Bayesian inference on high-dimensional multivariate binary data

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Abstract
It has become increasingly common to collect high-dimensional binary data; for example, with the emergence of new sampling techniques in ecology. In smaller dimensions, multivariate probit (MVP) models are routinely used for inferences. However, algorithms for fitting such models face issues in scaling up to high dimensions due to the intractability of the likelihood, involving an integral over a multivariate normal distribution having no analytic form. Although a variety of algorithms have been proposed to approximate this intractable integral, these approaches are difficult to implement and/or inaccurate in high dimensions. We propose a two-stage Bayesian approach for inference on model parameters while taking care of the uncertainty propagation between the stages. We use the special structure of latent Gaussian models to reduce the highly expensive computation involved in joint parameter estimation to focus inference on marginal distributions of model parameters. This essentially makes the method embarrassingly parallel for both stages. We illustrate performance in simulations and applications to joint species distribution modeling in ecology.

Keywords: Bayesian; Covariance; Divide-and-conquer; High-dimensional; Joint species distribution model; Laplace approximation; Parallel processing.

1 Introduction
High-dimensional multivariate binary data are routinely collected in many application areas. We are particularly motivated by joint species distribution modeling in ecology (Warton et al., *antik.chakraborty@duke.edu
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In this setting, data consist of a high-dimensional vector of indicators of occurrences of different species in a sample. Interest focuses on inferences on the dependence structure across species, as well as on covariate effects on the marginal occurrence probabilities. Automated sampling and species identification methods for insects and fungi have lead to routine collection of 1,000 – 100,000+ different species in a single study. Most statistical methods for multivariate binary data cannot be implemented due to the data dimensionality.

As a canonical model that is easily interpretable and routinely used in related contexts, we focus on the multivariate probit model (MVP) (Ashford and Sowden, 1970; Cox, 1972). The latent Gaussian formulation of the model leads to straightforward interpretation of the regression coefficients and also provides flexibility in modeling the dependence structure of binary responses. A key computational challenge for fitting such models lies in the evaluation of multivariate Gaussian orthant probabilities (Bock and Gibbons, 1996). Chib and Greenberg (1998) developed a data augmentation scheme simulating the latent variables from truncated multivariate Gaussian distributions for maximum likelihood estimation and Bayesian inference. Unfortunately, generating samples from high dimensional truncated Gaussian distributions is computationally prohibitive and remains an active area of research; see Pakman and Paninski (2014); Botev (2017) for developments.

Markov chain Monte Carlo (MCMC) algorithms based on simulating latent variables often suffer from poor mixing. This was shown formally in imbalanced binary data models by Johndrow et al. (2019). Andrieu and Roberts (2009) proposed pseudo marginal MCMC to avoid imputation of latent variables in models that have intractable marginal likelihoods integrating out the latent variables. Pseudo marginal MCMC replaces the marginal likelihood in a Metropolis-Hastings acceptance probability with an unbiased estimator obtained via importance sampling. Unfortunately, we have been unable to get pseudo marginal algorithms to work well in high dimensions, including for multivariate probit models.

Due to practical challenges with MCMC, approximate posterior inference algorithms have become popular for latent Gaussian models. A very successful example is the Integrated Nested Laplace Approximation (INLA) (Rue et al., 2009). However, current implementations of INLA available here do not allow for multivariate binary outcomes. One major issue is that INLA only allows low-dimensional parameters integrating out the latent Gaussian process, but in our setting we have a high-dimensional unknown correlation matrix and high-dimensional regression coefficients. A popular alternative is to use variational Bayes (Blei et al., 2017); however, the resulting posterior approximations have no guarantees in terms of accurate uncertainty quantification, and indeed are well known to badly underestimate posterior covariance in general.

Recently, Chen et al. (2018) proposed a fast computational algorithm to approximate
multivariate Gaussian orthant probabilities for deep MVP models. The method is appealing, especially in high dimensions, as it can be parallelized over the Monte Carlo samples and dimensions. However, there are two important issues. The method is very sensitive to the underlying correlation structure and as the dimension increases, exponentially more Monte Carlo samples are needed to produce the same level of accuracy. Pichler and Hartig (2020) build on this approximation technique but regularize the high-dimensional correlation matrix. Their approach inherits the problem with approximation inaccuracy and they do not address uncertainty quantification in statistical inferences.

In this article we develop a two-stage method for Bayesian inference for the MVP model. Our over-arching goals are to maintain accuracy in terms of estimation, uncertainty quantification and prediction without compromising on the computational budget. To achieve this, we focus on marginal inferences for model parameters in the MVP model; namely, regression coefficients for each outcome and correlation coefficients measuring pairwise dependence between outcomes. Two-stage inference methods have been popular for copula models in the frequentist literature (Shih and Louis, 1995). Several authors including Joe (2005); Ko and Hjort (2019) studied asymptotic properties of the resulting estimators. Joe (2005) studied asymptotic relative efficiency of the two-stage method compared to full maximum likelihood estimation and provided examples where the two-stage method achieves full efficiency. Adjusting for uncertainty in the first step is typically addressed by the two-stage variance estimator from Murphy and Topel (2002). Building on this line of work, Ting et al. (2020) recently proposed a two stage maximum likelihood method for MVP models where the regression parameters for each outcome are estimated marginally in the first stage and correlation parameters are estimated in the second stage for each pair of outcomes by plugging in estimates obtained in the first stage. Although the method is conceptually related to the work presented here, simply plugging in maximum likelihood estimates of the regression coefficients for the second stage estimates of the correlation structure can incur large bias in finite samples; see Section 4 for detailed comparisons. This in turn results in significant under/over coverage of confidence intervals for the correlation coefficients, with the performance getting worse as dimension increases.

A key innovation of our proposed approach is how we account for uncertainty in first stage estimation. In particular, we take into account the entire (approximate) distribution of the regression parameters in our inferences on the correlation parameters, leading to greatly improved finite sample performance. We prove that the resulting procedure achieves optimal rates in estimating both the regression parameters and the correlation coefficients. We also develop a hierarchical extension in which the regression coefficients for the different outcomes are drawn from a common Gaussian distribution to borrow information. This is especially useful when many of the binary outcomes are observed rarely - a typical scenario
in species sampling data. An approximation to the predictive distribution is provided in the supplementary materials.

2 Method

Multivariate binary outcome data consist of a vector \( y_i = (y_{i1}, \ldots, y_{iq})^T \) for samples \( i = 1, \ldots, n \), with \( y_{ij} \in \{0, 1\} \). In our motivating application, \( y_{ij} = 1 \) if the \( j \)th species is present in the \( i \)th sample, with \( y_{ij} = 0 \) otherwise. We also have covariate information \( x_i = (x_{i1}, \ldots, x_{ip})^T \) for each sample. In the species sampling application, \( q \) is large while \( p \) contains a small number of attributes of the sample; with this motivation, we focus on the problem of high-dimensional outcomes (large \( q \)) and low-dimensional covariates (small \( p \)).

A challenge with multivariate binary data is how to define the dependence structure. Two of the most common approaches are (1) define a generalized linear model (GLM) (e.g., logistic regression) for each outcome and then include common sample-specific latent factors in these models to induce dependence; and (2) define an underlying continuous variable model and induce dependence in the binary outcomes through dependence in these underlying variables. Although strategy (1) is common in the ecology literature, there are disadvantages that motivate our focus on the multivariate probit (MVP) model and strategy (2). A particularly concerning issue with GLM latent factor models is that the latent factor structure impacts the interpretation of the outcome-specific models, so that how we interpret covariate effects on the \( j \)th outcome depends on which other outcomes are included in the model.

The MVP does not have this issue, and is appealing in separating the marginal regression models for each outcome from the dependence structure between outcomes. This is accomplished with an underlying Gaussian variable model in which \( y_{ij} = \mathbb{1}(z_{ij} > 0) \), \( z_i = (z_{i1}, \ldots, z_{iq})' \in \mathbb{R}^q \) and these underlying variables have a simple multivariate normal linear model structure,

\[
  z_{ij} = x_i^T \beta_j + \epsilon_{ij}, \quad \epsilon_i = (\epsilon_{i1}, \ldots, \epsilon_{iq})^T \sim N(0, \Sigma),
\]

where \( \beta_j = (\beta_{j1}, \ldots, \beta_{jp})^T \) are regression coefficients specific to outcome \( j \), and \( \Sigma \) is a positive definite correlation matrix defining the dependence structure across outcomes. Marginally, a simple probit regression model is induced for each of the outcomes, with

\[
  \Pr(y_{ij} = 1|x_i) = \Phi(x_i^T \beta_j),
\]

where \( \Phi(\cdot) \) is the cumulative distribution function of a standard Gaussian random variable. Hence, we can interpret the \( \beta_j \)s based on (2), while the correlation coefficient \( \sigma_{jk} \) in element \((j, k)\) of matrix \( \Sigma \) controls the degree of dependence between \( y_{ij} \) and \( y_{ik} \).
We follow standard practice for multivariate probit models in assuming the data in the
different samples, \( y_i \) and \( y_i' \), are independent, so that the likelihood under (1) is
\[
\prod_{i=1}^{n} \text{pr}(y_i | x_i, B, \Sigma) = \prod_{i=1}^{n} \text{pr}(z_i \in E_i | x_i, B, \Sigma), \quad z_i \sim N(B^T x_i, \Sigma),
\]
where \( B = (\beta_1, \ldots, \beta_q) \) is the \( p \times q \) matrix of regression coefficients and \( E_i = \cap_j E_{ij} \subset \mathbb{R}^q \) with \( E_{ij} = \{ z : z > 0 \} \) if \( y_{ij} = 1 \) and vice versa. Working within a Bayesian framework, one endows the coefficient matrix with the prior \( \Pi_B(\cdot) \) and the correlation matrix \( \Sigma \) with the prior \( \Pi_\Sigma(\cdot) \). Initially, we shall assume that regression vectors \( \beta_j \) are independent \textit{apriori}, so that \( \Pi_B = \prod_{j=1}^{q} \Pi_j(\beta_j) \); extension to a hierarchical prior is considered in Section 2.3. The full posterior distribution of the model parameters is obtained as
\[
\Pi(B, \Sigma | y, X) \propto \Pi(\Sigma) \left\{ \prod_{j=1}^{q} \Pi_j(\beta_j) \right\} \left\{ \prod_{i=1}^{n} \text{pr}(z_i \in E_i) \right\}, \quad z_i \sim N(B^T x_i, \Sigma)
\]
Clearly, evaluating (4) becomes highly expensive as \( q \) increases because of the high dimensional integral involved in computing the likelihood for a given value of the parameters. This is true even when the focus is on inferences based on marginal posterior distributions \( \Pi_j(\beta_j | y, X) \) or \( \Pi(\sigma_{jk} | y, X) \).

To avoid computing the marginal likelihood integrating out \( \{z_i\} \), one can instantiate the latent data in a data augmentation (DA) algorithm. Chib and Greenberg (1998) develop a DA Gibbs sampler for the MVP model, which relies on a parameter-expanded version of the model replacing the correlation matrix \( \Sigma \) with a covariance matrix \( \Sigma^* \) and coefficients \( \beta_j \) with \( \beta_j^* \). One alternates between sampling the \( z_i \) vectors from their truncated multivariate normal conditional posteriors, sampling \( \beta_j^* \)’s from their multivariate normal conditional, and sampling \( \Sigma^* \) from an inverse-Wishart conditional under an inverse-Wishart prior. In a post-processing step, \( \beta_j \) is set to \( \beta_j^* \) divided by the square root of the \( j \)th diagonal element of \( \Sigma^* \) and \( \Sigma \) to the correlation matrix corresponding to covariance \( \Sigma^* \) to obtain posterior samples for the MVP parameters. While this approach can work well in low dimensions (small \( q \)), as \( q \) increases three problems arise: (1) inefficiency of sampling from a high-dimensional truncated multivariate normal; (2) poor performance of the inverse-Wishart prior for high-dimensional covariance/correlation matrices, and (3) worsening mixing, particularly when some binary outcomes are imbalanced (\( \text{pr}(y_{ij} = 1) \approx 0 \) or \( \approx 1 \)).

Our focus is on obtaining a much more computationally efficient and scalable alternative for approximating marginal posteriors of \( \beta_j \) and \( \sigma_{jk} \); in practice inference based on such posteriors is almost always the focus of Bayesian analyses. For example, in our motivating ecology applications to studies of species biodiversity, the focus is on interpreting the covari-
ate effects and correlations among species, and all such inferences can be based on marginal posteriors. In the next subsection we introduce such an approximation \( \Pi^*_j(\beta_j | y, X) \) for the marginal posterior of \( \beta_j \), while in the subsequent subsection we propose an approach to approximate the posteriors of \( \sigma_{jk} \).

### 2.1 First-stage inference

The approximator \( \Pi^*_j(\beta_j | y, X) \) is obtained by fitting a purposely misspecified likelihood. In particular, we replace the likelihood in (3) by the product of marginal likelihoods \( \prod_{i=1}^{n} \prod_{j=1}^{q} \text{pr}(z_{ij} \in E_{ij}) \); that is, we set \( \Sigma = I \). Since the prior also factors over the dimension, we immediately get that \( \Pi^*_j(\beta_j | y, X) \propto \text{pr}(z_{ij} \in E_{ij}) \Pi_j(\beta_j) \). This is equivalent to fitting univariate probit models to each outcome and allows for parallelization over the \( q \) outcomes. Set the \( j \)th column of the binary matrix \( y \) as \( y^{(j)} \) for \( j = 1, \ldots, q \). The approximating distribution \( \Pi^*_j(\beta_j | y, X) \) does not have a closed form expression. Working with the assumption that \( n \gg p \), though we do not assume \( n > q \), we set

\[
\Pi^*_j(\beta_j | y, X) = \Pi^*_j(\beta_j | y^{(j)}, X) \equiv N(\hat{\beta}_j, H_j)
\]

where \( H_j \) is the corresponding inverse Hessian. Since each \( \beta_j \) is a fixed-dimensional parameter, standard Bernstein-von Mises arguments lead to the Gaussian approximation. For the \( j \)th outcome, the mode \( \hat{\beta}_j \) can be obtained using the Newton-Raphson algorithm. The computational complexity of obtaining \( \hat{\beta}_j \) is \( O(M_j np^2) \), where \( M_j \) is the number of iterations until convergence of the Newton-Raphson algorithm. Hence, the complexity is linear in the number of outcomes \( q \).

