enough, \( \log(1/\tilde{q}_\tilde{S}) \leq \log(2e) = \log(2e) + L_0 s_0 \log p \).

The latter Kullback-Leibler divergence equals
\[
\mathrm{KL}(N_{\tilde{S}}(\mu_\tilde{S}, D_\tilde{S}) \| \Pi_{\tilde{S}}(\cdot | Y)) = E_{\mu_\tilde{S}, D_\tilde{S}} \left[ \log \frac{dN_{\tilde{S}}}{d\tilde{N}_{\tilde{S}}} (\mu_\tilde{S}, D_\tilde{S}) + \log \frac{d\tilde{N}_{\tilde{S}}}{d\Pi_{\tilde{S}}(\cdot | Y)} \right]
\]
(26)
for any covariance matrix $\Sigma_{\tilde{S}}$. For the first term in (26), the formula for the Kullback-Leibler divergence between two multivariate Gaussians gives

$$\text{KL}(N_{\tilde{S}}(\mu_{\tilde{S}}, D_{\tilde{S}})\|N_{\tilde{S}}(\mu_{\tilde{S}}, \Sigma_{\tilde{S}})) = \frac{1}{2} \left( \log(|\Sigma_{\tilde{S}}|/|D_{\tilde{S}}|) - |\tilde{S}| + \text{Tr}(\Sigma_{\tilde{S}}^{-1}D_{\tilde{S}}) \right),$$

where $|A|$ denotes the determinant of a square matrix $A$. Set now $\mu_{\tilde{S}} = (X_X^T X_{\tilde{S}})^{-1} X_{\tilde{S}} Y$, $\Sigma_{\tilde{S}} = (X_X^T X_{\tilde{S}})^{-1}$ as in (22) and define the diagonal matrix $D_{\tilde{S}}$ via $(D_{\tilde{S}})_{ii} = 1/(\Sigma^{-1})_{ii} = 1/(X_X^T X_{\tilde{S}})^{ii}$. This gives $\text{Tr}(\Sigma_{\tilde{S}}^{-1}D_{\tilde{S}}) = |\tilde{S}|$, so that it remains to control $1/2 \log(|\Sigma_{\tilde{S}}|/|D_{\tilde{S}}|) = 1/2 \log(|\Sigma_{\tilde{S}}||D_{\tilde{S}}^{-1}|)$. For our choice of $D_{\tilde{S}},$

$$|D_{\tilde{S}}^{-1}| = \prod_{j=1}^{|\tilde{S}|} (\Sigma_{\tilde{S}}^{-1})_{jj} = \prod_{j=1}^{|\tilde{S}|} (X_X^T X_{\tilde{S}})_{jj} \leq \|X\|^2|\tilde{S}|,$$

while for $\Lambda_{\min}(A)$ and $\Lambda_{\max}(A)$ the smallest and largest eigenvalues, respectively, of a matrix $A$ and using (25),

$$|\Sigma_{\tilde{S}}| \leq \Lambda_{\max}(X_X^T X_{\tilde{S}})^{|\tilde{S}|} = (1/\Lambda_{\min}(X_X^T X_{\tilde{S}}))^{1/|\tilde{S}|} \leq 1/(\|X\|\phi(|\tilde{S}|))^{2|\tilde{S}|}.$$

This yields that $\text{KL}(N_{\tilde{S}}(\mu_{\tilde{S}}, D_{\tilde{S}})\|N_{\tilde{S}}(\mu_{\tilde{S}}, \Sigma_{\tilde{S}})) \leq |\tilde{S}| \log(1/\phi(|\tilde{S}|)) \leq L_0 s_0 \log(1/\phi(L_0 s_0)) = o(s_0 \log p)$.

