Asymptotically Exact Variational Bayes for High-Dimensional Binary Regression Models

Augusto Fasano, Daniele Durante and Giacomo Zanella
Department of Decision Sciences, Bocconi University

Abstract

State-of-the-art methods for Bayesian inference on regression models with binary responses are either computationally impractical or inaccurate in high dimensions. To cover this gap we propose a novel variational approximation for the posterior distribution of the coefficients in high-dimensional probit regression. Our method leverages a representation with global and local variables but, unlike for classical mean-field assumptions, it avoids a fully factorized approximation, and instead assumes a factorization only for the local variables. We prove that the resulting variational approximation belongs to a tractable class of unified skew-normal distributions that preserves the skewness of the actual posterior and, unlike for state-of-the-art variational Bayes solutions, converges to the exact posterior as the number of predictors $p$ increases. A scalable coordinate ascent variational algorithm is proposed to obtain the optimal parameters of the approximating densities. As we show with both theoretical results and an application to Alzheimer’s data, such a routine requires a number of iterations converging to 1 as $p \to \infty$, and can easily scale to large $p$ settings where expectation-propagation and state-of-the-art Markov chain Monte Carlo algorithms are computationally impractical.

Keywords: Bayesian Computation, High-Dimensional Probit Regression, Data Augmentation, Variational Bayes, Truncated Normal Distribution, Unified Skew-Normal Distribution.

1 Introduction

The absence of tractable posterior distributions in several Bayesian models, and the recent abundance of high-dimensional datasets have motivated a growing interest in strategies for scalable learning of approximate posteriors, beyond classical sampling-based Markov chain Monte Carlo (MCMC) methods (e.g., Green et al., 2015). Deterministic approximations, such as variational Bayes (VB) (Blei et al., 2017) and expectation-propagation (EP) (Minka, 2001), provide powerful approaches to improve computational efficiency in posterior inference. However, in high-dimensional models these methods still face open problems in terms of scalability and quality of the posterior approximation. Notably, such issues also arise in basic predictor-dependent models for binary responses (Agresti, 2013), which are routinely used and provide a building block in several hierarchical models (e.g.,
Chipman et al., 2010; Rodriguez and Dunson, 2011). Recalling a recent review by Chopin and Ridgway (2017), the problem of posterior computation in binary regression is particularly challenging when the number of predictors \( p \) becomes large. Indeed, while standard sampling-based algorithms and deterministic approximations can easily deal with small \( p \) problems, these strategies are impractical when \( p \) is large; e.g., \( p > 1000 \).

Classical specifications of Bayesian regression models for binary data assume that the dichotomous responses \( y_i \in \{0; 1\}, i = 1, \ldots, n \), are conditionally independent realizations from a Bernoulli variable \( \text{Bern}[\text{g}(\mathbf{x}_i^\top \beta)] \), given a fixed \( p \)-dimensional vector of predictors \( \mathbf{x}_i = (x_{i1}, \ldots, x_{ip})^\top \in \mathbb{R}^p \), \( i = 1, \ldots, n \), and the associated coefficients \( \beta = (\beta_1, \ldots, \beta_p)^\top \in \mathbb{R}^p \). The mapping \( g(\cdot) : \mathbb{R} \to (0, 1) \) is commonly specified to be either the logit or probit link, thus obtaining \( \text{pr}(y_i = 1 \mid \beta) = \left[ 1 + \exp(-\mathbf{x}_i^\top \beta) \right]^{-1} \) in the first case, and \( \text{pr}(y_i = 1 \mid \beta) = \Phi(\mathbf{x}_i^\top \beta) \) in the second, where \( \Phi(\cdot) \) is the cumulative distribution function of a standard normal. In performing Bayesian inference under these models, it is common practice to specify Gaussian priors for the coefficients \( \beta \), and then update such priors with the likelihood of the observed data \( \mathbf{y} = (y_1, \ldots, y_n)^\top \) to obtain the posterior \( p(\beta \mid \mathbf{y}) \), which is used for point estimation, uncertainty quantification and prediction. However, the apparent absence of conjugacy in this Bayesian updating motivates the use of computational strategies relying either on Monte Carlo integration or on deterministic approximations (Chopin and Ridgway, 2017).

A popular class of MCMC methods that has been widely used in applications of Bayesian regression for binary data leverages augmented data representations which allow the implementation of tractable Gibbs samplers relying on conjugate full-conditional distributions. In Bayesian probit regression this strategy exploits the possibility of expressing the binary data \( y_i \in \{0; 1\}, i = 1, \ldots, n \), as dichotomized versions of an underlying regression model for Gaussian responses \( z_i \in \mathbb{R}, i = 1, \ldots, n \), thereby restoring conjugacy between the Gaussian prior for the coefficients \( \beta \) and the augmented data, which are in turn sampled from truncated normal full-conditionals (Albert and Chib, 1993). More recently, Polson et al. (2013) proposed a related strategy for logit regression which is based on a representation of the logistic likelihood as a scale mixture of Gaussians with respect to Pólya-gamma augmented variables \( z_i \in \mathbb{R}^+, i = 1, \ldots, n \). Despite their simplicity, these methods face well-known computational and mixing issues in high-dimensional settings, especially with imbalanced datasets (Johndrow et al., 2019). We refer to Chopin and Ridgway (2017) for a discussion of related data-augmentation strategies (Holmes and Held, 2006; Frühwirth-Schnatter and Frühwirth, 2007) and alternative sampling methods, such as adaptive Metropolis–Hastings (Roberts and Rosenthal, 2001; Haario et al., 2001) and Hamiltonian Monte Carlo (Hoffman and Gelman, 2014), among others.
While these strategies address some disadvantages of data-augmentation Gibbs samplers, they are still computationally impractical in large $p$ applications (Chopin and Ridgway, 2017; Durante, 2019).

A possible solution to scale-up computations is to consider deterministic approximations of the posterior distribution. In binary regression contexts, two strategies that have gained growing popularity are mean-field (MF) VB with global and local variables (Jaakkola and Jordan, 2000; Consonni and Marin, 2007; Durante and Rigon, 2019), and EP (Chopin and Ridgway, 2017). The first class of methods approximates the joint posterior density $p(\beta, z | y)$ for the global parameters $\beta = (\beta_1, \ldots, \beta_p)^T$ and the local augmented data $z = (z_1, \ldots, z_n)^T$ with an optimal factorized density $q^*_{MF}(\beta) \prod_{i=1}^n q^*_{MF}(z_i)$ which is the closest in Kullback–Leibler divergence (Kullback and Leibler, 1951) to $p(\beta, z | y)$, among all the approximating densities in the mean-field family $Q_{MF} = \{ q_{MF}(\beta, z) : q_{MF}(\beta, z) = q_{MF}(\beta) q_{MF}(z) \}$. Optimization typically proceeds via coordinate ascent variational inference methods (CAVI) which can scale easily to large $p$ settings. However, MF-VB is known to underestimate posterior uncertainty and often leads to Gaussian approximations which affect the quality of inference if the actual posterior is non-Gaussian (Kuss and Rasmussen, 2005). As we will show in Sections 2 and 3, this issue can have dramatic implications in the setting considered in this article. Also EP provides Gaussian approximations (Chopin and Ridgway, 2017), but typically improves the quality of VB via a moment matching of approximate marginals that have the same factorized form of the actual posterior. These gains come, however, with a computational cost which makes EP not practical for high-dimensional settings with, e.g., $p > 1000$. Indeed, recalling a concluding remark by Chopin and Ridgway (2017), the lack of scalability to large $p$ is common to most state-of-the-art methods for Bayesian computation in binary regression models. An exception is provided by the recent contribution of Durante (2019), which proves that in Bayesian probit regression with Gaussian priors the posterior actually belongs to the class of unified skew-normal (SUN) distributions (Arellano-Valle and Azzalini, 2006). These variables have several closure properties which facilitate posterior inference in large $p$ settings. However, the calculation of relevant functionals for inference and prediction requires the evaluation of cumulative distribution functions of $n$-variate Gaussians or sampling from $n$-variate truncated normals, thus making these results impractical in a variety of applications with sample size $n$ greater than a few hundreds (Durante, 2019).

In this article we address most of the aforementioned issues by proposing a new partially factorized mean-field approximation (PFM) for Bayesian probit regression which avoids assuming independence between the global variables $\beta$ and the augmented data $z$. Unlike EP (Chopin and Ridgway, 2017), the proposed PFM-VB scales easily to $p \gg 1000$ settings, and, unlike for the compu-
tational strategies proposed in Durante (2019), it only requires evaluation of distribution functions of univariate Gaussians. Moreover, despite having a computational cost comparable to standard MF-VB for probit models (Consonni and Marin, 2007), the proposed PFM-VB leads to a substantially improved approximation of the posterior in large $p$ settings, which reduces bias in locations and variances, and crucially incorporates skewness. Optimization proceeds via a simple CAVI algorithm and provides a tractable SUN approximating density. The methodology is discussed in Section 2, where we also provide theoretical results showing that the PFM-VB approximation converges to the exact posterior as $p \to \infty$, and that the number of iterations required by the CAVI to find the optimum converges to 1 as $p \to \infty$. Insightful negative results on the accuracy of standard MF-VB approximations, that suggest caution against maximum a posteriori inferences in high-dimensional contexts, are also provided. The proposed methods are evaluated on an Alzheimer’s application with $p = 9036$ in Section 3. Concluding remarks and proofs can be found in Section 4 and in Appendix A, respectively. Finally, Appendix B discusses the computational complexity of the proposed inference and optimization strategies which can crucially be performed at an $O(pn \cdot \min\{p,n\})$ cost. Codes and tutorials to implement the proposed methods and reproduce the analyses are available at https://github.com/augustofasano/Probit-PFMVB.

## 2 Approximate Bayesian Inference for Probit Models

Recalling Section 1, we focus on posterior inference for the classical Bayesian probit regression model defined as

$$
(y_i \mid \mathbf{\beta}) \sim \text{Bern}[\Phi(\mathbf{x}_i^\top \mathbf{\beta})], \text{ independently for } i = 1, \ldots, n, \text{ with } \mathbf{\beta} \sim N_p(0, \nu^2 \mathbf{I}_p). \quad (1)
$$

In (1), each $y_i$ is a binary variable whose success probability depends on a $p$-dimensional vector of observed predictors $\mathbf{x}_i = (x_{i1}, \ldots, x_{ip})^\top$ under a probit mapping. The coefficients $\mathbf{\beta} = (\beta_1, \ldots, \beta_p)^\top$ regulate the effect of each predictor and are assigned independent Gaussian priors $\beta_j \sim N(0, \nu^2)$, for every $j = 1, \ldots, p$. Although our contribution can be naturally generalized to a generic multivariate Gaussian prior for $\mathbf{\beta}$, we consider here the simpler setting with $\mathbf{\beta} \sim N_p(0, \nu^2 \mathbf{I}_p)$ to ease notation and presentation. In fact, this choice is arguably the most common in routine implementations of Bayesian probit models (e.g., Chopin and Ridgway, 2017).

Model (1) also has a simple constructive representation based on Gaussian augmented data, which has been broadly used in the development of MCMC (Albert and Chib, 1993) and VB (Consonni and Marin, 2007).
Marin, 2007) methods. More specifically, (1) can be obtained by marginalizing out the augmented data \( z = (z_1, \ldots, z_n)^T \) in the model

\[
y_i = 1(z_i > 0), \quad \text{with } (z_i | \beta) \sim N(x_i^T \beta, 1), \text{ independently for } i = 1, \ldots, n, \text{ and } \beta \sim N_p(0, \nu^2 I_p). \tag{2}
\]

Recalling Albert and Chib (1993), the above construction leads to closed-form full-conditionals for \( \beta \) and \( z \), thus allowing the implementation of a Gibbs sampler where \( p(\beta | z, y) = p(\beta | z) \) is a Gaussian density, and each \( p(z_i | \beta, y) = p(z_i | \beta, y_i) \) is the density of a truncated normal, for \( i = 1, \ldots, n \).

We refer to Albert and Chib (1993) for more details regarding such a strategy. Our focus here is on large \( p \) settings where classical MCMC is often impractical, thus motivating more scalable methods relying on approximate posteriors. In Section 2.1, we discuss standard MF-VB strategies for Bayesian probit models (Consonni and Marin, 2007) which rely on representation (2), and prove that in large \( p \) settings these approaches lead to poor approximations of the exact posterior that underestimate not only the variance but also the location, thus leading to unreliable inference and prediction. In Section 2.2, we address these issues via a new partially factorized variational approximation that has substantially improved practical and theoretical performance in large \( p \) settings, especially when \( p \gg n \).

