Bayesian sparse multiple regression for simultaneous rank reduction and variable selection

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Abstract

We develop a Bayesian methodology aimed at simultaneously estimating low-rank and row-sparse matrices in a high-dimensional multiple-response linear regression model. We consider a carefully devised shrinkage prior on the matrix of regression coefficients which obviates the need to specify a prior on the rank, and shrinks the regression matrix towards low-rank and row-sparse structures. We provide theoretical support to the proposed methodology by proving minimax optimality of the posterior mean under the prediction risk in ultra-high dimensional settings where the number of predictors can grow sub-exponentially relative to the sample size. A one-step post-processing scheme induced by group lasso penalties on the rows of the estimated coefficient matrix is proposed for variable selection, with default choices of tuning parameters. We additionally provide an estimate of the rank using a novel optimization function achieving dimension reduction in the covariate space. We exhibit the performance of the proposed methodology in an extensive simulation study and a real data example.

Key Words: Bayesian; High dimension; Shrinkage prior; Posterior concentration; Dimension reduction; Variable selection.

Short title: Bayesian sparse multi-task learner
1 Introduction

Studying the relationship between multiple response variables and a set of predictors has broad applications ranging from bioinformatics, econometrics, time series analysis to growth curve models. The least squares solution in a linear multiple response regression problem is equivalent to performing separate least squares on each of the responses (Anderson, 1984) and ignores any potential dependence among the responses. In the context of multiple response regression, a popular technique to achieve parsimony and interpretability is to consider a reduced-rank decomposition of the coefficient matrix, commonly known as reduced rank regression (Anderson, 1951; Izenman, 1975; Velu & Reinsel, 2013). Although many results exist about the asymptotic properties of reduced rank estimators (Anderson, 2002), formal statistical determination of the rank remains difficult even with fixed number of covariates and large sample size. The problem becomes substantially harder when a large number of covariates are present, and has motivated a series of recent work on penalized estimation of low rank matrices, where either the singular values of the coefficient matrix (Chen et al., 2013; Yuan et al., 2007), or the rank itself (Bunea et al., 2011) is penalized. Theoretical evaluations of these estimators focusing on adaptation to the oracle convergence rate when the true coefficient matrix is of low rank has been conducted (Bunea et al., 2011). It has also been noted (Bunea et al., 2012) that the convergence rate can be improved when the true coefficient matrix has zero rows and variable selection is incorporated within the estimation procedure. Methods that simultaneously handle rank reduction and variable selection include Bunea et al. (2012); Chen & Huang (2012); Yuan et al. (2007). To best of our knowledge, uncertainty characterization for the parameter estimates from these procedures is currently not available.

The first fully systematic Bayesian treatment of reduced rank regression was carried out in Geweke (1996), where conditioned on the rank, independent Gaussian priors were placed on the elements of the coefficient matrix. While formal Bayesian model selection can be performed to determine the rank (Geweke, 1996), calculation of marginal likelihoods for various candidate ranks gets computationally burdensome with increasing dimensions. The problem of choosing the rank is not unique to reduced rank regression and is ubiquitous in situations involving low rank decompositions, with factor models being a prominent example. Lopes & West (2004) placed a prior on the number of factors and proposed a computationally intensive reversible jump algorithm (Green,
1995) for model fitting. As an alternative, Bhattacharya & Dunson (2011) proposed to increasingly shrink the factors starting with a conservative upper bound and adaptively collapsing redundant columns inside their MCMC algorithm. Recent advancements in Bayesian matrix factorization have taken a similar approach; see for example, Alquier (2013); Babacan et al. (2011); Lim & Teh (2007); Salakhutdinov & Mnih (2008).

From a Bayesian point of view, a natural way to select variables in a single-response regression framework is to use point mass mixture priors (George & McCulloch, 1993; Scott et al., 2010) which allow a subset of the regression coefficients to be exactly zero. These priors were also adapted to multiple response regression by several authors (Bhadra & Mallick, 2013; Brown et al., 1998; Lucas et al., 2006; Wang, 2010). Posterior inference with such priors involves a stochastic search over an exponentially growing model space and is computationally expensive even in moderate dimensions. To alleviate the computational burden, a number of continuous shrinkage priors have been proposed in the literature which mimic the operating characteristics of the discrete mixture priors. Such priors can be expressed as Gaussian scale mixtures (Polson & Scott, 2010), leading to block updates of model parameters; see Bhattacharya et al. (2016a) for a review of such priors and efficient implementations in high-dimensional settings. To perform variable selection with these continuous priors, several methods for post-processing the posterior distribution have been proposed (Bondell & Reich, 2012; Hahn & Carvalho, 2015; Kundu et al., 2013).

In this article we simultaneously address the problems of dimension reduction and variable selection in high-dimensional reduced rank models from a Bayesian perspective. We develop a novel shrinkage prior on the coefficient matrix which encourages shrinkage towards low-rank and row-sparse matrices. The shrinkage prior is induced from appropriate shrinkage priors on the components of a full-rank decomposition of the coefficient matrix, and hence bypasses the need to specify a prior on the rank. We provide theoretical understanding into the operating characteristics of the proposed prior in terms of a novel prior concentration result around rank-reduced and low-sparse matrices. The prior concentration result is utilized to prove minimax concentration rates of the posterior under the fractional posterior framework of Bhattacharya et al. (2016c) in a ultrahigh-dimensional setting where the number of predictor variables can grow sub-exponentially in the sample size.

The continuous nature of the prior enables efficient block updates of parameters inside a Gibbs
sampler. In particular, we adapt an algorithm for sampling structured multivariate Gaussians from Bhattacharya et al. (2016a) to efficiently sample a high-dimensional matrix in a block. We propose two independent post-processing schemes to achieve row sparsity and rank reduction with encouraging performance. A key feature of our post-processing schemes is to exploit the posterior summaries to offer careful default choices of tuning parameters, resulting in a procedure which is completely free of tuning parameters. The resulting row-sparse and rank-reduced coefficient estimate is called a Bayesian sparse multi-task learner (BSML). We illustrate the superiority of BSML over its competitors through a detailed simulation study and the methodology is applied to a Yeast cell cycle data set.

2 Bayesian sparse multitask learner

2.1 Model and Prior Specification

Suppose, for each observational unit \(i = 1, \ldots, n\), we have a multivariate response \(y_i \in \mathbb{R}^q\) on \(q\) variables of interest, along with information on \(p\) possible predictors \(x_i \in \mathbb{R}^p\), a subset of which are assumed to be important in predicting the \(q\) responses. Let \(X \in \mathbb{R}^{n \times p}\) denote the design matrix whose \(i\)th row is \(x_i^T\), and \(Y \in \mathbb{R}^{n \times q}\) the matrix of responses with the \(i\)th row as \(y_i^T\). The multivariate linear regression model is,

\[
Y = XC + E, \quad E = (e_1^T, \ldots, e_n^T)^T,
\]

where we follow standard practice to center the response and exclude the intercept term. The rows of the error matrix are independent, with \(e_i \sim N(0, \Sigma)\). Our main motivation is the high-dimensional case where \(p \geq \max\{n, q\}\), although the method trivially applies to \(p < n\) settings as well. We shall also assume the dimension of the response \(q\) to be modest relative to the sample size.

The basic assumption in reduced rank regression is that \(\text{rank}(C) = r \leq \min(p, q)\), whence \(C\) admits a decomposition \(C = B_xA_x^T\) with \(B_x \in \mathbb{R}^{p \times r}\) and \(A_x \in \mathbb{R}^{q \times r}\). While it is possible to treat \(r\) as a parameter and assign it a prior distribution inside a hierarchical formulation, posterior inference on \(r\) requires calculation of intractable marginal likelihoods or resorting to complicated reversible jump Markov chain Monte Carlo algorithms. To avoid specifying a prior on \(r\), we work within a parameter-expanded framework (Liu & Wu, 1999) to consider a potentially full-rank decomposition.
\( C = B A^T \) with \( B \in \mathbb{R}^{p \times q} \) and \( A \in \mathbb{R}^{q \times q} \), and assign shrinkage priors to \( A \) and \( B \) to shrink out the redundant columns when \( C \) is indeed low rank. This formulation embeds all reduced-rank models inside the full model; if a conservative upper bound \( q^* \leq q \) on the rank is known, the method can be modified accordingly. The role of the priors on \( B \) and \( A \) is important to encourage appropriate shrinkage towards reduced-rank models, which is discussed below.