Note that the second term in (26) is identical to the expression (23), except that the expectation is taken under $\theta_{\tilde{S}} \sim N_{\tilde{S}}(\mu_{\tilde{S}}, D_{\tilde{S}})$ instead of $\theta_{\tilde{S}} \sim N_{\tilde{S}}(\mu_{\tilde{S}}, \Sigma_{\tilde{S}})$. One may therefore use the exact same arguments as in Lemma 3 with the only difference occurring in the second term in (24), where one instead has $\lambda E_{0} D_{\tilde{S}} \|\theta_{\tilde{S}}\|_1 \leq \lambda |\tilde{S}|^{1/2}(E_{0, D_{\tilde{S}}} \|\theta_{\tilde{S}}\|_2^2)^{1/2} = \lambda |\tilde{S}|^{1/2} \text{Tr}(D_{\tilde{S}})^{1/2}$. For $e_i$ the $i^{th}$ unit vector in $\mathbb{R}^p$,

$$\text{Tr}(D_{\tilde{S}}) = \sum_{i \in \tilde{S}} \frac{1}{(X_X^T X_{\tilde{S}})^{ii}} = \sum_{i \in \tilde{S}} \frac{1}{\|X e_i\|^2} \leq \sum_{i \in \tilde{S}} \frac{1}{\|X\|^2 \|\phi(1)^2\}} = \frac{|\tilde{S}|}{\|X\|^2 \phi(1)^2},$$

so that $\lambda |\tilde{S}|^{1/2} \text{Tr}(D_{\tilde{S}})^{1/2} \leq 4L_0 s_0 \sqrt{\log p}/\phi(1) = o(s_0 \log p)$, thereby completing the proof. \qedsymbol

**Lemma 6.** Under the conditions of Lemma 2(ii), the variational posterior $\tilde{\Pi}$ arising from the family (8) of spike-and-slab distributions satisfies

$$\sup_{\theta_0, \phi(S_0) \geq c_0, \phi(S_0) \geq c_0, |S_0| \leq s_0, |S_0| \leq d_0 mc(X)^{-1}} \left( 1 + \frac{12}{\lambda} \frac{1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\|^2 \log p}}{1 + \frac{\lambda}{\phi(S_0)^2} \frac{\lambda}{\|X\|^2 \log p}} \right)s_0 \log p \leq 1 + o(1).$$

**Proof.** Since $Q_{MF} \subset P_{MF}$, we have $\text{KL}(\tilde{\Pi}||\Pi(\cdot|Y)) \leq \text{KL}(\tilde{Q}||\Pi(\cdot|Y))$. The result then follows from Lemma 5. \qedsymbol

### 8.3 Contraction rates for the original posterior distribution

The contraction rate for the original posterior distribution has been studied in depth in Castillo et al. [13], where they establish oracle type bounds. However, since their results are not stated with exponential bounds as needed in (18), we must reformulate their results in order to apply them in our Theorem 7. The required exponential bounds in fact follow from
their proofs, but they are not stated as such there. We recall here the required results and, since [13] is a rather technical article, we provide a brief explanation why the exponential bounds hold. That in what follows, a slightly wider choice of parameter \( \lambda \) is allowed than in [5]. The next result says that the posterior concentrates on models of dimension up to a factor of the true dimension.

**Lemma 7** (Theorem 10 of [13]). Suppose \( \|X\|/p \leq \lambda \leq 4\|X\|\sqrt{\log p} \) and the prior \( \pi_p \) satisfies [4]. Then for \( p \) large enough and any \( \theta_0 \in \mathbb{R}^p \) and \( M > 0 \), with \( s_0 = |S_{\theta_0}| \),

\[
E_{\theta_0} \Pi \left( \theta : |S_\theta| > s_0 + \frac{4M}{A_4} \left( 1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\|\sqrt{\log p}} \right) s_0 |Y| \right) 1_{T_0} \leq C(A_2, A_4) \exp \left( -(M-2) \left( 1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\|\sqrt{\log p}} \right) s_0 \log p \right),
\]

where \( T_0 \) is the event in [19].

**Proof.** Following the proof of Theorem 10 of [13], one obtains using the second display on p. 2008 of [13] with \( \beta^* = \beta^0 = \theta_0 \) that for \( \lambda = 2\|X\|\sqrt{\log p} \) and any measurable set \( B \subseteq \mathbb{R}^p \),

\[
\sup_{\theta_0 \in \mathbb{R}^p} E_{\theta_0} \Pi(B|Y) 1_{T_0} \leq \left( \frac{c p^{2s_0}}{\pi_p(s_0)} \frac{\lambda p^2}{\|X\|^2 \phi(S_0)^2} \right) \int_B e^{-\lambda |\theta - \theta_0|_{1,1}^1} d\Pi(\theta)^{1/2}.
\]