### 2.1 Mean-field variational Bayes with global and local variables

Recalling Blei et al. (2017), mean-field VB with global and local variables aims at providing a tractable approximation for the joint posterior density \( p(\beta, z | y) \) of the global parameters \( \beta = (\beta_1, \ldots, \beta_p)^T \) and the local variables \( z = (z_1, \ldots, z_n)^T \), within the MF class of factorized densities \( Q_{MF} = \{q_{MF}(\beta, z) : q_{MF}(\beta, z) = q_{MF}(\beta)q_{MF}(z) \} \). The optimal VB solution \( q_{MF}^*(\beta)q_{MF}^*(z) \) within this family is the one that minimizes the Kullback–Leibler (KL) divergence (Kullback and Leibler, 1951) defined as

\[
KL[q_{MF}(\beta, z) \mid \mid p(\beta, z | y)] = E_{q_{MF}(\beta, z)}[\log q_{MF}(\beta, z)] - E_{q_{MF}(\beta, z)}[\log p(\beta, z | y)], \quad q_{MF}(\beta, z) \in Q_{MF}. \tag{3}
\]

Alternatively, it is possible to obtain \( q_{MF}^*(\beta)q_{MF}^*(z) \) by maximizing

\[
\text{ELBO}[q_{MF}(\beta, z)] = E_{q_{MF}(\beta, z)}[\log p(\beta, z, y)] - E_{q_{MF}(\beta, z)}[\log q(\beta, z)], \quad q_{MF}(\beta, z) \in Q_{MF}, \tag{4}
\]

since the ELBO coincides with the negative KL up to an additive constant. Recall also that the KL divergence is always non-negative. See Armagan and Zaretzki (2011) for the expression of \( \text{ELBO}[q_{MF}(\beta, z)] \) under (2). The maximization of (4) is typically easier than the minimization of
Indeed, recalling Albert and Chib (1993) it easily follows that the full-conditionals under model (2) consequence of the conditional independence of normal distribution having mean $\mu$ where $\sigma$ is simple to implement in Bayesian models having tractable full-conditional densities $p(\beta | z, y)$ and $p(z | \beta, y)$. This is the case of the augmented-data representation (2) for the probit model in (1). Indeed, recalling Albert and Chib (1993) it easily follows that the full-conditionals under model (2) are

$$
(\beta | z, y) \sim N_p(V X' z, V), \quad V = (\nu^{-2}I_p + X'X)^{-1},
$$

$$
(z_i | \beta, y) \sim \begin{cases} 
    \text{TN}[x_i' \beta, 1, (0, +\infty)], & \text{if } y_i = 1, \\
    \text{TN}[x_i' \beta, 1, (-\infty, 0)], & \text{if } y_i = 0,
\end{cases} \quad \text{independently for } i = 1, \ldots, n, 
$$

where $X$ is the $n \times p$ design matrix with rows $x_i'$, whereas $\text{TN}[\mu, \sigma^2, (a, b)]$ denotes a generic univariate normal distribution having mean $\mu$, variance $\sigma^2$, and truncation to the interval $(a, b)$. An important consequence of the conditional independence of $z_1, \ldots, z_n$ given $\beta$ and $y$, is that $q^{(t)}_{\text{MF}}(z) = \prod_{i=1}^n q^{(t)}_{\text{MF}}(z_i)$ and thus the optimal MF-VB solution always factorizes as $q^{*}_{\text{MF}}(\beta) = q^{*}_{\text{MF}}(\beta) \prod_{i=1}^n q^{*}_{\text{MF}}(z_i)$. Replacing the densities of the above full-conditionals in the CAVI outlined in (5), it can be easily noted that $q^{(t)}_{\text{MF}}(\beta)$ and $q^{(t)}_{\text{MF}}(z_i), i = 1, \ldots, n$, are Gaussian and truncated normal densities, respectively, with parameters as in Algorithm 1 (Consonni and Marin, 2007). Note that the actual parametric form of the optimal approximating densities follows directly from (5), without pre-specifying it.

Algorithm 1 relies on simple steps which basically require only updating of $\bar{\beta}$ via matrix operations, and, unlike for EP, is computationally feasible in high-dimensional settings; see e.g., Table 1. Due to the Gaussian form of $q^{*}_{\text{MF}}(\beta)$ also the calculation of the approximate posterior moments and predictive probabilities is straightforward. The latter quantities can be easily expressed as

$$
\Pr_{\text{MF}}(y_{\text{new}} = 1 | y) = \int \Phi(x_{\text{new}}' \beta) q^{*}_{\text{MF}}(\beta) d\beta = \Phi(x_{\text{new}}' \bar{\beta}^* (1 + x_{\text{new}}' V x_{\text{new}})^{-1/2}],
$$

where $x_{\text{new}} \in \mathbb{R}^p$ are the covariates of the new observation, and $\bar{\beta}^* = E_{q^{*}_{\text{MF}}(\beta)}(\beta)$. However, as shown by the asymptotic results in Theorem 1, MF-VB can lead to poor approximations of the posterior in high dimensions as $p \to \infty$, causing serious concerns on the quality of inference and
Algorithm 1: CAVI algorithm to obtain $q_{\text{MP}}^*(\beta, z) = q_{\text{MP}}^*(\beta) \prod_{i=1}^n q_{\text{MP}}^*(z_i)$

for $t$ from 1 until convergence of ELBO[$q_{\text{MP}}^{(t)}(\beta, z)$] do

[1] Set $q_{\text{MP}}^{(t)}(\beta) = \phi_p(\beta - \bar{\beta}^{(t)}; \nu X^T z^{(t-1)})$, where $z^{(t-1)}$ has elements $z_i^{(t-1)} = x_i^T \beta^{(t-1)} + (2y_i - 1)\phi(x_i^T \beta^{(t-1)})\Phi((2y_i - 1)x_i^T \beta^{(t-1)})^{-1}$ for every $i = 1, \ldots, n$. In the above expression, $\phi_p(\beta - \mu; \Sigma)$ is the density of a generic $p$-variate Gaussian for $\beta$ with mean $\mu$ and variance-covariance matrix $\Sigma$.

[2] Set $q_{\text{MP}}^{(t)}(z_i) = \frac{\phi(z_i - x_i^T \beta^{(t)})}{\Phi((2y_i - 1)x_i^T \beta^{(t)})} \Pi[(2y_i - 1)z_i > 0]$ for every $i = 1, \ldots, n$.

Output: $q_{\text{MP}}^*(\beta, z) = q_{\text{MP}}^*(\beta) \prod_{i=1}^n q_{\text{MP}}^*(z_i)$.

prediction. Throughout the paper, the asymptotic results are derived under the following random design assumption.

A 1. Assume that the predictors $x_{ij}, i = 1, \ldots, n, j = 1, \ldots, p$, are independent random variables with $E(x_{ij}) = 0$, $E(x_{ij}^2) = \sigma^2_x$ and $\sup_{ij} E(x_{ij}^4) < \infty$.

The above random design assumption is common to asymptotic studies of regression models (see e.g., Brown et al., 2002; Reiβ, 2008; Qin and Hobert, 2019). Moreover, the zero mean and the constant variance assumption is a natural requirement in the context of binary regression, where the predictors are typically standardized following the recommended practice in the literature (e.g., Gelman et al., 2008; Chopin and Ridgway, 2017). In Section 3, we will show how empirical evidence on a real dataset, where this assumption might not hold, is still coherent with the theoretical results stated below.

Theorem 1. Under A1, we have that $\liminf_{p \to \infty} \text{KL}[q_{\text{MP}}^*(\beta) \mid p(\beta \mid y)] > 0$ almost surely (a.s.). Moreover, $\|E_{q_{\text{MP}}^*(\beta)}(\theta)\| \xrightarrow{a.s.} 0$ as $p \to \infty$, where $\| \cdot \|$ is the usual Euclidean norm. On the contrary, $\|E_{p(\beta \mid y)}(\theta)\| \xrightarrow{a.s.} c\sqrt{n}\nu > 0$ as $p \to \infty$, where $c = 2 \int_0^\infty z\phi(z)dz$ is a strictly positive constant.

According to Theorem 1, MF-VB provides an approximate density $q_{\text{MP}}^*(\beta)$ which leads to an expectation for $\beta$ that, unlike the true posterior expectation, converges to 0 as $p \to \infty$. Therefore, MF-VB causes over-shrinkage of the approximate posterior means and also an unsatisfactory approximation of the entire posterior density $p(\beta \mid y)$ in high-dimensional settings. For instance, recalling the expression of the approximate predictive probabilities in (7), the over-shrinkage of $\bar{\beta}^*$ towards 0 causes rapid concentration of $\text{pr}_{\text{MP}}(y_{\text{new}} = 1 \mid y)$ around 0.5, thereby inducing bias. As shown in
Section 3, the magnitude of such a bias can be dramatic, making (7) unreliable in high-dimensional settings.

As discussed in the proof of Theorem 1 and in Armagan and Zaretzki (2011), $\hat{\beta}^*$ is also the mode of the actual posterior $p(\beta \mid y)$. Hence, the above results suggest that, despite its popularity (Chopin and Ridgway, 2017; Gelman et al., 2008), the posterior mode should be avoided as a point estimate in large $p$ settings. As a consequence, also Laplace approximation would provide unreliable inference since this approximation is centered at the posterior mode. These results are in apparent contradiction with the fact that the marginal posterior densities $p(\beta_j \mid y)$ often exhibit negligible skewness and their modes $\arg \max p(\beta_j \mid y)$ are typically close to the corresponding mean $E_{p(\beta_j \mid y)}(\beta_j)$; see e.g., Figure 2. However, the same is not true for the joint posterior density $p(\beta \mid y)$, where little skewness is sufficient to induce a dramatic difference between the joint posterior mode, $\arg \max p(\beta \mid y)$, and the posterior expectation; see e.g., Figure 3. In this sense, the results in Theorem 1 point towards caution in assessing Gaussianity of high-dimensional distributions based on the shape of their marginal distributions.

Motivated by the above considerations, in Section 2.2 we develop a new PFM-VB with global and local variables that solves the aforementioned issues without increasing computational costs. In fact, the computational cost of our procedure is the same of MF-VB but, unlike for such a strategy, we obtain a substantially improved approximation that provably converges to the exact posterior as $p \to \infty$. The magnitude of these improvements is outlined in the empirical studies in Section 3.

2.2 Partially factorized variational Bayes with global and local variables

A natural strategy to improve the performance of MF-VB is to relax the factorization assumptions on the approximating densities in a way that still allows simple optimization and inference. To accomplish this goal, we consider a partially factorized representation $Q_{pfm} = \{q_{pfm}(\beta, z) : q_{pfm}(\beta, z) = q_{pfm}(\beta \mid z) \prod_{i=1}^n q_{pfm}(z_i)\}$ which does not assume independence among the parameters $\beta$ and the local variables $z$, thus providing a more flexible family of approximating densities. This new enlarged family $Q_{pfm}$ allows to incorporate more structure of the actual posterior relative to $Q_{mf}$, while retaining tractability. In fact, following Holmes and Held (2006) and recalling that $V = (\nu^{-2}I_p + X'X)^{-1}$, the joint density $p(\beta, z \mid y)$ under the augmented model (2) can be factorized as $p(\beta, z \mid y) = p(\beta \mid z)p(z \mid y)$, where $p(\beta \mid z) = \phi_p(\beta - VXz; V)$ and $p(z \mid y) \propto \phi_n(z; I_n + \nu^2XX') \prod_{i=1}^n 1[(2y_i - 1)z_i > 0]$ denote the densities of a $p$-variate Gaussian and an $n$-variate truncated normal, respectively. The main source of intractability in this factorization of
the posterior is the truncated Gaussian density, which requires the evaluation of cumulative distribution functions of $n$-variate Gaussian with full variance-covariance matrix for inference (Genz, 1992; Horrace, 2005; Chopin, 2011; Pakman and Paninski, 2014; Botev, 2017; Durante, 2019). The independence assumption among the augmented data in $Q_{PFM}$ avoids the intractability that would arise from the multivariate truncated normal density $p(z \mid y)$, while being fully flexible on $q_{PFM}(\beta \mid z)$. Crucially, the optimal MF-VB approximation $q^*_MF(\beta, z)$ belongs to $Q_{PFM}$ and thus, by minimizing $KL[q_{PFM}(\beta, z) \mid p(\beta, z \mid y)]$ in $Q_{PFM}$, we are guaranteed to obtain an improved approximation of the joint posterior density relative to MF-VB, as stated in Proposition 1.

