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Lisha Chen^a & Jianhua Z. Huang^b

^a Department of Statistics, Yale University, New Haven, CT, 06511

^b Department of Statistics, Texas A&M University, College Station, TX, 77843-3143

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Sparse Reduced-Rank Regression for Simultaneous Dimension Reduction and Variable Selection

Lisha CHEN and Jianhua Z. HUANG

The reduced-rank regression is an effective method in predicting multiple response variables from the same set of predictor variables. It reduces the number of model parameters and takes advantage of interrelations between the response variables and hence improves predictive accuracy. We propose to select relevant variables for reduced-rank regression by using a sparsity-inducing penalty. We apply a group-lasso type penalty that treats each row of the matrix of the regression coefficients as a group and show that this penalty satisfies certain desirable invariance properties. We develop two numerical algorithms to solve the penalized regression problem and establish the asymptotic consistency of the proposed method. In particular, the manifold structure of the reduced-rank regression coefficient matrix is considered and studied in our theoretical analysis. In our simulation study and real data analysis, the new method is compared with several existing variable selection methods for multivariate regression and exhibits competitive performance in prediction and variable selection.

KEY WORDS: Group lasso penalty; Low rank matrix approximation; Multivariate regression; Penalized least squares; Sparsity; Stiefel manifold.

1. INTRODUCTION

We have seen a growing number of applications where several response variables are predicted or explained by a common set of predictors. For example, researchers in an autism study are interested in predicting multiple clinical characterization variables using patients' attentional pattern summarized in multidimensional eye-tracking data. In a genetic study, it is interesting to model gene expression level at multiple time points using multiple transcription factors. One might also model the returns of multiple stocks at once using a set of econometric variables.

For such multiple-response problems, one can naively perform separate linear regression on each response by ignoring the possible interrelations between response variables. However, we expect that this naive solution can be much improved. In this article, we ask the question of how to improve the interpretability and predictability of the linear model by selecting important predictors and taking advantage of the correlations between response variables. Our question has two aspects. One is dimension reduction, that is, to combine the predictor variables into fewer features that can be explained as latent factors that drive the variation in the multiple response variables. The other is variable selection, that is, to identify the relevant predictor variables and discard irrelevant variables when deriving those latent factors.

We develop a sparse reduced-rank regression (SRRR) method for multivariate regression by addressing these two aspects of the question. The dimension reduction aspect of multivariate regression is taken care of by the so-called reduced-rank regression (RRR) (Izenman 1975; Reinsel and Velu 1998). RRR makes a restriction on the rank of the regression coefficient matrix. The rank constraint implies that the effective number of parameters

to be estimated is reduced and the efficiency of estimation is thus improved. It also implies that the coefficient matrix can be expressed as the product of two lower rank matrices. The predictors multiplied by one of the lower rank matrices produces the lower dimensional factors that drive the variation in the multiple responses. The variable selection aspect is addressed by adding a penalty to the least squares fitting criterion to enforce the sparsity of the reduced-rank coefficient matrix. We focus in this article on sparsity-inducing penalty for the purpose of variable selection. Note that the Ky-Fan norm penalty has been used for factor selection and shrinkage in multivariate regression (Yuan et al. 2007), but it is not applicable for variable selection.

Different from the single response regression that has been extensively studied in the literature (Tibshirani 1996; Yuan and Lin 2006; Wang and Leng 2008), the variable selection for multivariate regression considered here is not only supervised jointly by all predictors but also integrated with the dimension reduction procedure. We use some invariance consideration to decide on a reasonable sparsity-inducing penalty in a penalized regression formulation (Section 2). The resulting penalty is a group-lasso type penalty that treats each row of the regression coefficient matrix as a group. Two numerical algorithms are developed for computation and tuning parameter selection methods are proposed (Section 3). One important difference between our setting and the well-studied single response setting is that the range of the regression coefficient matrix is not a linear space and has certain manifold structure. We address this issue by making good use of the Stiefel manifold representation in our theoretical analysis (Section 4). In an asymptotic analysis, we obtain the consistency result in terms of parameter estimation and variable selection (Section 5). It is well known that RRR contains many classical multivariate regression models as special cases, including principal component and factor analysis, canonical correlation analysis, linear discriminant analysis, and correspondence analysis; see chapter 6 of Izenman (2008).

Lisha Chen is Assistant Professor, Department of Statistics, Yale University, New Haven, CT 06511 (E-mail: lisha.chen@yale.edu). Jianhua Z. Huang is Professor, Department of Statistics, Texas A&M University, College Station, TX 77843-3143 (E-mail: jianhua@stat.tamu.edu). Huang's work was partially supported by grants from the National Science Foundation (NSF; DMS-0907170, DMS-1007618, DMS-1208952) and Award Number KUS-CI-016-04, made by King Abdullah University of Science and Technology (KAUST). The authors thank Joseph Chang, Dean Foster, Zhihua Qiao, Lyle Ungar, and Lan Zhou for helpful discussions. They also thank two anonymous reviewers, an associate editor and the co-editor Jun Liu for constructive comments.

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Therefore, our sparse RRR method provides a unified treatment of variable selection for these methods.

Variable selection for multivariate regression has started to attract attention recently. Several methods have been proposed in the literature, including the L_2 SVS (Simila and Tikka 2007), L_∞ SVS (Turlach, Venables, and Wright 2005), RemMap (Peng et al. (2010)), and SPLS (Chun and Keles 2010). The first three of these methods also use a sparsity-inducing penalty but none of them considers the reduced-rank structure. Our SRRR method is compared with these methods and a separate penalized regression method in a simulation study and shows competitive performance (Section 6). The SRRR method is illustrated using a yeast cell cycle dataset in Section 7.

2. SPARSE REDUCED-RANK REGRESSION

2.1 Multivariate Linear Regression and the Reduced-Rank Model

Suppose we have multiple response variables Y_1, Y_2, \dots, Y_q and multiple predictor variables X_1, X_2, \dots, X_p . The linear model assumes a linear relationship between each response variable and the predictors, that is,

$$Y_j = \sum_{k=1}^p X_k C_{kj} + \epsilon_j, \quad j = 1, 2, \dots, q.$$

In the model above, we have omitted the intercept term without loss of generality, since the intercept can be removed by assuming that the response variables and predictor variables have mean zero. We also assume that the q error terms ϵ_j 's are random variables with mean zero. With n observations, we can write the model in matrix notation as

$$\mathbf{Y} = \mathbf{X}\mathbf{C} + \mathbf{E}, \quad (1)$$

where \mathbf{Y} is the $n \times q$ response matrix, \mathbf{X} is the $n \times p$ predictor matrix, \mathbf{C} is the $p \times q$ matrix of regression coefficients, and \mathbf{E} is the $n \times q$ error matrix. Each row of \mathbf{X} and \mathbf{Y} corresponds to an observation. The generalization of the least squares criterion to the multiple response case is

$$\begin{aligned} \text{RSS}(\mathbf{C}) &= \sum_{j=1}^q \sum_{i=1}^n \left(y_{ij} - \sum_{k=1}^p x_{ik} C_{kj} \right)^2 \\ &= \text{tr}[(\mathbf{Y} - \mathbf{X}\mathbf{C})^T (\mathbf{Y} - \mathbf{X}\mathbf{C})] \\ &= \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2, \end{aligned} \quad (2)$$

where $\|\cdot\|$ denotes the Frobenius norm for a matrix or the Euclidean norm for a vector. The ordinary least squares (OLS) estimate of \mathbf{C} is

$$\hat{\mathbf{C}}_{\text{OLS}} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{Y}. \quad (3)$$

Note that the OLS estimate (3) for multiple responses is equivalent to performing separate OLS estimation for each response variable, and it does not make use of the fact that the multiple responses are likely correlated. In practice, however, it is often the case that the multiple regressions that are considered together have correlated response variables. One way of taking advantage of possible interrelationships between response variables is to impose a constraint on the rank of \mathbf{C} , that is,

$$\text{rank}(\mathbf{C}) = r, \quad r \leq \min(p, q), \quad (4)$$

resulting in the RRR model (Reinsel and Velu 1998). An immediate implication of the reduced-rank restriction is that there are a number of linear constraints on regression coefficients, and hence, the effective number of parameters is reduced and the estimation efficiency is improved. It also follows from the rank constraint that \mathbf{C} can be expressed as a product of two rank r matrices as follows

$$\mathbf{C} = \mathbf{B}\mathbf{A}^T,$$

where \mathbf{B} is of dimension $p \times r$ and \mathbf{A} is of dimension $q \times r$. The model (1) therefore can be rewritten as

$$\mathbf{Y} = (\mathbf{X}\mathbf{B})\mathbf{A}^T + \mathbf{E}, \quad (5)$$

where $\mathbf{X}\mathbf{B}$ is of reduced dimension with only r components. These r linear combinations of the predictor variables can be interpreted as unobservable latent factors that drive the variation in the responses. We expect that the correlations between the q responses are taken into account in the model as they are modeled by r ($r \leq q$) common latent factors. We therefore achieve the dimensionality reduction of the predictor variables.