Setting now \( B = \{ \theta : |S_\theta| > R \} \) for \( R > s_0 \), the third display on p. 2008 of [13] shows that

\[
\int_B e^{-\lambda |\theta - \theta_0|_{1,1}^1} d\Pi(\theta) \leq \pi_p(s_0)^4 \left( \frac{4A_2}{p^{A_4}} \right)^{R+1-s_0} \sum_{j=0}^{\infty} \left( \frac{4A_2}{p^{A_4}} \right)^j \leq C(A_2, A_4) \pi_p(s_0)^4 \left( \frac{4A_2}{p^{A_4}} \right)^{R+1-s_0}
\]

for \( p \) large enough. Substituting this into the second last display and using that \( \bar{\lambda}^2 = 4\|X\|^2 \log p \),

\[
\sup_{\theta_0 \in \mathbb{R}^p} E_{\theta_0} \Pi(B|Y) 1_{T_0} \leq C(A_2, A_4) e^{1/2} (2p)^{s_0} e^{16\lambda \log p} \left( \frac{4A_2}{p^{A_4}} \right)^{R+1-s_0}.
\]

Choosing \( R = (2\delta + 1)s_0 - 1 \), the right-hand side equals

\[
C(A_2, A_4) \exp \left\{ (\log 2 + \delta \log(4A_2)) s_0 + (1 + 16\lambda/(\bar{\lambda}\phi(S_0)^2) - \delta A_4) s_0 \log p \right\}.
\]

Further picking \( \delta = 2M(1 + 16\lambda/(\bar{\lambda}\phi(S_0)^2))/A_4 \), the right-hand side is then bounded by \( C(A_2, A_4) \exp\{-s_0(M-2)/(1 + 16\lambda/(\bar{\lambda}\phi(S_0)^2))s_0 \log p\} \) for \( p \) large enough as required. \( \square \)

**Lemma 8** (Theorem 3 of [13]). Suppose \( \|X\|/p \leq \lambda \leq 4\|X\|\sqrt{\log p} \) and the prior \( \pi_p \) satisfies [4]. Then for \( p \) large enough and any \( L > 0 \), there exists a constant \( M > 0 \) depending only on \( A_4 \), such that for all \( \theta_0 \in \mathbb{R}^p \) and \( s_0 = |S_{\theta_0}| \),

\[
E_{\theta_0} \Pi \left( \theta : \|X(\theta - \theta_0)\|_2 > \frac{M \sqrt{s_0 \log p}}{\psi_{L+2}(S_0)} (L^{1/2} + 1) \left( 1 + \frac{1}{\phi(S_0)} \right) |Y| \right) 1_{T_0} \leq C \exp \left( -L \left( 1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\|\sqrt{\log p}} \right) s_0 \log p \right)
\]

\[
+ C \exp \left( -\frac{1}{\psi_{L+2}(S_0)^2} \left( 1 + \frac{4(L+2)}{A_4} \left( 1 + \frac{8}{\phi(S_0)^2} \frac{\lambda}{\|X\|\sqrt{\log p}} \right) \right) s_0 \log p \right),
\]

34
where $C = C(A_2, A_4)$. Moreover,

$$E_{\theta_0} \Pi \left( \theta : \| \theta - \theta_0 \|_2 > \frac{M \sqrt{s_0 \log p}}{\| X \|_{\psi_{L+2}(S_0)^2}} (L^{1/2} + 1) \left( 1 + \frac{1}{\phi(S_0)} \| X \| \sqrt{\log p} \right) \right) 1_{\overline{\tau}_0}$$

satisfies the same inequality.

The above result is a modified version of the oracle inequality in Theorem 3 of [13] with $S_* = S_0$. Since it is not stated as above in [13], we briefly explain why this is true.

**Proof.** Unless otherwise stated, we use here the notation from [13]. As on p. 2008 of [13], define the event $E = \{ \theta : |S_0| \leq D_* \}$ for

$$D_* = D_*(L) = s_0 + \frac{4(L + 2)}{A_4} \left( 1 + \frac{16}{\phi(S_0)^2} \right) s_0$$

(27)

with $\bar{\lambda} = 2\| X \| \sqrt{\log p}$ [recall we take here $S_* = S_0$ so that $s_* = s_0$]. Note that we take different constants than in (6.7) of [13] to obtain the required exponential tail bound. Lemma 7 yields

$$E_{\theta_0} \Pi(E^c | Y) 1_{\overline{\tau}_0} = E_{\theta_0} \Pi(\theta : |S_0| > D_* | Y) 1_{\overline{\tau}_0} \leq C(A_2, A_4) \exp(-L(1 + \frac{16}{\phi(S_0)^2}) s_0 \log p)$$