### 2.2 Second stage inference

Having obtained \( \Pi^*_j(\beta_j | y, X) \) we move on to the more challenging problem of inference on the correlation matrix \( \Sigma \). We focus on the marginal posterior distribution \( \Pi(\sigma_{jk} | y, X) \) of the correlation between pairs of outcomes. An approximation to \( \Pi(\sigma_{jk} | y, X) \) is proposed by considering a bivariate probit model between the pairs \( (j, k) \) which in turn depends on the approximations obtained in the first stage, \( \Pi^*_j(\beta_j | y, X) \) and \( \Pi^*_k(\beta_k | y, X) \). While frequentist analogues of two stage estimation generally plug in maximum likelihood estimates of \( \beta_j \) and \( \beta_k \) obtained in the first stage (Joe, 2005; Yi et al., 2011; Ko and Hjort, 2019; Ting et al., 2020), we include \( \Pi^*_j(\beta_j | y, X) \) and \( \Pi^*_k(\beta_k | y, X) \), the approximate posterior distributions of the regression coefficients, in the form of updated prior distributions on
(\beta_j, \beta_k). More precisely, in the second stage, the updated prior distribution \( \Pi^*_{jk}(\beta_j, \beta_k) \) is set as \( \Pi^*_{jk}(\beta_j \mid y, X)\Pi^*_{k}(\beta_k \mid y, X) \). Since we focus our inference on \( \sigma_{jk} \) instead of the entire correlation matrix \( \Sigma \), here we work with marginal priors \( \Pi^*_{jk}(\sigma_{jk}) \) on \( \sigma_{jk} \). In our numerical experiments, we set \( \Pi^*_{jk}(\sigma_{jk}) \) as the uniform prior on \([-1, 1]\) although the proposed method can accommodate any prior that is continuous on \([-1, 1]\). Let \( \Pi^*_{jk}(\sigma_{jk} \mid y, X) \) be the approximate marginal posterior distribution of \( \sigma_{jk} \). We have,

\[
\Pi^*_{jk}(\sigma_{jk} \mid y, X) = \Pi^*_{jk}(\sigma_{jk} \mid y^{(j)}, y^{(k)}, X) = \prod_{i=1}^{n} \Pr(z_{ij} \in E_{ij}, z_{ik} \in E_{ik} \mid \sigma_{jk})\Pi(\sigma_{jk})
\]

\[
= \frac{\Pi(\sigma_{jk})}{\Pr(y^{(j)}, y^{(k)})} \prod_{i=1}^{n} \int \Pr(z_{ij} \in E_{ij}, z_{ik} \in E_{ik} \mid \sigma_{jk}, \beta_j, \beta_k) \Pi(\beta_j, \beta_k) d\beta_j d\beta_k
\]

\[
\approx \frac{\Pi(\sigma_{jk})}{\Pr(y^{(j)}, y^{(k)})} \prod_{i=1}^{n} \int \Pr(z_{ij} \in E_{ij}, z_{ik} \in E_{ik} \mid \sigma_{jk}, \beta_j, \beta_k) \Pi^*_{jk}(\beta_j \mid y, X)\Pi^*_{k}(\beta_k \mid y, X) d\beta_j d\beta_k
\]

\[
= \frac{\Pi(\sigma_{jk})}{C_{jk}} \prod_{i=1}^{n} \int \left\{ \int_{(E_{ij}, E_{ik})} \Pr(z_{ij}, z_{ik}) dz_{ij} \right\} \Pi^*_{jk}(\beta_j \mid y, X)\Pi^*_{k}(\beta_k \mid y, X) d\beta_j d\beta_k,
\]

where \( C_{jk} = \Pr(y^{(j)}, y^{(k)}) \) and \( \Pr(z_{ij}, z_{ik}) \) is the pdf of a bivariate Gaussian distribution with mean vector \((x^T_i \beta_j, x^T_i \beta_k)\), variance 1 and correlation coefficient \( \sigma_{jk} \). Using Fubini’s theorem, we interchange the order of integration in the above display to marginalize out \( \beta_j \) and \( \beta_k \) to obtain an updated distribution of the latent variables \((z_{ij}, z_{ik})\). Hence, we have

\[
\Pi^*_{jk}(\sigma_{jk} \mid y, X) = \frac{1}{C_{jk}} \prod_{i=1}^{n} \Pr(\tilde{z}_{ij} \in E_{ij}, \tilde{z}_{ik} \in E_{ik})\Pi(\sigma_{jk}),
\]

where \((\tilde{z}_{ij}, \tilde{z}_{ik}) \sim N(\tilde{\mu}_{jk}, \tilde{\Sigma}_{jk})\), \( \tilde{\mu}_{jk} = (x^T_i \tilde{\beta}_j, x^T_i \tilde{\beta}_k) \), and \( \tilde{\Sigma}_{jk} = \{(1 + x^T_i H_j x_i, \sigma_{jk})^T; (\sigma_{jk}, 1 + x^T_i H_k x_i)^T\}\). In Section 3 we show that \( \Pi^*_{jk}(\sigma_{jk} \mid y, X) \) can be approximated by a univariate Gaussian distribution with appropriate mean and variance. We obtain the mean \( \hat{\sigma}_{jk} \) and variance \( s^2_{jk} \) of \( \Pi^*_{jk}(\sigma_{jk} \mid y, X) \) using Gauss-Legendre quadrature and set \( \Pi^*_{jk}(\sigma_{jk} \mid y, X) \equiv N(\hat{\sigma}_{jk}, s^2_{jk}) \). For each pair of outcomes \((j, k)\), the computational complexity to obtain the mean and variance of \( \Pi^*_{jk}(\sigma_{jk} \mid y, X) \) using \( m \) quadrature points is \( \mathcal{O}(2mn) \) which implies \( \mathcal{O}(q^2mn) \) complexity for all pairs.

Under our working assumption that \( q \gg n > p \), the combined complexity of the two stages of the proposed method scale as \( \mathcal{O}(nq^2) \) to obtain the approximate marginals of the regression coefficients and the correlation coefficients. Data augmented MCMC samplers need to sample the latent variable \( z_i \) for each data point at every iteration, having a best case complexity of \( \mathcal{O}(nq^2) \) (Pakman and Paninski, 2014). This is highly expensive when one has to run the sampler for thousands of iterations. Unlike MCMC, we need to do the calculations only once and computations can be trivially parallelized.
2.3 Extension to hierarchical setting

In this section we extend the MVP model to a hierarchical setting, with the goal being to borrow information across the different outcomes to obtain more accurate estimates of the outcome-specific regression coefficients and cross outcome correlations. In our motivating application, this is particularly important to enable accurate inferences on the coefficients for rare species that are only observed a small number of times in the entire dataset. For example, in the breeding bird survey data in Lindström et al. (2015), out of the 141 bird species observed at 599 locations, 19 bird species were observed in less than 12 locations. Estimating probit regression coefficients for these species without borrowing of information will invariably lead to very high standard errors. To accommodate these situations, we consider the following hierarchy where the outcome specific regression coefficients $\beta_j$ are assumed to be drawn from a common Gaussian distribution,

\[
y_i \mid B, \Sigma, X, \eta, \Omega \sim \text{MVP} (B^T x_i, \Sigma), \ i = 1, \ldots, n,
\]

\[
\beta_j \mid \eta, \Omega \overset{iid}{\sim} \text{N}(\eta, \Omega), \ \Sigma = (\sigma_{jk}), \ \sigma_{jk} \sim \Pi(\sigma_{jk}), \ j, k = 1, \ldots, q,
\]

\[
(\eta, \Omega) \mid \eta_0, \nu_0, \gamma_0, \Lambda_0 \sim \text{NIW} (\eta_0, \nu_0, \gamma_0, \Lambda_0), \quad (7)
\]

where NIW($\eta_0, \nu_0, \gamma_0, \Lambda_0$) represents a Normal-Inverse Wishart distribution defined as $\Omega \sim \text{IW}(\gamma_0, \Lambda_0)$ and $\eta|\Omega \sim \text{N}(\eta_0, \nu_0^{-1}\Omega)$.

Although the hierarchical model has the advantage of reducing mean square errors in estimation through borrowing of information, efficient computation is more challenging due to the dependence between the $\beta_j$s for different outcomes, which is induced through shared dependence on $(\eta, \Omega)$. A natural way to maintain computational scalability is to consider empirical Bayes (Morris, 1983) estimates $(\hat{\eta}, \hat{\Omega})$ of $(\eta, \Omega)$ wherein one marginalizes over $\beta_j$s under the hierarchy (7). After marginalization, the distribution of the latent variables $z_i$ is $N(\Gamma_1^T x_i, \Sigma + \Gamma_2)$, where $\Gamma_1^{p \times q} = (\eta, \eta, \ldots, \eta)$ and $\Gamma_2 = \Sigma + \text{diag}(x_i^T \Omega x_i)$. Unfortunately, as $\Omega$ is now involved in the dependence structure of the latent $z_i$s, it becomes necessary in estimating $\Omega$ to evaluate multivariate Gaussian orthant probabilities or simulate from truncated multivariate Gaussian random variables in conducting data augmentation. Hence, in estimating $\Omega$, we encounter the same computational bottlenecks as discussed previously.

We address this issue by considering the approximate likelihood considered in Section 2.1. Under this approximate likelihood, the joint posterior distribution of $\beta_j$’s and $(\eta, \Omega)$ is

\[
\Pi(\beta_1, \ldots, \beta_q, \eta, \Omega \mid y, X) \propto \prod_{i=1}^n \prod_{j=1}^q \text{pr}(z_{ij} \in E_{ij} \mid \beta_j) \prod_{j=1}^q \Pi(\beta_j \mid \eta, \Omega) \Pi(\eta, \Omega). \quad (8)
\]

Sampling from the joint posterior can be easily implemented alternating between the full
conditionals $\Pi(\beta_j \mid \eta, \Omega, y, X)$, $\Pi(\eta \mid \beta_1, \ldots, \beta_q, \Omega, y, X)$ and $\Pi(\Omega \mid \beta_1, \ldots, \beta_q, \eta, y, X)$ for $j = 1, \ldots, q$. Here, we approximate $\Pi(\beta_j \mid \eta, \Omega, y, X)$ by their corresponding Laplace approximations. The details are given in Algorithm 1, which we call the first stage conditional sampler. Conditional on $(\eta, \Omega)$, sampling the $\beta_j$s requires the same complexity as mentioned in Section 2.1 whereas sampling $(\eta, \Omega)$ can be done in $O(qp^3)$ complexity. In our experience, the sampler mixes really fast with approximately 10 effective samples per second for $(n, p, q) = (200, 5, 100)$ when run on a 64 bit Intel i7-8700K CPU @3.7 GHz processor. Having obtained samples from the posterior distributions of $(\eta, \Omega)$, we simply plug-in the average $(\hat{\eta}, \hat{\Omega})$ of these quantities so that conditional on the plug-in estimates the proposed two-stage procedure can be implemented in a straightforward manner.

This conditional sampler is different from implementing MCMC for the entire model. We use the special dependence structure of hierarchy (7). As the prior on $\beta_j$ is unrelated to $\Sigma$, we base inference on $(\eta, \Omega)$ on the likelihood contribution relevant to the $\beta_j$s using a product of independent univariate probit likelihoods as in our previous first stage inferences. Implementing an “exact” Gibbs sampler is massively more computationally expensive in alternating from simulating the latent $z_i$s from high-dimensional truncated Gaussians and drawing from the full conditional distributions of $\beta_j$, $\Sigma$ and $(\eta, \Omega)$.

**Algorithm 1: First stage conditional sampler**

Initialize $(\eta, \Omega)$.

1. Given $(\eta, \Omega)$ obtain marginal Laplace approximations $N(\hat{\beta}_j, H_j)$ for $j = 1, \ldots, q$ with the prior $\Pi(\beta_j) \sim N(\eta, \Omega)$.

2. Draw $\beta_j \sim N(\hat{\beta}_j, H_j)$ independently for $j = 1, \ldots, q$.

3. Update $(\eta, \Omega) \sim \text{NIW}(\nu_0, \nu_q, \gamma_0, \Lambda_0)$ where $\nu_0 = \nu_0 + q$, $\gamma_0 = \gamma_0 + q$, $\bar{\beta} = (\sum_{j=1}^q \beta_j)/q$, $\eta_q = (\nu_0 \eta_0 + q \bar{\beta})/\nu_q$, $S = \sum_{j=1}^q (\beta_j - \bar{\beta})(\beta_j - \bar{\beta})^T$ and $\Lambda_q = \Lambda_0 + S + (\nu_0 q/\nu_q) \sum_{j=1}^q (\beta_j - \eta_0)(\beta_j - \eta_0)^T$.

3 Theory

Suppose $\theta = (B, \Sigma) \in \Theta$. In this section, we assume data are generated from the MVP model with true parameters $\theta^* = (B^*, \Sigma^*)$ and provide asymptotic results for $\Pi_j^*(\beta_j \mid y, X)$ and $\Pi_{jk}^*(\sigma_{jk} \mid y, X)$ assuming fixed number of covariates $p$. Our results hold irrespective of whether one allows the number of outcomes $q$ to grow with the sample size or not. In particular, we are interested in two key aspects of these approximations: (1) concentration - whether the posteriors converge to a point mass at the true parameter value and (2) shape - whether the posteriors are asymptotically normal. We recognize the likelihoods in both stages of our proposed method as versions of composite likelihood (Lindsay, 1988).
and leverage results from Miller (2019) to establish these properties of the approximate marginal likelihoods. Asymptotic validity of the Laplace approximations of $\Pi_j^*(\beta_j \mid y, X)$ is also proved paralleling the classical results of Geisser et al. (1990) for posteriors obtained without likelihood misspecification.