For fixed r , we estimate the rank-constrained \mathbf{C} by solving the optimization problem

$$\min_{\mathbf{C}: \text{rank}(\mathbf{C})=r} \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2, \quad (6)$$

or equivalently,

$$\min_{\mathbf{A}, \mathbf{B}: \text{rank}(\mathbf{A})=r, \text{rank}(\mathbf{B})=r} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T\|^2. \quad (7)$$

Denote $\mathbf{S}_{xx} = (1/n)\mathbf{X}^T \mathbf{X}$, $\mathbf{S}_{xy} = (1/n)\mathbf{X}^T \mathbf{Y}$, and $\mathbf{S}_{yx} = (1/n)\mathbf{Y}^T \mathbf{X}$. The matrices \mathbf{A} and \mathbf{B} that solve (7) are determined only up to nonsingular transformations. A set of solution is provided by

$$\hat{\mathbf{A}}^{(r)} = \mathbf{V}, \quad \hat{\mathbf{B}}^{(r)} = \mathbf{S}_{xx}^{-1} \mathbf{S}_{xy} \mathbf{V},$$

where $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_r]$ and \mathbf{v}_j is the eigenvector of $\mathbf{S}_{yx} \mathbf{S}_{xx}^{-1} \mathbf{S}_{xy}$ corresponding to the j th largest eigenvalue λ_j . This solution satisfies the identifiability conditions that $\mathbf{A}^T \mathbf{A} = \mathbf{I}_r$ and $\mathbf{B}^T \mathbf{S}_{xx} \mathbf{B}$ being diagonal.

2.2 Sparse Reduced-Rank Regression Through Penalized Least Squares

We now develop our method of variable selection for RRR using penalized regression. RRR allows the responses to borrow strength from each other through a set of common latent factors to improve prediction accuracy. However, each latent factor is a linear combination of all predictors. When a large number of predictor variables are available, some of them might not be useful for prediction. Thus, we would like to perform variable selection, or to exclude the redundant predictors when forming the latent factors. Note that excluding a predictor corresponds to setting as zero an entire row of the matrix \mathbf{B} . Inspired by the penalized regression with a grouped lasso penalty (Yuan and Lin 2006), we consider the following optimization problem:

$$\min_{\mathbf{A}, \mathbf{B}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T\|^2 + \sum_{i=1}^p \lambda_i \|\mathbf{B}^i\| \quad \text{such that} \quad \mathbf{A}^T \mathbf{A} = \mathbf{I}, \quad (8)$$

where the superscript denotes a row of the matrix so that \mathbf{B}^i is a row vector, the constraint $\mathbf{A}^T \mathbf{A} = \mathbf{I}$ is introduced for identifiability purposes, and $\lambda_i > 0$ are penalty parameters

whose choice will be discussed in Section 3.5. In (8), each row of \mathbf{B} is treated as a group and $\|\mathbf{B}^i\| = 0$ is equivalent to setting the i th row of \mathbf{B} as zeros. Thus, the group lasso penalty encourages rowwise sparsity on the \mathbf{B} matrix. An alternative way of introducing sparsity is to directly use the lasso penalty (Tibshirani 1996) on the entire matrix \mathbf{B} that encourages elementwise sparsity. We will show below that the group lasso penalty has a certain invariance property that the lasso penalty does not have. Note that the collection of $\mathbf{B}\mathbf{A}^T$ does not form a linear space, and its manifold structure needs to be respected in the optimization and in the theoretical analysis of the property of the corresponding estimator (see Sections 4 and 5 for more details). This is the key difference of (8) to the original group lasso problem (Yuan and Lin 2006).

The solution to the optimization problem (8) is not unique. Suppose $(\hat{\mathbf{A}}, \hat{\mathbf{B}})$ is a solution. For a $r \times r$ orthogonal matrix \mathbf{Q} , let $\tilde{\mathbf{A}} = \hat{\mathbf{A}}\mathbf{Q}$ and $\tilde{\mathbf{B}} = \hat{\mathbf{B}}\mathbf{Q}$. It follows from the fact $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}$ that $\tilde{\mathbf{B}}\tilde{\mathbf{A}}^T = \hat{\mathbf{B}}\hat{\mathbf{A}}^T$ and $\|\tilde{\mathbf{B}}^i\| = \|\hat{\mathbf{B}}^i\|$. Thus, $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}})$ is also a solution of (8). On the other hand, suppose $(\hat{\mathbf{A}}, \hat{\mathbf{B}})$ and $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}})$ are two solutions of (8). Since both $\hat{\mathbf{A}}$ and $\tilde{\mathbf{A}}$ are of full column rank r , there is nonsingular $r \times r$ matrix \mathbf{Q} such that $\tilde{\mathbf{A}} = \hat{\mathbf{A}}\mathbf{Q}$. The orthogonality constraint implies that

$$\mathbf{I}_r = \tilde{\mathbf{A}}^T \tilde{\mathbf{A}} = \mathbf{Q}^T \hat{\mathbf{A}}^T \hat{\mathbf{A}} \mathbf{Q} = \mathbf{Q}^T \mathbf{Q},$$

which in turn implies that \mathbf{Q} is an orthogonal matrix. Using $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}$ and $\|\tilde{\mathbf{B}}^i\| = \|\hat{\mathbf{B}}^i \mathbf{Q}^T\|$, we obtain that $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}})$ also minimizes $\|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{Q}^T(\mathbf{A}\mathbf{Q}^T)^T\|^2 + \sum_{i=1}^p \lambda_i \|\mathbf{B}^i \mathbf{Q}^T\|$. Since $\hat{\mathbf{A}} = \tilde{\mathbf{A}}\mathbf{Q}^T$, it follows that $(\hat{\mathbf{A}}, \hat{\mathbf{B}})$ minimize $\|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{Q}^T \hat{\mathbf{A}}^T\|^2 + \sum_{i=1}^p \lambda_i \|\mathbf{B}^i \mathbf{Q}^T\|$. Thus, fixing \mathbf{A} at $\hat{\mathbf{A}}$, both $\hat{\mathbf{B}}$ and $\tilde{\mathbf{B}}\mathbf{Q}^T$ minimize the convex function $\|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T\|^2 + \sum_{i=1}^p \lambda_i \|\mathbf{B}^i\|$, and therefore, $\hat{\mathbf{B}} = \tilde{\mathbf{B}}\mathbf{Q}^T$, or $\tilde{\mathbf{B}} = \hat{\mathbf{B}}\mathbf{Q}$. We have obtained the following result regarding the property of the optimization problem.

Lemma 1. The solution to the optimization problem (8) is unique up to an $r \times r$ orthogonal matrix. More precisely, suppose $(\hat{\mathbf{A}}, \hat{\mathbf{B}})$ is a solution of (8). $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}})$ is also a solution of (8) if and only if there is an orthogonal matrix \mathbf{Q} such that $\tilde{\mathbf{A}} = \hat{\mathbf{A}}\mathbf{Q}$ and $\tilde{\mathbf{B}} = \hat{\mathbf{B}}\mathbf{Q}$.