**Proposition 1.** Let $q^*_MF(\beta, z)$ and $q^*_PFM(\beta, z)$ be the optimal approximations for $p(\beta, z \mid y)$ from (2), under PFM-VB and MF-VB, respectively. Since $q^*_MF(\beta, z) \in Q_{PFM}$ and $q^*_PFM(\beta, z)$ minimizes $KL[q(\beta, z) \mid p(\beta, z \mid y)]$ in $Q_{PFM}$, then $KL[q^*_PFM(\beta, z) \mid p(\beta, z \mid y)] \leq KL[q^*_MF(\beta, z) \mid p(\beta, z \mid y)]$.

This result suggests that PFM-VB may provide a promising direction to improve quality of posterior approximation. However, to be useful in practice, the solution $q^*_PFM(\beta, z)$ should be simple to derive and the approximate posterior $q^*_PFM(\beta) = \int_{\mathbb{R}^n} q^*_PFM(\beta \mid z) \prod_{i=1}^{n} q^*_PFM(z_i)\mathrm{d}z = \mathbb{E}_{q^*_PFM}(z)[q^*_PFM(\beta \mid z)]$ of direct interest should be available in tractable form. Theorem 2 and Corollary 1 show that this is possible.

**Theorem 2.** Under the augmented model in equation (2), the KL divergence between $q^*_PFM(\beta, z) \in Q_{PFM}$ and $p(\beta, z \mid y)$ is minimized at $q^*_PFM(\beta \mid z) \prod_{i=1}^{n} q^*_PFM(z_i)$ with

$$q^*_PFM(\beta \mid z) = p(\beta \mid z) = \phi_p(\beta - \mathbf{V}\mathbf{X}^\top z; \mathbf{V}), \quad \mathbf{V} = (\nu^{-2}\mathbf{I}_p + \mathbf{X}^\top \mathbf{X})^{-1},$$

$$q^*_PFM(z_i) = \frac{\phi(z_i - \mu^*_i \sigma^*_2)}{\Phi([2y_i - 1]\mu^*_i \sigma^*_2)]}(2y_i - 1)z_i > 0, \quad \sigma^*_2 = (1 - \mathbf{x}_i^\top \mathbf{V}\mathbf{x}_i)^{-1}, \quad i = 1, \ldots, n, \ (8)$$

where $\mu^* = (\mu^*_1, \ldots, \mu^*_n)^\top$ solves the system $\mu^*_i - \sigma^*_2 \mathbf{x}_i^\top \mathbf{V}\mathbf{x}_i \mathbf{z}^*_i = 0, \ i = 1, \ldots, n$, with $\mathbf{X}_{-i}$ denoting the design matrix without the $i$th row, while $\mathbf{z}^*_i$ is an $n-1$ vector obtained by removing the $i$th element $\tilde{z}_i = \mu^*_i + (2y_i - 1)\sigma^*_2 \phi(\mu^*_i / \sigma^*_2) \Phi([2y_i - 1]\mu^*_i / \sigma^*_2)^{-1}, \ i = 1, \ldots, n$, from the vector $\mathbf{z}^* = (\tilde{z}^*_1, \ldots, \tilde{z}^*_n)^\top$.

In Theorem 2, the solution for $q^*_PFM(\beta \mid z)$ follows by noting that $KL[q_{PFM}(\beta, z) \mid p(\beta, z \mid y)] = KL[q_{PFM}(z) \mid p(z \mid y)] + \mathbb{E}_{q_{PFM}(z)}[KL[q_{PFM}(\beta \mid z) \mid p(\beta \mid z)]$ due to the chain rule for the KL divergence. Thus, the second summand is 0 if and only if $q^*_PFM(\beta \mid z) = p(\beta \mid z)$. The expressions for $q^*_PFM(z_i), \ i = 1, \ldots, n, \ i$ are instead a direct consequence of the closure under conditioning property of multivariate truncated Gaussians (Horrace, 2005) which allows to recognize the kernel of a univariate truncated normal in the optimal solution $\exp[\mathbb{E}_{q^*_PFM}(z_{-i})[\log[p(z_i \mid z_{-i}, y)]]]$ (Blei et al., 2017) for
\( q_{\text{PFM}}^*(z_i) \); see Appendix A for the detailed proof. Algorithm 2 outlines the steps of the CAVI to obtain \( q_{\text{PFM}}^*(\beta, z) \). As for classical CAVI (Blei et al., 2017), this routine optimizes the ELBO sequentially with respect to each density \( q_{\text{PFM}}^*(z_i) \), keeping fixed the others at their most recent update, thus producing a strategy that iteratively solves the system of equations for \( \mu^* \) in Theorem 2 via simple expressions. Indeed, since the form of the approximating densities is already available as in Theorem 2, the steps in Algorithm 2 reduce to update the vector of parameters \( \mu^* \) via simple functions and matrix operations.

As stated in Corollary 1, the optimal \( q_{\text{PFM}}^*(\beta) \) of interest can be easily derived from \( q_{\text{PFM}}^*(\beta | z) \) and \( \prod_{i=1}^n q_{\text{PFM}}^*(z_i) \), and coincides with the density of a tractable SUN (Arellano-Valle and Azzalini, 2006).

**Corollary 1.** Under (8), the approximate density \( q_{\text{PFM}}^*(\beta) \) for \( \beta \) coincides with that of the variable

\[
\left( u(0) + VX^T[I_n(2y - 1)]\sigma^* u(1) \right),
\]

where \( u(0) \sim N_p(VX^T\mu^*, V) \), and \( u(1) = (u_1(1), \ldots, u_n(1))^\top \) denotes an \( n \)-dimensional random vector of independent univariate truncated normals \( u_i^{(1)} \sim TN[0, 1, -(2y_i - 1)\mu_i^* / \sigma_i^*, + \infty], \) \( i = 1, \ldots, n \).

Hence, recalling Arellano-Valle and Azzalini (2006) and Azzalini and Capitanio (2014), \( q_{\text{PFM}}^*(\beta) \) is the density of the unified skew-normal distribution SUN\(_{p,n}(\xi, \Omega, \Delta, \gamma, \Gamma) \), with parameters

\[
\begin{align*}
\xi &= VX^T\mu^*, \\
\Omega &= \omega\Omega\omega = V + VX^T\sigma^{-2}XV, \\
\Delta &= \omega^{-1}VX^T[I_n(2y - 1)]\sigma^*, \\
\gamma &= [I_n(2y - 1)]\sigma^{*-1}\mu^*,
\end{align*}
\]

where \( \sigma^* = \text{diag}(\sigma_1^*, \ldots, \sigma_n^*) \), and \( \omega \) denotes a \( p \times p \) diagonal matrix containing the square roots of the diagonal elements in the covariance matrix \( \Omega \), whereas \( \Omega \) denotes the associated correlation matrix.

**Algorithm 2:** CAVI algorithm to obtain \( q_{\text{PFM}}^*(\beta, z) = q_{\text{PFM}}^*(\beta | z) \prod_{i=1}^n q_{\text{PFM}}^*(z_i) \)

1. Set \( q_{\text{PFM}}^*(\beta | z) = \phi_p(\beta - VX^Tz; V) \) with \( V = (\nu^{-2}I_p + VX^T)^{-1} \), and initialize \( \mu_i^{(0)} \in \mathbb{R} \), \( i = 1, \ldots, n \).
2. **for** \( t \) from 1 until convergence of ELBO(\( q_{\text{PFM}}^{(t)}(\beta, z) \)) **do**
   
   **for** \( i \) from 1 to \( n \) **do**

   \[
   q_{\text{PFM}}^{(t)}(z_i) = \frac{\phi(z_i - \mu_i^{(t)}; \sigma_i^{*2})}{\Phi[(2y_i - 1)\mu_i^{(t)} / \sigma_i^{*}]} \mathcal{I}[2y_i - 1] > 0, \]

   with \( \sigma_i^{*2} = 1 - x_i^T Vx_i \), and \( \mu_i^{(t)} = \sigma_i^{*2} x_i^T VX_i(z_i^{(t)}, \ldots, z_{i-1}^{(t)}, z_{i+1}^{(t)}, \ldots, z_n^{(t)-1})^\top \) where the generic \( z_i^{(t)} \) is defined as \( z_i^{(t)} \) in Theorem 2 replacing \( \mu_i^* \) with \( \mu_i^{(t)} \).

**Output:** \( q_{\text{PFM}}^*(\beta, z) = q_{\text{PFM}}^*(\beta | z) \prod_{i=1}^n q_{\text{PFM}}^*(z_i) \) and, as a consequence of Corollary 1, also \( q_{\text{PFM}}^*(\beta) \).
The results in Corollary 1 follow by noticing that, under (8), the approximate density for $\beta$ is the convolution of a $p$-variate Gaussian and an $n$-variate truncated normal, thereby producing the density of a SUN (Arellano-Valle and Azzalini, 2006; Azzalini and Capitanio, 2014). This class of random variables generalizes the multivariate Gaussian family via a skewness-inducing mechanism controlled by the matrix $\Delta$ which weights the skewing effect produced by an $n$-variate truncated normal with covariance matrix $\Sigma$ (Arellano-Valle and Azzalini, 2006; Azzalini and Capitanio, 2014). Besides introducing asymmetric shapes in multivariate Gaussians, the SUN has several closure properties which facilitate inference. However, the evaluation of functionals requires the calculation of cumulative distribution functions of $n$-variate Gaussians (Arellano-Valle and Azzalini, 2006; Azzalini and Capitanio, 2014), which is prohibitive when $n$ is large, unless $\Sigma$ is diagonal. Recalling Durante (2019), this issue makes Bayesian inference rapidly impractical under the exact posterior $p(\beta \mid y)$ when $n$ is more than a few hundreds, since $p(\beta \mid y)$ is a SUN density with non-diagonal $\Sigma_{\text{post}}$. Instead, the factorized form $\prod_{i=1}^{n} q_{\text{PFM}}(z_i)$ for $q_{\text{PFM}}(z)$ leads to a SUN approximate density for $\beta$ in Corollary 1, which crucially relies on a diagonal $\Sigma = I_n$. Such a result allows approximate posterior inference for every $n$ and $p$ via tractable expressions. In particular, recalling the stochastic representation in (9), the first two central moments of $\beta$ and the predictive distribution are derived in Proposition 2.

**Proposition 2.** If $q_{\text{PFM}}^*(\beta)$ is the SUN density in Corollary 1, then

$$
\mathbb{E}_{q_{\text{PFM}}^*(\beta)}(\beta) = VX^T\bar{z}^*, \quad \text{var}_{q_{\text{PFM}}^*(\beta)}(\beta) = V + VX^T[\sigma^*]^2 - (\bar{z}^* - \mu^*)^T I_n \bar{z}^*] XV, \quad (10)
$$

where $\bar{z}^*$, $\mu^*$ and $\sigma^*$ are quantities defined in Theorem 2. Moreover, the posterior predictive probability $pr_{\text{PFM}}(y_{\text{NEW}} = 1 \mid y) = \int \Phi(x_{\text{NEW}}^T \beta) q_{\text{PFM}}^*(\beta) \, d\beta$ for a new observation with covariates $x_{\text{NEW}}$ is

$$
pr_{\text{PFM}}(y_{\text{NEW}} = 1 \mid y) = \mathbb{E}_{q_{\text{PFM}}^*(\beta)} \{ \Phi(x_{\text{NEW}}^T V X^T z (1 + x_{\text{NEW}}^T V x_{\text{NEW}})^{-1/2}) \}, \quad (11)
$$

where, according to Theorem 2, $q_{\text{PFM}}^*(z)$ can be expressed as the product $\prod_{i=1}^{n} q_{\text{PFM}}^*(z_i)$ of univariate truncated normal densities $q_{\text{PFM}}^*(z_i) = \phi(z_i - \mu_i^*; \sigma_i^* (2y_i - 1)\mu_i^*/\sigma_i^*)^{-1} \mathbb{I}_{[ \{ (2y_i - 1)z_i > 0 \}]}$, $i = 1, \ldots, n$.

**Algorithm 3:** Strategy to sample from the approximate SUN posterior in Corollary 1

1. Draw $u^{(0)} \sim N_p(V X^T \mu^*, V)$.
2. Draw $u^{(1)}_i \sim TN(0, 1, [- (2y_i - 1)\mu_i^*/\sigma_i^*, +\infty])$, $i = 1, \ldots, n$. Set $u^{(1)} = (u^{(1)}_1, \ldots, u^{(1)}_n)^T$.
3. Compute $\beta = u^{(0)} + VX^T[I_n (2y - 1)\sigma^* u^{(1)}]$.