We consider independent standard normal priors on the entries of \( A \). As an alternative, a uniform prior on the Stiefel manifold (Hoff, 2009) of orthogonal matrices can be used. However, our numerical results suggested significant gains in computation time using the Gaussian prior over the uniform prior with no discernible difference in statistical performance. The Gaussian prior allows an efficient block update of \( \text{vec}(A) \), whereas the algorithm of Hoff (2009) involves conditional Gibbs update of each column of \( A \). Our theoretical results also suggest that the shrinkage provided by the Gaussian prior is optimal when \( q \) is modest relative to \( n \), the regime we operate in. We shall henceforth denote \( \Pi_A \) to denote the prior on \( A \), i.e., \( a_{hk} \sim \mathcal{N}(0, 1) \) independently for \( h, k = 1, \ldots, q \).

Recalling that the matrix \( B \) has dimension \( p \times q \), with \( p \) potentially larger than \( n \), stronger shrinkage is warranted on the columns of \( B \). We use independent horseshoe priors (Carvalho et al., 2010) on the columns of \( B \), which can be represented hierarchically as

\[
\begin{align*}
    b_{jh} \mid \lambda_{jh}, \tau_h & \sim \mathcal{N}(0, \lambda_{jh}^2 \tau_h^2), \\
    \lambda_{jh} & \sim \text{Ca}_+(0, 1), \\
    \tau_h & \sim \text{Ca}_+(0, 1),
\end{align*}
\]

independently for \( j = 1, \ldots, p \) and \( h = 1, \ldots, q \), where \( \text{Ca}_+(0, 1) \) denotes the truncated standard half-Cauchy distribution with density proportional to \( (1 + t^2)^{-1} \mathbb{1}_{(0, \infty)}(t) \). We shall denote the prior on the matrix \( B \) induced by the hierarchy in (2) by \( \Pi_B \).

We shall primarily restrict attention to settings where \( \Sigma \) is diagonal, \( \Sigma = \text{diag}(\sigma_1^2, \ldots, \sigma_q^2) \), noting that extensions to non-diagonal \( \Sigma \) can be incorporated in a straightforward fashion. For example, for moderate \( q \), a conjugate inverse-Wishart prior can be used as a default. Furthermore, if \( \Sigma \) has a factor model or Gaussian Markov random field structure, they can also be incorporated using standard techniques (Bhattacharya & Dunson, 2011; Rue, 2001). The cost-per-iteration of the Gibbs sampler retains the same complexity as in the diagonal \( \Sigma \) case; see §3 for more details. In the diagonal case, we assign independent improper priors \( \pi(\sigma_h^2) \propto \sigma_h^{-2} \), \( h = 1, \ldots, q \) on the diagonal elements, and call the resulting prior \( \Pi_{\Sigma} \).
The model augmented with the above priors now takes the shape

\[ Y = XBA^T + E, \quad e_i \sim N(0, \Sigma), \quad (3) \]

\[ B \sim \Pi_B, \quad A \sim \Pi_A, \quad \Sigma \sim \Pi_\Sigma. \quad (4) \]

We shall refer to the induced prior on \( C = BA^T \) by \( \Pi_C \).

2.2 Concentration results

In this section, we establish a minimax posterior concentration result under the prediction loss when the number of covariates are allowed to grow sub-exponentially in \( n \). To best of our knowledge, this is the first such result in Bayesian reduced rank regression models. We are also not aware of a similar result in any model involving the horseshoe or another polynomial tailed shrinkage prior in ultrahigh-dimensional settings. Armagan et al. (2013) applied the general theory of posterior consistency (Ghosal et al., 2000) to linear models with growing number of covariates and established consistency for the horseshoe prior with a sample size dependent hyperparameter choice when \( p = o(n) \). Results (Ghosh & Chakrabarti, 2017; van der Pas et al., 2014) that quantify rates of convergence focus exclusively on the normal means problem, with their proofs crucially exploiting an exact conjugate representation of the posterior mean.

In this article, we study concentration properties of the posterior distribution in model (3) in \( p \gg n \) settings. To aid the theoretical analysis, we adopt the fractional posterior framework of Bhattacharya et al. (2016c), where a fractional power of the likelihood function is combined with a prior using the usual Bayes formula to arrive at a fractional posterior distribution. It is sufficient to verify a prior mass condition on Kullback–Leibler neighborhoods of the true parameter for the fractional posterior to concentrate at the true parameter, obviating the construction of sieves and verification of prior tail conditions to prove consistency of the actual posterior (Ghosal et al., 2000). Our key contribution is the development of a novel non-asymptotic prior concentration result for the horseshoe prior around sparse vectors in Lemma S1 in the supplemental document. The only other instance of a similar prior concentration result in \( p \gg n \) settings that we are aware of is for the Dirichlet–Laplace prior (Pati et al., 2014). We believe our prior concentration result will be of independent interest in various other models involving the horseshoe prior. We first list the assumptions needed for our concentration result.

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Assumption 2.1 (Growth of number of covariates). \( \log p/n \leq \gamma \) for some \( \gamma \in (0, 1) \).

Assumption 2.2 (Response covariance). The error covariance \( \Sigma \) is known, and without loss of generality, assume \( \Sigma = I_q \).

Assumption 2.3 (True coefficient matrix). The true coefficient matrix \( C_0 \) admits the decomposition \( C_0 = B_0 A_0^T \) where \( B_0 \in \mathbb{R}^{p \times r_0} \) and \( A_0 \in \mathbb{R}^{q \times r_0} \) for some \( r_0 = \kappa q \), \( \kappa \in (0, 1] \). We additionally assume that \( A_0 \) is semi-orthogonal, i.e. \( A_0^T A_0 = I_{r_0} \), and all but \( s \) rows of \( B_0 \) are identically zero for some \( s = o(p) \). Finally, \( \max_{j,h} |C_{0jh}| < T \) for some \( T > 0 \).

Assumption 2.4. The number of response variables \( q \) is fixed.

Assumption 2.5 (Design matrix). For \( X_j \) the \( j \)th column of \( X \), \( \max_{1 \leq j \leq p} \|X_j\| \asymp n \).

Fix \( \alpha \in (0, 1) \). Recall the prior \( \Pi_C \) on \( C \) defined after equation (4). The \( \alpha \)-fractional posterior for \( C \) under model (3) is given by

\[
\Pi_{n,\alpha}(C) \propto e^{-\alpha \text{tr}((Y-XC)(Y-XC)^T)/2} \Pi_C(C),
\]

where we used Assumption 2 to set \( \Sigma = I_q \). Assuming the data is generated with a true coefficient matrix \( C_0 \), we wish to show that the \( \alpha \)-fractional posterior \( \Pi_{n,\alpha}(\cdot) \) concentrates around \( C_0 \) under the averaged prediction loss \( \|XC - XC_0\|^2_F/(nq) \), where \( \|\cdot\|^2_F \) denotes the Frobenius norm of a matrix. Theorem 2.6 states a non-asymptotic concentration bound for \( \Pi_{n,\alpha} \) below.

Theorem 2.6. Fix \( \alpha \in (0, 1) \) and let \( \Pi_{n,\alpha} \) be defined as in (5). Suppose assumptions 1-5 are satisfied. Let \( \epsilon_n = \{(qr_0 + r_0s \log p)/n\}^{1/2} \). Then for any \( D \geq 2 \) and \( t > 0 \),

\[
\Pi_{n,\alpha} \left( C \in \mathbb{R}^{p \times q} : \frac{1}{nq} \|XC - XC_0\|^2_F \geq \frac{2(D+3t)}{\alpha(1-\alpha)} \epsilon_n^2 \mid Y \right) \leq e^{-t\epsilon_n^2}
\]

holds with probability at least \( 1 - 2/(\{(D - 1 + t)\epsilon_n^2\} \) under the true distribution.
A proof of Theorem 2.6 is provided in the Appendix. An immediate consequence is that the posterior mean \( \mathbb{E} = \int C \Pi_{n,\alpha}(dC) \) satisfies \( \| X \mathbb{E} - X C_0 \|_F^2/(nq) \lesssim K \epsilon_n^2 \) with large probability for some constant \( K > 0 \). It then follows from Bunea et al. (2012) that the posterior mean achieves the minimax rate as a frequentist estimate.