According to this lemma, \mathbf{B} is determined only up to an orthogonal transformation, and thus, setting to zero a single element of \mathbf{B} does not have a clear meaning. We now show that our formulation ensures meaningful variable selection, because different solutions of the optimization problem correspond to selection of the same set of predictors. To formalize this idea, we need the following definition. Note that each row of \mathbf{B} corresponds to a column of \mathbf{X} .

Definition 1. If the entire row j of \mathbf{B} is zero, then the predictor variable X_j is called a nonactive variable, otherwise it is called an active variable.

Suppose $(\hat{\mathbf{A}}, \hat{\mathbf{B}})$ and $(\tilde{\mathbf{A}}, \tilde{\mathbf{B}})$ are two solutions of (8). By switching the order of variables, we can write $\tilde{\mathbf{B}} = (\tilde{\mathbf{B}}_1^T, \mathbf{0})^T$ such that $\tilde{\mathbf{B}}_1$ does not include rows with all zeros. According to Lemma 1, there exists an orthogonal matrix \mathbf{Q} such that $\tilde{\mathbf{B}} = (\tilde{\mathbf{B}}_1^T, \mathbf{0})^T \mathbf{Q} = ((\tilde{\mathbf{B}}_1 \mathbf{Q})^T, \mathbf{0})^T$. Note that none of the rows of $\tilde{\mathbf{B}}_1 \mathbf{Q}$ is entirely zero; for any row $\tilde{\mathbf{B}}_1^i$ in the matrix $\tilde{\mathbf{B}}_1$, $\tilde{\mathbf{B}}_1^i \mathbf{Q} = \mathbf{0}$ if and only if $\tilde{\mathbf{B}}^i = \mathbf{0}$. Therefore, the active variables determined

by $\tilde{\mathbf{B}}$ are the same as those by $\hat{\mathbf{B}}$. We summarize this result below as a lemma.

Lemma 2. The set of active variables obtained by solving the optimization problem (8) is uniquely determined.

This lemma provides some support to our use of group lasso penalty since it guarantees the identifiability of variable selection. It is easy to see that elementwise sparsity of \mathbf{B} does change when \mathbf{B} is multiplied by a rotation matrix.

3. NUMERICAL SOLUTION AND TUNING

This section presents two algorithms for solving the optimization problem (8), both iteratively optimizing with respect to \mathbf{A} and \mathbf{B} . This section also discusses methods for specifying the tuning parameters.

3.1 Overview of the Iterative Optimization

For fixed \mathbf{B} , the optimization problem reduces to

$$\min_{\mathbf{A}} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T\| \quad \text{such that} \quad \mathbf{A}^T \mathbf{A} = \mathbf{I}, \quad (9)$$

which is an orthogonal Procrustes problem (Gower and Dijksterhuis 2004). The solution is $\hat{\mathbf{A}} = \mathbf{U}\mathbf{V}^T$, where \mathbf{U} and \mathbf{V} are obtained from singular value decomposition $\mathbf{Y}^T \mathbf{X}\mathbf{B} = \mathbf{U}\mathbf{D}\mathbf{V}^T$, where \mathbf{U} is $q \times r$ and \mathbf{V} is $r \times r$.

Now we consider optimization over \mathbf{B} for fixed \mathbf{A} . Since \mathbf{A} has orthonormal columns, there is a matrix \mathbf{A}^\perp with orthonormal columns such that $(\mathbf{A}, \mathbf{A}^\perp)$ is an orthogonal matrix. Then we have

$$\begin{aligned} \|\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T\|^2 &= \|(\mathbf{Y} - \mathbf{X}\mathbf{B}\mathbf{A}^T)(\mathbf{A}, \mathbf{A}^\perp)\|^2 \\ &= \|\mathbf{Y}\mathbf{A} - \mathbf{X}\mathbf{B}\|^2 + \|\mathbf{Y}\mathbf{A}^\perp\|^2. \end{aligned} \quad (10)$$

The second term does not involve \mathbf{B} . Therefore for fixed \mathbf{A} , the optimization problem (8) reduces to

$$\min_{\mathbf{B}} \|\mathbf{Y}\mathbf{A} - \mathbf{X}\mathbf{B}\|^2 + \sum_{i=1}^p \lambda_i \|\mathbf{B}^i\|. \quad (11)$$

Below, we present two methods for solving this problem.

3.2 Subgradient Method

We use the subgradient method to solve (11) (Friedman et al. 2007). The subgradient equations with respect to \mathbf{B}^l , the l th row of \mathbf{B} , are

$$2\mathbf{X}_l^T (\mathbf{X}\mathbf{B} - \mathbf{Y}\mathbf{A}) + \lambda_l s_l = 0, \quad l = 1, 2, \dots, p,$$

where $s_l = \mathbf{B}^l / \|\mathbf{B}^l\|$ if $\|\mathbf{B}^l\| \neq 0$, and s_l is an r vector satisfying $\|s_l\| < 1$ if $\|\mathbf{B}^l\| = 0$. If $\|\mathbf{B}^l\| = 0$, the subgradient equations for \mathbf{B}^l become

$$2\mathbf{X}_l^T \left(\sum_{k \neq l}^p \mathbf{X}_k \mathbf{B}^k - \mathbf{Y}\mathbf{A} \right) + \lambda_l s_l = 0.$$

Solving for s_l , one gets

$$s_l = -\frac{2}{\lambda_l} \mathbf{X}_l^T \left(\sum_{k \neq l}^p \mathbf{X}_k \mathbf{B}^k - \mathbf{Y}\mathbf{A} \right) = -\frac{2}{\lambda_l} \mathbf{X}_l^T \mathbf{R}_l,$$

where $\mathbf{R}_l = \mathbf{Y}\mathbf{A} - \sum_{k \neq l}^p \mathbf{X}_k \mathbf{B}^k$, which in turn is used to check whether $\|s_l\| < 1$. If $\|s_l\| < 1$ holds, set $\|\mathbf{B}^l\| = 0$. Otherwise,

\mathbf{B}^l can be solved from the first-order conditions. We can transform the first-order condition with respect to \mathbf{B}^l ($\mathbf{B}^l \neq 0$) to

$$-2\mathbf{X}_l^T(\mathbf{R}_l - \mathbf{X}_l\mathbf{B}^l) + \lambda_l \frac{\mathbf{B}^l}{\|\mathbf{B}^l\|} = 0,$$

which has the solution

$$\mathbf{B}^l = \left(\mathbf{X}_l^T \mathbf{X}_l + \frac{\lambda_l}{2\|\mathbf{B}^l\|} \right)^{-1} \mathbf{X}_l^T \mathbf{R}_l. \quad (12)$$

Note that the right-hand side involves $\|\mathbf{B}^l\|$ and therefore we need to obtain $\|\mathbf{B}^l\|$ to get \mathbf{B}^l . Denote $c = \|\mathbf{B}^l\|$ and we can obtain an equation of c using (12). It is easy to see that this equation has the solution $c = (\|\mathbf{X}_l^T \mathbf{R}_l\| - \lambda_l/2)/\|\mathbf{X}_l\|^2$. Plug this solution into the right-hand side of (12) to get

$$\mathbf{B}^l = \frac{1}{\|\mathbf{X}_l\|^2} \left(1 - \frac{\lambda_l}{2\|\mathbf{X}_l^T \mathbf{R}_l\|} \right) \mathbf{X}_l^T \mathbf{R}_l.$$

Combining this result with that for $\mathbf{B}^l = 0$, we obtain that the optimal solution of (11) is

$$\mathbf{B}^l = \frac{1}{\mathbf{X}_l^T \mathbf{X}_l} \left(1 - \frac{\lambda_l}{2\|\mathbf{X}_l^T \mathbf{R}_l\|} \right)_+ \mathbf{X}_l^T \mathbf{R}_l. \quad (13)$$

This is a vector version of the soft-thresholding rule.