**Output:** a draw $\beta$ from the approximate posterior with density as in (9).
Hence, unlike for inference under the exact posterior (Durante, 2019), calculation of relevant approximate moments such as those in equation (10), only requires the evaluation of cumulative distribution functions of univariate Gaussians. Similarly, the predictive probabilities in equation (11) can be easily evaluated via efficient Monte Carlo methods based on samples from \( n \) independent univariate truncated normals with density \( q_{\text{pfm}}^*(z_i) \), \( i = 1, \ldots, n \). Moreover, leveraging (9), samples from the approximate posterior \( q_{\text{pfm}}^*(\beta) \) can directly be obtained via a linear combination between realizations from a \( p \)-variate Gaussian and from \( n \) univariate truncated normals, as shown in Algorithm 3. This strategy allows to study complex approximate functionals of \( \beta \) through simple Monte Carlo methods. If instead the focus is only on \( q_{\text{pfm}}^*(\beta_j) \), \( j = 1, \ldots, p \), one can avoid the cost of simulating from the \( p \)-variate Gaussian in Algorithm 3 and just sample from the marginals of \( u^{(0)} \) in the additive representation of the sum to get samples from \( q_{\text{pfm}}^*(\beta_j) \) for \( j = 1, \ldots, p \) at an \( O(pn \cdot \min\{p, n\}) \) cost.

We conclude the presentation of PFM-VB by studying its properties in high-dimensional settings as \( p \to \infty \). As discussed in Section 2.1, MF-VB (Consonni and Marin, 2007) provides poor Gaussian approximations of the posterior density in high dimensions, which do not include asymmetric shapes usually found in Bayesian binary regression (Kuss and Rasmussen, 2005), and affect quality of inference and prediction. By relaxing the MF assumption we obtain, instead, an approximate density which includes skewness and matches the exact posterior for \( \beta \) when \( p \to \infty \), as stated in Theorem 3.

**Theorem 3.** Under A1, we have that \( \text{KL}[q_{\text{pfm}}^*(\beta) \mid p(\beta \mid y)] \overset{a.s.}{\to} 0 \) as \( p \to \infty \).

Hence, in the high dimensional settings where current computational strategy are impractical (Chopin and Ridgway, 2017), inference and prediction under the approximation provided by PFM-VB is practically feasible, and provides essentially the same results as those obtained under the exact posterior. For instance, Corollary 2 states that, unlike for MF-VB, PFM-VB is guaranteed to provide increasingly accurate approximations of posterior predictive probabilities as \( p \to \infty \).

**Corollary 2.** Let \( \Pr(y_{\text{new}} = 1 \mid y) = \int \Phi(x_\text{new}^\top \beta)p(\beta \mid y)d\beta \) be the exact posterior predictive probability for a new unit with predictors \( x_{\text{new}} \in \mathbb{R}^p \), then, under A1, we have that \( \sup_{x_{\text{new}} \in \mathbb{R}^p} |\Pr_{\text{PFM}}(y_{\text{new}} = 1 \mid y) - \Pr(y_{\text{new}} = 1 \mid y)| \overset{a.s.}{\to} 0 \) as \( p \to \infty \). On the contrary, \( \lim \inf_{p \to \infty} \sup_{x_{\text{new}} \in \mathbb{R}^p} |\Pr_{\text{MF}}(y_{\text{new}} = 1 \mid y) - \Pr(y_{\text{new}} = 1 \mid y)| > 0 \) almost surely as \( p \to \infty \).

Corollary 2 implies that, under A1, the error made by PFM-VB in terms of approximation of posterior predictive probabilities goes to 0 as \( p \to \infty \), regardless of the choice of \( x_{\text{new}} \in \mathbb{R}^p \). On
the contrary, under MF-VB there always exists, for every \( p \), some \( x_{\text{new}} \) such that the corresponding posterior predictive probability is not accurately approximated.

Finally, as stated in Theorem 4, the number of iterations required by the CAVI in Algorithm 2 to produce the optimal solution \( q^{(t)}_{\text{PFM}}(\beta) \) converges to 1 as \( p \to \infty \).

**Theorem 4.** Let \( q^{(t)}_{\text{PFM}}(\beta) = \int_{\mathbb{R}^n} q^{(t)}_{\text{PFM}}(\beta \mid z) \prod_{i=1}^{n} q^{(t)}_{\text{PFM}}(z_i) \, dz \) denote the approximate density for \( \beta \) produced at iteration \( t \) by Algorithm 2. Then, under \( A1 \), \( \text{KL}[q^{(1)}_{\text{PFM}}(\beta) \mid | p(\beta \mid y)] \to 0 \) as \( p \to \infty \).

According to Theorem 4, the CAVI in Algorithm 2 converges essentially in one iteration as \( p \to \infty \). Thus the computational complexity of the entire PFM-VB routine is provably equal to that of a single CAVI iteration, which is dominated by the \( \mathcal{O}(pn \cdot \min\{p, n\}) \) cost of computing \( XVX^\top \) via its expression, when \( n > p \), or using Woodbury’s identity for \( V \), when \( p > n \). This identity for \( V \) is useful also for the calculation of the functionals in Proposition 2 which can be achieved at the same cost; see also Appendix B. More complex functionals of the joint approximate posterior can be instead obtained at higher costs via Monte Carlo methods based on Algorithm 3. Finally, we shall emphasize that also the computational complexity of approximate inference under MF-VB is dominated by the \( \mathcal{O}(pn \cdot \min\{p, n\}) \) pre-computation cost of calculating \( XVX^\top \). However, according to our empirical findings, the number of CAVI iterations to reach convergence seems to increase with \( p \) under MF-VB.

In Section 3, we discuss how the theoretical results presented in Sections 2.1 and 2.2 match closely the empirical behavior observed in a real-world application to Alzheimer’s data.

## 3 High-Dimensional Probit Regression for Alzheimer’s Data

As shown in Chopin and Ridgway (2017), state-of-the-art computational methods for Bayesian binary regression, such as Hamiltonian Monte Carlo (Hoffman and Gelman, 2014), VB (Consonni and Marin, 2007) and EP (Chopin and Ridgway, 2017) are feasible and powerful procedures in small-to-moderate \( p \) settings, but become rapidly impractical or inaccurate in large \( p \) contexts, such as \( p > 1000 \). The overarching focus of the present article is to close this gap and, consistent with this aim, we consider a large \( p \) study to quantify the drawbacks encountered by the aforementioned strategies along with the improvements provided by the proposed PFM-VB method.

Following the above remarks, we focus on an application to model presence or absence of Alzheimer’s disease in its early stages as a function of demographic data, genotype and assay results.
The original dataset is available in the R library `AppliedPredictiveModeling` and arises from a study of the Washington University to determine if biological measurements from cerebrospinal fluid are useful in modeling and predicting early stages of Alzheimer’s disease (Craig-Schapiro et al., 2011). In the original article, the authors consider a variety of machine learning procedures to improve the flexibility relative to a basic binary regression model. Here, we avoid excessively complex black-box algorithms and rely on an interpretable probit regression (1), which improves flexibility by simply adding pairwise interactions, thus obtaining $p = 9036$ predictors collected for 333 individuals. Following Gelman et al. (2008) and Chopin and Ridgway (2017) the original measurements have been standardized to have mean 0 and standard deviation 0.5, before entering such variables and their interactions in the probit regression. In general, we recommend to always standardize the predictors when implementing PFM-VB since this choice typically reduces the correlation between units and thus also between the associated latent variables $z_i$, making the resulting variational approximation more accurate. We shall also emphasize that the sample size of this study is low relative to those that can be easily handled under PFM-VB. In fact, this moderate $n$ is required to make inference under the exact posterior, which serves here as a benchmark, still feasible (Durante, 2019).

In performing Bayesian inference under the above probit model, we follow the guidelines in Gelman et al. (2008) and rely on independent weakly informative Gaussian priors with mean 0 and standard deviation 5 for each coefficient $\beta_j$, $j = 1, \ldots, 9036$. These priors are then updated with the likelihood of $n = 300$ units, after holding out 33 individuals to study the behavior of the posterior predictive probabilities in such large $p$ settings, along with the performance of the overall approximation of the posterior. Table 1 provides insights on the computational time of MF-VB and PFM-VB, and highlights the bottlenecks encountered by relevant routine-use competitors. These include the `rstan` implementation of Hamiltonian Monte Carlo, the `ep` algorithm in the R library `EPGLM`, and the Monte Carlo strategy based on 20000 independent draws from the exact SUN posterior using the algorithm in Durante (2019). As expected, these strategies are clearly impractical in such settings. In particular, `stan` and `ep` suffer from the large $p$, whereas sampling from the exact posterior is still feasible, but requires a non-negligible computational effort due to the moderately large $n$. Variational inference under MF-VB and PFM-VB is orders of magnitude faster and, hence, provides the only viable approach in such settings. These results motivate our main focus on the quality of MF-VB and PFM-VB approximations in Figures 1–3, taking as benchmark Monte Carlo inference based on 20000 independent samples from the exact SUN posterior. In this example PFM-VB requires only 7 CAVI iterations to converge, instead of 212 as for MF-VB. This result is in line
Table 1: Computational time of state-of-the-art routines in the Alzheimer’s application. This includes the running time of the sampling or optimization procedure and the time to compute means, standard deviations and predictive probabilities, for those routines that were feasible.

| Computational time in minutes | STAN | EP | SUN | MF-VB | PFM-VB |
|------------------------------|------|----|-----|-------|--------|
| > 360.00                     | > 360.00 | 92.71 | 0.05 | 0.05  |

Figure 1: For MF-VB and PFM-VB, histograms of the log-Wasserstein distances between the $p = 9036$ approximate marginal densities provided by the two VB methods and the exact posterior marginals. These distances are computed via Monte Carlo based on 20000 samples from the approximate and exact marginals. To provide insights on Monte Carlo error, the dashed vertical lines represent the quantiles $2.5\%$ and $97.5\%$ of the log-Wasserstein distances between two different samples of 20000 draws from the exact posterior marginals. According to these histograms, PFM-VB improves the quality of MF-VB and, in practice, it matches almost perfectly the exact posterior since it provides distances within the range of values obtained by comparing two different samples of 20000 draws from the same exact posterior marginals. Hence, most of the variability in the PFM-VB histogram is arguably due to Monte Carlo error.

Figure 1 shows the histograms of the log-Wasserstein distances among the $p = 9036$ exact posterior marginals and the associated approximations under MF-VB and PFM-VB. Such quantities are computed with the R function `wasserstein1d`, which uses 20000 values sampled from the approximate and exact marginals. According to these histograms, PFM-VB improves the quality of MF-VB and, in practice, it matches almost perfectly the exact posterior since it provides distances within the range of values obtained by comparing two different samples of 20000 draws from the same exact posterior marginals. Hence, most of the variability in the PFM-VB histogram is arguably due to Monte Carlo error.

These results are in line with Theorems 1 and 3, and are also confirmed by Figure 2 which compares graphically the quality of the marginal approximation for the coefficients associated with
Figure 2: Quality of marginal approximation for the coefficients associated with the highest and lowest Wasserstein distance from the exact posterior under MF-VB and PFM-VB, respectively. The shaded grey area denotes the density of the exact posterior marginal, whereas the dotted and dashed lines represent the approximate densities provided by MF-VB and PFM-VB, respectively.

Figure 3: Scatterplots comparing the posterior expectations, standard deviations and predictive probabilities computed from 20000 values sampled from the exact SUN posterior, with those provided by the MF-VB (light grey circles) and PFM-VB (dark grey triangles).

As is clear from Figure 2, PFM-VB produces approximations which perfectly overlaps with the exact posterior in all cases, including also the worst-case scenario with the highest Wasserstein distance.
Consistent with Theorem 1, MF-VB has instead a reduced quality mostly due to a tendency to dramatically shrink towards zero the locations of the actual posterior. This behavior is displayed in the first panel of Figure 3, which compares the posterior expectations computed from 20000 values sampled from the exact SUN posterior with those provided by the closed-form expressions under MF-VB and PFM-VB reported in Section 2. Also the standard deviations are slightly under-estimated relative to PFM-VB that notably removes bias also in the second order moments. Consistent with the results in Figures 1–2, the slight variability of the PFM-VB estimates in the second panel of Figure 3 is arguably due to Monte Carlo error. We conclude by assessing quality in the approximation of the exact posterior predictive probabilities for the 33 held-out individuals. These measures are fundamental for prediction and, unlike for the first two marginal moments, their evaluation depends on the behavior of the entire posterior since it relies on an non-linear mapping of a linear combination of the parameters $\beta$. In the third panel of Figure 3, the proposed PFM-VB essentially matches the exact posterior predictive probabilities, thus providing reliable classification and uncertainty quantification. Instead, as expected from the theoretical results in Corollary 2, MF-VB over-shrinks these quantities towards 0.5.