### 3.1 Preliminaries

We assume the data $Y = (y_1, \cdots, y_n)^T$ are generated by an MVP model under true parameters $\theta^* = (\Sigma^*, B^*)$, where $B^* \in \mathbb{R}^{p \times q}$ and $\Sigma^* \in \mathcal{S}^q$, the cone of positive definite matrices. Given two densities $p$ and $q$ with respect to the Lebesgue measure, the total variation distance is defined as $\|p - q\|_1 = \int |p(u) - q(u)|du$. The density function of the standard Gaussian distribution is $\phi(\cdot)$. For a two dimensional covariance matrix $\Sigma$, let $\phi_{\Sigma}(\cdot)$ and $\Phi_{\Sigma}(\cdot)$ denote the density and distribution function of a bivariate Gaussian distribution with mean $(0, 0)^T$; i.e. $\phi_{\Sigma}(x) = (2\pi)^{-1/2}|\Sigma|^{-1/2}\exp\{-x^T\Sigma^{-1}x/2\}$ and $\Phi_{\Sigma}(x) = \int_{-\infty}^{x} \phi_{\Sigma}(u)du$ for $x, u \in \mathbb{R}^2$. For two vectors $x, y$ we write $x \odot y$ for their Hadamard product. For two positive sequences $a_n$ and $b_n$, we write $a_n \sim b_n$ to denote that $a_n/b_n \to 1$ as $n \to \infty$. We use $\|v\|$ for the Euclidean norm of a real valued vector $v$.

### 3.2 Assumptions

The following assumptions are made on the parameter space, design matrix and prior distributions.

**Assumption 3.1** (Regularity). Let $B \in \Xi \subset \mathbb{R}^{p \times q}$ where $\Xi$ is an open bounded subset of Euclidean $\mathbb{R}^{p \times q}$.

**Assumption 3.2** (Regularity). There exists a real interval $(M_1, M_2) \subset (-1, 1)$ such that for every $\{j, k\}$ $\sigma_{jk}^* \in (M_1, M_2)$ for $1 \leq j, k \leq q$.

**Assumption 3.3** (Prior support). Let $\pi_j$ be the prior probability density of $\beta_j$ with respect to the Lebesgue measure for $1 \leq j \leq q$. Then for each $j$, $\pi_j(\cdot)$ is continuous at $\beta_j^*$ and there exists an $\epsilon > 0$ such that $\pi_j(\beta_j^*) > \epsilon > 0$ uniformly in $j$. Let $\pi_{jk}(\cdot) : (-1, 1) \to \mathbb{R}$ be the prior probability density of $\sigma_{jk}$ with respect to Lebesgue measure, then $\pi_{jk}(\cdot)$ is continuous at $\sigma_{jk}^*$ and there exists an $\epsilon > 0$ such that $\pi_{jk}(\sigma_{jk}^*) > \epsilon > 0$ for every $1 \leq j, k \leq q$.

**Assumption 3.4** (Design matrix). The Euclidean norms of the rows $x_i$ of $X$, i.e. $\|x_i\|_2$, are uniformly bounded in $i$ and $\lim_{n \to \infty} n^{-1}\sum_{i=1}^{n} x_i x_i^T$ is a finite nonsingular matrix. Furthermore the empirical distribution of $\{x_i\}$ converges to a distribution function. Assumption 3.1 together with Assumption 3.4 imply there exists a real number $M \in \mathbb{R}$ such that $|x_i^T \beta_j| \leq M$ almost surely for every $1 \leq i \leq n$ and $1 \leq j \leq q$. 

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Assumptions 3.1 and 3.2 are standard in classical asymptotic theory of maximum likelihood estimation for parametric models (Van der Vaart, 2000). The prior support assumption, i.e. Assumption 3.3, ensures positive prior probability around true parameter values. Common priors that satisfy the prior support condition on the Euclidean space include the Gaussian prior. Assumption 3.4 on the design matrix is also used in (Amemiya, 1985, Theorem 9.2.2) in establishing asymptotic normality of maximum likelihood estimators for univariate probit regression.

3.3 First-stage Analysis

We analyze the posterior distribution of $\beta_j$ asymptotically, for any $1 \leq j \leq q$. The misspecified likelihood used in Section 2.1, where we replace $\Sigma$ by the identity matrix, can be viewed as a product of marginal likelihoods and thus falls under the umbrella of composite likelihoods (Lindsay, 1988). Properties of estimators derived by maximizing composite likelihoods, such as consistency and asymptotic normality, are well established; see Varin et al. (2011) for a survey. Miller (2019) provide sufficient conditions under which posterior distributions obtained by combining a composite likelihood derived from a correct model combined with a suitable prior concentrate at the true parameter value and exhibit asymptotic normality.

In Theorem 3.5 we show that $\Pi^*_j(\beta_j \mid y, X)$ is asymptotically normal centered at the maximum composite likelihood estimator and the Laplace approximation we employ is valid. Our proof relies on the observation that the marginal distribution of $y^{(j)}$ is the same under the joint model (3) and the independence model obtained by plugging in $\Sigma = I$ in (3); under both models $y^{(j)}$ follows a univariate probit model conditional on $\beta_j$. The proof guarantees that the maximum composite likelihood estimator converges to $\beta^*_j$. This also implies a parametric contraction rate $O_{P_{\theta^*}}(n^{-1/2})$ for $\Pi^*_j(\beta_j \mid y, X)$, i.e., $\Pi^*_j \left( \| \beta_j - \beta^*_j \| > \frac{M_n}{n} \mid y, X \right) \to 0$ for every $M_n \to +\infty$.

Let the log-likelihood of $\beta_j$ under the independence model be $\ell(\beta_j) = \sum_{i=1}^{n} \ell_i(\beta_j)$, where $\ell_i(\beta_j)$ is the likelihood contribution of the $i$th data point. Then,

$$\ell(\beta_j) = \sum_{i=1}^{n} \log pr(z_{ij} \in E_{ij}) = \sum_{i=1}^{n} \left[ y^{(j)}_i \log \Phi(x_i^T \beta_j) + (1 - y^{(j)}_i) \log \left( 1 - \Phi(x_i^T \beta_j) \right) \right]. \quad (9)$$

Define $p_{nj}(\beta_j) = -\ell(\beta_j)/n$ and $d_n = \int \exp\{-np_{nj}(\beta_j)\Pi(\beta_j)\} d\beta_j$, so that $\Pi^*_j(\beta_j \mid y, X) = \exp\{-np_{nj}(\beta_j)\Pi(\beta_j)\}/d_n$. We shall write $\Phi_{ij}, \Phi^*_{ij}, \phi_{ij}, \phi^*_{ij}$ as shorthand for $\Phi(x_i^T \beta_j), \Phi(x_i^T \beta^*_j), \phi(x_i^T \beta_j), \phi(x_i^T \beta^*_j)$, respectively. Following the analysis in Theorem 9.2.2 of Amemiya (1985), $p_{nj} \to p_j$ pointwise in $P_{\theta^*}$-probability, where
\[ p_j(\beta_j) = \lim_{n \to \infty} n^{-1} \sum_{i=1}^{n} \Phi_j^* \log \Phi_{ij} + \lim_{n \to \infty} n^{-1} \sum_{i=1}^{n} (1 - \Phi_j^*) \log (1 - \Phi_{ij}) \] (10)

Also, let

\[ p'_j(\beta_j) = \lim_{n \to \infty} n^{-1} \sum_{i=1}^{n} \Phi_j^* \phi_{ij} x_i - \lim_{n \to \infty} n^{-1} \sum_{i=1}^{n} 1 - \Phi_j^* \phi_{ij} x_i \] (11)

\[ p''_j(\beta_j) = \lim_{n \to \infty} n^{-1} \sum_{i=1}^{n} \left( \frac{(\phi_j)^2}{\Phi^*_j(1 - \Phi^*_j)} \right) x_i x'_i. \] (12)

\textbf{Theorem 3.5.} If Assumptions 3.1, 3.3 and 3.4 hold, then there exists a sequence \( \beta_j \to \beta^* \) such that \( p_{nj}(\beta_j) = 0 \) for all \( n \) sufficiently large, and \( p_{nj}(\beta_j) \to p_j(\beta^*_j) \) in probability. Let \( R_j = p'_j(\beta^*_j) \), then

\[ d_n \sim \exp\left\{ -np_{nj}(\beta_j) \right\} \pi(\beta_j^*) \left( \frac{2\pi}{n} \right)^{p/2}. \]

Furthermore, if we let \( g_{nj} \) to be the density of \( \sqrt{n}(\beta_j - \beta^*_j) \) with \( \beta_j \sim \Pi_j^*(\beta_j | y, X) \), then

\[ \| g_{nj} - \phi_{R_j^{-1}} \|_1 \to 0, \text{ in } P_{\theta^*} \text{- probability}, \]

where \( \phi_{R_j^{-1}} \) is the density of a \( p \)-dimensional Gaussian distribution centered at 0 with covariance matrix \( R_j \).

The proof is provided in the supplementary document. While this result establishes that the approximate marginal posteriors concentrate around \( \beta^*_j \) and are asymptotically normal, in general this does not guarantee nominal coverage of credible intervals obtained from \( \Pi_j^*(\beta_j | y, X) \). This is because the maximum composite likelihood estimator \( \sqrt{n}(\beta_j - \beta^*_j) \) asymptotically follows \( N(0, R_j^{-1} V_j R_j^{-1}) \) where \( V_j = E_{\theta^*}(u_{\beta_j}(y^{(j)}, \beta^*_j) u_{\beta_j}(y^{(j)}, \beta^*_j)^T) \) and \( u_{\beta_j}(y^{(j)}, \beta^*_j) = \nabla_{\beta_j} \big|_{\beta_j = \beta^*_j} \ell(\beta_j) \). Hence, \( \Pi_j^*(\beta_j | y, X) \) has correct asymptotic frequentist coverage iff \( R_j = V_j \) which happens when each of the marginal likelihoods are correctly specified (Ko and Hjort, 2019). This is true if the joint multivariate probit model is the true data-generating model.

\textbf{Theorem 3.6.} Under Assumptions 3.1 - 3.4 define a Borel-measurable sequence of sets \( W_{n,l} = \left\{ \beta_{j,l} : \beta_{j,l} - (R_{j,l}^{-1/n})^{1/2} v_{1-\alpha/2} \leq \beta_{j,l} \leq \beta_{j,l} + (R_{j,l}^{-1/n})^{1/2} v_{1-\alpha/2} \right\} \), where \( \Phi(v_{1-\alpha/2}) = 1 - \alpha/2 \) for \( 0 \leq \alpha \leq 1 \) and \( 1 \leq j \leq q \) and \( \beta_{j,l} \) is the \( l \)-th element of \( \beta_j \). Then

\[ P_{\theta^*} \left( \beta_{j,l}^* \in W_{n,l} \right) \to \Phi \left( v_{1-\alpha/2} \right) - \Phi \left( -v_{1-\alpha/2} \right) = \alpha. \]

\textbf{Proof.} We have \( P_{\theta^*} \left( \beta_{j,l}^* \in W_{n,l} \right) = P_{\theta^*} \left\{ \sqrt{n} \left( R_{j,l}^{-1/2} \right)^{1/2} (\tilde{\beta}_{j,l} - \beta_{j,l}^*) \in [-v_{1-\alpha/2}, v_{1-\alpha/2}] \right\} \to \Phi \left( v_{1-\alpha/2} \right) \)
− Φ(−v_{1−\frac{α}{2}}), which follows from Theorem 3.5.

3.4 Second-Stage Analysis

In our second stage analysis, we use the likelihood \( \prod_{j=1}^{q-1} \prod_{k=(j+1)}^{q} \Pr(z_{ij} \in E_{ij}, z_{ik} \in E_{ik}) \) for the \( i \)th data point which can be seen as a pairwise composite likelihood. As a result, the results of Miller (2019) can be used to study concentration and asymptotic normality of \( \Pi_{jk}^*(\sigma_{jk} \mid y, X) \). Intuitively, if \( \hat{\sigma}_{jk} \) is the maximum composite likelihood estimator from the bivariate margins then \( \Pi_{jk}^*(\sigma_{jk} \mid y, X) \), when suitably scaled, is close to a Gaussian distribution centered at \( \hat{\sigma}_{jk} \). Treating \( \sigma_{jk} \) as the parameter of interest, these bivariate margins are correctly specified when the latent \( (z_{ij}, z_{ik}) \sim N(\mu_{jk}^*, \Sigma_{jk}) \) where \( \mu_{jk}^* = (x_i^T \beta_j^*, x_i^T \beta_k^*) \) and \( \Sigma_{jk} = \{(1, \sigma_{jk})^T; (\sigma_{jk}, 1)^T\} \). However, in incorporating the uncertainty associated with estimating the regression coefficients \( (\beta_j, \beta_k) \), we fit the likelihood \( N(\hat{\mu}_{jk}, \hat{\Sigma}_{jk}) \), \( \hat{\mu}_{jk} = (x_i^T \hat{\beta}_j, x_i^T \hat{\beta}_k) \), and \( \hat{\Sigma}_{jk} = \{(1 + x_i^T H_j x_i, \sigma_{jk})^T, (\sigma_{jk}, 1 + x_i^T H_k x_i)^T\} \). Although the quantities \( \mu_{jk} \) and \( \hat{\Sigma}_{jk} \) depend on \( i \), we use this notation for simplicity. We denote the parameter involving the \( j \)th and \( k \)th outcomes by \( \theta_{jk} = \{\beta_j^T, \beta_k^T, \text{vec}(\Sigma_{jk})^T\} \) and its true value \( \theta_{jk}^* = \{\beta_j^T, \beta_k^T, \text{vec}(\Sigma_{jk})^T\} \).