The discussion above leads to the following algorithm:

Algorithm 1: Numerical algorithm using subgradient method

Input: $\mathbf{X}, \mathbf{Y}, \lambda$

Output: \mathbf{A}, \mathbf{B}

while value of objective function (8) not converged **do**

 For fixed \mathbf{B} , solve \mathbf{A} by SVD as in Procrustes problem indicated by (9).

while \mathbf{B} not converged **do**

for each l **do**

 solve \mathbf{B}^l by (13)

 check whether \mathbf{B} has converged

 check whether objective function has converged

3.3 Variational Method

An alternative method to optimize (11) over \mathbf{B} for fixed \mathbf{A} is the variational method that makes use of the following result

$$\min_c \frac{1}{2} \left(cx^2 + \frac{1}{c} \right) = |x|.$$

According to this result, optimizing the objective function in (11) over \mathbf{B} is equivalent to optimizing the following objective function jointly over \mathbf{B} and $\mu_i, i = 1, \dots, p$,

$$f = \|\mathbf{Y}\mathbf{A} - \mathbf{X}\mathbf{B}\|^2 + \sum_{i=1}^p \frac{\lambda_i}{2} \left(\mu_i \|\mathbf{B}^i\|^2 + \frac{1}{\mu_i} \right), \quad (14)$$

which can be done iteratively. For fixed \mathbf{B} , the optimal μ_i is

$$\mu_i = 1/\|\mathbf{B}^i\|, \quad i = 1, \dots, p. \quad (15)$$

For fixed μ_i , the first-order condition for \mathbf{B}^i is

$$\frac{\partial f}{\partial \mathbf{B}^i} = -2\mathbf{X}_i^T(\mathbf{Y}\mathbf{A} - \mathbf{X}\mathbf{B}) + \lambda_i \mu_i \mathbf{B}^i = 0, \quad i = 1, 2, \dots, p.$$

Collect all these conditions and express them in the matrix form to obtain

$$-\mathbf{X}^T(\mathbf{Y}\mathbf{A} - \mathbf{X}\mathbf{B}) + \frac{1}{2} \text{diag}(\lambda_1 \mu_1, \dots, \lambda_p \mu_p) \mathbf{B} = 0.$$

Solving for \mathbf{B} yields

$$\mathbf{B} = \left\{ \mathbf{X}^T \mathbf{X} + \frac{1}{2} \text{diag}(\lambda_1 \mu_1, \dots, \lambda_p \mu_p) \right\}^{-1} \mathbf{X}^T \mathbf{Y}\mathbf{A}. \quad (16)$$

One iterates between (15) and (16) until convergence. The variational method seldom produces $\|\mathbf{B}^i\|$ that is exactly zero, so one needs to set a threshold for $\|\mathbf{B}^i\|$ to obtain the sparsity.

3.4 Comparison of the Two Algorithms

We compare the computational complexity of the two algorithms. Updating \mathbf{A} is done in the same fashion in both methods so we consider only the steps for updating \mathbf{B} . In the following calculation, we ignore one-time computations such as that for $\mathbf{X}^T \mathbf{X}$ and $\mathbf{X}^T \mathbf{Y}$ and focus on the terms that appear in the iterative steps. Moreover, we assume that the rank number r is a fixed small constant. For the variational method, (15) requires $2pr$ operations and (16) requires $O(p^3)$ (for inversion) + pqr (for $(\mathbf{X}^T \mathbf{Y})\mathbf{A}$) + p^2r operations. Since r is small, the computational complexity for each iteration of the variational method is $O(pq + p^3)$. For the subgradient method, calculation of \mathbf{R}_l requires $O(npr + nqr)$ operations, subsequent calculation of $\mathbf{X}_l^T \mathbf{R}_l$ requires $O(nr)$ operations and thus calculation of \mathbf{B}_l using (13) requires $O(npr + nqr)$ operations. Since there are p of \mathbf{B}_l 's, the computational complexity for one iteration of the subgradient method is $O(nrpq + nrp^2)$, or $O(npq + np^2)$ when r is a small number. It is clear that the variational method is computationally less expensive when $n \gg p$. If q is smaller or not much bigger than p , the subgradient method is computationally less costly when $p \gg n$.

3.5 Tuning

The cross-validation (CV) or K -fold CV can be used to select the rank number (or the number of factors) r and the penalty parameters. The parameters that give a smaller CV error are preferred. From the simulation study to be reported in Section 6, we observed that the fivefold CV works very well in selecting the correct rank number when the data are generated from a reduced-rank model; see Table 3. In practice, the reduced-rank model is usually an approximation, and the CV error may continue to decline as a function of the rank number. Borrowing an idea from the principal components analysis, we can use the scree plot of the CV error to select an appropriate rank number; see Section 7 for an illustration using a real-world dataset.

Since selection of p penalty parameters requires computationally intensive optimization, we propose two strategies to reduce the number of tuning parameters: one uses a single penalty parameter by setting λ_i 's all equal; the other uses the idea of adaptive lasso (Zou 2006). The adaptive lasso penalty requires a pilot estimator $\tilde{\mathbf{C}}$ and sets $\lambda_i = \lambda \|\tilde{\mathbf{C}}^i\|^{-\gamma}$, where $\|\tilde{\mathbf{C}}^i\|^{-\gamma}$'s are referred to as the adaptive weights and $\lambda, \gamma > 0$ are two tuning parameters that can be selected using CV. Our experience suggests that it is sufficient to choose γ from a small set of candidates such as $\{0.5, 1, 2, 4, 8\}$. When $n > p$, the solution of the unpenalized version of (8) provides a pilot estimator. When

$n \leq p$, the solutions of unpenalized RRR or ordinary multivariate regression are not well defined. For this case, a reasonable pilot estimator can be the solution of (8) with a single penalty parameter, which in turn is chosen by CV.

4. GEOMETRY OF THE REDUCED-RANK MODEL

This section discusses some geometry facts of reduced-rank model, which will play an important role in obtaining the asymptotic results in the next section. Let \mathbf{C}_* be the rank- r coefficient matrix used to generate the data according to model (1) and $\mathbf{C}_* = \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T$ be its reduced singular value decomposition, where \mathbf{U}_* and \mathbf{V}_* are, respectively, $p \times r$ and $q \times r$ rank- r matrices with orthonormal columns and \mathbf{D}_* is a $r \times r$ nonnegative diagonal matrix. Although this reparameterization is not globally identifiable (considering, e.g., $\tilde{\mathbf{U}}_* = -\mathbf{U}_*$ and $\tilde{\mathbf{V}}_* = -\mathbf{V}_*$), it is identifiable up to the sign switch of each column of \mathbf{U}_* and \mathbf{V}_* . Let \mathbf{C} be a $p \times q$ matrix in the neighborhood of \mathbf{C}_* on the manifold of rank- r matrices. We now derive a local reparameterization of \mathbf{C} .