4 Discussion and Future Research Directions

This article highlights notable issues in state-of-the-art methods for approximate Bayesian inference in high-dimensional binary regression, and proposes a partially factorized mean-field variational Bayes strategy which provably covers these open gaps. Our basic idea is to relax the mean-field assumption in a way which approximates more closely the factorization of the actual posterior, but still allows simple optimization and inference. The theoretical results confirm that the proposed strategy is an optimal solution in large $p$ settings, especially when $p \gg n$, and the empirical studies suggest that the theory provides useful insights also in applications not necessarily meeting the assumptions.

While our contribution provides an important advancement in a non-Gaussian regression context where previously available Bayesian computational strategies are unsatisfactory (Chopin and Ridgway, 2017), the results in this article open new avenues for future research. For instance, the theoretical issues of MF-VB and MAP estimators presented in Section 2.1 for large $p$ settings point to the need of further theoretical studies on the use of MF-VB and MAP estimators in high-dimensional regression with non-Gaussian responses. In these contexts, our general idea of relying on a partially
factorized approximating family could provide a viable strategy to solve potential issues of current approximations, as long as simple optimization is possible and the approximate posterior density for the global parameters can be derived in closed-form via marginalization of the local variables. This strategy could be also useful in Bayesian models relying on hierarchical priors for $\beta$ that facilitate variable selection and improved shrinkage. Albeit interesting, this setting goes beyond the scope of the article.

Finally, it would be certainly relevant to extend the asymptotic results in Theorems 1, 3 and 4 to settings in which $n$ grows with $p$ at some rate. In particular, we conjecture that $n$ growing sublinearly with $p$ is a sufficient condition to obtain asymptotic-exactness results analogous to Theorem 3. The theoretical results could also be relatively easily extended to cases where the prior variance $\nu^2$ varies with $p$, and in particular we expect Theorems 3 and 4 to still hold under mild assumptions on the dependence of $\nu^2$ on $p$.

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A Proofs

We start by proving some general lemmas that will be useful for the proofs of Theorems 1, 3 and 4. A key one is a variant of the strong law of large numbers, which is a classical result that follows from Khintchine–Kolmogorov convergence theorem and Kronecker’s lemma.

**Lemma A.1.** Let $(w_j)_{j \geq 1}$ be a sequence of independent random variables with mean 0 and variance bounded over $j$. Then $p^{-1/2-\delta} \sum_{j=1}^{p} w_j \overset{a.s.}{\rightarrow} 0$ as $p \rightarrow \infty$ for every $\delta > 0$.

**Lemma A.2.** Under A1, for any $\delta > 0$ we have $(\sigma_x^2 p)^{-1} X X^\top \overset{a.s.}{=} I_n + o(p^{-1/2+\delta})$ and $(\nu^2 \sigma_x^2 p)^{-1} (I_n + \nu^2 X X^\top) \overset{a.s.}{\rightarrow} I_n$ as $p \rightarrow \infty$.

**Proof.** By A1, $(x_{ij}^2)_{j \geq 1}$ are independent random variables with mean $\sigma_x^2$ and variance bounded over $j$. Thus $p^{1/2-\delta}[(\sigma_x^2 p)^{-1} X X^\top - I_n]_{ii} = p^{-1/2-\delta} \sum_{j=1}^{p} (\sigma_x^2 x_{ij}^2 - 1) \overset{a.s.}{\rightarrow} 0$ by Lemma A.1. Similarly, when
\[ i \neq i', (x_{ij}x_{i'j'})_{j \geq 1} \text{ are independent random variables with mean 0 and variance } \sigma_i^2 < \infty. \]

Thus
\[ p^{1/2-\delta}[(\sigma^2_{x}p)^{-1}XX^\top - I]_{ii'} = \sigma_i^{-2}p^{-1/2-\delta} \sum_{j=1}^p x_{ij}x_{i'j'} \xrightarrow{a.s.} 0 \]
as \( p \to \infty \) by Lemma A.1. It follows that \((\sigma^2_{x}p)^{-1}XX^\top \xrightarrow{a.s.} I_n + o(p^{-1/2+\delta})\) as \( p \to \infty \), which implies also \((\nu^2\sigma^2_{x}p)^{-1}(I_n + \nu^2XX^\top) = (\nu^2\sigma^2_{x}p)^{-1}I_n + (\sigma^2_{x}p)^{-1}XX^\top \xrightarrow{a.s.} I_n \) as \( p \to \infty \).

\[ \square \]

**Lemma A.3.** Let \( H = XX^\top \), then under A1, we have \((\nu^2\sigma^2_{x}p)(I_n - H) \xrightarrow{a.s.} I_n \) as \( p \to \infty \). Thus, for \( p \to \infty \), \( H_{ii} \xrightarrow{a.s.} 1 - (\nu^2\sigma^2_{x}p)^{-1} + o(p^{-1}) \) for all \( i = 1, \ldots, n \), and \( H_{ii'} \xrightarrow{a.s.} o(p^{-1}) \) for all \( i \neq i' \).

Proof. Since \( V = (\nu^2I_p + XX^\top)^{-1} \), by applying the Woodbury’s identity to \((I_n + \nu^2XX^\top)^{-1}\), we obtain \((I_n + \nu^2XX^\top)^{-1} = I_n - \nu^2X(I_p + \nu^2X^\top)^{-1}X^\top = I_n - X(\nu^2I_p + X^\top)^{-1}X^\top = I_n - H \). Thus \([(\nu^2\sigma^2_{x}p)(I_n - H)]^{-1} = (\nu^2\sigma^2_{x}p)^{-1}(I_n + \nu^2XX^\top) \xrightarrow{a.s.} I_n \) as \( p \to \infty \) by Lemma A.2 and the thesis follows by the continuity of the inverse operator over the set of non-singular \( n \times n \) matrices.

\[ \square \]

**Lemma A.4.** Let \( \mu_l^{(p)} \to 0 \) and \( \Sigma_l^{(p)} \to I_n \) as \( p \to \infty \) for \( l = 1, 2 \), where \( \mu_l^{(p)} \in \mathbb{R}^n \) and \( \Sigma_l^{(p)} \in \mathbb{R}^{n^2} \), \( l = 1, 2 \). Then \( \text{KL}(\text{TN}(\mu_1^{(p)}, \Sigma_1^{(p)}, A)) || \text{TN}(\mu_2^{(p)}, \Sigma_2^{(p)}, A)) \to 0 \) as \( p \to \infty \), where \( A \) is an orthant of \( \mathbb{R}^n \).

Proof. By definition, \( \text{KL}(\text{TN}(\mu_1^{(p)}, \Sigma_1^{(p)}, A)) || \text{TN}(\mu_2^{(p)}, \Sigma_2^{(p)}, A)) \) is equal to
\[
\log\left(\psi_2^{(p)} - \psi_1^{(p)} + \frac{1}{2} \log(\det(\Sigma_1^{(p)})^{-1} - \det(\Sigma_2^{(p)})) + (\psi_1^{(p)}2\pi)^{-n/2}\det(\Sigma_1^{(p)})^{-1/2} \int_A f_p(u)du\right),
\]
where \( \psi_i^{(p)} = \text{pr}(u_i^{(p)} \in A) \) with \( u_i^{(p)} \sim N_n(\mu_i^{(p)}, \Sigma_i^{(p)}) \), for \( l = 1, 2, \) and
\[
\begin{align*}
g_p(u) &= g_p(u) \exp[-0.5(u - \mu_i^{(p)})^\top(\Sigma_i^{(p)})^{-1}(u - \mu_i^{(p)})], \quad \text{with} \\
g_p(u) &= -0.5[(u - \mu_i^{(p)})^\top(\Sigma_i^{(p)})^{-1}(u - \mu_i^{(p)}) - (u - \mu_i^{(p)})^\top(\Sigma_i^{(p)})^{-1}(u - \mu_i^{(p)})].
\end{align*}
\]

Since \( \mu^{(p)} \to 0 \) and \( \Sigma^{(p)} \to I_n \) as \( p \to \infty \), we have that \( N_n(\mu_i^{(p)}, \Sigma_i^{(p)}) \to N_n(0, I_n) \) in distribution and \( \psi_i^{(p)} \to 2^{-n} \) by Portmanteau theorem, which implies \( \log\left(\psi_1^{(p)} - \psi_2^{(p)}\right) \to 0 \). In addition, by the continuity of \( \det(\cdot) \), we have \( \det(\Sigma_i^{(p)}) \to \det(I_n) = 1 \) as \( p \to \infty \), and thus \( \log(\det(\Sigma_1^{(p)})^{-1} - \det(\Sigma_2^{(p)})) \to 0 \) as \( p \to \infty \). Moreover, \( \Sigma_i^{(p)} \to I_n \) implies that all the eigenvalues of \( \Sigma_i^{(p)} \) converge to 1 as \( p \to \infty \) for \( l = 1, 2 \), and thus are eventually bounded away from 0 and \( \infty \). Therefore, there exist positive, finite constants \( m, M \) and \( k \) such that \( m\|u - \mu_i^{(p)}\|^2 \leq (u - \mu_i^{(p)})^\top(\Sigma_i^{(p)})^{-1}(u - \mu_i^{(p)}) \leq M\|u - \mu_i^{(p)}\|^2 \) for \( l = 1, 2 \) and \( p \geq k \). Calling \( b = \sup_{p \geq 1, i \in \{1,2\}} \|\mu_i^{(p)}\| < \infty \), and using standard properties of norms, we obtain, for \( l = 1, 2 \) and \( p \geq k \),
\[
\begin{align*}
m(\|u\|^2 - 2b\|u\|) \leq (u - \mu_i^{(p)})^\top(\Sigma_i^{(p)})^{-1}(u - \mu_i^{(p)}) \leq (M\|u\|^2 + Mb),
\end{align*}
\]
from which we immediately obtain that, for \( p \geq k \), \( |f_p(u)| \leq (M\|u\|^2 + Mb) \exp(-m\|u\|^2/2 + b\|u\|) \), where the latter is an integrable function on \( \mathbb{R}^n \). Therefore we can apply the dominated convergence theorem and obtain \( \lim_{p \to \infty} \int_A f_p(u)du = \int_A \lim_{p \to \infty} f_p(u)du = 0 \) as desired.

\[ \square \]
A.1 Proof of Theorem 1

Let \( \tilde{\beta}^* = \arg \max_{\beta \in \mathbb{R}^p} \ell(\beta) \), where \( \ell(\beta) = -(2\nu^2)^{-1}\|\beta\|^2 + \sum_{i=1}^n \log \Phi[(2y_i - 1)x_i^T\beta] \) denotes the log-posterior up to an additive constant under (1). Note that \( \tilde{\beta}^* \) is unique because \( \ell(\beta) \) is strictly concave (Haberman, 1974).

Lemma A.5. Under A1, we have \( \|\tilde{\beta}^*\| \xrightarrow{a.s.} 0 \) as \( p \to \infty \).

Proof. Since \( \log \Phi[(2y_i - 1)x_i^T\beta] < 0 \) for every \( i = 1, \ldots, n \), we have \( \ell(\beta) < -(2\nu^2)^{-1}\|\beta\|^2 \) and thus \( \|\beta\|^2 < -(2\nu^2)\ell(\beta) \) for any \( \beta \in \mathbb{R}^p \). It follows that \( \|\tilde{\beta}^*\|^2 < -(2\nu^2)\ell(\tilde{\beta}^*) = -(2\nu^2)\sup_{\beta \in \mathbb{R}^p} \ell(\beta) \).