Define \( r_{ij} = 2y_{ij} - 1, r_{ik} = 2y_{ik} - 1 \) and \( r_i = (r_{ij}, r_{ik})^T \). Let \( \Sigma_{jk} = \{(1 + x_i^T H_j x_i, r_{ij} r_{ik} \sigma_{jk})^T; (r_{ij} r_{ik} \sigma_{jk}, 1 + x_i^T H_k x_i)^T\} \) for all \( i \), and \( \ell_{jk}^i(\sigma_{jk}; \hat{\mu}_{jk}, \hat{\Sigma}_{jk}) = \ell_{jk}^i(\sigma_{jk}) = \log\{\Phi_{\Sigma_{jk}}(r_i \circ \hat{\mu}_{jk})\} \). We write \( \Phi_{\Sigma_{jk}} \) and \( \phi_{\Sigma_{jk}} \) as shorthand for \( \Phi_{\Sigma_{jk}}(r_i \circ \hat{\mu}_{jk}) \) and \( \phi_{\Sigma_{jk}}(r_i \circ \hat{\mu}_{jk}) \), respectively. Then define \( \hat{\sigma}_{jk} \) to be the two-stage M-estimator obtained as the solution of

\[
\sum_{i=1}^{n} \nabla_{\sigma_{jk}} \ell_{jk}^i(\sigma_{jk}; \hat{\mu}_{jk}, \hat{\Sigma}_{jk}) = 0. \tag{13}
\]

We then have the following asymptotic result on \( \Pi_{jk}^*(\sigma_{jk} \mid y, X) \).

**Theorem 3.7.** If Assumptions 3.1 to 3.4 hold, then there exists a solution \( \hat{\sigma}_{jk} \) of (13) for all sufficiently large \( n \) with \( \hat{\sigma}_{jk} \to \sigma_{jk}^* \) in \( P_{\theta^*} \)-probability. Let \( \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} E_{\theta^*} \left( \frac{\partial^2 \ell_{jk}^i}{\partial \sigma_{jk}} \right) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Var}_{\theta^*} \left( \frac{\partial \ell_{jk}^i}{\partial \sigma_{jk}} \right) \). If \( g_{njk} \) is the density of \( \sqrt{n}(\sigma_{jk} - \hat{\sigma}_{jk}) \), where \( \sigma_{jk} \sim \Pi_{jk}^*(\sigma_{jk} \mid y, X) \), then

\[
\|g_{njk} - \phi_{R_{jk}^{-1}}\|_1 \to 0 \quad \text{in} \quad P_{\theta^*} \quad \text{probability},
\]

where \( \phi_{R_{jk}^{-1}} \) is the density of a univariate Gaussian centered at 0 with variance \( R_{jk}^{-1} \).

The proof is given in the appendix. Theorem 3.7 says that the approximate marginal posterior \( \Pi_{jk}^*(\sigma_{jk} \mid y, X) \) behaves like \( N(\hat{\sigma}_{jk}, R_{jk}^{-1}) \) for sufficiently large \( n \). In Lemma S.3.1 we show that asymptotically \( \hat{\sigma}_{jk} \) has a Gaussian distribution centered at \( \sigma_{jk}^* \) but with a larger
variance. This inflation of the variance results from the extra uncertainty induced by using \((\hat{\beta}_j, \hat{\beta}_k)\) and \((1 + x_i^T \hat{\beta}_j x_i, 1 + x_i^T \hat{\beta}_k x_i)\) in (13). Such inflation in two stage estimators has been observed previously (Murphy and Topel, 2002). To define the correct variance of \(\hat{\sigma}_{jk}\), we first define the following quantities:

\[
R_j^k = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n \text{Cov}_{\theta^*} \left\{ \nabla_{\beta_j} \ell_i(x_i^T \beta_j) \right\}_{\beta_j = \beta_j^*}, \nabla_{\sigma_j} \ell_i^j(x_i^T \sigma_j; \mu_j, \Sigma_j) \bigg|_{\sigma_j = \sigma_j^*} \bigg|_{\beta_j = \beta_j^*}, \\
R_k^j = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n \text{Cov}_{\theta^*} \left\{ \nabla_{\beta_k} \ell_i(x_i^T \beta_k) \right\}_{\beta_k = \beta_k^*}, \nabla_{\sigma_j} \ell_i^j(x_i^T \sigma_j; \mu_j, \Sigma_j) \bigg|_{\sigma_j = \sigma_j^*} \bigg|_{\beta_k = \beta_k^*}, \\
V_{jk} = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n \text{Cov}_{\theta^*} \left\{ \nabla_{\beta_j} \ell_i(x_i^T \beta_j) \right\}_{\beta_j = \beta_j^*}, \nabla_{\beta_k} \ell_i(x_i^T \beta_k) \bigg|_{\beta_k = \beta_k^*}, \\
Q_{jk} = -\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n E_{\theta^*} \left\{ \partial^2 \ell_i^j(x_i^T \beta_j; \mu_j, \Sigma_j) \right\}_{\theta_j = \theta_j^*} \bigg|_{\beta_j = \beta_j^*}, \\
Q_{kj} = -\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^n E_{\theta^*} \left\{ \partial^2 \ell_i^j(x_i^T \beta_j; \mu_j, \Sigma_j) \right\}_{\theta_j = \theta_j^*} \bigg|_{\beta_k = \beta_k^*}.
\]

Detailed expressions of these quantities are provided in Section S.5 of the supplementary document where we show that \(R_j^k\) and \(R_k^j\) are zero for all \(1 \leq j \neq k \leq q\). The existence of all limits in the above display is guaranteed by Assumption 3.4. Also, recall the definition of \(R_j\) from Theorem 3.5 for any arbitrary \(j\). In Lemma S.3.1 we show that \(\sqrt{n}(\hat{\sigma}_{jk} - \sigma_{jk}^*) \xrightarrow{d} N(0, \tau_{jk})\) where

\[
\tau_{jk} = R_{jk}^{-1} + R_{jk}^{-1} \left( Q_{jk}^j R_{jk}^{-1} Q_{jk}^j R_{jk}^{-1} \right) R_{jk}^{-1} + R_{jk}^{-1} \left( Q_{kj}^k R_{kj}^{-1} Q_{kj}^k R_{kj}^{-1} \right) R_{jk}^{-1} + 2 R_{jk}^{-1} Q_{jk}^j R_{jk}^{-1} V_{jk} R_{kj}^{-1} Q_{kj}^k R_{kj}^{-1}.
\]

The extra terms in (14) correspond to the variances incurred by estimating \(\beta_j\), \(\beta_k\) and the covariance. Due to this miscalibration in the variance, intervals computed from \(\Pi_{jk}^* (\sigma_{jk} | y, X)\) will typically have under coverage since \(\tau_{jk} > R_{jk}^{-1}\) (Miller, 2019, Section 4.1).

**Theorem 3.8.** Under Assumptions 3.1 - 3.4 define a Borel-measurable sequence of sets \(S_n = \{ \sigma_{jk} : \bar{\sigma}_{jk} - (R_{jk}^{-1} / n)^{1/2} v_{1-\alpha} \leq \sigma_{jk} \leq \bar{\sigma}_{jk} + (R_{jk}^{-1} / n)^{1/2} v_{1-\alpha} \} \), where \(\Phi(v_{1-\alpha}) = 1 - \alpha/2\) for \(0 \leq \alpha \leq 1\) and \(1 \leq j, k \leq q\). Suppose \(\tau_{jk}\) is as defined in (14). Then,

\[
P_{\theta^*} (\sigma_{jk}^* \in S_n) \rightarrow \Phi \left( \sqrt{R_{jk}^{-1} / \tau_{jk} z_{1-\alpha}} \right) - \Phi \left( -\sqrt{R_{jk}^{-1} / \tau_{jk} z_{1-\alpha}} \right) < \alpha
\]

**Proof.** Let \(U_n = \sqrt{n}(\hat{\sigma}_{jk} - \bar{\sigma}_{jk})\). Let the cdf of \(U_n\) be \(F_{U_n}(\cdot)\) and \(F_{U_n}(\cdot)\) be a continuous function on the real line. From Lemma S.3.1, we have \(U_n \xrightarrow{d} N(0, \tau_{jk})\). Hence, \(F_{U_n}(u) \rightarrow \)
\[ \Phi(u/\sqrt{\tau_{jk}}) \text{ as } n \to \infty \text{ for every } u \in \mathbb{R}. \] Thus,

\[ P_{\theta^*} \left( U_n \in \left[ -\sqrt{\frac{R_{jk}^{-1} v_1}{2}}, \sqrt{\frac{R_{jk}^{-1} v_1}{2}} \right] \right) = F_{U_n} \left( \sqrt{\frac{R_{jk}^{-1} v_1}{2}} \right) - F_{U_n} \left( -\sqrt{\frac{R_{jk}^{-1} v_1}{2}} \right) \]

\[ \to \Phi \left( \sqrt{\frac{R_{jk}^{-1}/\tau_{jk} v_1}{2}} \right) - \Phi \left( -\sqrt{\frac{R_{jk}^{-1}/\tau_{jk} v_1}{2}} \right) < \alpha, \]

since \( \tau_{jk} > R_{jk}^{-1} \).

The extent of under coverage clearly depends on the ratio \( R_{jk}^{-1}/\tau_{jk} \). To that end, consider

\[
\frac{\tau_{jk}}{R_{jk}^{-1}} = 1 + \frac{Q_j^k R_j^{-1} Q_j^{kT}}{R_{jk}} + \frac{Q_k^j R_k^{-1} Q_k^{jT}}{R_{jk}} + 2 \frac{Q_j^k R_j^{-1} V_j^k R_k^{-1} Q_k^{jT}}{R_{jk}}. \tag{15}
\]

An upper bound on the ratio \( \tau_{jk}/R_{jk}^{-1} \) can be obtained by bounding each term in (15) separately. Rewrite \( Q_j^k = \sum_{i=1}^{n} (a_i x_i / n)^T \) and \( R_j = \sum_{i=1}^{n} (b_i x_i x_i^T / n) \) where \( a_i = -E_{\theta^*} \left( \frac{\partial^2 \ell_i}{\partial \sigma_{jk} \partial \beta_j} \right) \) and \( b_i = -E_{\theta^*} \left( \frac{\partial \ell_i}{\partial \beta_j} \right) \). Then by Lemma S.4.2 in the supplementary materials, we have \( Q_j^k R_j^{-1} Q_j^{kT} \leq p \max_i a_i^2 b_i \). By symmetry, \( Q_k^j R_j^{-1} Q_k^{jT} \leq p \max_i a_i^2 b_i \). Finally, let

\[ Q_j^k R_j^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla \beta_j \ell_i^j (x_i^T \beta_j^*) = W_n. \]

Then by the Cauchy-Schwartz inequality we get

\[ 2 \lim_{n \to \infty} \text{Cov}(W_n, W_n) = 2Q_j^k R_j^{-1} V_j^k R_k^{-1} Q_k^{jT} \leq 2 \lim_{n \to \infty} \sqrt{\text{Var}(W_n) \text{Var}(W_n)} = 2 \sqrt{Q_j^k R_j^{-1} Q_j^{kT}} \sqrt{Q_k^j R_k^{-1} Q_k^{jT}} \leq 2p \max_i a_i^2 b_i. \]

Combining the results we get

\[
\frac{\tau_{jk}}{R_{jk}^{-1}} = 1 + \frac{Q_j^k R_j^{-1} Q_j^{kT}}{R_{jk}} + \frac{Q_k^j R_k^{-1} Q_k^{jT}}{R_{jk}} + 2 \frac{Q_j^k R_j^{-1} V_j^k R_k^{-1} Q_k^{jT}}{R_{jk}} \leq 1 + 4p \max_i \frac{a_i^2}{b_i}, \tag{16}
\]

where \( \max_i \frac{a_i^2}{b_i} \) is finite due to Assumptions 3.1 - 3.4. The bound is proportional to the number of covariates and to a transformation of the true correlation \( \sigma_{jk} \).

To remove this bias, a natural remedy is to consider a consistent estimator of \( \tau_{jk} \) and construct intervals based on this variance. Unfortunately, this involves an additional \( \mathcal{O}(p^2 q^2) \) complexity. Fortunately, in practice in all our simulations, we found the bias to be negligible, so that bias removal is not practically worth the additional computational expense.
4 Simulation results

4.1 Statistical accuracy and uncertainty quantification

We evaluate performance of the non-hierarchical (bigMVP) and hierarchical (bigMVP\textsubscript{h}) versions of the proposed method through simulation studies. We compare these results to the data augmented MCMC sampler (DA) of Chib and Greenberg (1998) and the two-stage frequentist method (TSF) of Ting et al. (2020). We consider sample sizes \( n = 200, 500 \), fix the number of covariates to \( p = 5 \) and vary the number of outcomes as \( q = 10, 15, 20, 100, 200 \). The MCMC sampler and the TSF method were too computationally intensive for \( q = 100, 200 \). Hence, for these choices of \( q \), we only report results from our proposed method.

The metrics on which the methods are evaluated are estimation error and uncertainty quantification. Given data \( y, X \) simulated assuming parameters \( \theta^* = (B^*, \Sigma^*) \), we compute the estimation error as \( \| \hat{B} - B^* \|_F/pq \) (E1) and \( \| \hat{\Sigma} - \Sigma^* \|_F/q^2 \) (E2) for any estimator \( \hat{B} \) and \( \hat{\Sigma} \).

For DA \( \hat{B} \) and \( \hat{\Sigma} \) are the estimated posterior means, for TSF we take the maximum (composite) likelihood estimator as \( \hat{B} \) and \( \hat{\Sigma} \) and for bigMVP and bigMVP\textsubscript{h} we take \( \hat{B} = (\hat{\beta}_1, \ldots, \hat{\beta}_q) \) and \( \hat{\Sigma} = (\hat{\sigma}_{jk}) \).