Let $\mathbf{C} = \mathbf{UDV}^T$ be the reduced singular value decomposition, where \mathbf{U} and \mathbf{V} are, respectively, $p \times r$ and $q \times r$ rank- r orthonormal matrices and \mathbf{D} is a $r \times r$ nonnegative diagonal matrix. According to the Stiefel manifold representation of orthonormal matrices (Edelman, Arias, and Smith 1998), the manifold of $p \times r$ orthonormal matrices can be represented as

$$\{\mathbf{U} = \exp(1, \mathbf{U}_* \mathbf{G}_u + \mathbf{H}_u) : \mathbf{G}_u \text{ is } r \times r, \mathbf{G}_u = -\mathbf{G}_u^T, \mathbf{H}_u \text{ is } p \times r, \mathbf{U}_*^T \mathbf{H}_u = \mathbf{0}\},$$

where $\exp(t, \mathbf{J}_u)$ is the exponential map that defines a geodesic emanating from \mathbf{U}_* in the tangent direction \mathbf{J}_u . The exponential map can be expressed as $\exp(t, \mathbf{J}_u) = \mathbf{U}_* \mathbf{M}(t, \mathbf{J}_u) + \mathbf{Q} \mathbf{N}(t, \mathbf{J}_u)$, where $\mathbf{Q} \mathbf{R} = (\mathbf{I} - \mathbf{U}_* \mathbf{U}_*^T) \mathbf{J}_u$ is the compact QR decomposition (\mathbf{Q} is $p \times r$, \mathbf{R} is $r \times r$), and $\mathbf{M}(t, \mathbf{J}_u)$ and $\mathbf{N}(t, \mathbf{J}_u)$ are $r \times r$ matrices given by the matrix exponential

$$\begin{bmatrix} \mathbf{M}(t, \mathbf{J}_u) \\ \mathbf{N}(t, \mathbf{J}_u) \end{bmatrix} = \exp \left\{ t \begin{bmatrix} \mathbf{U}_*^T \mathbf{J}_u & -\mathbf{R}^T \\ \mathbf{R} & 0 \end{bmatrix} \right\} \begin{bmatrix} \mathbf{I}_r \\ \mathbf{0} \end{bmatrix}.$$

Similarly, the manifold of $q \times r$ orthonormal matrices can be represented as

$$\{\mathbf{V} = \exp(1, \mathbf{V}_* \mathbf{G}_v + \mathbf{H}_v) : \mathbf{G}_v \text{ is } r \times r, \mathbf{G}_v = -\mathbf{G}_v^T, \mathbf{H}_v \text{ is } q \times r, \mathbf{V}_*^T \mathbf{H}_v = \mathbf{0}\},$$

where $\exp(t, \mathbf{J}_v)$ is the exponential map that defines a geodesic emanating from \mathbf{V}_* in the tangent direction \mathbf{J}_v . The nonnegative diagonal matrix \mathbf{D} can be parameterized as $\mathbf{D} = \mathbf{D}_* \exp(\mathbf{K})$, where \mathbf{K} is an $r \times r$ diagonal matrix whose diagonal elements are not constrained.

Using the definition of the matrix exponential and Taylor series expansion, we obtain the following first-order approximations for perturbations along the manifolds:

$$\mathbf{U} - \mathbf{U}_* = \exp(1, \mathbf{U}_* \mathbf{G}_u + \mathbf{H}_u) - \mathbf{U}_* = \mathbf{U}_* \mathbf{G}_u + \mathbf{H}_u + O(\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2), \quad (17)$$

$$\mathbf{V} - \mathbf{V}_* = \exp(1, \mathbf{V}_* \mathbf{G}_v + \mathbf{H}_v) - \mathbf{V}_* = \mathbf{V}_* \mathbf{G}_v + \mathbf{H}_v + O(\|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2), \quad (18)$$

$$\mathbf{D} - \mathbf{D}_* = \mathbf{D}_* \exp(\mathbf{K}) - \mathbf{D}_* = \mathbf{D}_* \mathbf{K} + O(\|\mathbf{K}\|^2). \quad (19)$$

We say that two matrix norms are equivalent if their ratio is bounded away from zero and infinity. Note that $\|\mathbf{U}_* \mathbf{G}_u + \mathbf{H}_u\|^2 = \|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2$ and $\|\mathbf{V}_* \mathbf{G}_v + \mathbf{H}_v\|^2 = \|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2$. Thus, (17)–(19) imply the following result.

Lemma 3. $\|\mathbf{U} - \mathbf{U}_*\|$ and $\|\mathbf{V} - \mathbf{V}_*\|$ are locally equivalent to $\{\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2\}^{1/2}$ and $\{\|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2\}^{1/2}$, respectively. If the diagonal elements of \mathbf{D}_* are bounded away from zero and infinity, $\|\mathbf{D} - \mathbf{D}_*\|$ is locally equivalent to $\|\mathbf{K}\|$.

The next result gives the first-order approximation of $\mathbf{C} = \mathbf{UDV}^T$ in a neighborhood of $\mathbf{C}_* = \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T$. The proof relies on (17)–(19) and is given in the Appendix.

Lemma 4. The following holds:

$$\begin{aligned} \mathbf{UDV}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T &= \mathbf{U}_* (\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v) \mathbf{V}_*^T + \mathbf{U}_* \mathbf{D}_* \mathbf{H}_v^T + \mathbf{H}_u \mathbf{D}_* \mathbf{V}_*^T + \mathbf{U}_* \mathbf{D}_* \mathbf{K} \mathbf{V}_*^T \\ &\quad + O(\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2 + \|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2 + \|\mathbf{K}\|^2). \end{aligned} \quad (20)$$

Note that the four leading terms in (20) are orthogonal to each other. The orthogonality of the terms involving \mathbf{H}_u and \mathbf{H}_v follows from $\mathbf{U}_*^T \mathbf{H}_u = \mathbf{0}$ and $\mathbf{V}_*^T \mathbf{H}_v = \mathbf{0}$. To show the orthogonality of the two terms not involving \mathbf{H}_u and \mathbf{H}_v , note that

$$\langle \mathbf{U}_* (\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v) \mathbf{V}_*^T, \mathbf{U}_* \mathbf{D}_* \mathbf{K} \mathbf{V}_*^T \rangle = \langle \mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v, \mathbf{D}_* \mathbf{K} \rangle.$$

Because of the antisymmetry, the diagonal elements of \mathbf{G}_u and \mathbf{G}_v are all zero. Since \mathbf{D}_* and \mathbf{K} are diagonal matrices, the above inner product is zero. The orthogonality also implies that

$$\begin{aligned} \|\mathbf{U}_* (\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v) \mathbf{V}_*^T + \mathbf{U}_* \mathbf{D}_* \mathbf{H}_v^T + \mathbf{H}_u \mathbf{D}_* \mathbf{V}_*^T + \mathbf{U}_* \mathbf{D}_* \mathbf{K} \mathbf{V}_*^T\|^2 &= \text{tr}\{(\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v)^T (\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v)\} + \text{tr}(\mathbf{D}_* \mathbf{H}_u^T \mathbf{H}_u \mathbf{D}_*) \\ &\quad + \text{tr}(\mathbf{D}_* \mathbf{H}_v^T \mathbf{H}_v \mathbf{D}_*) + \text{tr}(\mathbf{D}_* \mathbf{K}^2 \mathbf{D}_*). \end{aligned} \quad (21)$$

Let d_i denote the i th diagonal element of \mathbf{D}_* . The next result is proved in the Appendix.

Lemma 5. We have that

$$\begin{aligned} \frac{1}{2} \left\{ \min_{i < j} (d_i - d_j)^2 \right\} (\|\mathbf{G}_u\|^2 + \|\mathbf{G}_v\|^2) &\leq \|\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v\|^2 \leq 2 \left(\max_i d_i^2 \right) (\|\mathbf{G}_u\|^2 + \|\mathbf{G}_v\|^2). \end{aligned}$$

To summarize the developments so far, the manifold of rank- r matrices is locally reparameterized as $\Theta = (\mathbf{G}_u, \mathbf{H}_u, \mathbf{G}_v, \mathbf{H}_v, \mathbf{K})$, where \mathbf{G}_u , \mathbf{G}_v , \mathbf{H}_u , \mathbf{H}_v , and \mathbf{K} are specified as above and $\Theta_* = \mathbf{0}$ is the parameter value corresponding to the true coefficient matrix \mathbf{C}_* . Define $\|\Theta\|^2 = \|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2 + \|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2 + \|\mathbf{K}\|^2$. Lemma 4, (21), and Lemma 5 together imply the following result:

Lemma 6. If the diagonal elements of \mathbf{D}_* are all distinct, positive, and bounded, then the distance $\|\mathbf{C} - \mathbf{C}_*\|$ is locally equivalent to the norm $\{\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2 + \|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2 + \|\mathbf{K}\|^2\}^{1/2}$.

5. ASYMPTOTIC ANALYSIS

In this section, we study the asymptotic behavior of the estimator obtained as the solution of problem (8) when the sample size n goes to infinity and p and q are fixed constants.