A main ingredient of the proof is a novel non-asymptotic prior concentration result for the prior \( \Pi_C \). Building on a sequence of results, we prove in Lemma S4 of the supplementary document that if \( C_0 \) satisfies Assumption 3, then

\[
\Pi_C(C : \|C - C_0\|_F < \epsilon_n) \geq e^{-K \epsilon_n^2},
\]

where \( K \) is a positive constant. The implication is that the prior places sufficient mass to minimax neighborhoods of the truth, which drives the concentration of the fractional posterior \( \Pi_{n,\alpha} \).

We expect the concentration results to hold as well for the actual posterior, i.e., when \( \alpha = 1 \), which, however, is well beyond the scope of the current paper. For model (3), raising the likelihood to a fractional power only results in a change in the (co)variance term, and hence our Gibbs sampler can be easily adapted to sample from the fractional posterior. Our numerical investigations found the point estimates to be virtually indistinguishable from the actual posterior when the fractional power \( \alpha \) is close to one, e.g., 0.95 or 0.99, justifying our choice of the theoretical environment. It was also theoretically shown in Bhattacharya et al. (2016c) that as \( \alpha \to 1- \), the fractional posterior converges weakly to the usual posterior.

### 3 Posterior Computation

Exploiting the conditional conjugacy of the proposed prior, we develop a straightforward and efficient Gibbs sampler to update the model parameters in (3) from their full conditional distributions. We use vectorization to update parameters in blocks. Specifically, in what follows, we will make multiple usage of the following identity. For matrices \( \Phi_1, \Phi_2, \Phi_3 \) with appropriate dimensions, and \( \text{vec}(A) \) denoting column-wise vectorization, we have,

\[
\text{vec}(\Phi_1\Phi_2\Phi_3) = (\Phi_3^T \otimes \Phi_1)\text{vec}(\Phi_2) = (\Phi_3^T \Phi_2^T \otimes I_k)\text{vec}(\Phi_1),
\]

where the matrix \( \Phi_1 \) has \( k \) rows and \( \otimes \) denotes the Kronecker product.
Letting $\theta \mid -$ denote the full conditional distribution of a parameter $\theta$ given other parameters and the data, the Gibbs sampler cycles through the following steps, sampling parameters from their full conditional distributions:

**Step 1.** To sample $B \mid -$, use (6) to vectorize $Y = XBA^T + E$ to obtain,

$$y = (X \otimes A)\beta + e,$$

where $\beta = \text{vec}(B^T) \in \mathbb{R}^{pq \times 1}$, $y = \text{vec}(Y^T) \in \mathbb{R}^{nq \times 1}$, and $e = \text{vec}(E^T) \sim N_{nq}(0, \tilde{\Sigma})$ with $\tilde{\Sigma} = \text{diag}(\Sigma, \ldots, \Sigma)$. Multiplying both sides of (7) by $\tilde{\Sigma}^{-1/2}$ yields $\tilde{y} = \tilde{X}\beta + \tilde{e}$ where $\tilde{y} = \tilde{\Sigma}^{-1/2}y$, $\tilde{X} = \tilde{\Sigma}^{-1/2}(X \otimes A)$ and $\tilde{e} = \tilde{\Sigma}^{-1/2}e \sim N_{nq}(0, I_{nq})$. Thus, the full conditional distribution $\beta \mid - \sim N_{pq}(\Omega_B^{-1}A\tilde{X}^T\tilde{y}, \Omega_B^{-1}A)$, where $\Omega_B = (\tilde{X}^T\tilde{X} + \Lambda^{-1})$ with $\Lambda = \text{diag}(\lambda_{11}^2, \ldots, \lambda_{1q}^2, \ldots, \lambda_{p1}^2, \ldots, \lambda_{pq}^2)$. 

Naively sampling from the full conditional of $\beta$ has complexity $O(p^3q^3)$ which becomes highly expensive for moderate values of $p$ and $q$. Bhattacharya et al. (2016a) recently developed an algorithm to sample from a class of structured multivariate normal distributions whose complexity scales linearly in the ambient dimension. We adapt the algorithm in Bhattacharya et al. (2016a) as follows:

(i) Sample $u \sim N(0, \Lambda)$ and $\delta \sim N(0, I_{nq})$ independently.

(ii) Set $v = \tilde{X}u + \delta$.

(iii) Solve $(\tilde{X}^T\tilde{X} + I_{nq})w = (\tilde{y} - v)$ to obtain $w$.

(iv) Set $\beta = u + \Lambda\tilde{X}^Tw$.

It follows from Bhattacharya et al. (2016a) that $\beta$ obtained from steps (i) - (iv) above produce a sample from the desired full conditional distribution. One only requires matrix multiplications and linear system solvers to implement the above algorithm, and no matrix decomposition is required. It follows from standard results (Golub & van Loan, 1996) that the above steps have a combined complexity of $O(q^3\max\{n^2, p\})$, a substantial improvement over $O(p^3q^3)$ when $p \gg \max\{n, q\}$.

**Step 2.** To sample $A \mid -$, once again vectorize $Y = XBA^T + E$, but this time use the equality of the first and the third terms in (6) to obtain,

$$y = (XB \otimes I_q)a + e,$$

where $e$ and $y$ are the same as in step 1, and $a = \text{vec}(A) \in \mathbb{R}^{q^2 \times 1}$. The full conditional posterior distribution $a \mid - \sim N(\Omega_A^{-1}X_s\tilde{y}, \Omega_A^{-1})$, where $\Omega_A = (X_s^TX_s + I_{q^2})$, $X_s = \tilde{\Sigma}^{-1/2}(XB \otimes I_{q^2})$ and
\[ \tilde{y} = \tilde{\Sigma}^{-1/2}y. \] To sample from the full conditional of \( a \), we use the algorithm from §3.1.2 of Rue (2001). Compute the Cholesky decomposition \( (X^T X + q^2) = LL^T \). Solve the system of equations:

\[ Lv = X^T \tilde{y}, \quad L^T m = v, \quad \text{and} \quad L^T w = z, \]

where \( z \sim N(0, I_q^2) \). Finally obtain a sample as \( a = m + w \).

**Step 3.** To sample \( \sigma^2_h|_- \), observe that \( \sigma^2_h|_- \sim \text{inverse-Gamma}(n/2, S_h/2) \) independently across \( h \), where \( S_h = \{Y_h - (XBA^T)_h\}^T\{Y_h - (XBA^T)_h\} \), with \( \Phi_h \) denoting the \( h \)th column of a matrix \( \Phi \).

**Step 4.** The global and local scale parameters \( \lambda_{jh} \)'s and \( \tau_h \)'s have independent conditional posteriors across \( j \) and \( h \), which can be sampled via a slice sampling scheme provided in the online supplement to Polson et al. (2014). We illustrate the sampling technique for a generic local shrinkage parameter \( \lambda_{jh} \); a similar scheme works for \( \tau_h \). Setting \( \eta_{jh} = \lambda^{-2}_{jh} \), the slice sampler proceeds by sampling \( u_{jh} | \eta_{jh} \sim \text{Unif}(0, 1/(1 + \eta_{jh})) \) and then sampling \( \eta_{jh} | u_{jh} \sim \text{Exp}(2\tau^2_h/b^2_{jh})I\{\eta_{jh} < (1 - u_{jh})/u_{jh}\} \), a truncated exponential distribution.

The Gibbs sampler above can be trivially modified to accommodate non-diagonal \( \Sigma \). Steps 1-2 do not assume any structure for \( \Sigma \). The matrix \( \Sigma^{-1/2} \) can be computed in \( O(q^3) \) steps using standard algorithms, which does not increase the overall complexity of steps 1 and 2 since \( q < n \ll p \) by assumption. Step 3 will change depending on the prior on \( \Sigma \); for example, a conjugate update is retained under an inverse-Wishart prior on \( \Sigma \). Modifications to situations where \( \Sigma \) has a graphical/factor model structure is also straightforward.