In simulating the data we consider two different settings for the regression coefficients and the correlation matrix. For the coefficient matrix we consider the two cases 1) (Dense) \( \beta_{ij}^* \sim N(0, 1) \) and the intercept term \( \beta_{0j}^* \sim N(0, 1) \) for \( l = 1, \ldots, p \), \( j = 1, \ldots, q \) and 2) \( \beta_{ij}^* \sim N(0, 1) \) and the intercept term is set to \( \beta_{0j}^* = -3 \) so that many outcomes are rarely observed. For the correlation matrix we first generate a covariance matrix \( \Gamma \) and then set the corresponding correlation matrix as \( \Sigma = D^{-1}\Gamma D^{-1} \) where \( D = \text{diag}(\Gamma_{11}^{1/2}, \ldots, \Gamma_{qq}^{1/2}) \). The settings we consider are 1) (Factor) generate \( \Gamma^* = \Lambda \Lambda^T + I_q \), where \( \Lambda \) is a \( q \times k \) matrix with \( k = 3 \) and \( \lambda_{jl} \sim N(0, 1) \) and 2) (Block) \( \Gamma^* = \text{diag}(\Gamma_1^*, \Gamma_2^*, \ldots) \), where each \( \Gamma_l = LL^T \) with the elements of \( L \) generated from a \( N(0, 1) \) distribution; the size of each \( \Gamma_l \) is taken to be \( 5 \times 5 \). Elements of the design matrix are simulated from \( N(0, 1) \). To implement the hierarchical extension of the proposed method, the initial conditional sampler is run 200 times of which the first 50 samples are discarded. For each setting, the logarithm of the errors averaged over 30 independent replications are displayed in Figure 1; corresponding numerical values are given in Table S.1 of the supplementary materials.

In terms of estimating the regression coefficients, the proposed method performs better across all settings compared to the other methods. The improvement over the data augmented MCMC sampler is especially stark when many binary outcomes are rare, potentially due to very poor mixing in the rare outcome case (Johndrow et al., 2019). In terms of performance in estimating the correlation matrix, the data augmented sampler and the proposed method are very close in all the settings, but in this case the frequentist two-stage method has much larger errors, particularly when outcomes are rare. We further investigate the
Figure 1: Boxplot of logarithm of Frobenius errors in estimating \((B, \Sigma)\) for the hierarchical (bigMVP_h), non-hierarchical (bigMVP), data augmented MCMC sampler (DA) and two-stage frequentist method (TSF) method for \(q = 10, 15, 20\). The prefix bigMVP for the proposed method is removed due to space constraints.

The proposed method’s ability to accurately quantify uncertainty for the correlation matrix. We compare with the two-stage frequentist method and leave out the data augmented sampler for these experiments due to the very high computing time. Variance of the parameters for the two-stage method in Ting et al. (2020) is computed following Hardin (2002) which adjusts for the two-step nature of the method. For individual parameters, \(\sigma_{jk}\) where \(j, k = 1, \ldots, q\), we compute a marginal confidence interval from estimated variance-covariance matrices for Ting et al. (2020). Similarly, we compute credible intervals for these parameters for our proposed method.

We consider the same combination of data generating parameters and for each of these settings we generate 10 different values of \(\theta^*\). Then, for each of these values of \(\theta^*\), we generate 100 data sets and calculate how many of these intervals contain the true parameter values. The average coverage for 95% confidence/credible intervals across all the parameter values and all correlation coefficients is reported in Table S.2 of the supplement. A visual summary of the results is provided in Figure 2. For all cases considered, the proposed method provides very close to nominal coverage but the corresponding frequentist method has severe under coverage when many of the binary outcomes are rare. This illustrates the advantage of incorporating the entire approximate distribution of the regression coefficients in the second-stage estimation. When the outcomes are relatively more common, the coverage of the frequentist method does improve, although it is still not close to the nominal level.

### 4.2 Runtime

We compare the runtime of the proposed method with the recently developed fast MVP method in Pichler and Hartig (2020) which uses the algorithm from Chen et al. (2018) to
compute Gaussian orthant probabilities in parallel and imposes an elastic net penalty on the correlation matrix for handling large numbers of outcomes. We leave out the frequentist two-stage approach of Ting et al. (2020) as their code is not publicly available (authors declined our request) and the code used to produce results for their method in the previous subsection is not optimized. In our runtime analysis we vary the sample size \( n \) over a grid from 50 to 500 with increments of 50 and for each sample size we consider 3 different choices of the number of outcomes: \( q = 0.1n, 0.3n, 0.5n \). The number of covariates \( p = 5 \) and the true regression matrix \( B^* \) is simulated according the “dense” case listed in the previous subsection. The true correlation matrix is set as \( \Sigma^* = \rho I^T + (1 - \rho)I_q \) with \( \rho = 0.5 \). For each value of \((n, q)\) we repeated the procedures 20 times and report the average runtime and average error where the error for each run is computed as \( \|\hat{B} - B^*\|_F/pq + \|\hat{\Sigma} - \Sigma^*\|_F/q^2 \).

The results are reported in Figure S6, based on analyses conducted on an Intel i7-8700K CPU with 3.7 GHz processor; the corresponding plot showing the errors are provided in the supplement. Our proposed method improves upon the computing time by an order of magnitude while also performing better in estimation accuracy, especially in small sample sizes. In addition, unlike the competing fast MVP method, our approach provides standard errors and uncertainty intervals (credible intervals in our case).

5 Applications

We apply the proposed methodology to two data sets in this section:

1. **Bird data.** Lindström et al. (2015) compiled these data from the national bird monitoring programs in Finland, Sweden and Norway. In total \( q = 141 \) bird species were sampled using line transects (Finland and Sweden) and point counts (Norway).
formation on 21 covariates related to land cover, climate and other factors were also collected. We follow Norberg et al. (2019) in including \( p = 5 \) covariates obtained from an initial principal components analysis on the 21 covariates.

2. Vegetation data. These data on arctic vegetation come from a community ecology survey conducted in northern Norway (Niittynen and Luoto, 2018). The data consist of \( q = 242 \) different species of plants, bryophytes and lichens and 6 environmental covariates related to soil, topography and climate were also recorded. We follow Norberg et al. (2019) to include \( p = 4 \) covariates after an initial principal components analysis.

We compare the results with the regularized MVP model of Pichler and Hartig (2020) and the two-stage frequentist (TSF) method of Ting et al. (2020). In our analysis, we fit the models using \( n = 600 \) training points for both datasets. For the bird data the hierarchical version of the proposed method provided a 3 times speedup compared to Pichler and Hartig (2020), whereas for the vegetation data the speedup was by a factor of 5. The computation time for the TSF method was very high in both cases; in our implementation of TSF, we follow the authors suggestion of using the `optim()` function in R, which may lead to substantial computational overhead. The estimated pairwise correlations for all possible pairs of species are shown in Figure 4; corresponding figures showing results from Ting et al. (2020) are in the supplementary material. The sjSDM approach of Pichler and Hartig (2020) does not always produce valid pairwise correlations; some values are outside \([-1, 1]\) in Figure 4. Estimates of the regression coefficients are close for the methods, as shown in the right panel of Figure 4 for the bird data.
Discussion

Our proposed bigMVP Bayesian method provides huge computational benefits compared to sampling based methods without compromising on statistical accuracy. The hierarchical extension leads to very substantial gains in practical performance over frequentist competitors, enabling borrowing of information across outcomes, leading to a particularly substantial improvement in performance for rare outcomes. Our proposed approach is supported by theoretical guarantees showing the performance improves with sample size. The focus of this theory is on marginal posterior distributions for the parameters, which is the emphasis of inference in our motivating application areas.

There are several interesting future directions from both methodological and application perspectives. In ecology, species occurrence data typically come with important spatial information. Extending the model and corresponding methodology to incorporate spatial dependence is straightforward. Consider $q$ dimensional binary outcomes indexed by spatial locations $s$, that is, we observe $y(s)$ and $X(s)$ for each location. Assuming the underlying correlation structure of the species is the same across locations, one only needs to replace the first and second stage likelihoods by their spatial versions. This approach can be extended to additionally account for spatio-temporal dependence. A more challenging problem is to incorporate covariate-dependent correlation; for example, in ecology the dependence between species can vary according to the habitat. The proposed method can also be extended to handle species count data under a latent Gaussian assumption.

SUPPLEMENTARY MATERIAL

The supplementary document contains an approximation scheme to pairwise marginal predictive distribution following the proposed method, it’s performance on test data for the
bird and vegetation data, proofs of Theorem 3.5 and several other technical results. Codes to implement the proposed method are made available here.

A Appendix

A.1 Proof of Theorem 3.7

We will rely on Theorem 3.2 of Miller (2019) to prove this result. We set \((j,k) = 1,2\) without loss of generality. Before proceeding to the main body of the proof, we introduce the definition of equi-Lipschitz as in Miller (2019). A family of functions \(h_n : E \to F\), where \(E\) and \(F\) are subsets of a normed space, is L-equi-Lipschitz if there exists an \(L > 0\) such that such that for all \(n \in \mathbb{N}\), \(x, y \in E\), we have \(\|h_n(x) - h_n(y)\| \leq L\|x - y\|\). We write \(\theta_{12}^* = (\beta_1^T, \beta_2^T, \text{vec}^T(\Sigma_{12}))\) where \(\beta_1\) and \(\beta_2\) are fixed on their respective true values and its consistent estimator \(\hat{\theta}_{12} = (\hat{\beta}_1, \hat{\beta}_2, \text{vec}(\hat{\Sigma}_{12}))\) for any \(\sigma_{12} \in (-1, 1)\). Recall the definitions of \(\hat{\Sigma}_{jk}\) and \(\Sigma_{jk}\) from Section 3. We will first prove the pointwise convergence of \(p_{n,12}(\sigma_{12})\) in \(P_{\theta^*}\). We write

\[
p_{n,12}(\sigma_{12}) = -\left[\frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}, \Sigma_{12}) - \frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}^*, \Sigma_{12})\right]\text{part (a)} - \frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}^*, \Sigma_{12})\text{part (b)}.
\]

We will show that in the preceding display part (a) converges to 0 and part (b) converges to some limit in \(P_{\theta^*}\). To prove part (a) converges to 0, we fix a small enough, convex and open neighborhood \(U\) of \(\theta_{12}^*\) and define \(h_n(\theta_{12}) := \frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}, \Sigma_{12})\). Under Assumption 3.1, 3.2 and 3.4, we have \(\sup_n \sup_{\theta_{12} \in U} \|\frac{\partial h_n(\theta_{12})}{\partial \theta_{12}}\| < \infty\). From Lemma S.4.1, for any \(\sigma_{12} \in (-1, 1), \ h_n(\theta_{12})\) is L-equi-Lipschitz in \(\theta_{12}\) for any \(\theta_{12} \in U\). Thus, for any \(\xi > 0\), we have

\[
\limsup_{n \to \infty} P_{\theta^*}\left\{\left|\frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}, \Sigma_{12}) - \frac{1}{n} \sum_{i=1}^{n} \ell_i^{12}(\sigma_{12}; \mu_{12}^*, \Sigma_{12})\right| > \xi\right\} = \limsup_{n \to \infty} P_{\theta^*}\left\{h_n(\theta_{12}) - h_n(\theta_{12}^*) > \xi\right\} \\
\leq \limsup_{n \to \infty} P_{\theta^*}\left\{L \|\hat{\theta}_{12} - \theta_{12}^*\| > \xi\right\} + \limsup_{n \to \infty} P_{\theta^*}\left\{\hat{\theta}_{12} \notin U\right\} = 0,
\]

where the last equality holds since \(\hat{\theta}_{12}\) is consistent for \(\theta_{12}^*\). The convergence of part (b) is implied by Kolmogorov’s strong law for independent but not identically distributed random variable series (Theorem 7.3.3 of Resnick (2019)), which requires that \(\frac{1}{n} \sum_{i=1}^{n} \text{Var}(\ell_i^{12}(\sigma_{12}; \mu_{12}^*, \Sigma_{12})) < \infty\). Such requirement can be guaranteed by the bounded parameter assumption (Assumption 3.1), bounded design matrix assumption (Assumption 3.4) and correlation assumption.
(Assumption 3.2), which guarantees that $\ell_i^{12}(\sigma_{12}; \mu_{12}, \Sigma_{12})$ is uniformly bounded for every $i$. Now that part (a) converges to 0 and part (b) converges in $P_{\theta^*}$, we have that $p_n(\sigma_{12})$ converges to some limit in $P_{\theta^*}$ for every $\sigma_{12} \in (-1, 1)$. We denote such pointwise limit by $p_{12}(\sigma_{12})$, i.e., $p_{12}(\sigma_{12}) = -\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} E_{\theta^*}(\ell_i^{12})$.

Similar to the proof of Theorem 3.5, we need to verify certain conditions so that the conclusion of the theorem hold. In the current context this involves verifying the following conditions - A) $p''_{n12}(\sigma_{12})$ is uniformly bounded for $\sigma_{12} \in E \subseteq (-1, 1)$ where $E \subseteq \mathbb{R}^p$ is some open, convex and bounded set and $\sigma_{12}^* \in E$, B) $p''(\sigma_{12}^*) = R_{12} > 0$, C) Each $p_{n12}(\sigma_{12})$ is convex in $E$ and D) $p''(\sigma_{12}^*) = 0$.