Asymptotic analysis that allows p and/or q to grow with n is left for future research; see, however, Zou and Zhang (2009) for some relevant results for the univariate regression case. The following assumptions are made for the asymptotic results.

C1. There is a positive definite matrix Σ such that $\mathbf{X}\mathbf{X}^T/n \rightarrow \Sigma$ as $n \rightarrow \infty$.

C2. The first p_0 variable is important and the rest are irrelevant, that is, $\|\mathbf{C}_*^i\| > 0$ if $i \leq p_0$ and $\|\mathbf{C}_*^i\| = 0$ if $i > p_0$, where \mathbf{C}_*^i is the i th row of \mathbf{C}_* .

Theorem 1. (Consistency of parameter estimation.) Suppose $\lambda_i/\sqrt{n} = \lambda_{n,i}/\sqrt{n} \rightarrow 0$ for all $i \leq p_0$. Then, (i) there is a local minimizer $\hat{\mathbf{C}}$ of (22) that is \sqrt{n} -consistent in estimating \mathbf{C}_* ; (ii) letting $\hat{\mathbf{C}} = \hat{\mathbf{U}}\hat{\mathbf{D}}\hat{\mathbf{V}}^T$ be the singular value decomposition, $\hat{\mathbf{U}}$, $\hat{\mathbf{D}}$, and $\hat{\mathbf{V}}$ are \sqrt{n} -consistent in estimating \mathbf{U}_* , \mathbf{D}_* , and \mathbf{V}_* , respectively.

The proof of this theorem makes use of the geometric results in the previous section. Let $\mathbf{C} = \mathbf{B}\mathbf{A}^T$. If $\mathbf{A}^T\mathbf{A} = \mathbf{I}$, then $\|\mathbf{C}^i\| = \|\mathbf{B}^i\|$, where \mathbf{C}^i is the i th row of \mathbf{C} . Thus, the optimization problem (8) is equivalent to the minimization of the criterion function

$$Q(\mathbf{C}) = \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2 + \sum_{i=1}^p \lambda_{n,i} \|\mathbf{C}^i\| \quad (22)$$

subject to the constraint $\text{rank}(\mathbf{C}) = r$. With a slight abuse of notation, we use $Q(\Theta)$ to denote the optimizing objective function (22) in terms of the new parameterization given in the previous section. If we can show that for any positive number ε , there is a sufficiently large α such that

$$\liminf_n \Pr \left\{ \inf_{\|\Theta\| = n^{-1/2}\alpha} Q(\Theta) > Q(\Theta_*) \right\} > 1 - \varepsilon, \quad (23)$$

then with probability tending to one, there exists a local minimizer $\hat{\Theta}$ of $Q(\Theta)$ located in the interior of the ball $\{\Theta : \|\Theta\| \leq n^{-1/2}\alpha\}$, and thus, the corresponding $\hat{\mathbf{C}}$ is \sqrt{n} -consistent, in the light of Lemma 6. Details of the proof of Theorem 1 is given in the Appendix.

Theorem 2. (Consistency of variable selection.) If $\lambda_{n,i}/\sqrt{n} \rightarrow 0$ for $i \leq p_0$ and $\lambda_{n,i}/\sqrt{n} \rightarrow \infty$ for $i > p_0$, then

$$P(\hat{\mathbf{C}}^i = \mathbf{0}) = \Pr(\hat{\mathbf{U}}^i = \mathbf{0}) \rightarrow 1, \quad i > p_0.$$

The proof of this theorem is given in the Appendix. Theorem 2 in particular implies that an adaptive lasso penalty similar to that in Zou (2006) will yield consistency of variable selection. Specifically, let $\lambda_{n,i} = \lambda \|\tilde{\mathbf{C}}^i\|^{-\gamma}$, $\lambda, \gamma > 0$, if $\tilde{\mathbf{C}}$ is a consistent estimate of \mathbf{C}_* , then the conditions on $\lambda_{n,i}$ are satisfied and consistency of variable selection therefore holds. The unpenalized least squares reduced-rank estimator can be used as the pilot estimator $\tilde{\mathbf{C}}$, since it is consistent and asymptotically normally distributed (Anderson 1999).

6. SIMULATION STUDY

In this section, we use simulated data to illustrate the proposed SRRR method and compare it with five related methods that were proposed in the literature for variable selection in multivariate regression.

6.1 Related Methods

The first three methods all solve certain penalized least squares problems but with different penalty functions. The L_2 SVS (Simila and Tikka 2007) method solves the following optimization problem:

$$\min_{\mathbf{C}} \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2 + \lambda \sum_{i=1}^p \|\mathbf{C}^i\|,$$

where \mathbf{C}^i is the i th row of \mathbf{C} . The L_2 SVS is most closely related to our method, SRRR, but it has no low rank constraint on \mathbf{C} . The L_∞ SVS (Turlach, Venables, and Wright, 2005) method solves a similar optimization problem as L_2 SVS but with a different penalty. The optimization problem is

$$\min_{\mathbf{C}} \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2 + \lambda \sum_{i=1}^p \|\mathbf{C}^i\|_\infty,$$

where $\|\mathbf{C}^i\|_\infty = \max(|C_{i1}|, \dots, |C_{ip}|)$ is the L_∞ -norm of the i th row of \mathbf{C} . Because of the L_∞ -penalty, a predictor variable would be selected if it is useful for one response. In contrast to L_2 SVS, $\|\mathbf{C}^i\|_\infty$ rather than $\|\mathbf{C}^i\|$ is used to measure the effect of the i th variable on the responses. As a result, the selection of the i th variable depends on its strongest effect on each one of the responses but not its overall effect. Therefore, we expect this method will select more variables than L_2 SVS, which is confirmed by our simulation study. The RemMap (Peng et al. 2010) method imposes both rowwise and elementwise sparsity of \mathbf{C} by solving the following optimization problem:

$$\min_{\mathbf{C}} \|\mathbf{Y} - \mathbf{X}\mathbf{C}\|^2 + \lambda_1 \sum_{i=1}^p \|\mathbf{C}^i\|_1 + \lambda_2 \sum_{i=1}^p \|\mathbf{C}^i\|.$$

All three of these methods encourage rowwise sparsity of \mathbf{C} . But none of them imposes the reduced-rank structure as we do in SRRR.

Another method is the SPLS method (Chun and Keles 2010) which is based on partial least squares (PLS). A PLS method tries to find the multidimensional direction in the predictor space that explains the maximum multidimensional variance direction in the response space. The SPLS (sparse PLS) encourages sparsity in the direction vector by imposing L_1 constraint on the optimization criterion for PLS. Because it identifies significant latent components, the SPLS essentially employs a reduced-rank structure though in a different way from the SRRR. Unlike the SRRR, SPLS does not directly target on prediction of the responses and thus we expect that SPLS has disadvantages in terms of prediction, as we will observe in both simulation and real data examples.

The last method is to apply separate regressions with variable selection using lasso (referred to as SepLasso). Unlike the other methods we mentioned above, this method ignores the possible interrelation between the responses and fits each of them separately. Although this method is not expected to be competitive, it serves as a good benchmark for all multivariate methods.

6.2 Adaptive Weighting

For a fair comparison, a single penalty parameter is used for SRRR when comparing it with the five methods listed in the

previous subsection. The adaptive weighting for SRRR as discussed in Section 3.5 is also evaluated, along with the same adaptive weighting scheme for L_2 SVS. They are referred to as adaptive SRRR and adaptive L_2 SVS in this article. The adaptive weighting for other methods is not considered either because there is no existing implementation or because it is not straightforward how to incorporate it into the existing methods.