(28)

for every $\theta_0 \in \mathbb{R}^p$. Let

$$\Pi^E(\cdot) = \Pi(\cdot \cap E)/\Pi(E)$$

be the prior conditioned to $E$ and denote by $\Pi^E(\cdot | Y)$ the posterior distribution arising from the prior $\Pi^E$. By a standard inequality ([34], p. 142),

$$\| \Pi(\cdot | Y) - \Pi^E(\cdot | Y) \|_{TV} = \sup_A | \Pi(A | Y) - \Pi^E(A | Y) | \leq 2 \Pi(E^c | Y),$$

where the supremum is taken over all measurable sets $A \subseteq \mathbb{R}^p$. Using the last display and (28), we may therefore work on the restricted prior $\Pi^E$.

Using definition (17), note that $\overline{\psi}_{L+2}(S_0) = \overline{\psi}(D_* + s_0)$. Continuing through the proof, the third last display on p. 2009 of [13] (note that up to this point, the definition of $D_*$ only affects the definition of the compatibility type constants) gives

$$\Pi^E(\theta \in E : \| X(\theta - \theta_0) \|_2 > R | Y) 1_{\overline{\tau}_0} \leq \frac{e}{\pi_p(0)A_1^2 p^{(2 + A_4)s_0} e^{|s_0|^2(X)_{L+2}(s_0)^2}} e^{-\bar{\lambda}^2 \sum_{s=0}^{p} \pi_p(s)2^s},$$

where again $\bar{\lambda} = 2\| X \| \sqrt{\log p}$. Using condition (4), $\sum_{s=0}^{p} \pi_p(s)2^s \leq \pi_p(0) \sum_{s=0}^{p} (2A_2p^{-A_4})^s \leq \pi_p(0)C(A_2, A_4)$ for $p$ large enough. Using this and the value of $\lambda$, the last display is bounded by

$$C(A_2, A_4) \exp \left\{ -s_0 \log A_1 + (2 + A_3)s_0 \log p + \frac{128(D_* + s_0) \log p}{\overline{\psi}_{L+2}(S_0)^2} - \frac{1}{8} R^2 \right\}.$$}

Taking $R^2 = \overline{M}^2(D_* + s_0) \log p/\overline{\psi}_{L+2}(S_0)^2$, we thus have that for $p$ large enough, $\Pi^E(\theta \in E : \| X(\theta - \theta_0) \|_2 > R | Y) 1_{\overline{\tau}_0} \leq C(A_2, A_4) \exp(-\lambda(D_* + s_0) \log p/\overline{\psi}_{L+2}(S_0)^2)$ upon taking $\overline{M} > 0$ large enough. Using the definition (27) of $D_*$, that $\lambda/\bar{\lambda} \leq 2$ and the inequality $\sqrt{x+y} \leq \sqrt{x} + \sqrt{y}$ for any $x, y \geq 0$,

$$(D_* + s_0)^{1/2} \leq C s_0^{1/2} (L^{1/2} + 1)(1 + 1/\phi(S_0))$$

35
for a constant $C > 0$ depending only on $A_1$, yielding $R \leq C M \sqrt{\delta_0 \log \psi}(L^{1/2} + 1)(1 + 1/\phi(S_0))/\tilde{\psi}_{L+2}(S_0)$ as required. This establishes the required inequality for prediction error $\|X(\theta - \theta_0)\|_2$.

For $\ell_2$-loss, note that $\|X(\theta - \theta_0)\|_2 \geq \tilde{\phi}(|S_0 - \theta_0|) \|X\| \|\theta - \theta_0\|_2 \geq \tilde{\psi}_{L+2}(S_0) \|X\| \|\theta - \theta_0\|_2$ for any $\theta \in E$. The result then follows from that for prediction error and that $\tilde{\psi}_{L+2}(S_0) \geq \tilde{\psi}_{L+2}(S_0)$ by Lemma 1.

\section{Additional methodological details}

\subsection{Proofs for the variational algorithm}

We provide here derivations for the formulas used in the CAVI implementation of our variational algorithm in Section 4.