We now prove that \( \sup_{\beta \in \mathbb{R}^p} \ell(\beta) \xrightarrow{a.s.} 0 \) as \( p \to \infty \). Define \( \tilde{\beta} = (\tilde{\beta}_j)_{j=1}^p \in \mathbb{R}^p \) as

\[
\tilde{\beta}_j = p^{-2/3}(2y_{nj/p} - 1)x_{nj/p,j}, \quad j = 1, \ldots, p,
\]

where \( \lceil a \rceil \) denotes the smallest integer larger or equal to \( a \). It follows that

\[
p^{-1/3}x_i^T\tilde{\beta} = p^{-1}(2y_i - 1)\sum_{j \in D_i} x_{ij}^2 + p^{-1}\sum_{j \notin D_i} \zeta_{ij},
\]

where \( D_i = \{j \in \{1, \ldots, p\} : (i-1)p/n < j \leq ip/n \} \) and \( \zeta_{ij} = x_{ij}x_{nj/p,j}(2y_{nj/p} - 1) \). Since \( (x_{ij}^2)_{j \in D_i} \) and \( (\zeta_{ij})_{j \notin D_i} \) are independent variables with bounded variance, the size of \( D_i \) is asymptotic to \( n^{-p} \) as \( p \to \infty \) and \( E(\zeta_{ij}) = 0 \) for \( j \notin D_i \), Lemma A.1 implies that \( \lim_{p \to \infty} p^{-1/3}x_i^T\tilde{\beta} \xrightarrow{a.s.} n^{-1}(2y_i - 1)\sigma_x^2 \).

Assuming \( \sigma_x^2 > 0 \) without loss of generality (when \( \sigma_x^2 = 0 \) it holds \( \tilde{\beta}^* \xrightarrow{a.s.} 0 \) it follows that \( x_i^T\tilde{\beta} \xrightarrow{a.s.} +\infty \) if \( y_i = 1 \) and \( x_i^T\tilde{\beta} \xrightarrow{a.s.} -\infty \) if \( y_i = 0 \) as \( p \to \infty \) and therefore \( \sum_{i=1}^n \log \Phi[(2y_i - 1)x_i^T\tilde{\beta}] \xrightarrow{a.s.} 0 \) as \( p \to \infty \). Moreover \( \|\tilde{\beta}\|^2 = p^{-1/3}(p^{-1}\sum_{j=1}^p x_{nj/p,j}^2) \xrightarrow{a.s.} 0 \) as \( p \to \infty \) by Lemma A.1. Thus \( 0 \geq \sup_{\beta \in \mathbb{R}^p} \ell(\beta) \geq \ell(\tilde{\beta}) \xrightarrow{a.s.} 0 \) as \( p \to \infty \) as desired. \( \square \)

Lemma A.6. Let \( q_1 \) and \( q_2 \) be probability distributions on \( \mathbb{R}^p \). Then, for any \( x_{\text{new}} \in \mathbb{R}^p \), we have \( \text{KL}[q_1 \mid \mid q_2] \geq 2\|p_{q_1} - p_{q_2}\|^2 \), where \( p_{q_1} = \int \Phi(x_{\text{new}}^T\beta)q_1(\beta)d\beta \) for \( l = 1, 2 \).

Proof. By Pinsker’s inequality, \( \text{KL}[q_1 \mid \mid q_2] \geq 2\text{TV}[q_1, q_2]^2 \) where \( \text{TV}[\cdot, \cdot] \) denotes the total variation distance between probability distributions. Recall that \( \text{TV}[q_1, q_2] = \sup_{h: \mathbb{R}^p \to [0,1]} |\int_{\mathbb{R}^p} h(\beta)q_1(\beta)d\beta - \int_{\mathbb{R}^p} h(\beta)q_2(\beta)d\beta|. \) Taking \( h(\beta) = \Phi(x_{\text{new}}^T\beta) \) in the above equation we obtain the desired statement. \( \square \)

Theorem 1. As noted in Armagan and Zaretzki (2011), the CAVI algorithm for MF-VB is equivalent to an EM algorithm for \( p(\beta|y) \) with missing data \( z \), which in this case is guaranteed to converge to the unique maximizer of \( p(\beta|y) \) by, e.g., Theorem 3.2 of McLachlan and Krishnan (2007) and the
fact that \( p(\beta | y) \) is strictly concave (Haberman, 1974). Therefore \( \mathbb{E}_{q_{\text{tar}}(\beta)}(\beta) = \bar{\beta}^* \) and Lemma A.5 implies that \( \|\mathbb{E}_{q_{\text{tar}}(\beta)}(\beta)\| \xrightarrow{a.s.} 0 \) as \( p \to \infty \).

We now show that \( \|\mathbb{E}_{p(\beta | y)}(\beta)\|^2 \xrightarrow{a.s.} \nu^2 nc^2 \) as \( p \to \infty \). By the law of total expectation \( \mathbb{E}_{p(\beta | y)}(\beta) = \mathbf{V} \mathbf{X}^\top \mathbb{E}_{p(z | y)}(z) \). It follows that \( \|\mathbb{E}_{p(\beta | y)}(\beta)\|^2 = \mathbb{E}_{p(z | y)}(z)^\top \mathbf{X} \mathbf{V} \mathbf{X} \mathbb{E}_{p(z | y)}(z) \). Applying the Woodbury’s identity to \( \mathbf{V} \) we have \( \mathbf{V} \mathbf{X}^\top = \nu^2 \mathbf{X}^\top (\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top)^{-1} \). Therefore, we can write \( \sigma_{z, p}^2 \mathbf{X} \mathbf{V} \mathbf{X}^\top = \mathbf{S}^\top (\sigma_{z, p}^2)^{-1} \mathbf{X}^\top \mathbf{S} \) with \( \mathbf{S} = \nu^2 \sigma_{z, p}^2 (\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top)^{-1} \) and deduce \( \sigma_{z, p}^2 \mathbf{X} \mathbf{V} \mathbf{X}^\top \xrightarrow{a.s.} \mathbf{I}_n \) as \( p \to \infty \) from Lemma A.2. Multiplying and dividing by \( \sigma_{z, p}^2 \) in the expression for \( \|\mathbb{E}_{p(\beta | y)}(\beta)\|^2 \), it also follows that \( \lim_{p \to \infty} \|\mathbb{E}_{p(\beta | y)}(\beta)\|^2 \xrightarrow{a.s.} \lim_{p \to \infty} \| (\sigma_{z, p}^2)^{-1/2} \mathbb{E}_{p(z | y)}(z) \|^2 \). Since \( (z | y) \sim \mathcal{T}N(0, (\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top), \mathbb{A}) \), it holds \( [(\nu^2 \sigma_{z, p}^2)^{-1/2} z | y) \sim \mathcal{T}N(0, (\nu^2 \sigma_{z, p}^2)^{-1}(\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top), \mathbb{A}) \]. Then,

\[
\mathbb{E}_{p(z | y)}([\nu^2 \sigma_{z, p}^2]^{-1/2} z) = \frac{1}{\psi(p)} \int_{\mathbb{A}} \hat{u}_i \phi_n(\hat{u}; [\nu^2 \sigma_{z, p}^2]^{-1}(\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top))] d\hat{u},
\]

where \( \psi(p) = \text{pr}(u(u) \in \mathbb{A}) \) for \( u(u) \sim N_n(0, (\nu^2 \sigma_{z, p}^2)^{-1}(\mathbf{I}_n + \nu^2 \mathbf{X} \mathbf{X}^\top)) \). Thus, Lemma A.2 together with a domination argument similar to the one used in the proof of Lemma A.4 imply that, as \( p \to \infty \),

\[
(\nu^2 \sigma_{z, p}^2)^{-1/2} \mathbb{E}_{p(z | y)}(z) \xrightarrow{a.s.} \nu^2 \sum_{i=1}^n c_i^2 = \nu^2 nc^2.
\]

Finally, we show that \( \lim_{p \to \infty} \mathbb{K}L[q_{\text{tar}}^* (\beta) \mid p(\beta | y)] \xrightarrow{a.s.} 0 \). Lemma A.6 implies \( \mathbb{K}L[q_{\text{tar}}^* (\beta) \mid p(\beta | y)] \geq 2 |\text{pr}_{\text{MF}} - \text{pr}_{\text{SUN}}|^2 \), where \( \text{pr}_{\text{SUN}} = \int \Phi(x_{\text{NEW}}^\top \beta)p(\beta | y) \) d\beta and \( \text{pr}_{\text{MF}} = \int \Phi(x_{\text{NEW}}^\top \beta)q_{\text{tar}}^*(\beta) \) d\beta.

To accomplish this goal, we consider \( x_{\text{NEW}}^\top = (\nu^2 \sigma_{z, p}^2)^{-1/2} \mathbf{X}^\top \mathbf{H}^{-1} \delta \), with \( \delta = (2y_1 - 1, 0, \ldots, 0)^\top \), and show that \( \lim_{p \to \infty} |\text{pr}_{\text{MF}} - \text{pr}_{\text{SUN}}| > 0 \). Here we can assume without loss of generality that \( \mathbf{H} \xrightarrow{a.s.} \mathbf{I}_n \) as \( p \to \infty \) by Lemma A.3 and the set of \( n \times n \) non-singular matrices is open. This implies that \( \mathbf{H} \) is eventually invertible as \( p \to \infty \) almost surely. By definition of \( x_{\text{NEW}} \) we have

\[
\|x_{\text{NEW}}\|^2 = x_{\text{NEW}}^\top x_{\text{NEW}} = \nu^{-2} \delta^\top \mathbf{H}^{-1} (\sigma_{z, p}^2)^{-1} \mathbf{X} \mathbf{X}^\top \mathbf{H}^{-1} \delta \xrightarrow{a.s.} \nu^{-2} \|\delta\|^2 = \nu^{-2} \text{ as } p \to \infty,
\]

because \( \mathbf{H}^{-1} \xrightarrow{a.s.} \mathbf{I}_n \) and \( (\sigma_{z, p}^2)^{-1} \mathbf{X} \mathbf{X}^\top \xrightarrow{a.s.} \mathbf{I}_n \) as \( p \to \infty \) by Lemmas A.3 and A.2, respectively. By (7) we have \( \text{pr}_{\text{MF}} = \Phi[x_{\text{NEW}}^\top \bar{\beta}^* (1 + x_{\text{NEW}}^\top \mathbf{X} x_{\text{NEW}})^{-1/2}] \), and by Cauchy-Schwarz inequality and \( x_{\text{NEW}}^\top \mathbf{V} x_{\text{NEW}} \geq 0 \) we have \( |x_{\text{NEW}}^\top \bar{\beta}^* (1 + x_{\text{NEW}}^\top \mathbf{X} x_{\text{NEW}})^{-1/2}| \leq \|x_{\text{NEW}}\|\|\bar{\beta}^*\|^2 \xrightarrow{a.s.} 0 \) as \( p \to \infty \), where the latter convergence follows from \( \|x_{\text{NEW}}\| \xrightarrow{a.s.} 1 \) and \( \|\bar{\beta}^*\| \xrightarrow{a.s.} 0 \). Thus \( \text{pr}_{\text{MF}} \xrightarrow{a.s.} 0.5 \) as \( p \to \infty \).

Consider now \( \text{pr}_{\text{SUN}} \). With derivations analogous to those of equation (11), we can express \( \text{pr}_{\text{SUN}} = \mathbb{E}_{p(z | y)} \{ \Phi[x_{\text{NEW}}^\top \mathbf{V} z (1 + x_{\text{NEW}}^\top \mathbf{V} x_{\text{NEW}})^{-1/2}] \} \). By definition of \( x_{\text{NEW}} \), we have that \( x_{\text{NEW}}^\top \mathbf{V} x_{\text{NEW}} = (\nu^2 \sigma_{z, p}^2)^{-1} \delta^\top \mathbf{H}^{-1} \delta \xrightarrow{a.s.} 0 \) as \( p \to \infty \) since \( \mathbf{H}^{-1} \xrightarrow{a.s.} \mathbf{I}_n \) by Lemma A.3 and \( \|\delta\| = 1 \). Moreover, \( x_{\text{NEW}}^\top \mathbf{V} z = \delta^\top (\nu^{-1} \sigma_{z, p}^{-1} - 1/2) z \) and \( \nu^{-1} \sigma_{z, p}^{-1} \xrightarrow{a.s.} 0 \) as \( p \to \infty \),
almost surely. Combining these results with Slutsky’s lemma and the fact that \( \Phi(\cdot) \) is bounded and continuous, it follows that 
\[
E_{p(z|x)}\{\Phi^{\top}(x_{\text{NEW}}^\top VX^\top z(1 + x_{\text{NEW}}^\top VX_{\text{NEW}})^{-1/2})\} \rightarrow E_{p(z)}[\Phi(\delta^\top z)] \text{ with } z \sim TN(\mathbf{0}, \mathbf{I}, \mathbf{A}).
\]
Thus \( pr_{\text{sun}} \rightarrow E_{p(z)}[\Phi(2y_th - 1)\tilde{z}] = \int_0^\infty \Phi(z)2\phi(z)dz > 0.5 \) as \( p \to \infty \). It follows that 
\[
\lim_{p \to \infty} KL[q^*_\text{PMM}(\beta) \mid p(\beta \mid y)] \geq 2\lim_{p \to \infty} |pr_{\text{SPM}} - pr_{\text{sun}}|^2 > 0 \text{ almost surely as } p \to \infty.
\]

\section*{A.2 Proof of Theorem 2, Corollary 1 and Proposition 2}

\textbf{Theorem 2.} Leveraging the chain rule of the KL divergence we have that 
\[
KL[q^*_\text{PMM}(\beta, z) \mid p(\beta, z \mid y)] = KL[q^*_\text{PMM}(z) \mid p(z \mid y)] + E_{q^*_\text{PMM}(z)}\{KL[q^*_\text{PMM}(\beta \mid z) \mid p(\beta \mid z)]\},
\]
where \( q^*_\text{PMM}(\beta|z) \) appears only in the second summand. This quantity is always non-negative and coincides with zero, for every \( q^*_\text{PMM}(z) \), if and only if \( q^*_\text{PMM}(\beta \mid z) = p(\beta \mid z) = \phi_p(\beta - VX^\top z; V) \).