**Condition A:** The analysis in verifying this condition is similar to its counterpart in the proof of Theorem 3.5. We define $\kappa_{i12} = r_{i1} r_{i2} \sigma_{12}$ and write $p''_{n12}(\sigma_{12})$ as

$$p''_{n12}(\sigma_{12}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial^3 \ell_i^{12}(\sigma_{12}; \tilde{\mu}_{12}, \tilde{\Sigma}_{12})}{\partial \kappa_{i12}^3} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial^3 \ell_i^{12}(\sigma_{12}; \tilde{\mu}_{12}, \tilde{\Sigma}_{12})}{\partial \kappa_{i12}^3}.$$

where

$$\frac{\partial^3 \ell_i^{12}(\sigma_{12}; \tilde{\mu}_{12}, \tilde{\Sigma}_{12})}{\partial \kappa_{i12}^3} = U \left\{ \Phi_{\Sigma_{12}}(\kappa_{i12}), \phi_{\Sigma_{12}}(\kappa_{i12}), \phi'_{\Sigma_{12}}(\kappa_{i12}), \phi''_{\Sigma_{12}}(\kappa_{i12}) \right\}.$$

In the preceding display $U \left\{ \Phi_{\Sigma_{12}}(\kappa_{i12}), \phi_{\Sigma_{12}}(\kappa_{i12}), \phi'_{\Sigma_{12}}(\kappa_{i12}), \phi''_{\Sigma_{12}}(\kappa_{i12}) \right\}$ involves polynomial functions of $\Phi_{\Sigma_{12}}(\kappa_{i12}), \phi_{\Sigma_{12}}(\kappa_{i12}), \phi'_{\Sigma_{12}}(\kappa_{i12}), \phi''_{\Sigma_{12}}(\kappa_{i12})$. Because of Assumption 3.2, $\sigma_{12}$ is bounded away from both -1 and 1, hence, $\Sigma_{12}$ is strictly positive definite with probability 1. Therefore, $\Phi_{\Sigma_{12}}(\kappa_{i12})$ is bounded away from 0 for every $\sigma_{12} \in E$ and $1 \leq i \leq n$. Assumption 3.1 and 3.4 imply that $\tilde{\mu}_{12}$ is bounded, so that $\Phi_{\Sigma_{12}}(\kappa_{i12}), \phi_{\Sigma_{12}}(\kappa_{i12}), \phi'_{\Sigma_{12}}(\kappa_{i12}), \phi''_{\Sigma_{12}}(\kappa_{i12})$ are bounded for every $\sigma_{12} \in E$ and $1 \leq i \leq n$ since $\Sigma_{12}$ is strictly positive definite with probability 1. Therefore, $U \left\{ \Phi_{\Sigma_{12}}(\kappa_{i12}), \phi_{\Sigma_{12}}(\kappa_{i12}), \phi'_{\Sigma_{12}}(\kappa_{i12}), \phi''_{\Sigma_{12}}(\kappa_{i12}) \right\}$ is also uniformly bounded in $i$. Since $\Phi_{\Sigma_{12}}$ is bounded away from 0 uniformly and $U(\cdot)$ is uniformly bounded in $i$, $\frac{\partial^3 \ell_i^{12}(\sigma_{i12}; \tilde{\mu}_{12}, \tilde{\Sigma}_{12})}{\partial \kappa_{i12}^3}$ is uniformly bounded and thus $p''_{n12}(\sigma_{12})$ is uniformly bounded in $n$.

**Condition B:** We have

$$p''(\sigma_{12}^*) = R_{12} = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Var}_{\theta^*} \left( \frac{\partial \ell_i^{12}}{\partial \sigma_{12}} \right) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Var}_{\theta^*} \left( \frac{\phi_{\Sigma_{12}}^{r_{i1} r_{i2}}}{\phi_{\Sigma_{12}}} \right),$$

where $\text{Var}_{\theta^*} \left( \frac{\phi_{\Sigma_{12}}}{\phi_{\Sigma_{12}}} r_{i1} r_{i2} \right) = \sigma_{12} r_{i1} = -1, 1 \sum_{r_{i1} = -1}^{1} \sigma_{12} r_{i1} = -1, 1 \phi_{\Sigma_{12}}^{r_{i1} r_{i2}}$. Because $\sigma_{12} \in (-1, 1)$ and $\tilde{\mu}_{12}$ is uniformly bounded for every $i$, $\phi_{\Sigma_{12}}^{r_{i1} r_{i2}}$ is uniformly bounded away from 0 for every $i$. Therefore, $R_{12} = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Var}_{\theta^*} \left( \frac{\phi_{\Sigma_{12}}}{\phi_{\Sigma_{12}}} r_{i1} r_{i2} \right) > 0$.

**Condition C:** It suffices to prove $p_{n12}(\sigma_{12})$ is convex in $E$ with probability arbitrarily
closed to 1 for all sufficiently large $n$. First, we have

$$p_{i12}''(\sigma_{12}) = -\frac{1}{n} \sum_{i=1}^{n} \frac{\partial^2 p_{i12}}{\partial \sigma_{12}^2}(\sigma_{12}) = -\frac{1}{n} \sum_{i=1}^{n} \left[ \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} - \left( \frac{\phi_{\Sigma_{12}}}{\Phi_{\Sigma_{12}}} \right)^2 \right].$$

We will prove the first term in the preceding display converges to 0 when $\theta_{12}^{**} = \theta_{12}^*$ in $P_{\theta^*}$, i.e., $-\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} \right) P_{\theta^*} \rightarrow 0$. We write $T_i(\tilde{\theta}_{12}) = \left( \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} \right)$ for every $i$ so that we will need to prove that when $\theta_{12}^{**} = \theta_{12}^*$, $\frac{1}{n} \sum_{i=1}^{n} T_i(\tilde{\theta}_{12}) \rightarrow 0$ for every $\sigma_{12} \in (-1, 1)$. To that end, we write

$$\frac{1}{n} \sum_{i=1}^{n} T_i(\tilde{\theta}_{12}) = \left\{ \frac{1}{n} \sum_{i=1}^{n} T_i(\tilde{\theta}_{12}) - \frac{1}{n} \sum_{i=1}^{n} T_i(\theta_{12}^*) \right\} + \frac{1}{n} \sum_{i=1}^{n} T_i(\theta_{12}^*)$$

and prove part (a) and (b) in the preceding display all converge to 0 in $P_{\theta^*}$. Fix a neighborhood $U$ of $(\mu_{12}, \Sigma_{12})$. Then for every $\xi > 0$ we have

$$\limsup_{n \to \infty} P_{\theta^*} \left\{ \left| \frac{1}{n} \sum_{i=1}^{n} T_i(\tilde{\theta}_{12}) - \frac{1}{n} \sum_{i=1}^{n} T_i(\theta_{12}^*) \right| > \xi \right\} \leq \limsup_{n \to \infty} P_{\theta^*} \left\{ L \left\| \tilde{\theta}_{12} - \theta_{12}^* \right\| > \xi \right\} + \limsup_{n \to \infty} P_{\theta^*} \left\{ \tilde{\theta}_{12} \notin U \right\} = 0 \quad (17)$$

The preceding display is implied by the fact that $\tilde{\theta}_{12}$ is a consistent estimator of $\theta$. Thus, part (a) converges to 0 in $P_{\theta^*}$. To prove part (b) converges to 0 in $P_{\theta^*}$, it can be easily verified that $E_{\theta^*} [T_i(\theta_{12}^*)] = 0$. Then, by the Kolmogorov’s strong law, we have $\frac{1}{n} \sum_{i=1}^{n} T_i(\theta_{12}^*) \rightarrow 0$.

Combining part (a) and part (b), when $\theta_{12}^{**} = \theta_{12}^*$, $-\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} \right) P_{\theta^*} \rightarrow 0$. The L-equi-Lipschitz property also guarantees that for any $\epsilon > 0$, if we choose $E_{\theta}^*$ to be small enough, for any $\sigma_{12} \in E$

$$\lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} \right) \exists \text{ and } \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \left( \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} \frac{\partial \sigma_{12}}{\Phi_{\Sigma_{12}}} \right) > -\epsilon \quad (18)$$

in $P_{\theta^*}$. From Assumption 3.1, 3.2 and 3.4, we also have that $\frac{\phi_{\Sigma_{12}}}{\Phi_{\Sigma_{12}}}$ is bounded away from 0 uniformly for every $i$ and so is $\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\phi_{\Sigma_{12}}}{\Phi_{\Sigma_{12}}} \right)^2$. We can choose a small enough $\epsilon$ such that for all sufficiently large $n$,

$$\frac{1}{n} \sum_{i=1}^{n} \left( \frac{\phi_{\Sigma_{12}}}{\Phi_{\Sigma_{12}}} \right)^2 > 2\epsilon \quad (19)$$
Combining (18) and (19), with probability arbitrary closed to 1 and all \( n \) sufficiently large, we have
\[
p''_{n12}(\sigma_{12}) = -\frac{1}{n} \sum_{i=1}^{n} \left[ \frac{\partial \phi_{\Sigma_{12}}}{\partial \sigma_{12}} - \left( \frac{\phi_{\Sigma_{12}}}{\Phi_{\Sigma_{12}}} \right)^2 \right] \geq 2\epsilon - \epsilon = \epsilon > 0,
\]
for every \( \sigma_{12} \in E \) which implies that with probability arbitrary closed to 1, \( p_{n12}(\sigma_{12}) \) is convex for all sufficiently large \( n \).

**Condition D:** Define \( \Sigma^*_{12} = \{(1, r_{i1} r_{i2} \sigma^*_{12})^T; (r_{i1} r_{i2} \sigma^*_{12}, 1)^T\} \). Then we have
\[
E_{\theta^*} \left( \frac{\phi_{\Sigma^*_{12}}}{\Phi_{\Sigma^*_{12}}} r_{i1} r_{i2} \right) = \sum_{r_{i1} = -1, 1} \sum_{r_{i2} = -1, 1} r_{i1} r_{i2} \phi_{\Sigma^*_{12}} (r_{i1} x_i^T \beta^*_1, r_{i2} x_i^T \beta^*_2) = 0.
\]
Therefore,
\[
p'_{12}(\sigma^*_{12}) = \lim_{n \to \infty} -\frac{1}{n} \sum_{i=1}^{n} E_{\theta^*} \left( \frac{\phi_{\Sigma^*_{12}}}{\Phi_{\Sigma^*_{12}}} r_{i1} r_{i2} \right) = \lim_{n \to \infty} -\frac{1}{n} \sum_{i=1}^{n} E_{\theta^*} \left( \frac{\phi_{\Sigma^*_{12}}}{\Phi_{\Sigma^*_{12}}} r_{i1} r_{i2} \right) = 0.
\]

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Yi, G. Y., L. Zeng, and R. J. Cook (2011). A robust pairwise likelihood method for incomplete longitudinal binary data arising in clusters. Canadian Journal of Statistics 39(1), 34–51.
S.1 Marginal pairwise prediction

Although our focus is on inference on the model parameters, it can nonetheless be useful to obtain predictive distributions as key components of model assessments and comparisons. As obtaining a joint predictive rule for all $q$ outcomes is necessarily computationally demanding when $q$ is large, we focus on prediction of an arbitrary pair of outcomes in a new sample $t$ having covariate value $x_t$.

Fix a pair $(j,k)$. Then from our proposed two-stage approach, we have access to the approximate marginal posterior distributions $\Pi^*_j(\beta_j \mid y, X)$, $\Pi^*_k(\beta_k \mid y, X)$ and $\Pi^*_{jk}(\sigma_{jk} \mid y, X)$. Let $\theta_{jk} = (\beta_j, \beta_k, \sigma_{jk})$. Given a new test point $x_t$, the marginal predictive distribution for this pair is

$$p_{jk}(y_t^{(j)}, y_t^{(k)} \mid y, X) = \int p_{jk}(y_t^{(j)}, y_t^{(k)} \mid \theta_{jk}, y, X) \Pi(\theta_{jk} \mid y, X) d\theta_{jk},$$

(S.1)

where we approximate the joint posterior $\Pi(\theta_{jk} \mid y, X)$ by a product of the marginals, $\Pi(\theta_{jk} \mid y, X) \approx \Pi^*_j(\beta_j \mid y, X)\Pi^*_k(\beta_k \mid y, X)\Pi^*_{jk}(\sigma_{jk} \mid y, X)$. The first component inside the integral in (S.1) can be written as $p_{jk}(y_t^{(j)}, y_t^{(k)} \mid \theta_{jk}, y, X) = \int p_{jk}(y_t^{(j)}, y_t^{(k)} \mid z_t^{(j)}, z_t^{(k)}, \theta_{jk}, y, X) dz_t^{(j)} dz_t^{(k)}$, where $(z_t^{(j)}, z_t^{(k)})$ are the corresponding latent variables for the test point $x_t$. Hence, we focus on the predictive distribution of the latent variables $(z_t^{(j)}, z_t^{(k)})$. Under the MVP model, $(z_t^{(j)}, z_t^{(k)}) \mid \theta_{jk}, y, X$ has a bivariate Gaussian distribution with mean $\mu_t = (x_t^T \beta_j, x_t^T \beta_k)$, unit variance and correlation $\sigma_{jk}$. Since the posterior distributions of the regression coefficients are Gaussian, we can easily marginalize over them to
obtain that \((z_t^{(j)}, z_t^{(k)}) \mid \sigma_{jk} \sim N(\tilde{\mu}_t, \tilde{\Sigma}_t)\), where \(\tilde{\mu}_t = (x_t^\top \hat{\beta}_j, x_t^\top \hat{\beta}_k)\) and the diagonal elements of \(\tilde{\Sigma}_t\) are \(1 + x_t^\top H_j x_t, 1 + x_t^\top H_k x_t\). To obtain the distribution of \((z_t^{(j)}, z_t^{(k)}) \mid y, X\), it remains to marginalize over \(\sigma_{jk}\) where \(\sigma_{jk} \sim N(\hat{\sigma}_{jk}, \sigma_{jk}^2)\). In Section 3.4, we show that \(\Pi(\sigma_{jk} \mid y, X) \xrightarrow{d} \delta_{\sigma_{jk}}\); a consequence of the total variation convergence of Theorem 3.7 where \(\sigma_{jk}^*\) is the true value of the correlation between outcomes \(j\) and \(k\). Hence, \(\hat{\sigma}_{jk} \xrightarrow{P} \sigma_{jk}^*\). Write the marginal density \((z_t^{(j)}, z_t^{(k)}) \mid \sigma_{jk}, y, X\) as the expectation over \(\Pi(\sigma_{jk} \mid y, X)\), that is \(p(z_t^{(j)}, z_t^{(k)}) \mid y, X = E_{\sigma_{jk}} p(z_t^{(j)}, z_t^{(k)} \mid \sigma_{jk}, y, X)\). Then by Assumption 3.2 the conditional density \(p(z_t^{(j)}, z_t^{(k)} \mid \sigma_{jk}, y, X)\) is bounded and integrable. Thus, by the dominated convergence theorem, \(p(z_t^{(j)}, z_t^{(k)} \mid \sigma_{jk}, y, X) \rightarrow p(z_t^{(j)}, z_t^{(k)} \mid \sigma_{jk}^*, y, X)\) of which a reasonable approximation is provided by \(p(z_t^{(j)}, z_t^{(k)} \mid \hat{\sigma}_{jk}, y, X)\). With all the above ingredients, we approximate \(p(z_t^{(j)}, z_t^{(k)} \mid y, X)\) by \(N(\tilde{\mu}_t, \tilde{\Sigma}_t)\), where \(\tilde{\mu}_t\) is as defined before and \(\tilde{\Sigma}_t\) has the same diagonal elements as \(\hat{\Sigma}_t\) and the off-diagonal elements are \(\hat{\sigma}_{jk}\). Finally, a predictive sample for \((y_t^{(j)}, y_t^{(k)})\) can be drawn by first drawing the latent variables \((z_t^{(j)}, z_t^{(k)}) \sim N(\tilde{\mu}_t, \tilde{\Sigma}_t)\) and then thresholding these latent variables. In our numerical experiments, this provided reliable approximations to the predictive distribution. For example, when \((n, p, q) = (150, 5, 2)\) and with 50 test points, the approximation maintained an average 1% error rate in estimating the posterior predictive mean for different values of the underlying correlation coefficient in \([-1, 1]\); here we treated the posterior predictive mean computed using the data augmented MCMC sampler as our benchmark.