Proof of (15): We compute the Kullback-Leibler divergence between $P_{\mu,\sigma,\gamma}$ and the posterior $\Pi(\cdot|Y)$, conditional on $z_i = 1$, as a function of $\mu_i$ and $\sigma_i$. Since the variational probability distribution of $\theta_i$ conditional on $z_i = 1$ (i.e. $P_{\mu_i,\sigma_i|z_i=1}$) is singular to the Dirac measure $\delta_0$, in the Radon-Nikodym derivative $dP_{\mu_i,\sigma_i|z_i=1}/d\Pi_i$, where $\Pi_i$ is the prior for $\theta_i$, it suffices to consider only the continuous part of the prior measure in the denominator. Write $\Pi(\theta|Y) = D_\Pi^{-1}e^{-|Y - X\theta|^2/2}d\Pi(\theta)$ with $D_\Pi$ the normalizing constant. Using all of these and the prior product structure, $KL(P_{\mu,\sigma,\gamma}|z_i=1\Pi(\cdot|Y))$ equals, as a function of $\mu_i$ and $\sigma_i$,

\[ E_{\mu,\sigma,\gamma|z_i=1} \left[ \frac{1}{2} \|Y - X\theta\|^2 + \log D_\Pi + \log \frac{dP_{\mu_i,\sigma_i,\gamma_i} \otimes N(\mu_i, \sigma_i^2)}{d\Pi_i \otimes \overline{w}\text{Lap}(\lambda)} \right] = E_{\mu,\sigma,\gamma|z_i=1} \left[ \frac{1}{2} (Y - X\theta)^T (Y - X\theta) + \log \frac{dP_{\mu_i,\sigma_i,\gamma_i} \otimes N(\mu_i, \sigma_i^2)}{d\Pi_i} (\theta - \mu_i)^T - \log \sigma_i - \left(\frac{\theta_i - \mu_i}{2\sigma_i^2}\right)^2 + \lambda |\theta_i| \right] + C, \]

where $C > 0$ is independent of $\mu_i, \sigma_i$ and $\overline{w}_i = a_0/(a_0 + b_0)$ is the prior mean for $w_i$. Recall that the expected value of the folded normal distribution with parameters $\mu \in \mathbb{R}$ and $\sigma > 0$ is $\sigma \sqrt{2/\pi} e^{-\mu^2/(2\sigma^2)} + \mu(1 - 2\Phi(-\mu/\sigma))$. Using this and explicitly evaluating the expectation of the first term, the last display equals

\[ \mu_i \sum_{k \neq i} (X^T X)_{ik} \sigma_k \mu_k + \frac{1}{2} (X^T X)_{ii} (\sigma_i^2 + \mu_i^2) - (Y^T X)_i \mu_i + \lambda \sigma_i \sqrt{2/\pi} e^{-\mu_i^2/(2\sigma_i^2)} \]

\[ + \lambda \mu_i (1 - 2\Phi(-\mu_i/\sigma_i)) - \log \sigma_i + C', \]

where $C' > 0$ is again independent of $\mu_i, \sigma_i$. Minimizing the last display with respect to either $\mu_i$ or $\sigma_i$ (but not jointly) gives the same minimizers as minimizing $f_i$ and $g_i$ in (15).

Proof of (16): Similarly to the derivation of (15) above, the KL divergence between $P_{\mu,\sigma,\gamma}$ and $\Pi(\cdot|Y)$ as a function of $\gamma_i$ equals

\[ E_{\mu,\sigma,\gamma} \left[ \frac{1}{2} \|Y - X\theta\|^2 + \log \frac{dP_{\mu_i,\sigma_i,\gamma_i} \otimes N(\mu_i, \sigma_i^2)}{d\Pi_i} (\theta - \mu_i) + \log \frac{d(\gamma_i N(\mu_i, \sigma_i^2) + (1 - \gamma_i) \delta_0)}{d(\overline{w}_i\text{Lap}(\lambda) + (1 - \overline{w}_i) \delta_0)} (\theta_i) \right] + C, \]

where $C > 0$ is independent of $\gamma_i$ and $\overline{w}_i = a_0/(a_0 + b_0)$. Since on an event of $P_{\mu,\sigma,\gamma}$-probability
We collect here for completeness the variational algorithms for the spike-and-slab prior with component-wise variational Bayes for Gaussian slabs