The expression for \( q^*_\text{PMM}(z) = \prod_{i=1}^n q^*_\text{PMM}(z_i) \) is instead a direct consequence of the closure under conditioning property of the multivariate truncated Gaussian (Horrace, 2005; Holmes and Held, 2006). In particular, adapting the results in Holmes and Held (2006), it easily follows that 
\[
p(z_i \mid z_{-i}, y) \propto \phi[z_i - (1 - x_i^\top Vx_i)^{-1}x_i^\top VX_{-i}^\top y_{-i}; (1 - x_i^\top Vx_i)^{-1}] \mathbb{1}[(2y_i - 1)z_i > 0], \quad i = 1, \ldots, n,
\]
where \( X_{-i} \) is the design matrix without row \( i \). To obtain the expression for \( q^*_\text{PMM}(z_i), i = 1, \ldots, n, \) note that, recalling e.g., Blei et al. (2017), the optimal solution for \( q^*_\text{PMM}(z) \) which minimizes 
\[
KL[q^*_\text{PMM}(z) \mid p(z \mid y)]
\]
within family of distributions that factorize over \( z_1, \ldots, z_n \) can be expressed as 
\[
\prod_{i=1}^n q^*_\text{PMM}(z_i) \propto \exp[E_{q^*_\text{PMM}(z_{-i})}(\log[p(z_i \mid z_{-i}, y)])]
\]
for every \( i = 1, \ldots, n \). Combining such a result with the above expression for \( p(z_i \mid z_{-i}, y) \) we have that \( \exp[E_{q^*_\text{PMM}(z_{-i})}(\log[p(z_i \mid z_{-i}, y)])] \) is proportional to 
\[
\exp\left[-\frac{z_i^2 - 2z_i(1 - x_i^\top Vx_i)^{-1}x_i^\top VX_{-i}^\top \mathbb{E}_{q^*_\text{PMM}(z_{-i})}(z_{-i})}{2(1 - x_i^\top Vx_i)^{-1}}\right] \mathbb{1}[(2y_i - 1)z_i > 0], \quad i = 1, \ldots, n.
\]
The above quantity coincides with the kernel of a Gaussian distribution having variance \( \sigma^2_i = (1 - x_i^\top Vx_i)^{-1} \), expectation \( \mu^*_i = (\sigma^2_i x_i^\top Vx_i^\top \mathbb{E}_{q^*_\text{PMM}(z_{-i})}(z_{-i}) \) and truncation below zero if \( y_i = 1 \) or above zero if \( y_i = 0 \). Hence, each \( q^*_\text{PMM}(z_i) \) is the density of a truncated normal with parameters specified in Theorem 2. The proof is concluded after noticing that the expression for \( \tilde{z}^*_i = \mathbb{E}_{q^*_\text{PMM}(z_i)}(z_i), i = 1, \ldots, n, \) in Theorem 2 follows directly from the mean of truncated normals.

\textbf{Corollary 1.} From (8), we have that \( q^*_\text{PMM}(\beta) \) coincides with the density of a random variable that has the same distribution of \( \tilde{u}^{(0)} + VX^\top \tilde{u}^{(1)} \), where \( \tilde{u}^{(0)} \sim N_p(0, V) \) and \( \tilde{u}^{(1)} \) is from an \( n \)-variate Gaussian with mean vector \( \mu^* \), diagonal covariance matrix \( \sigma^2 \) and generic \( i \)th component truncated either
below or above zero depending of the sign of \((2y_i - 1)\), for \(i = 1, \ldots, n\). Since \(\tilde{u}^{(1)}\) has independent components, by standard properties of univariate truncated normal variables we obtain
\[
\tilde{u}^{(0)} + VX^\top \tilde{u}^{(1)} \overset{d}{=} u^{(0)} + VX^\top [I_n(2y - 1)] \sigma^* u^{(1)},
\]
where \(u^{(0)} \sim N_p(VX^\top \mu^*; V)\) and \(u^{(1)}\) is an \(n\)-variate Gaussian with mean vector \(0\), covariance matrix \(I_n\), and truncation below \(-|I_n(2y - 1)| \sigma^* \mu^*\). Calling \(\xi = VX^\top \mu^*\), \(\Omega = \omega \bar{\Omega} \omega = V + VX^\top \sigma^2 XV\), \(\Delta = \omega^{-1} VX^\top [I_n(2y - 1)] \sigma^*\), \(\gamma = [I_n(2y - 1)] \sigma^{-1} \mu^*\) and \(\Gamma = I_n\), as in Corollary 1, we have that
\[
u^{(0)} \sim N_p(0, \Omega - \Delta \Gamma^{-1} \Delta^\top),\]
and \(u^{(1)}\) distributed as a \(n\)-variate Gaussian random variable with mean vector \(0\), covariance matrix \(\Gamma\), and truncation below \(-\gamma\). Recalling Arellano-Valle and Azzalini (2006) and Azzalini and Capitanio (2014) such a stochastic representation coincides with the one of the unified skew-normal random variable SUN\(_{p,n}(\xi, \Omega, \Delta, \gamma, \Gamma)\).

\[\text{Proposition 2.}\]

To prove Proposition 2, first notice that by the results in equation (8) and in Theorem 2, \(z = (z_1, \ldots, z_n)^\top\) denotes a vector whose entries have independent truncated normal approximating densities. Hence, \(E_{q^{\text{tru}}(z_i)}(z_i) = \bar{z}_i^*\) and var\(_{q^{\text{tru}}(z_i)}(z_i) = \sigma_i^* [1 - (2y_i - 1)\eta_i^*/\sigma_i^* - \eta_i^2]\) with \(\eta_i = \phi(\mu_i^*/\sigma_i^*)\Phi([2y_i - 1]\mu_i^*/\sigma_i^*)^{-1}\) for \(i = 1, \ldots, n\). Using the parameters defined in Theorem 2, var\(_{q^{\text{tru}}(z_i)}(z_i)\) can be also re-written as var\(_{q^{\text{tru}}(z_i)}(z_i) = \sigma_i^* - (\bar{z}_i^* - \mu_i^*) \bar{z}_i^*.\) Therefore, \(E_{q^{\text{tru}}(z)}(z) = \bar{z}^*\) and var\(_{q^{\text{tru}}(z)}(z) = \sigma^2 - (\bar{z}^* - \mu^*)^\top I_n \bar{z}^*,\) where \(\bar{z}^*, \mu^*\) and \(\sigma^*\) are defined in Theorem 2 and Corollary 1. Combining these results with equation (8), and using the law of iterated expectations we have
\[
E_{q^{\text{tru}}(z)}(\beta) = E_{q^{\text{tru}}(z)}[E_{p(\beta|z)}(\beta)] = E_{q^{\text{tru}}(z)}(VX^\top z) = VX^\top E_{q^{\text{tru}}(z)}(z) = VX^\top \bar{z}^*,
\]
\[
\text{var}_{q^{\text{tru}}(z)}(\beta) = E_{q^{\text{tru}}(z)}[\text{var}_{p(\beta|z)}(\beta)] + \text{var}_{q^{\text{tru}}(z)}[E_{p(\beta|z)}(\beta)] = V + VX^\top \text{var}_{q^{\text{tru}}(z)}(z) XV
\]
\[
= V + VX^\top [\sigma^2 - (\bar{z}^* - \mu^*)^\top I_n \bar{z}^*] XV,
\]
thus proving equation (10).

To prove equation (11) it suffices to notice that \(\text{pr}_{\text{PMM}}(y_{\text{NEW}} = 1 \mid y) = E_{q^{\text{tru}}(\beta)}[\Phi(x_{\text{NEW}}^\top \beta)]\). Hence, by applying again the law of iterated expectations we have
\[
E_{q^{\text{tru}}(\beta)}[\Phi(x_{\text{NEW}}^\top \beta)] = E_{q^{\text{tru}}(z)}[E_{p(\beta|z)}[\Phi(x_{\text{NEW}}^\top \beta)]] = E_{q^{\text{tru}}(z)}[\Phi(x_{\text{NEW}}^\top VX^\top z(1 + x_{\text{NEW}}^\top VX_{\text{NEW}})^{-1/2})].
\]
The last equality follows from the fact that \(p(\beta | z)\) is a Gaussian density and hence \(E_{p(\beta|z)}[\Phi(x_{\text{NEW}}^\top \beta)]\) can be derived in closed-form; see e.g., Lemma 7.1 in Azzalini and Capitanio (2014).
A.3 Proof of Theorem 3 and Corollary 2

**Theorem 3.** As a consequence of the discussion after the statement of Theorem 2, the density \( q_{\text{FPM}}^*(z) \) minimizes the KL divergence to \( p(z|y) \) within the family of distributions that factorize over \( z_1, \ldots, z_n \). Thus \( \text{KL}[q_{\text{FPM}}^*(z)||p(z|y)] \leq \text{KL}[\text{TN}(0, \nu^2\sigma_x^2pI_n, A)||p(z|y)] \). Since the KL divergence is invariant with respect to bijective transformations and \( p(z|y) = \text{TN}(0, I_n + \nu^2XX^\top, A) \), then rescaling each \( z_i \) by \((\nu^2\sigma_x^2p)^{-1/2}\) we have \( \text{KL}[\text{TN}(0, \nu^2\sigma_x^2pI_n, A)||p(z|y)] = \text{KL}[\text{TN}(0, I_n, A)||\text{TN}(0, (\nu^2\sigma_x^2p)^{-1}(I_n + \nu^2XX^\top), A)] \). Lemma A.2 shows that \((\nu^2\sigma_x^2p)^{-1}(I_n + \nu^2XX^\top) \overset{a.s.}{\to} I_n \) and thus Lemma A.4 implies that \( \text{KL}[\text{TN}(0, I_n, A)||\text{TN}(0, (\nu^2\sigma_x^2p)^{-1}(I_n + \nu^2XX^\top), A)] \overset{a.s.}{\to} 0 \) as \( p \to \infty \). From this result it follows that \( \lim_{p \to \infty} \text{KL}[q_{\text{FPM}}^*(z)||p(z|y)] \overset{a.s.}{=} 0 \) as desired. \( \square \)

**Corollary 2.** Lemma A.6 and Theorem 3 also imply that \( \sup_{x_{\text{new}} \in \mathbb{R}^p} |pr_{\text{FPM}} - pr_{\text{SUN}}| \leq \{ \text{KL}[q_{\text{FPM}}(\beta)||p(\beta|y)]/2 \}^{1/2} \overset{a.s.}{\to} 0 \) as \( p \to \infty \). Moreover, in the proof of Theorem 1 it has been shown that setting \( x_{\text{new}} = (\nu^2\sigma_x^2)^{-1/2}X^\top H^{-1} \delta \) for every \( p \) leads to \( \lim_{p \to \infty} \inf |pr_{\text{MF}} - pr_{\text{SUN}}| = 0 \), from which it follows the second part of the corollary. \( \square \)

A.4 Proof of Theorem 4

**Lemma A.7.** Let \( y \in \{0; 1\} \) be a generic binary response and \( \bar{z}^* = \mu^* + (2y - 1)\sigma^*\phi(\mu^*/\sigma^*)\Phi((2y - 1)\mu^*/\sigma^*)^{-1} \), with \( \mu^* \in \mathbb{R} \) and \( \sigma^* \geq 0 \). Then \( \sup_{\mu^*, \sigma^*} (|\mu^*| + \sigma^*)^{-1} |\bar{z}^*| < \infty \).