S.1.1 Prediction performance in real data

We held out 50 test points for each dataset. The number of unique pairs of species for the bird data is 9870 and for the vegetation data is 29161. For each of these pairs of species we sampled 100 predictive samples following Section S.1. Suppose \(x_t\) is the test point and we are considering the \((j, k)\)-th pair of species. We computed the predictive mean for this test point and pair of species averaging over the 100 predictive samples. The predictive accuracy is then computed as the difference between the predictive mean and the observed species indicators at this test point. We additionally computed the class of these outcomes as 1 or 0 according to whether the predictive mean is above or below 0.5. We also computed similar predictions for these pairs by plugging in the corresponding frequentist two-stage estimates. The misclassification rate is then computed as the difference in observed values and predicted classes. For the pair \((j, k)\) and \(n_t\) test points we then obtained the average prediction error and misclassification error. We summarise the results in Table S.1. On the misclassification metric, the proposed method has lower error rate compared to the frequentist approach except for the maximum. In cases where the proposed method achieves lower error rate, rows 2-4 in Table S.1, it provides a minimum of 9% improvement but for the
maximum error where the frequentist approach performs better it has about 2% lower error rate. Furthermore, in pairs where at least one of the species is rare, the frequentist approach often estimates the correlation to be very close to either -1 or 1 shown in the cluster of points around the $y = 1, -1$ line in Figure S5. The hierarchical version of the proposed method do not have these computational issues.

|                  | Bird data          | Vegetation data    |
|------------------|--------------------|--------------------|
|                  | Prediction error   | Misclassification error |
|                  | bigMVP | TSF | bigMVP | TSF | bigMVP | TSF |
| Minimum          | 0.0005 | 0   | 0    | 0    | 0.0002 | 0   | 0    |
| 1st quartile     | 0.048  | 0.049 | 0.066 | 0.010 | 0      | 0    | 0.028 |
| Median           | 0.067  | 0.077 | 0.091 | 0.039 | 0.04   | 0.056 |
| 3rd quartile     | 0.08   | 0.097 | 0.107 | 0.064 | 0.077  | 0.089 |
| Maximum          | 0.117  | 0.165 | 0.161 | 0.117 | 0.16   | 0.158 |

Table S.1: Summary statistics of the pairwise prediction and misclassification errors for the bird data and vegetation data.
S.2 Proof of Theorem 3.5

In the proof, we write \( \beta_1 \) instead of \( \beta_j \) for convenience as the proof holds for any arbitrary \( j = 1, \ldots, q \). The theorem is a direct consequence of Theorem 3.2 of Miller (2019) and we shall verify all sufficient conditions of Theorem 3.2 from Miller (2019). Specifically, we will need to verify four conditions: A) \( p_n''(\beta_1) \) is uniformly bounded in \( E \) where \( E \subset \mathbb{R}^p \) is some open, convex and bounded set and \( \beta_1^* \in E \), B) \( p_n'((\beta_1^*) \) is positive definite, C) Each \( p_n \) is convex in \( E \) and D) \( p_n'(\beta_1^*) = 0 \). Recall \( r_{i1} = 2y_{i1} - 1 \) from Section 3.4.

**Condition A**) Letting \( \psi_{i1} = r_{i1}x_i^T\beta_1 \) we have,

\[
p_n''(\beta_1)_{i1i2i3} = -\frac{1}{n} \sum_{i=1}^{n} \frac{\partial^3 \ell_i}{\partial(\psi_{i1})^3} r_{i1}^3 x_{i1} x_{i2} x_{i3}.
\]

where

\[
\frac{\partial^3 \ell_i}{\partial(\psi_{i1})^3}(\psi_{i1}) = \frac{T(\Phi, \phi, \phi', \phi'')}{\Phi^3}(\psi_{i1}),
\]

and \( l_1, l_2, l_3 = 1, \ldots, p \). Here \( T(\Phi, \phi, \phi', \phi'') \) is a polynomial function of \( \Phi(\psi_{i1}), \phi(\psi_{i1}), \phi'(\psi_{i1}) \) and \( \phi''(\psi_{i1}) \). From Assumption 3.1 and 3.4, \( \{\psi_{i1}\} \) is bounded for every \( \beta_1 \in E \) so there exists an \( \epsilon > 0 \) such that \( \Phi(\psi_{i1}) > \epsilon > 0 \) for every \( i \). Moreover, since \( \{\psi_{i1}\} \) is bounded, \( \Phi(\psi_{i1}), \phi(\psi_{i1}), \phi'(\psi_{i1}) \) and \( \phi''(\psi_{i1}) \) are also bounded and so is \( T(\Phi, \phi, \phi', \phi'') \). Therefore, there exists an \( M > 0 \) such that for every \( \beta_1 \in E \)

\[
\left| \frac{\partial^3 \ell_i}{\partial(\psi_{i1})^3} r_{i1}^3 \right| \leq M \quad \text{a.s.}
\]

We then have

\[
|p_n''(\beta_1)_{i1i2i3}| \leq \frac{1}{n} \sum_{i=1}^{n} \left| \frac{\partial^3 \ell_i}{\partial(\psi_{i1})^3} \right| |x_{i1} x_{i2} x_{i3}| \leq \frac{M}{n} \sum_{i=1}^{n} |x_{i1} x_{i2} x_{i3}| \quad \text{a.s.}
\]

In addition, from Assumption 3.4 we have \( \frac{1}{n} \sum_{i=1}^{n} |x_{i1} x_{i2} x_{i3}| \) converges almost surely for every \( j, k, l \). Thus, \( |p_n''(\beta_1)_{i1i2i3}| \) is uniformly bounded for every \( \beta_1 \in E \) and \( l_1, l_2, l_3 = 1, \ldots, p \).

**Condition B**) \( p_n'(\beta_1^*) \) as defined in (12) and its positive definiteness is implied by Assumption 3.4.

**Condition C**) The convexity of every \( p_n \) is proved in Theorem 9.2.3 of Amemiya (1985).

**Condition D**) From (11), we also have that

\[
p_n'(\beta_1^*) = \lim_{n \to \infty} n^{-1} \left( \sum_{i=1}^{n} \frac{\Phi_{i1}}{\Phi_{i1}^*} \phi_{i1}^* x_i - \sum_{i=1}^{n} \frac{1 - \Phi_{i1}^*}{1 - \Phi_{i1}} \phi_{i1}^* x_i \right) = 0.
\]
S.3 Asymptotic normality of $\tilde{\sigma}_{jk}$

In Lemma S.3.1 we prove that the two-step M-estimator asymptotically has a Gaussian distribution. One critical step of Lemma S.3.1 is to use the asymptotic normality of the score functions of both stages, i.e.

$$
\begin{bmatrix}
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_1} \ell_i^1(x_i^T \beta_1^*) \\
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_2} \ell_i^2(x_i^T \beta_2^*) \\
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_i^{12}(\sigma_{12}^*; \mu_{12}^*; \Sigma_{12}^*)
\end{bmatrix} \xrightarrow{D} 
\begin{bmatrix}
R_1 \\
V_{12}^T R_2 \\
V_{12}^T R_2^2 R_1
\end{bmatrix},
$$

(S.2)

where $\mu_{12}^* = (x_1^T \beta_1^*, x_2^T \beta_2^*)$ and $\Sigma_{12}^* = \{(1, \sigma_{12}^*)^T; (\sigma_{12}^*, 1)^T\}$. Such asymptotic normality is implied by the multivariate (Lyapunov) Central Limit Theorem (CLT) since each term in the summation is independent and has a bounded third order moment implied by Assumption 3.4.

**Lemma S.3.1.** Under Assumptions 3.1, 3.2 and 3.4 the following asymptotic normality of two-step M-estimator $\tilde{\sigma}_{jk}$ holds:

$$
\sqrt{n}(\tilde{\sigma}_{jk} - \sigma_{jk}^*) \xrightarrow{d} N(0, \tau_{jk})
$$

where $\tau_{jk}$ is defined as

$$
\tau_{jk} := R_{jk}^{-1} + R_{jk}^{-1} \left( Q_j^k R_j^{-1} Q_j^{kT} \right) R_{jk}^{-1} + R_{jk}^{-1} \left( Q_k^j R_k^{-1} Q_k^{jT} \right) R_{jk}^{-1} + 2 R_{jk}^{-1} Q_j^k R_j^{-1} V_{jk} R_k^{-1} Q_k^{jT} R_{jk}^{-1}.
$$

**Proof.** We prove the result for $(j, k) = (1, 2)$. We first write down the estimation equations for both stages:

$$
\begin{aligned}
\sum_{i=1}^{n} \nabla_{\beta_1} \ell_i^1(x_i^T \hat{\beta}_1) &= 0 & \text{first stage estimation of } \beta_1, \\
\sum_{i=1}^{n} \nabla_{\beta_2} \ell_i^2(x_i^T \hat{\beta}_2) &= 0 & \text{first stage estimation of } \beta_2,
\end{aligned}
\tag{S.3}
$$

Let $\mu_{12}^* = (x_1^T \beta_1^*, x_2^T \beta_2^*)$ and $\Sigma_{12}^* = \{(1, \sigma_{12}^*)^T; (\sigma_{12}^*, 1)^T\}$. Then expand the third equation of (S.3) at $(\mu_{12}^*, \Sigma_{12}^*)$.

$$
-\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_i^{12}(\sigma_{12}^*; \mu_{12}^*, \Sigma_{12}^*) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_i^{12}(\hat{\beta} - \beta_1^*) + \frac{1}{n} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_i^{12}(\hat{\beta} - \beta_2^*)
$$
From Appendix where \( \hat{\delta}_{1i} = x_i^T H_1 x_i \) and \( \hat{\delta}_{2i} = x_i^T H_2 x_i \). We note here that since both \( \hat{\delta}_{1i} \) and \( \hat{\delta}_{1i} \) are of order \( O_{P_{\theta}}(n^{-1}) \), the third and fourth term of the right hand side of (S.4) are \( O_{P_{\theta}}(n^{-1/2}) \). Hence, rearranging the terms in (S.4), asymptotically we have,

\[
\sqrt{n}(\tilde{\sigma}_{12} - \sigma_{12}^*) = -R_{12}^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_{i}^{12}(\sigma_{12}^*; \mu_{12}^*, \Sigma_{12}^*) \\
+ R_{12}^{-1} Q_{12}^2 R_{12}^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_2} \ell_{i}^{2}(x_i^T \beta_2^*) \\
+ R_{12}^{-1} Q_{12}^2 R_{12}^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_2} \ell_{i}^{2}(x_i^T \beta_2^*). \tag{S.5}
\]

We also have from a simple application of the multivariate CLT that

\[
\begin{bmatrix}
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_1} \ell_{i}^{1}(x_i^T \beta_1^*) \\
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\beta_2} \ell_{i}^{1}(x_i^T \beta_2^*) \\
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \nabla_{\sigma_{12}} \ell_{i}^{12}(\sigma_{12}^*; \mu_{12}^*, \Sigma_{12}^*)
\end{bmatrix} \xrightarrow{D} \begin{bmatrix}
R_1 & V_{12} & R_{12}^{12} \\
V_{12}' & R_2 & R_{12}^{12} \\
R_{12}^{12} & R_{2}^{12} & R_{12}
\end{bmatrix}
\]

As a result, the right hand side of (S.5) converges to \( N(0, \tau_{12}) \) in distribution, where

\[
\tau_{12} = R_{12}^{-1} + R_{12}^{-1} \left( -2R_{12}^{12} R_{12}^{-1} Q_{12}^{12} + Q_{12}^{12} R_{12}^{-1} Q_{12}^{12} \right) R_{12}^{-1} \\
+ R_{12}^{-1} \left( -2R_{12}^{12} R_{12}^{-1} Q_{12}^{12} + Q_{12}^{12} R_{12}^{-1} Q_{12}^{12} \right) R_{12}^{-1} \\
+ 2R_{12}^{-1} Q_{12}^{12} R_{12}^{-1} V_{12} R_{2}^{-1} Q_{2}^{12} R_{12}^{-1}
\]

From Appendix S.5, we have \( R_{12}^{12} = R_{12}^{12} = 0 \). Therefore,

\[
\tau_{12} = R_{12}^{-1} + R_{12}^{-1} \left( Q_{12}^{12} R_{12}^{-1} Q_{12}^{12} \right) R_{12}^{-1} + R_{12}^{-1} \left( Q_{2}^{12} R_{2}^{-1} Q_{2}^{12} \right) R_{12}^{-1} \\
+ 2R_{12}^{-1} Q_{12}^{12} R_{12}^{-1} V_{12} R_{2}^{-1} Q_{2}^{12} R_{12}^{-1}
\]

6
S.4 Auxiliary results

**Lemma S.4.1** (Lemma S6.2 of Miller (2019)). Let $E \subseteq \mathbb{R}^D$ be open and convex, and let $f_n : E \to \mathbb{R}$ for $n \in \mathbb{N}$. For any $k \in \mathbb{N}$, if each $f_n$ has continuous $k$th-order derivatives and $(f_n^{(k)})$ is uniformly bounded, then $(f_n^{(k-1)})$ is equi-Lipschitz.