6.3 Simulation Setups and Evaluation Methods

In the simulation study, the data were generated using model (5), $\mathbf{Y} = \mathbf{XBA}^T + \mathbf{E}$. To be specific, the $n \times p$ matrix \mathbf{X} was generated from multivariate normal distribution $\mathcal{N}(0, \Sigma_x)$ and Σ_x has diagonal elements 1 and off-diagonal elements ρ_x . For the $p \times r$ component matrix \mathbf{B} , the elements of its first p_0 rows were generated from $\mathcal{N}(0, 1)$ and the rest $p - p_0$ rows were set to be zero. The elements of $q \times r$ matrix \mathbf{A} were generated from $\mathcal{N}(0, 1)$. The elements of the $n \times q$ random noise matrix \mathbf{E} were generated from $\mathcal{N}(0, \sigma^2 \Sigma_e)$ and Σ_e had diagonal elements 1 and off-diagonal elements ρ_e . The magnitude of the noise σ^2 is chosen so that the signal-to-noise ratio (SNR), $\text{trace}(\mathbf{C}^T \Sigma_x \mathbf{C}) / \text{trace}(\mathbf{E})$, equals 1. After the matrix \mathbf{Y} was obtained, we centered and standardized it and then applied the proposed SRRR method and the five related methods as well as adaptive SRRR and adaptive L_2 SVS. We compared predictive accuracy of these methods in terms of the mean squared error (MSE), defined as

$$\text{MSE} = \|\mathbf{X}(\hat{\mathbf{B}}\hat{\mathbf{A}}^T - \mathbf{B}\mathbf{A}^T)\|^2/nq. \quad (24)$$

We also compared all the methods in terms of sensitivity and specificity, which are commonly used measures to evaluate the accuracy of variable selection. The sensitivity refers to the ratio between the number of correct selection and the total number of relevant variables (p_0), which measures the ability of detecting the relevant variables. The specificity refers to the ratio between number of correct “deletions” and the total number of irrelevant variables ($p - p_0$), which measures the ability of detecting

irrelevant variables. If a method selects the relevant variables accurately, it will have both high sensitivity and high specificity. If a method tends to over-select, it will produce high sensitivity but low specificity. If a method tends to under-select, it will have low sensitivity but high specificity. Finally, we compared how accurate the low rank structure is estimated in terms of the number of selected factors for SRRR (and adaptive SRRR) and SPLS.

In the first set of simulations (Case 1), $n > p$. More specifically $n = 100$, $p = 30$, $p_0 = 10$, $q = 10$, and varying r , ρ_x , and ρ_e . The precise setups are described as follows.

Case 1a: We set $r = 3$, $\rho_x = 0$, and $\rho_e = 0$ in this baseline model that has a strong factor structure and this setup favors our method.

Case 1b: We set $r = 10$ and $\rho_x = \rho_e = 0$. In this setup, \mathbf{C} is of full rank and we intend to use this case to see if SRRR has robust performance when the low rank structure is violated.

Case 1c: Same as Case 1a but with $\rho_x = 0.5$. In this case, moderate amount of correlations among predictors is introduced.

Case 1d: Same as Case 1a but with $\rho_e = 0.5$. In this case, a moderate amount of correlations among error terms is introduced and ideally the weighted least square criterion should be considered. We used this case for robustness check for the ordinary least square criterion used by all methods considered in our comparative study. Rothman, Levina, and Zhu (2010) proposed multivariate regression with covariance estimation (MRCE) method that directly models the error correlation for sparse multivariate regression. Extension of SRRR that models covariance structure may lead to more efficient estimation and is left for future research.

The second set of simulations is concerned about higher dimensional cases with $p \geq n$. In particular, we consider the following two settings for n , p , p_0 , and q . The other parameters are equal to baseline values in Case 1a, that is, $r = 3$, $\rho_x = 0$, and $\rho_e = 0$.

Case 2a: $n = p = 100$, $p_0 = 30$, and $q = 10$.

Case 2b: $n = 100$, $p = 300$, $p_0 = 30$, and $q = 30$.

Table 1. Simulation examples (Section 6.3). Mean squared errors (MSE) for seven setups. Reported are the means and SEs (standard errors, in parentheses) based on 30 simulation runs

| $n = 100$ | | | Parameters | | | Mean squared error | | | | | | | |
|-----------|-------|-----|------------|----------|----------|--------------------|-----------|---------|---------|----------------|----------|---------|-------------|
| p | p_0 | q | r | ρ_x | ρ_e | SRRR | L_2 SVS | RemMap | SPLS | L_∞ SVS | SepLasso | aSRRR | a L_2 SVS |
| 30 | 10 | 10 | 3 | 0 | 0 | 0.044 | 0.087 | 0.096 | 0.085 | 0.100 | 0.123 | 0.038 | 0.064 |
| | | | | | | (0.002) | (0.002) | (0.003) | (0.004) | (0.003) | (0.003) | (0.002) | (0.002) |
| | | | 10 | 0 | 0 | 0.077 | 0.085 | 0.092 | 0.085 | 0.120 | 0.111 | 0.061 | 0.062 |
| | | | | | | (0.003) | (0.003) | (0.003) | (0.004) | (0.002) | (0.003) | (0.002) | (0.002) |
| | | | 3 | 0.5 | 0 | 0.045 | 0.066 | 0.066 | 0.079 | 0.074 | 0.101 | 0.044 | 0.062 |
| | | | | | | (0.002) | (0.002) | (0.002) | (0.003) | (0.002) | (0.002) | (0.002) | (0.002) |
| 100 | 30 | 10 | 3 | 0 | 0.5 | 0.053 | 0.09 | 0.099 | 0.099 | 0.104 | 0.12 | 0.047 | 0.069 |
| | | | | | | (0.002) | (0.003) | (0.003) | (0.006) | (0.003) | (0.003) | (0.002) | (0.002) |
| | | | 3 | 0 | 0 | 0.132 | 0.208 | 0.208 | 0.269 | 0.236 | 0.274 | 0.136 | 0.207 |
| | | | | | | (0.005) | (0.005) | (0.004) | (0.009) | (0.004) | (0.004) | (0.006) | (0.005) |
| | | | 3 | 0 | 0 | 0.091 | 0.223 | 0.228 | 0.223 | 0.253 | 0.334 | 0.092 | 0.181 |
| | | | | | | (0.002) | (0.005) | (0.004) | (0.009) | (0.004) | (0.004) | (0.006) | (0.004) |
| 100 | 100 | 10 | 10 | 0 | 0 | 0.26 | 0.261 | 0.238 | 0.362 | 0.353 | 0.247 | 0.294 | 0.306 |
| | | | | | | (0.003) | (0.003) | (0.004) | (0.004) | (0.002) | (0.004) | (0.004) | (0.005) |

Table 2. Simulation examples (Section 6.3). Average sensitivity (Se) and specificity (Sp) over 30 simulation runs

| $n = 100$ | | | Parameters | | | SRRR | | L_2 SVS | | RemMap | | SPLS | | L_∞ SVS | | SepLasso | | aSRRR | | a L_2 SVS | |
|-----------|-------|-----|------------|----------|----------|------|------|-----------|------|--------|------|------|------|----------------|------|----------|------|-------|------|-------------|------|
| p | p_0 | q | r | ρ_x | ρ_e | Se | Sp | Se | Sp | Se | Sp | Se | Sp | Se | Sp | Se | Sp | Se | Sp | Se | Sp |
| 30 | 10 | 10 | 3 | 0 | 0 | 1 | 0.42 | 1 | 0.4 | 1 | 0.23 | 0.94 | 0.94 | 1 | 0.1 | 1 | 0.02 | 1 | 0.82 | 1 | 0.74 |
| | | | 10 | 0 | 0 | 1 | 0.35 | 1 | 0.34 | 1 | 0.16 | 0.97 | 0.95 | 1 | 0.09 | 1 | 0.02 | 1 | 0.8 | 1 | 0.75 |
| | | | 3 | 0.5 | 0 | 0.99 | 0.62 | 1 | 0.52 | 1 | 0.46 | 0.9 | 0.94 | 1 | 0.29 | 1 | 0.08 | 0.98 | 0.69 | 0.96 | 0.73 |
| | | | 3 | 0 | 0.5 | 1 | 0.5 | 1 | 0.37 | 1 | 0.24 | 0.92 | 0.92 | 1 | 0.13 | 1 | 0.03 | 0.99 | 0.79 | 1 | 0.77 |
| 100 | 30 | 10 | 3 | 0 | 0 | 0.92 | 0.57 | 0.87 | 0.51 | 0.89 | 0.5 | 0.56 | 0.81 | 0.9 | 0.46 | 0.96 | 0.23 | 0.84 | 0.79 | 0.71 | 0.88 |
| 300 | 30 | 30 | 3 | 0 | 0 | 0.93 | 0.74 | 0.83 | 0.68 | 0.93 | 0.41 | 0.51 | 0.98 | 0.85 | 0.64 | 0.96 | 0.25 | 0.89 | 0.82 | 0.68 | 0.96 |
| 100 | 100 | 10 | 10 | 0 | 0 | 0.71 | NA | 0.77 | NA | 0.86 | NA | 0.6 | NA | 0.68 | NA | 0.89 | NA | 0.38 | NA | 0.41 | NA |

In the last simulation, the row-wise sparsity assumption in the coefficient matrix \mathbf{C} is violated. We use this setup to test the SRRR method in an unfavorable case.