Point estimates of \( C \), such as the posterior mean, or element-wise posterior median, are readily obtained from the Gibbs sampler along with a natural uncertainty quantification, which can be used for point and interval predictions. However, the continuous nature of our prior implies that such point estimates will be non-sparse and full rank with probability one, and hence not directly amenable for variable selection and rank estimation. Motivated by our concentration result in Theorem 2.6 that the posterior mean \( X\overline{C} \) increasingly concentrates around \( XC_0 \), we propose two simple post-processing schemes for variable selection and rank estimation below. The procedures are completely automated and do not involve any input of tuning parameters from the user’s end.
3.1 Post processing for variable selection

We first focus on variable selection. We define a row-sparse estimate \( \hat{C}_R \) for \( C \) as the solution to the optimization problem

\[
\hat{C}_R = \arg \min_{\Gamma \in \mathbb{R}^{p \times q}} \left\{ \|X\bar{C} - X\Gamma\|_F^2 + \sum_{j=1}^{p} \mu_j \|\Gamma^{(j)}\|_2 \right\},
\]

where \( \Phi^{(j)} \) represents the \( j \)th row of a matrix \( \Phi \), and the \( \mu_j \)'s are predictor specific regularization parameters. The objective function aims to find a row-sparse solution close to the posterior mean in terms of the prediction loss, with the sparsity driven by the group lasso penalty (Yuan & Lin, 2006). For a derivation of the objective function in (9) from a utility function perspective as in Hahn & Carvalho (2015), refer to the Appendix.

To solve (9), we set the sub-gradient of (9) with respect to \( \Gamma^{(j)} \) to zero and replace \( \|\Gamma^{(j)}\|_2 \) by a data dependent quantity to obtain the soft thresholding estimate,

\[
\hat{C}_R^{(j)} = \frac{1}{X_j^T X_j} \left( 1 - \frac{\mu_j}{2\|X_j^T R_j\|} \right) X_j^T R_j,
\]

where for \( x \in \mathbb{R}, x_+ = \max(x, 0) \), and \( R_j \) is the residual matrix obtained after regressing \( X\bar{C} \) on \( X \) leaving out the \( j \)th predictor, \( R_j = X\bar{C} - \sum_{k \neq j} X_k \hat{C}_R^{(k)} \). For practical implementation, we use \( \bar{C} \) as our initial estimate and make a single pass through each variable to update the initial estimate according to (10). With this initial choice, \( R_j = X_j \bar{C}^{(j)} \) and \( \|X_j^T R_j\| = \|X_j\|^2 \|ar{C}_j\| \). Derivation of (10) is deferred to the Appendix.

While the \( p \) tuning parameters \( \mu_j \) can be chosen by cross-validation, the computational cost explodes with \( p \) to search over a grid in \( p \) dimensions. Exploiting the presence of an optimal initial estimate in the form of \( \bar{C} \), we recommend default choices for the hyperparameters as \( \hat{\mu}_j = 1/\|\bar{C}_j\|^{-2} \).

When predictor \( j \) is not important, the minimax \( \ell_2 \)-risk for estimating \( C_0^{(j)} \) is \( (\log q)/n \), so that \( \|\bar{C}^{(j)}\| \asymp (\log q)/n \). Since \( \|X_j\|^2 \asymp n \) by assumption, \( \hat{\mu}_j/\|X_j^T R_j\| \asymp n^{1/2}/(\log q)^{3/2} \gg 1 \), implying a strong penalty for all irrelevant predictors.

Following Hahn & Carvalho (2015), posterior uncertainty in variable selection can be gauged if necessary by replacing \( \bar{C} \) with the individual posterior samples for \( C \) in (9).
3.2 Post processing for rank estimation

To estimate the rank, we threshold the singular values of $X\hat{C}_R$, with $\hat{C}_R$ obtained from (10). In situations where row sparsity is not warranted, $C$ can be used instead of $\hat{C}_R$. For $s_1, \ldots, s_q$ the singular values of $X\hat{C}_R$, and a threshold $\omega > 0$, define the thresholded singular values as $\nu_h = s_h I(s_h > \omega)$ for $h = 1, \ldots, q$. We estimate the rank as the number of nonzero thresholded singular values, that is, $\hat{r} = \sum_{h=1}^q I(\nu_h > 0) = \sum_{h=1}^q I(s_h > \omega)$. We use the largest singular value of $Y - X\hat{C}_R$ as the default choice of the threshold parameter $\omega$, a natural candidate for the maximum noise level in the model.

4 Simulation Results

We performed a thorough simulation study to assess the performance of the proposed method across different settings. For all our simulation settings the sample size $n$ was fixed at 100. We considered 3 different $(p, q)$ combinations, $(p, q) = (500, 10), (200, 30), (1000, 12)$. The data were generated from the model $Y = XC_0 + E$. Each row of the matrix $E$ was generated from a multivariate normal distribution with diagonal covariance matrix having diagonal entries uniformly chosen between 0.5 and 1.75. The columns of the design matrix $X$ were independently generated from $N(0, \Sigma_X)$. We considered two cases, $\Sigma_X = I_p$, and $\Sigma_X = (\sigma^X_{ij})$, $\sigma^X_{jj} = 1$, $\sigma^X_{ij} = 0.5$ for $i \neq j$. The true coefficient matrix $C_0 = B_* A_*^T$, with $B_* \in \mathbb{R}^{p \times r_0}$ and $A_* \in \mathbb{R}^{r \times r_0}$, with the true rank $r_0 \in \{3, 5, 7\}$. The entries of $A_*$ were independently generated from a standard normal distribution. We generated the entries in the first $s = 10$ rows of $B_*$ independently from $N(0, 1)$, and the remaining $(p - s)$ rows were set equal to zero.

As a competitor, we considered the sparse partial least squares (SPLS) approach due to Chun & Keleş (2010). Partial least squares minimizes the least square criterion between the response $Y$ and design matrix $X$ in a projected lower dimensional space where the projection direction is chosen to preserve the correlation between $Y$ and $X$ as well as the variation in $X$. Chun & Keleş (2010) suggested adding lasso type penalties while optimizing for the projection vectors for sparse high dimensional problems. Since SPLS returns a coefficient matrix which is both row sparse and rank reduced, we create a rank reduced matrix $\hat{C}_{RR}$ from $\hat{C}_R$ for a fair comparison. Recalling that $\hat{C}_R$ has zero rows, let $\hat{S}_R$ denote the sub-matrix corresponding to the non-zero rows of $\hat{C}_R$. Trun-
cate the singular value decomposition of $\hat{S}_R$ to the first $\hat{r}$ terms as obtained in §3.2. Insert back the zero rows corresponding to $\hat{C}_R$ in the resulting matrix to obtain $\hat{C}_{RR}$. Clearly, $\hat{C}_{RR} \in \mathbb{R}^{p \times q}$ so created is row sparse and has rank at most $\hat{r}$; we shall refer to $\hat{C}_{RR}$ as the Bayesian sparse multi-task learner (BSML). Matlab implementation of the proposed method can be found online at www.stat.tamu.edu/antik/software.html.

For an estimator $\hat{C}$ of $C$, we consider the mean square error, $\text{MSE} = \|\hat{C} - C_0\|_F^2/(pq)$, and the mean square prediction error, $\text{MSPE} = \|XC\hat{C} - XC_0\|_F^2/(nq)$ to measure its performance. The squared estimation and prediction errors of SPLS and $\hat{C}_{RR}$ for different settings are reported in table 1 along with the estimates of rank. In our simulations we used the default 10 fold cross validation in the cv.spls function from the R package spls. The SPLS estimator of the rank is the one for which the minimum cross validation error is achieved. We observed highly accurate estimates of the rank for the proposed method, whereas SPLS overestimated the rank in all the settings considered. The proposed method also achieved superior performance in terms of the two squared errors, improving upon SPLS by as much as 5 times in some cases. Additionally, we observed that the performance of SPLS deteriorated relative to BSML with increasing number of covariates.