**Proof.** By the triangle inequality

\[
(|\mu^*| + \sigma^*)^{-1} |\bar{z}^*| \leq 1 + (|\mu^*| + \sigma^*)^{-1} \sigma^*\phi(\mu^*/\sigma^*)/\Phi(-|\mu^*/\sigma^*|).
\]

If \( |\mu^*| \leq \sigma^* \) then \( |\bar{z}^*|/(|\mu^*| + \sigma^*) \leq 1 + 1 \times \phi(0)/\Phi(-1) < \infty \). If \( |\mu^*| > \sigma^* \), setting \( t = |\mu^*|/\sigma^* \) and using the bound \( \Phi(-t) \geq (2\pi)^{-1/2}t(t^2 + 1)^{-1} \exp(-t^2/2) \), which holds for every \( t > 0 \), we have

\[
(|\mu^*| + \sigma^*)^{-1} |\bar{z}^*| \leq 1 + |\mu^*|^{-1} \sigma^*\phi(t)/\Phi(-t) \\
\leq 1 + t^{-1} \exp(-t^2/2)(t^2 + 1)^{-1} \exp(-t^2/2) = 1 + t^{-2}(t^2 + 1) < 3
\]

where in the last inequality we used \( t > 1 \). Combining the above results it follows that \( \sup_{\mu^*, \sigma^*} (|\mu^*| + \sigma^*)^{-1} |\bar{z}^*| < \infty \) as desired. \( \square \)

**Lemma A.8.** For every \( i = 1, \ldots, n \), we have \( p^{-1/2} \mu_i^{(1)} \overset{a.s.}{\to} 0 \) as \( p \to \infty \), where \( \mu_i^{(1)} \) is defined as in Algorithm 2.
Proof. Lemma A.7 implies \( \sup_{\sigma_i} |z_i^{(0)}|/\sigma_i < \infty \) and, since \( \sigma_i \) is almost surely asymptotic to \( \sigma x \nu p^{1/2} \) as \( p \to \infty \) by Lemma A.3, it follows \( \sup_{p \geq 1} p^{-1/2}|z_i^{(0)}| \overset{a.s.}{\to} \infty \) for every \( i = 1, \ldots, n \). Note that we are implicitly assuming Algorithm 2 to have fixed initialization \( \mu_i^{(0)} \in \mathbb{R}, \ i = 1, \ldots, n \). We now prove that \( \lim_{p \to \infty} p^{-1/2} \mu_i = 0 \) and \( \sup_{p \geq 1} p^{-1/2}|z_i^{(1)}| \overset{a.s.}{\to} \infty \) for every \( i = 1, \ldots, n \) by induction on \( i \). When \( i = 1 \), recalling the definition of \( \mu_i^{(1)} \) in Algorithm 2, we have that \( |p^{-1/2} \mu_i^{(1)}| = |\sigma_i^{1/2} \sum_{i'=2}^n H_{ii'} p^{-1/2} z_i^{(0)}| \leq \sum_{i'=2}^n \sigma_i^{1/2} H_{ii'} |p^{-1/2}|z_i^{(0)}| \). Lemma A.3 and the fact that \( \sigma_i^2 \) is almost surely asymptotic to \( \nu^2 \sigma_i^2 p \), imply that \( \sigma_i^2 |H_{ii'}| \overset{a.s.}{\to} 0 \) for every \( i' \geq 2 \) as \( p \to \infty \). Combining the latter with \( \sup_{p \geq 1} p^{-1/2}|z_i^{(0)}| \overset{a.s.}{\to} \infty \), we obtain \( p^{-1/2} \mu_i^{(1)} \overset{a.s.}{\to} 0 \) as \( p \to \infty \). Combining the latter with Lemma A.7, we obtain \( \sup_{p \geq 1} p^{-1/2} z_i^{(1)} \overset{a.s.}{\to} \infty \). We thus proved the desired statements for \( i = 1 \).

When \( i > 1 \), by simple manipulations of the expressions in Algorithm 2, we can express \( \mu_i^{(1)}/\sigma_i \) as

\[
p^{-1/2} \mu_i^{(1)} = \sum_{i'=1}^{i-1} \sigma_i^2 H_{ii'} p^{-1/2} z_i^{(1)} + \sum_{i'=i+1}^{n} \sigma_i^2 H_{ii'} p^{-1/2} z_i^{(0)}.
\]

Now, for \( i' > i \) we have \( |\sigma_i^2 H_{ii'} p^{-1/2} z_i^{(0)}| \overset{a.s.}{\to} 0 \) by the same arguments of the \( i = 1 \) case above. For \( i' < i \) we have \( |\sigma_i^2 H_{ii'} p^{-1/2} z_i^{(1)}| \overset{a.s.}{\to} 0 \) by Lemma A.3, the fact that \( \sigma_i^2 \) is almost surely asymptotic to \( \sigma x \nu^2 p \) and \( \sup_{p \geq 1} p^{-1/2} z_i^{(1)} \overset{a.s.}{\to} \infty \) for \( i' < i \) by induction. It follows that \( \lim_{p \to \infty} p^{-1/2} \mu_i^{(1) \overset{a.s.}{\to} 0} \) and thus, by Lemma A.7, also that \( \sup_{p \geq 1} p^{-1/2} z_i^{(1)} \overset{a.s.}{\to} \infty \). The thesis follows by induction.

**Theorem 4.** The chain rule for KL divergences and the fact that \( q_{\text{pfm}}^{(1)}(\beta|z) = p(\beta|y,z) \) imply that

\[
\text{KL}[q_{\text{pfm}}^{(1)}(\beta)||p(\beta|y)] \leq \text{KL}[q_{\text{pfm}}^{(1)}(\beta,z)||p(\beta,z|y)] = \text{KL}[q_{\text{pfm}}^{(1)}(z)||p(z|y)].
\]

Since \( q_{\text{pfm}}^{(1)}(z) = \text{TN}(\mu, \sigma^{-2}, \mathcal{A}) \) and \( p(z|y) = \text{TN}[0, (I_n + \nu^2 XX^\top), \mathcal{A}] \), then rescaling by \( p^{-1/2} \) we have that

\[
\text{KL}[q_{\text{pfm}}^{(1)}(z)||p(z|y)] = \text{KL}[\text{TN}(p^{-1/2} \mu^{(1)}, p^{-1} \sigma^{-2}, \mathcal{A})||\text{TN}[0, p^{-1}(I_n + \nu^2 XX^\top), \mathcal{A}]].
\]

Lemma A.8 implies that \( p^{-1/2} \mu^{(1)} \overset{a.s.}{\to} 0 \), while Lemmas A.2 and A.3 imply that both \( p^{-1}(I_n + \nu^2 XX^\top) \) and \( p^{-1} \sigma^{-2} \) converge a.s. to \( \nu^2 \sigma_i^2 I_n \) as \( p \to \infty \). Therefore \( \text{KL}[\text{TN}(p^{-1/2} \mu^{(1)}, p^{-1} \sigma^{-2}, \mathcal{A})||\text{TN}[0, p^{-1}(I_n + \nu^2 XX^\top), \mathcal{A}]] \overset{a.s.}{\to} 0 \) by Lemma A.4, implying \( \text{KL}[q_{\text{pfm}}^{(1)}(\beta)||p(\beta|y)] \overset{a.s.}{\to} 0 \) as desired.

**B Computational cost of PFM-VB**

We now discuss the computational cost of PFM-VB, showing that the whole routine requires matrix pre-computations with \( O(np \cdot \min\{p,n\}) \) cost and iterations with \( O(n \cdot \min\{p,n\}) \) cost.

Consider first Algorithm 2. When \( p \geq n \), one can pre-compute \( XX^\top \) at \( O(np^2) \) cost by applying the Woodbury’s identity to \( V \), and then perform each iteration at \( O(n^2) \) cost. Instead, when \( p < n \,
one can pre-compute $\mathbf{XV}$ at $\mathcal{O}(p^2 n)$ cost, and then perform each iteration at $\mathcal{O}(pn)$ cost noting that

$$
\mu_i(t) = \sigma^2 \sum_{j=1}^{p} (\mathbf{XV})_{ij} \alpha_j^{(t,i)}, \quad \text{with} \quad \alpha_j^{(t,i)} = \sum_{i'=1}^{t-1} x_{i'j} z_{i't}^{(t)} + \sum_{i'=i+1}^{n} x_{i'j} z_{i't}^{(t-1)},
$$

where the vector $\alpha^{(t,i)} = (\alpha_1^{(t,i)}, \ldots, \alpha_p^{(t,i)})^\top$ can be computed at $\mathcal{O}(p)$ cost from $\alpha^{(t,i-1)}$ exploiting the recursive equations $\alpha_j^{(t,i)} = \alpha_j^{(t,i-1)} - x_{ij} z_i^{(t-1)} + x_{i-1,j} z_{i-1}^{(t)}$. Therefore, computing $\mu_i^{(t)}$ for $i = 1, \ldots, n$, which is the most expensive part of Algorithm 2, can be done in $\mathcal{O}(np)$ operations using $\mathbf{XV}$ and $\alpha^{(t,i)}$. With simple calculations one can check that also computing ELBO$(\ell_p^{(t)}|\beta, \mathbf{z})$ requires $\mathcal{O}(n \cdot \min\{p, n\})$ operations, as it involves quadratic forms of $n \times n$ matrices with rank at most $\min\{p, n\}$; see https://github.com/augustofasano/Probit-PFMVB for the full ELBO expression.

Given the output of Algorithm 2, the mean of $\beta$ under PFM-VB can be computed at $\mathcal{O}(pn \cdot \min\{p, n\})$ cost noting that, by (10), $E_{q_{\nu(m)}(\beta)} = \mathbf{VX}^\top \bar{\mathbf{z}}$ and that $\mathbf{VX}^\top$ can be computed at $\mathcal{O}(pn \cdot \min\{p, n\})$ cost using either its definition, when $p \leq n$, or the equality $\mathbf{VX}^\top = \nu^2 \mathbf{X}^\top (\mathbf{I}_n + \nu^2 \mathbf{XX}^\top)^{-1}$, when $p > n$. Given $\mathbf{VX}^\top$, one can compute the covariance matrix of $\beta$ under PFM-VB at $\mathcal{O}(p^2 n)$ cost using (10), and applying Woodbury’s identity to $\mathbf{V}$ when $p > n$. On the other hand, the marginal variances $\text{var}_{q_{\nu(m)}(\beta_j)}(\beta_j)$, $j = 1, \ldots, p$, can be obtained at $\mathcal{O}(pn \cdot \min\{p, n\})$ cost by first computing $\mathbf{VX}^\top$, and then exploiting (10) along with $V_{jj} = \nu^2 [1 - \sum_{i=1}^{n} (\mathbf{VX}^\top)_{ji} x_{ij}]$, which follows from $\mathbf{V}(\mathbf{I}_p + \nu^2 \mathbf{X}^\top \mathbf{X}) = \nu^2 \mathbf{I}_p$.

Finally, the Monte Carlo estimates of the approximate predictive probabilities $\Pr_{\text{PFM}}(y_{\text{new}} = 1 \mid \mathbf{y})$ in (11) can be computed at $\mathcal{O}(pn \cdot \min\{p, n\} + nR)$ cost, where $R$ denotes the number of Monte Carlo samples. Indeed, simulating i.i.d. realizations $\mathbf{z}^{(r)}$, $r = 1, \ldots, R$, from $q_{\nu(m)}(\mathbf{z})$ for has an $\mathcal{O}(nR)$ cost, while computing $\Phi[x_{\text{new}}^\top \mathbf{VX}^\top \mathbf{z}^{(r)} (1 + x_{\text{new}}^\top \mathbf{Vx}_{\text{new}})^{-1/2}]$ for $r = 1, \ldots, R$ has $\mathcal{O}(pn \cdot \min\{p, n\} + nR)$ cost because, given $\mathbf{VX}^\top$, the computation of $x_{\text{new}}^\top \mathbf{VX}^\top \mathbf{z}^{(r)}$ for $r = 1, \ldots, R$ requires $\mathcal{O}(pn + nR)$ operations, while the computation of $x_{\text{new}}^\top \mathbf{Vx}_{\text{new}}$ can be done in $\mathcal{O}(pn \cdot \min\{p, n\})$ operations using either its definition, when $p \leq n$, or Woodbury’s identity on $\mathbf{V}$, when $p > n$, leading to $x_{\text{new}}^\top \mathbf{Vx}_{\text{new}} = \nu^2 \|x_{\text{new}}\|^2 - \nu^2 (\mathbf{Xx}_{\text{new}})^\top (\mathbf{I}_n + \nu^2 \mathbf{XX}^\top)^{-1} (\mathbf{Xx}_{\text{new}})$.

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