\begin{equation}
\begin{aligned}
& E_{\mu, \sigma, \gamma} \left[ \frac{1}{2} \| Y - X \theta \|^2 + 1_{\{z_i=1\}} \log \frac{\gamma_i dN(\mu_i, \sigma_i^2)}{\text{Lap}(\lambda)}(\theta_i) + 1_{\{z_i=0\}} \log \frac{1 - \gamma_i}{1 - w_i} \right] + C \\
& = E_{\mu, \sigma, \gamma} \left[ \frac{1}{2} \| Y - X \theta \|^2 + 1_{\{z_i=1\}} \left( \log \frac{\sqrt{2}}{\sqrt{\pi} \sigma_i \lambda} - \frac{(\theta_i - \mu_i)^2}{2\sigma_i^2} + \lambda |\theta_i| \right) \right] \\
& \quad + \gamma_i \log \frac{\gamma_i}{w_i} + (1 - \gamma_i) \log \frac{1 - \gamma_i}{1 - w_i} + C \\
& = \gamma_i \left\{ \mu_i \sum_{k \neq i} (X^T X)_{ki} \gamma_k \mu_k + \frac{1}{2} (X^T X)_{ii} (\sigma_i^2 + \mu_i^2) - (Y^T X)_{i} \mu_i + \log \frac{\sqrt{2}}{\sqrt{\pi} \sigma_i \lambda} - \frac{1}{2} \right. \\
& \quad + \lambda \sigma_i \sqrt{2/\pi e^{-\mu_i^2/(2\sigma_i^2)}} + \lambda \mu_i (1 - 2\Phi(-\mu_i/\sigma_i)) + \log \frac{\gamma_i}{1 - \gamma_i} + \log \frac{b_0}{a_0} \left. \right\} + \log (1 - \gamma_i) + C
\end{aligned}
\end{equation}

where $C > 0$ may change from line to line and is independent of $\gamma_i$. Setting the derivative with respect to $\gamma_i$ of this last expression equal to zero and rearranging gives (16).

9.2 Algorithms for Gaussian slabs

We collect here for completeness the variational algorithms for the spike-and-slab prior with Gaussian slabs with which we have compared our method. First we give the component-wise update of the parameters as in [25], see Algorithm 2 below.

**Algorithm 2** Component-wise variational Bayes for Gaussian slabs

1. **Initialization:**
2. $\Delta_H := 1$
3. $\mu := (X^T X + I)^{-1} X^T Y$, $\sigma := (1, \ldots, 1)$, $\gamma = \left( \frac{a_0}{a_0 + b_0}, \ldots, \frac{a_0}{a_0 + b_0} \right)$
4. **while** $\Delta_H \geq 10^{-4}$ **do**
5. $\gamma_{old} := \gamma$
6. **for** $i = 1$ to $p$ **do**
7. $\mu_i := \sigma_i^2 (Y^T X)_i - \sum_{j \neq i} (X^T X)_{i,j} \mu_j \sigma_j$
8. $\sigma_i := 1/\sqrt{(X^T X)_{ii} + 1}$
9. $\gamma_i := \text{logit}^{-1}(\log(a_0/b_0) + \log \sigma_i + \mu_i^2/(2\sigma_i^2))$
10. $\Delta_H := \max_q |H(\gamma_q) - H(\gamma_{old,q})|$

In [22] the authors argue that coordinate-wise updates of the parameters can accumulate error from each step leading to a suboptimal procedure. To resolve this problem they propose simultaneously updating the entire parameter vectors $\mu$, $\sigma$ and $\lambda$ without using a CAVI type of algorithm. A version of their proposed algorithm is given in Algorithm 3, where $\text{diag}(v)$, $v \in \mathbb{R}^p$, creates a diagonal square matrix in $\mathbb{R}^{p \times p}$ with diagonal elements $v$ (see also Algorithm 1 of [38] with $\alpha = 1$, $\sigma = 1$ and $\nu_1 = 1$ for a related implementation). As in the other cases, we have taken the ridge regression estimator $(X^T X + I)^{-1} X^T Y$ as our initialization for $\mu$.