In terms of variable selection, both methods had specificity and sensitivity both close to one in all the simulation settings listed in table 1. Since SPLS consistently overestimated the rank, we further investigated the effect of the rank on variable selection. We focused on the simulation case $(p, q, r_0) = (1000, 12, 3)$, and fit both methods with different choices of the postulated rank between 3 and 9. For the proposed method, we set $q^* \in \mathbb{N}$ in §2.1 to be the postulated rank, that is, considered $B \in \mathbb{R}^{p \times q^*}$ and $A \in \mathbb{R}^{q \times q^*}$ for $q^* \in \{3, \ldots, 9\}$. For SPLS, we simply input $q^*$ as the number of hidden components inside the function spls. Figure 1 plots the sensitivity and specificity of BSML and SPLS as a function of the postulated rank. While the specificity is robust for either method, the sensitivity of SPLS turned out to be highly dependent on the rank. The left panel of figure 1 reveals that at the true rank, SPLS only identifies 40% of the significant variables, and only achieves a similar sensitivity as BSML when the postulated rank is substantially overfitted. BSML, on the other hand, exhibits a decoupling effect wherein the overfitting of the rank does not impact the variable selection performance.

We conclude this section with a simulation experiment carried out in a correlated response
setting. Keeping the true rank \( r_0 \) fixed at 3, the data were generated similarly as before except that the individual rows \( e_i \) of the matrix \( E \) was generated from \( N(0, \Sigma) \), with \( \Sigma_{ii} = 1, \Sigma_{ij} = 0.5, 1 \leq i \neq j \leq p \). To accommodate the non-diagonal error covariance, we placed a inverse-Wishart\((q, I_q)\) prior on \( \Sigma \). An associate editor pointed out the recent article (Ruffieux et al., 2017) which used spike-slab priors on the coefficients in a multiple response regression setting. They implemented a variational algorithm to posterior inclusion probabilities of each covariate, which is available from the \texttt{R} package \texttt{locus}. To select a model using the posterior inclusion probabilities, we used the median probability model (Barbieri & Berger, 2004); predictors with a posterior inclusion probability less than 0.5 were deemed irrelevant. We implemented their procedure with the prior \( \Sigma \), with \( \Sigma_{ij} = 1, \Sigma_{ij} = 0.5 \) for \( i \neq j \) (correlated). The method achieving superior performance for each setting is highlighted in bold.

Table 1: Estimation and predictive performance of the proposed method (BSML) versus SPLS across different simulation settings. We report the average estimated rank (\( \hat{r} \)), Mean Square Error, MSE (\( \times 10^{-4} \)) and Mean Square Predictive Error, MSPE, across 50 replicates. For each setting the true number of signals were 10 and sample size was 100. For each combination of \((p,q)\) the columns of the design matrix were generated from \( N(0, \Sigma_X) \). Two different choices of \( \Sigma_X \) was considered. \( \Sigma_X = I_p \) (independent) and \( \Sigma_X = (\sigma_{ij}^X, \sigma_{jj}^X = 1, \sigma_{ij}^X = 0.5 \) for \( i \neq j \) (correlated). The method achieving superior performance for each setting is highlighted in bold.

| Rank | Measures | \((200, 30)\) | \((500, 10)\) | \((1000, 12)\) |
|------|----------|---------------|---------------|---------------|
|      |          | Independent   | Correlated    | Independent   | Correlated    | Independent   | Correlated    |
|      |          | BSML          | SPLS          | BSML          | SPLS          | BSML          | SPLS          |
| 3    | \( \hat{r} \) | 3.0           | 7.9           | 3.0           | 9.4           | 3.0           | 9.7           | 3.0           | 8.8           | 3.2           | 9.4           | 3.4           | 8.9           |
|      | MSE      | 3             | 14            | 5             | 15            | 3             | 7             | 5             | 30            | 3             | 50            | 3             | 38            |
|      | MSPE     | 0.07          | 0.25          | 0.06          | 0.17          | 0.22          | 0.15          | 0.34          | 0.21          | 0.35          | 4.19          | 0.30          | 1.51          |
| 5    | \( \hat{r} \) | 5             | 9.7           | 4.9           | 12.2          | 4.9           | 9.9           | 4.8           | 9.8           | 5.1           | 9.9           | 5.1           | 9.9           |
|      | MSE      | 5             | 60            | 9             | 61            | 3             | 10            | 6             | 24            | 2             | 108           | 4             | 129           |
|      | MSPE     | 0.11          | 3.8           | 0.09          | 4.6           | 0.17          | 0.41          | 0.20          | 0.38          | 0.32          | 9.54          | 0.32          | 4.63          |
| 7    | \( \hat{r} \) | 6.9           | 10.3          | 6.9           | 15.8          | 6.8           | 10            | 6.7           | 9.7           | 6.8           | 10.2          | 6.6           | 11.5          |
|      | MSE      | 6             | 116           | 10            | 112           | 3             | 20            | 5             | 49            | 2             | 195           | 4             | 261           |
|      | MSPE     | 0.12          | 10.81         | 0.11          | 9.01          | 0.16          | 0.72          | 0.16          | 0.92          | 0.32          | 16.70         | 0.31          | 7.44          |
Figure 1: Average sensitivity and specificity across 50 replicates is plotted for different choices of the postulated rank. Here \((p, q, r_0) = (1000, 12, 3)\). Values for BSML (SPLS) are in bold (dashed).

Table 2: Variable selection performance of the proposed method in a non-diagonal error structure setting; \(e_i \sim \Sigma\), \(\sigma_{ii} = 1\), \(\sigma_{ij} = 0.5\). Sensitivity and specificity of BSML is compared with Ruffieux et al. (2017).

| \((p, q)\)     | Measure | \(r_0 = 3\) | \(r_0 = 3\) |
|---------------|---------|-------------|-------------|
| \((200,30)\)  | Sensitivity | 1           | 0.96        | 1           | 0.87        |
|               | Specificity | 0.90        | 0.84        | 0.77        | 0.67        |
| \((500,10)\)  | Sensitivity | 1           | 0.99        | 0.9         | 0.8         |
|               | Specificity | 0.99        | 0.99        | 0.80        | 0.64        |
| \((1000,12)\) | Sensitivity | 0.99        | 0.99        | 0.92        | 0.63        |
|               | Specificity | 0.99        | 0.99        | 0.80        | 0.64        |

5 Yeast Cell Cycle Data

Identifying transcription factors which are responsible for cell cycle regulation is an important scientific problem (Chun & Keleş, 2010). The yeast cell cycle data from Spellman et al. (1998) contains information from three different experiments on mRNA levels of 800 genes on an α-factor based experiment. The response variable is the amount of transcription (mRNA) which was measured every 7 minutes in a period of 119 minutes, a total of 18 measurements \((Y)\) covering two
cell cycle periods. The ChIP-chip data from Lee et al. (2002) on chromatin immunoprecipitation contains the binding information of the 800 genes for 106 transcription factors ($X$). We analyze this data available publicly from the R package spls which has the above information completed for 542 genes. The yeast cell cycle data was also analyzed in Chen & Huang (2012) via sparse reduced rank regression (SRRR). Scientifically 21 transcription factors of the 106 were verified by Wang et al. (2007) to be responsible for cell cycle regulation.

The proposed BSML procedure identified 33 transcription factors. Corresponding numbers for SPLS and SRRR were 48 and 69 respectively. Of the 21 verified transcription factors, the proposed method selected 14, whereas SPLS and SRRR selected 14 and 16 respectively. 10 additional transcription factors that regulate cell cycle were identified by Lee et al. (2002), out of which 3 transcription factors were selected by our proposed method. Figure 2 plots the posterior mean, BSML estimate $\hat{C}_{RR}$, and 95% symmetric pointwise credible intervals for two common effects ACE2 and SW14 which are identified by all the methods. Similar periodic pattern of the estimated effects are observed as well for all the other two methods in contention, perhaps unsurprisingly due to the two cell cycles during which the mRNA measurements were taken. Similar plots for the remaining 19 effects identified by our method are placed inside the supplemental document.