**Lemma S.4.2.** Let $\{x_i\}$ be a sequence of $p$-dimensional vectors where each $x_i \in \mathbb{R}^p$ and $\lim_{n \to \infty} n^{-1} \sum_{i=1}^n x_i x_i^T$ is a finite nonsingular matrix. For any $p \times p$ square matrix $A$, we let its trace $\text{tr}(A)$ be the sum of its diagonal elements, i.e., $\text{tr}(A) = \sum_{i=1}^p A_{ii}$. Let $\{a_i\}, \{b_i\}$ be real number sequences and $\{b_i\}$ are all positive. Then

$$\sum_{i=1}^n (a_i x_i)^T \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1} \sum_{i=1}^n (a_i x_i) \leq p \max_{i} \frac{a_i^2}{b_i}$$

**Proof.** We have,

$$\frac{1}{n} \sum_{i=1}^n (a_i x_i)^T \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1} \sum_{i=1}^n (a_i x_i) = \frac{1}{n} \text{tr} \left[ \sum_{i=1}^n (a_i x_i)^T \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1} \sum_{i=1}^n (a_i x_i) \right]$$

$$= \frac{1}{n} \text{tr} \left[ \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1/2} \sum_{i=1}^n (a_i x_i) \sum_{i=1}^n (a_i x_i)^T \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1/2} \right]$$

(S.6)

Also, the matrix

$$A = \sum_{i=1}^n \left[ a_i x_i - \frac{1}{n} \sum_{i=1}^n (a_i x_i) \right] \left[ a_i x_i - \frac{1}{n} \sum_{i=1}^n (a_i x_i) \right]^T = \sum_{i=1}^n a_i^2 x_i x_i^T - \frac{1}{n} \sum_{i=1}^n (a_i x_i) \sum_{i=1}^n (a_i x_i)^T$$

is positive definite. Plugging the preceding display back to (S.6), we have

$$\frac{1}{n} \text{tr} \left[ \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1/2} \sum_{i=1}^n (a_i x_i) \sum_{i=1}^n (a_i x_i)^T \left( \sum_{i=1}^n b_i x_i x_i^T \right)^{-1/2} \right]$$
\[
\leq \text{tr} \left[ \left( \sum_{i=1}^{n} b_i x_i x_i^T \right)^{-1/2} \left( \sum_{i=1}^{n} a_i^2 x_i x_i^T \left( \sum_{i=1}^{n} b_i x_i x_i^T \right)^{-1/2} \right) \right]
\]
\[
= \text{tr} \left[ \left( \sum_{i=1}^{n} b_i x_i x_i^T \right)^{-1} \left( \sum_{i=1}^{n} a_i^2 x_i x_i^T \right) \right]
\]
\[
\leq \max_i \frac{a_i^2}{b_i} \text{tr} \left[ \left( \sum_{i=1}^{n} b_i x_i x_i^T \right)^{-1} \left( \sum_{i=1}^{n} b_i x_i x_i^T \right) \right]
\]
\[
= p \max_i \frac{a_i^2}{b_i}
\]

\[\square\]

### S.5 Some Useful Quantities

Here, we present the detailed expressions of quantities used in Section 3. Recall that \(\Sigma_{12}^* = \{(1, r_i r_j \sigma_{12}^*)^T; (r_i r_j \sigma_{12}^*, 1)^T\}\). Let \(\mu_1^* = x_i^T \beta_1^*, \mu_2^* = x_i^T \beta_2^*\). We have,

\[
R_{12}^1 = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Cov}_{\theta^*} \left( \frac{\partial \ell_i^1}{\partial \beta_1}, \frac{\partial \ell_i^1}{\partial \sigma_{12}} \right) = 0 \quad (S.7)
\]

where

\[
\text{Cov}_{\theta^*} \left( \frac{\partial \ell_i^1}{\partial \beta_1}, \frac{\partial \ell_i^1}{\partial \sigma_{12}} \right) = E_{\theta^*} \left( \frac{\partial \ell_i^1}{\partial \beta_1} \frac{\partial \ell_i^1}{\partial \sigma_{12}} \right)
\]
\[
= E_{\theta^*} \left[ \frac{\phi(r_i r_j \mu_1^*)}{\Phi(r_i \mu_1^*)} r_i r_j \times \frac{\phi_{\Sigma_{12}^*} r_i r_j x_i}{\Phi_{\Sigma_{12}^*}} \right]
\]
\[
= E_{\theta^*} \left[ \frac{\phi(r_i r_j \mu_1^*)}{\Phi(r_i \mu_1^*)} \frac{\phi_{\Sigma_{12}^*} r_i r_j x_i}{\Phi_{\Sigma_{12}^*}} \right]
\]
\[
= \frac{\phi(\mu_1^*)}{\Phi(\mu_1^*)} \phi_{\Sigma_{12}^*}(\mu_1^*, \mu_2^*) - \frac{\phi(\mu_1^*)}{\Phi(\mu_1^*)} \phi_{\Sigma_{12}^*}(\mu_1^*, \mu_2^*)
\]
\[
+ \frac{\phi(-\mu_1^*)}{\Phi(-\mu_1^*)} \phi_{\Sigma_{12}^*}(\mu_1^*, \mu_2^*) - \frac{\phi(-\mu_1^*)}{\Phi(-\mu_1^*)} \phi_{\Sigma_{12}^*}(\mu_1^*, \mu_2^*)
\]
\[
\stackrel{(a)}{=} 0
\]
Similarly, \( R_{12}^2 = \lim_{n \to \infty} \frac{1}{n} \text{Cov}_{\theta^*} \left( \frac{\partial \ell_i}{\partial \sigma_{12}}, \frac{\partial \ell_i}{\partial \sigma_{12}} \right) = 0 \). For \( V_{12} \), we have

\[
V_{12}^2 = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \text{Cov} \left[ \frac{\phi(r_{1i} \mu_{1}^*)}{\Phi(r_{1i} \mu_{1}^*)} r_{1i}, \frac{\phi(r_{2i} \mu_{2}^*)}{\Phi(r_{2i} \mu_{2}^*)} r_{2i} \right] \tag{S.8}
\]

where

\[
\text{Cov} \left[ \frac{\phi(r_{1i} \mu_{1}^*)}{\Phi(r_{1i} \mu_{1}^*)} r_{1i}, \frac{\phi(r_{2i} \mu_{2}^*)}{\Phi(r_{2i} \mu_{2}^*)} r_{2i} \right] = E \left[ \frac{\phi(r_{1i} \mu_{1}^*)}{\Phi(r_{1i} \mu_{1}^*)} \frac{\phi(r_{2i} \mu_{2}^*)}{\Phi(r_{2i} \mu_{2}^*)} r_{1i} r_{2i} \right] = \sum_{r_{1i}=-1,1} \sum_{r_{2i}=-1,1} r_{1i} r_{2i} \frac{\phi(r_{1i} \mu_{1}^*)}{\Phi(r_{1i} \mu_{1}^*)} \frac{\phi(r_{2i} \mu_{2}^*)}{\Phi(r_{2i} \mu_{2}^*)} \Sigma_{12}^* (r_{1i} x_i^T \beta_{1}^*, r_{2i} x_i^T \beta_{2}^*),
\]

with \( \Sigma_{12}^* = \{(1, r_{1i} r_{2i} \sigma_{12}^*), (r_{1i} r_{2i} \sigma_{12}^*, 1)\} \). Now we turn to \( Q_{12}^1 \). We have

\[
Q_{12}^1 = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} -E_{\theta^*} \left( \frac{\partial^2 \ell_i^2}{\partial \sigma_{12} \partial \beta_i^T} \right)
\]

where

\[
- E_{\theta^*} \left( \frac{\partial^2 \ell_i^2}{\partial \sigma_{12} \partial \beta_i^T} \right) = \text{Cov}_{\theta^*} \left( \frac{\partial \ell_i^2}{\partial \sigma_{12}}, \frac{\partial \ell_i^2}{\partial \beta_i} \right)
= \text{Cov} \left( \frac{\phi_{\Sigma_{12}^*} r_{1i} r_{2i} \phi(r_{1i} \mu_{1}^*) \Phi(r_{1i} \mu_{1}^*)}{\Phi_{\Sigma_{12}^*}} \frac{r_{2i} \mu_{2}^* - \sigma_{12} \mu_{1}^*}{\sqrt{1 - (\sigma_{12}^*)^2}} x_i^T, \right)
= \sum_{r_{1i}=-1,1} \sum_{r_{2i}=-1,1} r_{2i} \phi(r_{1i} \mu_{1}^*) \Phi(r_{1i} \mu_{1}^*) \frac{r_{2i} \mu_{2}^* - \sigma_{12} \mu_{1}^*}{\sqrt{1 - (\sigma_{12}^*)^2}} \Phi_{\Sigma_{12}^*} (r_{1i} x_i^T \beta_{1}^*, r_{2i} x_i^T \beta_{2}^*) x_i^T \tag{S.9}
\]

Similarly,

\[
Q_{22}^2 = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} \sum_{r_{1i}=-1,1} \sum_{r_{2i}=-1,1} r_{1i} r_{2i} \phi(r_{1i} \mu_{1}^*) \Phi(r_{1i} \mu_{1}^*) \phi(r_{2i} \mu_{2}^*) \Phi(r_{2i} \mu_{2}^*) \frac{r_{1i} \mu_{1}^* - \sigma_{12} \mu_{2}^*}{\sqrt{1 - (\sigma_{12}^*)^2}} \Phi_{\Sigma_{12}^*} (r_{1i} x_i^T \beta_{1}^*, r_{2i} x_i^T \beta_{2}^*) x_i^T \tag{S.10}
\]

S.6 Simulation tables etc.
| $q$ | $n$ | NH E1 | NH E2 | DA E1 | DA E2 | TSF E1 | TSF E2 | DA E1 | DA E2 | TSF E1 | TSF E2 | DA E1 | DA E2 | TSF E1 | TSF E2 | DA E1 | DA E2 | TSF E1 | TSF E2 |
|-----|-----|-------|-------|-------|-------|--------|--------|-------|-------|--------|--------|-------|-------|--------|--------|-------|-------|--------|--------|
| 10  | 100 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 15  | 150 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 20  | 200 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 50  | 500 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 100 | 100 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 150 | 150 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |
| 200 | 200 | 0.007 | 0.008 | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  | 0.008 | 0.008 | 0.008  | 0.008  |

Table S.1: Comparison of the hierarchical (H) and non-hierarchical (NH) approach of the bigMVP approach versus the two-stage frequentist method (TSF) from Ting et al. (2020) and Bayesian implementation via the data augmented MCMC sampler (DA) in terms of error in estimating the coefficient matrix $B$ and correlation matrix $\Sigma$. 
Table S.2: Comparison of the hierarchical (H) and non-hierarchical (NH) approach of the bigMVP approach versus the two-stage frequentist method (TSF) from Ting et al. (2020) in terms of uncertainty quantification.

|       | (Dense, Factor) | (Rare, Factor) | (Dense, Block) | (Rare, Block) |
|-------|-----------------|----------------|----------------|--------------|
|       | NH   | H   | TSF | NH   | H   | TSF | NH   | H   | TSF | NH   | H   | TSF |
| n = 200 | q = 10 | 92.11 | 93.31 | 88.04 | 98.77 | 98.87 | 35.24 | 93.41 | 93.91 | 81.56 | 96.53 | 96.02 | 58.04 |
|        | q = 15 | 93.3 | 93.18 | 87.32 | 97.44 | 97.79 | 47.82 | 93.16 | 93.2 | 87.19 | 97 | 97.42 | 49.51 |
|        | q = 20 | 93.89 | 93.81 | 87.63 | 98 | 97.67 | 43.34 | 92.95 | 92.95 | 87.84 | 98.27 | 98.05 | 42.67 |
| n = 500 | q = 10 | 94.28 | 94.27 | 92.93 | 95.06 | 95.08 | 71.27 | 94.37 | 94.49 | 91.87 | 95.37 | 95.28 | 71.53 |
|        | q = 15 | 94.09 | 94.2 | 92.39 | 95.98 | 95.89 | 65.67 | 95.18 | 95.05 | 92.93 | 95.18 | 95.05 | 70.03 |
|        | q = 20 | 93.75 | 93.78 | 91.17 | 95.67 | 95.57 | 66.45 | 93.76 | 93.87 | 92.37 | 94.86 | 94.72 | 69.18 |

Figure S6: Estimation error of the hierarchical (red solid), non-hierarchical (green dashed) versus the fast regularized method (blue dotted) from Pichler and Hartig (2020) for different choices of the number of data points $n$ and the number of binary outcomes $q$. 