**References**

[1] Alquier, P., and Ridgway, J. Concentration of tempered posteriors and of their variational approximations. arXiv e-prints (Jun 2017), arXiv:1706.09293.
Algorithm 3 Batch-wise variational Bayes for Gaussian slabs

1: Initialization:
2: \( \Delta_H := 1 \)
3: \( \mu := (X^TX + I)^{-1}X^TY, \sigma := (1, \ldots, 1), \gamma = (1/p, \ldots, 1/p) \)
4: while \( \Delta_H \geq 10^{-4} \) do
5: \( \gamma_{old} := \gamma \)
6: \( \Gamma := \text{diag}(\gamma) \)
7: \( \mu := (X^TX + \Gamma)^{-1}X^TY \)
8: for \( i = 1 \) to \( p \) do
9: \( \sigma_i := 1/\sqrt{(X^TX)_{ii} + \gamma_i} \)
10: \( \gamma_i := \logit^{-1}(\logit(1/p) + \log \sigma_i + \mu_i^2/(2\sigma^2)) \)
11: \( \Delta_H := \max_i \{|H(\gamma_i) - H(\gamma_{old,i})|\} \)

[2] Archambeau, C., and Bach, F. R. Sparse probabilistic projections. In Advances in Neural Information Processing Systems 21, D. Koller, D. Schuurmans, Y. Bengio, and L. Bottou, Eds. Curran Associates, Inc., 2009, pp. 73–80.

[3] Blei, D. M., Kucukelbir, A., and McAuliffe, J. D. Variational inference: a review for statisticians. J. Amer. Statist. Assoc. 112, 518 (2017), 859–877.

[4] Blei, D. M., Ng, A. Y., and Jordan, M. I. Latent Dirichlet Allocation. J. Mach. Learn. Res. 3 (Mar. 2003), 993–1022.

[5] Boucheron, S., Lugosi, G., and Massart, P. Concentration inequalities. Oxford University Press, Oxford, 2013. A nonasymptotic theory of independence, With a foreword by Michel Ledoux.

[6] Breiman, L., and Friedman, J. H. Estimating optimal transformations for multiple regression and correlation. Journal of the American statistical Association 80, 391 (1985), 580–598.

[7] Bühlmann, P., and van de Geer, S. Statistics for high-dimensional data. Springer Series in Statistics. Springer, Heidelberg, 2011. Methods, theory and applications.

[8] Cai, T. T., and Jiang, T. Limiting laws of coherence of random matrices with applications to testing covariance structure and construction of compressed sensing matrices. Ann. Statist. 39, 3 (2011), 1496–1525.

[9] Carbonetto, P., and Stephens, M. Scalable variational inference for Bayesian variable selection in regression, and its accuracy in genetic association studies. Bayesian Anal. 7, 1 (2012), 73–107.

[10] Caron, F., and Doucet, A. Sparse Bayesian nonparametric regression. In Proceedings of the 25th International Conference on Machine Learning (New York, NY, USA, 2008), ICML ’08, ACM, pp. 88–95.

[11] Carvalho, C. M., Polson, N. G., and Scott, J. G. The horseshoe estimator for sparse signals. Biometrika 97, 2 (2010), 465–480.

[12] Castillo, I., and Roquain, E. On spike and slab empirical Bayes multiple testing. arXiv e-prints (Aug 2018), arXiv:1808.09748.

[13] Castillo, I., Schmidt-Hieber, J., and van der Vaart, A. Bayesian linear regression with sparse priors. Ann. Statist. 43, 5 (2015), 1986–2018.

[14] Castillo, I., and Szabo, B. Spike and slab empirical Bayes sparse credible sets. Bernoulli, to appear, arXiv:1808.07721.

[15] Castillo, I., and van der Vaart, A. Needles and straw in a haystack: posterior
concentration for possibly sparse sequences. *Ann. Statist.* 40, 4 (2012), 2069–2101.

[16] Donoho, D. L., Elad, M., and Temlyakov, V. N. Stable recovery of sparse overcomplete representations in the presence of noise. *IEEE Transactions on Information Theory* 52, 1 (Jan 2006), 6–18.

[17] Efron, B. Microarrays, empirical Bayes and the two-groups model. *Statist. Sci.* 23, 1 (2008), 1–22.

[18] George, E. I., and McCulloch, R. E. Variable selection via Gibbs sampling. *J. Amer. Statist. Assoc.* 88, 423 (1993), 881–889.

[19] Ghosal, S., Ghosh, J. K., and van der Vaart, A. W. Convergence rates of posterior distributions. *Ann. Statist.* 28, 2 (2000), 500–531.