The proposed automatic rank detection technique estimated a rank of 1 which is significantly different from SRRR (4) and SPLS (8). The singular values of $Y - X\hat{C}_{R}$ showed a significant drop in magnitude after the first four values which agrees with the findings in Chen & Huang (2012). The 10-fold cross validation error with a postulated rank of 4 for BSML was 0.009 and that of SPLS was 0.19.

We repeated the entire analysis with a non-diagonal $\Sigma$, which was assigned an inverse-Wishart prior. No changes in the identification of transcription factors or rank estimation were detected.
Figure 2: Estimated effects of ACE2 and SWI4, two of 33 transcription factors with non-zero effects on cell cycle regulation. Both have been scientifically verified by Wang et al. (2007). Dotted lines correspond to 95% posterior symmetric credible intervals, bold lines represent the posterior mean and the dashed lines plot values of the BSML estimate $\hat{C}_{RR}$.

Appendix

Proof of theorem 2.6

Proof. For $C \in \mathbb{R}^{p \times q}$, we write $p_C^{(n)}$ to denote the density of $Y|X$ which is proportional to $e^{-\alpha \text{tr}((Y-XC)(Y-XC)^T)/2}$. For any $C^* \in \mathbb{R}^{p \times q}$ we define a $\epsilon$-neighborhood as,

$$B_n(C^*, \epsilon) = \left\{ C \in \mathbb{R}^{p \times q} : \int p_C^{(n)} \log(p_C^{(n)}/p_C^{(n)}) d\mu^{(n)} \leq n\epsilon^2 \right\},$$

and finally we let the Rényi divergence of order $\alpha$ as,

$$D_\alpha^{(n)}(C, C_0) = D_\alpha^{(n)}(p_C^{(n)}, p_{C_0}^{(n)}) = \frac{1}{\alpha - 1} \log \int \{p_C^{(n)}\}^\alpha \{p_{C_0}^{(n)}\}^{1-\alpha} d\mu^{(n)}$$

We start by characterizing $B_n(C_0, \epsilon)$ and $D_\alpha^{(n)}(C, C_0)$ in terms of $X$ and $C$. It is easy to observe that $B(C_0, \epsilon) \supseteq A(C_0, \epsilon) = \left\{ C \in \mathbb{R}^{p \times q} : \frac{1}{nq} \|XC - XC_0\|_F^2 \leq \epsilon^2 \right\}$ for all $\epsilon > 0$. We also have,

$$D_\alpha^{(n)}(C, C_0) = \frac{\alpha}{2} \|XC - XC_0\|_F^2.$$

We now provide an upper bound to the mean prediction error $\|XC - XC_0\|_F^2$. We have,

$$\|X(C - C_0)\|_F^2 \leq \|X\|_F^2 \|C - C_0\|_F^2 \leq q \max_{1 \leq j \leq p} \|X_j\|_F^2 \|C - C_0\|_F^2 = nq \|C - C_0\|_F^2,$$

where the first inequality follows from the Cauchy-Schwartz inequality and the last equality holds due to assumption 5, for a sufficiently large $n$. 

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We proceed with a prior concentration result on $B_n(C_0, \epsilon_n)$ with $\epsilon_n = \{(qr_0 + r_0s \log p)/n\}^{1/2}$. We prove in Lemma S4 in the supplemental document that $\Pi_C(B_n) \geq \Pi_C(A_n) \geq \Pi_C \{C : \|C - C_0\|^2_F \leq \epsilon_n^2/M \} \geq e^{-Kn\epsilon_n^2}$ for some positive constant $K$. The statement of the theorem then follows from Theorem 3.2 of Bhattacharya, Pati, Yang (2016).

**Derivation of (9)**

Suppose $Y^* \in \mathbb{R}^{n \times q}$ be $n$ future observations with design points $X$ so that given $C$, $Y^*$ can be decomposed into $Y^* = XC + E^*$ where $E^*$ has the same distribution as $E$ in (1). We define the utility function in terms of loss of predicting these $n$ new future observations. To encourage sparsity in rows of a coefficient matrix $\Gamma$ that balances the prediction we add a group lasso penalty (Yuan & Lin, 2006) to this utility function. We define the utility function as,

$$L(Y^*, \Gamma) = \|Y^* - X\Gamma\|^2_F + \sum_{j=1}^p \mu_j \|\Gamma^{(j)}\|_2$$

where the $p$ tuning parameters $\mu_j$ control the penalty for selecting each predictor variable and $\Phi^{(j)}$ represents the $j^{th}$ row of any matrix $\Phi$. Intuitively we want $\mu_j$ to be small if the $j^{th}$ predictor is important and vice versa. The expected risk, $E\{L(Y^*, \Gamma)\}$, after integrating over the space of all such future observations given $C$ and $\Sigma$, is

$$L(\Gamma, C, \Sigma) = q \operatorname{tr}(\Sigma) + \|XC - X\Gamma\|^2_F + \sum_{j=1}^p \mu_j \|\Gamma^{(j)}\|_2.$$  (14)

Finally we take expectation of this quantity with respect to $\pi(C, \Sigma \mid Y, X)$ and drop the constant terms to obtain (9).

**Derivation of (10)**

We let $\Phi_j$ and $\Phi^{(j)}$ denote the $j^{th}$ column and row of a generic matrix $\Phi$. Using the subgradient of (9) with respect to $\Gamma^{(j)}$ (Friedman et al., 2007), we have

$$2X_j^T(X\Gamma - XC) + \mu_j \alpha_j = 0, \quad j = 1, \ldots, p,$$  (15)

where $\alpha_j = \Gamma^{(j)}/\|\Gamma^{(j)}\|$ if $\|\Gamma^{(j)}\| \neq 0$ and $\|\alpha_j\| < 1$ when $\|\Gamma^{(j)}\| = 0$. For $\Gamma^{(j)} = 0$ we can rewrite (15) as, $2X_j^T(\sum_{k \neq j} X_k \Gamma^{(k)} - XC) + \mu_j \alpha_j = 0$ which imply that $\alpha_j = -2X_j^T R_j/\mu_j$, where $R_j$ is the residual matrix obtained after regressing $XC$ on $X$ leaving out the $j^{th}$ predictor, $R_j =$
\( X \mathcal{C} - \sum_{k \neq j} X_k \Gamma^{(k)} \). We can use this to set \( \Gamma^{(j)} \) to zero: if \( \alpha_j < 1 \) set \( \Gamma^{(j)} = 0 \). Otherwise we have

\[
2 X_j^T (X_j \Gamma^{(j)} - R_j) + \mu_j \Gamma^{(j)}/\|\Gamma^{(j)}\| = 0.
\]

Solving for \( \Gamma^{(j)} \) in the above equation we then get,

\[
\Gamma^{(j)} = \left( X_j^T X_j + \frac{\mu_j}{2\|\Gamma^{(j)}\|} \right)^{-1} X_j^T R_j.
\] (16)

This solution is dependent on the unknown quantity \( \|\Gamma^{(j)}\| \). However, taking norm on both sides in (16) we get a value of \( \|\Gamma^{(j)}\| \) which does not involve any unknown quantities: \( \|\Gamma^{(j)}\| = (\|X_j^T R_j\| - \mu_j/2)/X_j^T X_j \). Substituting this in (16) we get, \( \Gamma^{(j)} = (X_j^T X_j)^{-1} \left( 1 - \mu_j/2\|X_j^T R_j\| \right) X_j^T R_j \).

Finally, combining the case when \( \Gamma^{(j)} = 0 \), we have (10).

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Convention

Equations defined in this document are numbered (S1), (S2) etc, while (1), (2) etc refer to those defined in the main document. Similar for lemma, theorems etc.

S.1 Proof of theorem 2.6

We establish few results in the following sequence of lemmas needed to prove Theorem 1. Recall $Ca^+(0, 1)$ denotes the half-Cauchy distribution with density proportional to \((1 + t^2)^{-1}1_{(0, \infty)}(t)\).

For a vector $\beta \in \mathbb{R}^p$, let $\Pi_{\text{HS}}$ denote the prior on $\beta$ defined by the hierarchy,

\[
\beta_j \mid \lambda_j, \tau \sim N(0, \lambda_j^2 \tau^2), \quad (j = 1, \ldots, p)
\]

\[
\lambda_j \sim Ca^+(0, 1), \quad (j = 1, \ldots, p) \tag{S.1}
\]

\[
\tau \sim Ca^+(0, 1).
\]

We first state a novel prior concentration result for the horseshoe prior which bounds from below the probability assigned to an Euclidean neighborhood of a sparse vector.
Lemma S.1.1. Suppose $\beta_0 \in l_0 [s; p]$ where $l_0 [s; p] = \{ \beta_0 \in \mathbb{R}^p : \#(1 \leq j < p : \beta_{0j} \neq 0) \leq s \}$. Let $S = \{ j : \beta_{0j} \neq 0 \}$ so that $|S| \leq s$. Assume $s = o(p)$ and $\log p/n \leq \gamma$ for some $\gamma \in (0, 1)$ and max $|\beta_{0j}| \leq M$ for some $M > 0$ and for $j \in S$. Suppose $\beta \sim \Pi_{HS}$. Define $\delta = \{(s \log p)/n\}^{1/2}$. Then we have, for some positive constant $K$,

$$
\Pi_{HS}(\|\beta - \beta_0\|_2 < \delta) \geq e^{-Ks \log p}.
$$

Proof. Using the conditional formulation of prior (S.1) we have,

$$
\Pi_{HS}(\|\beta - \beta_0\|_2 < \delta) = \int_{\tau} pr(\|\beta - \beta_0\|_2 < \delta | \tau) f(\tau) d\tau
$$

(S.2)

where $I_{\tau} = [\tau_0/2, \tau_*]$ with $\tau_* = (s/p)^{3/2} (\log p/n)^{1/2}$. We first provide lower bound of the conditional probability $pr(\|\beta - \beta_0\|_2 < \delta | \tau \in I_{\tau})$ by dividing it into two terms and providing lower bounds for each of them. For $\tau \in I_{\tau}$ we have,

$$
pr(\|\beta - \beta_0\| < \delta | \tau) \geq \prod_{j \in S} pr\left( |\beta_j - \beta_{0j}| < \frac{\delta}{2\sqrt{s}} | \tau \right) \prod_{j \in s^c} pr\left( |\beta_j| < \frac{\delta}{2\sqrt{p}} | \tau \right)
$$

(S.3)

$$
= \left\{ pr\left( |\beta_j - \beta_{0j}| < \frac{\delta}{2\sqrt{s}} | \tau \right) \right\}^s \left\{ pr\left( |\beta_j| < \frac{\delta}{2\sqrt{p}} | \tau \right) \right\}^{p-s}.
$$

We proceed with $pr(|\beta_j| < \delta/2\sqrt{p} | \tau)$ for $\tau \in I_{\tau}$. We have, with $R = 1/\sqrt{2\pi^3}$ and $\delta_* = \delta/2\sqrt{p}$,

$$
pr(|\beta_j| < \delta_* | \tau) \geq \frac{R}{2\tau} \int_{-\delta_*}^{\delta_*} \log \left( 1 + \frac{4\tau^2}{\beta_j^2} \right) d\beta_j
$$

$$
= \frac{R}{\tau} \int_0^{\delta_*} \log \left( 1 + \frac{4\tau^2}{\beta_j^2} \right) d\beta_j \geq \frac{R}{\tau} \int_0^{\delta_*} \frac{4\tau^2/\beta_j^2}{1 + 4\tau^2/\beta_j^2} d\beta_j
$$

$$
= 4R\tau \int_0^{\delta_*} \frac{1}{\beta_j^2 + 4\tau^2} d\beta_j = 2K \arctan \frac{\delta_*}{2\tau}
$$

$$
\geq 2R \left( \frac{\pi}{2} - \frac{2\tau}{\delta_*} \right) \geq R \left( \frac{\pi}{2} - \frac{2\tau_*}{\delta_*} \right) = R \left( \frac{1}{2} - \frac{4s}{\pi p} \right),
$$

where we have used the inequalities $\log(1 + x) \geq x/(x + 1)$ for $x > -1$ and $\arctan x > (\pi/2 - 1/x)$ in succession.
For \( pr(\| \beta_j - \beta_{0j} \| < \delta_0 | \tau) \) with \( \tau \in I_{\tau_*} \), we have, letting \( \delta_0 = 2^{-1}\{(\log p)/n\}^{1/2} \),

\[
pr(\| \beta_j - \beta_{0j} \| < \delta_0 | \tau) = \sqrt{2\pi}^{-3/2} \int_{\lambda_j} \int_{|\beta_j - \beta_{0j}| < \delta_0} \exp\{-\beta_j^2/(2\lambda_j^2\tau^2)\} \frac{1}{\lambda_j \tau(1 + \lambda_j^2)} d\lambda_j d\beta_j \\
\geq \sqrt{2\pi}^{-3/2} \int_{|\beta_j - \beta_{0j}| < \delta_0} \int_{1/\tau_*}^{4/\tau_*} \exp\{-\beta_j^2/(2\lambda_j^2\tau^2)\} \frac{1}{\lambda_j \tau(1 + \lambda_j^2)} d\lambda_j d\beta_j \\
\geq (2\pi)^{-3/2} \int_{|\beta_j - \beta_{0j}| < \delta_0} \exp(-\beta_j^2/2) \int_{1/\tau_*}^{4/\tau_*} \frac{1}{1 + \lambda_j^2} d\lambda_j d\beta_j,
\]

since for \( \lambda_j \in [1/\tau_*, 4/\tau_*] \), \( 1/\lambda_j \tau \geq 1/4 \) and \( \exp\{-\beta_j^2/(2\lambda_j^2\tau^2)\} \geq \exp(-\beta_j^2/2) \). Continuing,

\[
pr(\| \beta_j - \beta_{0j} \| < \delta_0 | \tau) \geq (2\pi)^{-3/2} \frac{3\tau_*}{16 + \tau_*^2} \int_{|\beta_j - \beta_{0j}| < \delta_0} \exp(-\beta_j^2/2) d\beta_j \\
\geq (2\pi)^{-3/2} \frac{3\tau_*}{16 + \tau_*^2} \exp\{-2(M + 1)^2/2\}\delta_0 \\
\approx K_* \left( \frac{s}{p} \right)^{3/2} \frac{\log p}{n},
\]

for some positive constant \( K_* \). Substituting these bounds in S.3, we have,

\[
pr(\| \beta - \beta_0 \| < \delta | \tau \in I_{\tau_*}) \geq e^{-K_*\log p}, \tag{S.4}
\]

where \( K \) is a positive constant. The proof is completed upon observing that \( pr(\tau \in I_{\tau_*}) \approx \tau_*/2 \), so that with a slight abuse of notation we get,

\[
\Pi_{HS}(\| \beta - \beta_0 \| < \delta) \geq e^{-K_*\log p}, \tag{S.5}
\]

for some positive constant \( K \).

Recall the prior \( \Pi_B \) from the main document. If a matrix \( B \in \mathbb{R}^{p \times q} \sim \Pi_B \) then each column of \( B \) is a draw from \( \Pi_{HS} \). In the following Lemma we generalize Lemma S.1.1 to provide a lower bound on the probability the prior \( \Pi_B \) assigns to Frobenius neighborhoods of \( B_0 \in \mathbb{R}^{p \times r_0} \). By assumption 3 the \( h \)-th column of \( B_0 \), \( b_h \in l_0[s; p] \). In order to make the Frobenius neighborhood well defined we append \((q - r_0)\) zero columns to the right of \( B_0 \) and set \( B_{0*} = (B_0 | O^{p \times (q - r_0)}) \).