[20] Hoffman, M. D., Blei, D. M., Wang, C., and Paisley, J. Stochastic variational inference. *J. Mach. Learn. Res.* 14 (2013), 1303–1347.

[21] Horn, R. A., and Johnson, C. R. *Matrix analysis*, second ed. Cambridge University Press, Cambridge, 2013.

[22] Huang, X., Wang, J., and Liang, F. A variational algorithm for Bayesian variable selection. *ArXiv e-prints* (Feb. 2016), arXiv:1602.07640.

[23] Ishwaran, H., Rao, J., and Kogalur, U. spikeslab: Prediction and variable selection using spike and slab regression, 2013. R package version 1.1.5.

[24] Johnstone, I. M., and Silverman, B. W. Needles and straw in haystacks: empirical Bayes estimates of possibly sparse sequences. *Ann. Statist.* 32, 4 (2004), 1594–1649.

[25] Logsdon, B. A., Hoffman, G. E., and Mezey, J. G. A variational Bayes algorithm for fast and accurate multiple locus genome-wide association analysis. *BMC bioinformatics* 11, 1 (2010), 58.

[26] Lounici, K. Sup-norm convergence rate and sign concentration property of Lasso and Dantzig estimators. *Electron. J. Stat.* 2 (2008), 90–102.

[27] Lu, Y., Stuart, A., and Weber, H. Gaussian approximations for probability measures on $\mathbb{R}^d$. *SIAM/ASA J. Uncertain. Quantif.* 5, 1 (2017), 1136–1165.

[28] Mitchell, T. J., and Beauchamp, J. J. Bayesian variable selection in linear regression. *J. Amer. Statist. Assoc.* 83, 404 (1988), 1023–1036. With comments by James Berger and C. L. Mallows and with a reply by the authors.

[29] Ormerod, J. T., You, C., and Müller, S. A variational Bayes approach to variable selection. *Electron. J. Stat.* 11, 2 (2017), 3549–3594.

[30] Pati, D., Bhattacharya, A., and Yang, Y. On statistical optimality of variational Bayes. In *Proceedings of the Twenty-First International Conference on Artificial Intelligence and Statistics* (Playa Blanca, Lanzarote, Canary Islands, 09–11 Apr 2018), A. Storkey and F. Perez-Cruz, Eds., vol. 84 of *Proceedings of Machine Learning Research*, PMLR, pp. 1579–1588.

[31] Ročková, V., and George, E. I. EMVS: the EM approach to Bayesian variable selection. *J. Amer. Statist. Assoc.* 109, 506 (2014), 828–846.

[32] Tipping, M. E. Sparse Bayesian learning and the relevance vector machine. *J. Mach. Learn. Res.* 1, 3 (2001), 211–244.

[33] Titsias, M. K., and Lázaro-Gredilla, M. Spike and slab variational inference for multi-task and multiple kernel learning. In *Advances in neural information processing systems* (2011), pp. 2339–2347.

[34] van der Vaart, A. W. *Asymptotic statistics*, vol. 3 of *Cambridge Series in Statistical and Probabilistic Mathematics*. Cambridge University Press, Cambridge, 1998.

[35] van Erven, T., and Szabo, B. Fast exact Bayesian inference for sparse signals in the
normal sequence model. *arXiv e-prints* (Oct 2018), arXiv:1810.10883.

[36] Wang, Y., and Blei, D. M. Frequentist consistency of variational Bayes. *J. Amer. Statist. Assoc.*, to appear, arXiv:1705.03439.

[37] West, M. Bayesian factor regression models in the “large p, small n” paradigm. In *Bayesian statistics, 7 (Tenerife, 2002)*. Oxford Univ. Press, New York, 2003, pp. 733–742.

[38] Yang, Y., Pati, D., and Bhattacharya, A. α-variational inference with statistical guarantees. *Ann. Statist.*, to appear, arXiv:1710.03266.

[39] Zhang, A. Y., and Zhou, H. H. Theoretical and computational guarantees of mean field variational inference for community detection. *ArXiv e-prints* (Oct. 2017), arXiv:1710.11268.

[40] Zhang, F., and Gao, C. Convergence rates of variational posterior distributions. *ArXiv e-prints* (Dec. 2017), arXiv:1712.02519.

[41] Zhao, P., and Yu, B. On model selection consistency of Lasso. *J. Mach. Learn. Res.* 7 (2006), 2541–2563.