**Lemma S.1.2.** Let the entries of \( B_{0*} \in \mathbb{R}^{p \times q} \) satisfy \( |B_{0*}| \leq M \) for some positive constant \( M \). Suppose \( B \) is a draw from \( \Pi_B \). Define \( \delta_B = \{(r_0 s \log p)/n\}^{1/2} \). Then for some positive constant \( K \) we have,

\[
\Pi_B(\| B - B_{0*} \|_F < \delta_B) \geq e^{-K r_0 s \log p}.
\]
Proof. Observe that, since by assumption 3, $r_0 = \kappa q$ for some $\kappa \in (0, 1)$,

$$
\Pi_B(\|B - B_0\|_F < \delta_B) \geq \prod_{h=1}^{q} \Pi_{\text{HS}}(\|b_h - b_{0h}\|_2 < q^{-1/2}\delta_B)
$$

$$
= \prod_{h=1}^{q} \Pi_{\text{HS}}[\|b_h - b_{0h}\|_2 < \alpha (s \log p/n)^{1/2}]
$$

$$
= \prod_{h=1}^{q} \Pi_{\text{HS}}[\|b_h - b_{0h}\|_2 < \alpha (s \log p/n)^{1/2}] \prod_{h=r_0+1}^{q} \Pi_{\text{HS}}[\|b_h - b_{0h}\|_2 < \alpha (s \log p/n)^{1/2}]
$$

From Lemma S.1.1 we have, $\Pi_{\text{HS}}(\|b_h - b_{0h}\|_2 < \alpha (s \log p/n)^{1/2}) \geq e^{-K_1 s \log p}$. Arguments along the same line of lemma S.1.1 can also be applied to obtain that, $\Pi_{\text{HS}}(\|b_h\|_2 < \alpha (s \log p/n)^{1/2}) \geq e^{-K_2 \log p}$ for some positive $K_2$. Combining these two lower bounds in the above display we have,

$$
\Pi_B(\|B - B_0\|_F < \delta_B) \geq e^{-K_1 r_0 s \log p} e^{-K_2 (q - r_0) \log p}.
$$

Since $r_0 = \kappa q$, the result follows immediately with $K = K_1 + (1/\kappa - 1)K_2$.

Similar to the previous lemma, the following result provides a lower bound on the probability assigned to Frobenius neighborhoods of $A_0$ by the prior $\Pi_A$. Again we append $(q - r_0)$ columns at the right of $A_0$ and set $A_{0*} = (A_0 \mid O^{q \times (q - r_0)})$.

**Lemma S.1.3.** Suppose the matrix $A \sim \Pi_A$. Let $\delta_A = (q r_0 / n)^{1/2}$. Then for some positive constant $K$ we have,

$$
\Pi_A(\|A - A_{0*}\|_F < \delta_A) \geq e^{-K q r_0}.
$$

Proof. First we use vectorization to obtain $\Pi_A(\|A - A_0\|_F < \delta_A) = \Pi_A(\|a - a_0\|_2 < \delta_A)$, where $a, a_0 \in \mathbb{R}^d$. Using Anderson’s lemma (Bhattacharyya et al., 2016b) for multivariate Gaussian distributions, we then have,

$$
\Pi_A(\|a - a_0\|_2 < \delta_A) \geq e^{-\|a_0\|^2/2} p_r(\|a\|_2 < \delta_A/2)
$$

$$
= e^{-r_0/2} p_r(\|a\|_2 < \delta_A/2).
$$
The quantity \( pr(\|a\| < \delta_A/2) \) can be bounded from below as,

\[
pr(\|a\|_2 < \delta_A/2) \geq \{pr(\|a_j\| < \delta_A/q)\}^{q^2} \geq me^{-f_A^2(\delta_A/q)^2} \approx e^{-q^2},
\]

where \( m \) is a positive constant. Since \( r_0 = \kappa q \), it follows that \( \Pi_A(\|A - A_0\|_F < \delta_A) \geq e^{-Kq r_0} \) for some positive \( K \).

\[
\Pi_C(\|C - C_0\|_F < \delta_C) \geq e^{-K(q r_0 + r_0 s \log p)}.
\]

Our final result will concern the prior mass assigned to Frobenius neighborhoods of \( C \in \mathbb{R}^{p \times q} \). As in the main document we write \( \Pi_C \) for prior on \( C = B A^T \) induced from \( \Pi_B \) and \( \Pi_A \).

**Lemma S.1.4.** Suppose \( C_0 \) satisfies assumption 3. Let \( C \sim \Pi_C \) with \( \Pi_C \) as defined above. Define \( \delta_C = (q r_0 + r_0 s \log p)/n \)^{1/2}. Then for some positive constant \( K \),

\[
\Pi_C(\|C - C_0\|_F < \delta_C) \geq e^{-K(q r_0 + r_0 s \log p)}.
\]

**Proof.** Using the triangle inequality followed by the fact that for two matrices \( P \) and \( Q \), \( \|PQ\|_F \leq s_{\text{max}}(P)\|Q\|_F \) where \( s_{\text{max}}(P) \) is the largest singular value of \( P \), we have,

\[
\|C - C_0\|_F = \|B A^T - B_0 A_0^T\|_F = \|B A^T - B_0 A^T + B_0 A^T - B_0 A_0^T\|_F
\]

\[
= \|(B - B_0) A^T + B_0 (A - A_0)\|_F
\]

\[
\leq s_{\text{max}}(A)\|(B - B_0)\|_F + s_{\text{max}}(B_0)\|A - A_0\|_F,
\]

where \( s_{\text{max}}(A) \) and \( s_{\text{max}}(B_0) \) are the largest singular values of \( A \) and \( B_0 \) respectively. From standard random matrix theory it is well known that for a random matrix of dimension \( m \times n \) with independent Gaussian entries, the largest singular admits a high probability upper bound; for every \( t \geq 0 \), \( s_{\text{max}}(A) \leq \sqrt{m} + \sqrt{n} + t \) with probability at least \( 1 - 2 \exp(-t^2/2) \) (Vershynin, 2010). Also since the elements of \( B_0 \) are bounded, so is \( s_{\text{max}}(B_0) \), say by \( \xi \). For a sufficiently large positive number \( L \) and for \( A \in E = \{A : s_{\text{max}}(A) \leq 2\sqrt{q} + L\} \) we then have,

\[
\|C - C_0\|_F \leq (2\sqrt{q} + L)\|B - B_0\|_F + \xi\|A - A_0\|_F.
\]

Thus we have, \( \Pi_C(\|C - C_0\|_F < \delta_C) \geq \Pi_C\{(2\sqrt{q} + L)\|B - B_0\|_F + \xi\|A - A_0\|_F < \delta_C\} \). Since \( \delta_C = (q r_0 + r_0 s \log p)/n \)^{1/2} \( \geq 2^{-1/2}\{(r_0 s \log p/n)^{1/2} + (q r_0)^{1/2}\} = 2^{-1/2}(\delta_B + \delta_A) \), the probability
\[ \Pi_C(\|C - C_0\|_F < \delta_C) \geq \Pi_B(\|B - B_0\|_F < m_1\delta_B)\Pi_A(\|A - A_0\|_F < m_2\delta_A), \] where \( m_1 \) and \( m_2 \) are positive constants.

From lemma S.1.2 it follows that, \( \Pi_B(\|B - B_0\|_F < m_1\delta_B) \geq e^{-K_1r_0s\log p} \) and from lemma S.1.3 we have, \( \Pi_A(\|A - A_0\|_F < m_2\delta_A/\beta) \geq e^{-K_2qr_0} \). Hence \( \Pi_C(E \cap \{ C : \|C - C_0\|_F < \delta_C \}) \geq e^{-K(qr_0+r_0s\log p)} \). Since for two sets \( E_1 \) and \( E_2 \), \( pr(E_1 \cup E_2) \geq pr(E_1) + pr(E_2) - 1 \), the Lemma is proved.

**Yeast cell cycle data**

The yeast cell cycle data consists of mRNA measurements \( Y \), measured every 7 minutes in a period of 119 minutes. The covariates \( X \) are binding information on 106 transcription factors. When applied to this data, the proposed method identified 33 transcription factors out of 106 that driving the variation in mRNA measurements. 14 of the identified transcription factors are among the 21 scientifically verified (Lee et al., 2002). In the main document we provided estimated effects of two of the 21 scientifically verified transcription factors. Here we plot the estimated effects of the remaining transcriptions factors that were scientifically verified.
Figure S3: Estimated effects of the 19 of 21 scientifically verified transcription factors selected by the proposed method. Effects of other two, viz. ACE2 and SWI4 are included in the main manuscript. Red lines correspond to 95% posterior symmetric credible intervals, black lines represent the posterior mean and the blue dashed line plots values of the BSML estimate $\hat{C}_{RR}$. 