Case 3: \mathbf{C} has element-wise sparsity with 70% randomly assigned zero elements. The other parameters are set as follows: $n = p = 100$, $p_0 = 100$, and $r = q = 10$.

6.4 Simulation Results

We applied all eight methods to each of the seven setups. We used fivefold CV to choose tuning parameter(s) for all methods. In particular for SRRR and SPLS, the tuning parameters include λ and the number of factors r . For the adaptive methods, tuning parameters also include γ . The performance of all methods was measured using the criteria detailed in the previous subsection. The performance of the fitted model was measured using the MSE defined in (24) where \mathbf{X} is based on 1000 test samples. Summary of MSE for each method is given in Table 1. The first six columns provide fair comparison of our SRRR with five other methods, as all of them use the same tuning strategy without adaptive weights. In all cases except Case 1b (violation of low rank assumption) and the last one (violation of row-wise sparsity), SRRR produces considerably smaller average MSE among all methods, and the reduction of MSE is usually substantial. For Case 1b, there is no factor structure, so it is understandable that using SRRR has no clear advantage over using L_2 SVS. For the last case where elementwise sparsity is imposed, RemMap performs the best without surprise because its form of penalty accommodates both rowwise and element-wise sparsity structure; our SRRR does a reasonably good job in

this case. The separate lasso regression is not competitive with any multivariate methods considered; it gives the largest MSE except in the last case.

Table 2 reports sensitivity and specificity, for each method. All methods except SPLS tend to over-select indicated by high sensitivity but low specificity, and our SRRR has the highest specificity among all methods. It is noted in earlier work (Peng et al. 2010) that using CV as a tuning criterion to achieve best prediction performance often leads to over-selection, indicated by low specificity. SPLS does an excellent job in variable selection when $n > p$, but its sensitivity becomes the worst among all methods when $p \geq n$. The separate lasso regression and L_∞ SVS give the lowest specificity. The SRRR performs toward the top based on the overall evaluation of sensitivity and specificity.

Table 3 shows that the fivefold CV can select the number of factors r quite accurately for the SRRR and adaptive SRRR method.

The effect of adaptive weighting can be seen by comparing the first and the last two columns of Tables 1 and 2. Adaptive weighting improves the accuracy of prediction and variable selection for both SRRR and L_2 SVS in all setups where $n > p$. For cases where $p \geq n$, the adaptive weighting produces similar prediction accuracy as the unweighted version and tends to have lower sensitivity but higher specificity. That the adaptive weighting has the tendency of under-selecting relevant variables can be explained by the fact that the variables filtered out in the first stage will get infinitely large weights in the penalty term and therefore cannot be included in the final model. It is an interesting research topic to explore whether the use of a different pilot estimator will improve the performance of adaptive weighting in $p \geq n$ cases.

Table 3. Simulation examples (Section 6.3). Average number of factors selected for the SRRR, adaptive SRR, and SPLS, based on 30 simulation runs

| $n = 100$ | | | Parameters | | | Number of factors | | |
|-----------|-------|-----|------------|----------|----------|-------------------|------|-------|
| p | p_0 | q | r | ρ_x | ρ_e | SRRR | SPLS | aSRRR |
| 30 | 10 | 10 | 3 | 0 | 0 | 3 | 5 | 3.1 |
| | | | 10 | 0 | 0 | 7.1 | 8.6 | 7.4 |
| | | | 3 | 0.5 | 0 | 3.1 | 3.2 | 3.4 |
| | | | 3 | 0 | 0.5 | 3 | 5.1 | 3 |
| 100 | 30 | 10 | 3 | 0 | 0 | 3.1 | 4.2 | 3 |
| 300 | 30 | 30 | 3 | 0 | 0 | 3 | 7.2 | 3.1 |
| 100 | 100 | 10 | 10 | 0 | 0 | 9.3 | 5.2 | 9 |

7. REAL DATA EXAMPLE: YEAST CELL CYCLE DATASET

This data analysis is concerned with identifying transition factors (TF) that regulate the RNA transcript levels of yeast genes within the eukaryotic cell cycle. Spellman et al. (1998) identified 800 cell-cycle-regulated genes by three independent synchronization methods. We use data generated by the α factor arrest method where RNA levels were measured every 7 min for 119 min with a total of 18 time points covering two cell cycles (Y). The genes whose RNA levels varied periodically were identified as cell-cycle-regulated genes. The chromatin immunoprecipitation data (Lee et al. 2002) contain binding information of

Table 4. Yeast cell cycle data. Mean squared prediction error (MSPE) is based on half-splitting the data into training and test sets. Mean and SE of test errors are reported. Stability results report the times of each TF being selected over 100 runs of fivefold CV. False positive rate is the average percent of false selection over 100 random permutations

| | | SRRR | aSRRR | L_2 SVS | RemMap | SPLS |
|----------------|-----------|---------|---------|-----------|---------|---------|
| MSPE | mean | 0.189 | 0.188 | 0.190 | 0.189 | 0.197 |
| | (SE) | (0.001) | (0.001) | (0.001) | (0.001) | (0.001) |
| Stability | [90, 100] | 69 | 60 | 59 | 94 | 12 |
| | | (16) | (16) | (17) | (21) | (7) |
| | (10, 90) | 10 | 0 | 36 | 0 | 24 |
| | [0, 10] | 27 | 46 | 11 | 12 | 70 |
| False positive | | 2.10 | 1.74 | 2.91 | 4.39 | 7.36 |

these 800 genes for a total of 106 TFs (X). We use a smaller dataset analyzed by Chun and Keles (2010), which includes 524 of the 800 genes, after excluding the genes with missing RNA levels or binding information. The data are publicly available in the R package “spl.”

We applied SRRR and adaptive SRRR to these data. We also considered L_2 SVS, RemMap, and SPLS—the three other methods that showed competitive performance in our simulation study. Five-fold CV was used for selecting tuning parameters, including the number of factors r for SRRR, adaptive SRRR, and SPLS. For each fivefold random partition of the data, we obtained a trace plot of the minimum CV error for $r = 1, 2, \dots, 10$, where the minimum CV error corresponds to the best penalty parameters selected by CV. Figure 1 shows 20 such traces for 20 random partitions. For SRRR and adaptive SRRR, the trace plots flatten out from $r = 4$ onwards and thus we set $r = 4$ for further analysis. For SPLS, the “elbow” shape is less pronounced and we feel that $r = 6$ is the most natural choice.

For comparison of prediction accuracy, we randomly split the data into two halves, one as the training set and another as the test set. We used the training set to identify the best penalty parameters and then used the corresponding model to predict on the test data. The top row of Table 4 reports the means and standard errors of squared prediction errors from 50 random

splits. All methods except SPLS perform very similarly in terms of prediction errors. The larger prediction error of SPLS is due to the fact that it tends to under-select.

For the purpose of variable selection comparison, we fit the entire dataset using the optimal penalty parameters selected by the fivefold CV and kept track on whether each of 106 TFs is chosen in the fitted model. To account for the variability introduced by random partitions of CV, this experiment was done 100 times and we identified the TFs that were consistently included or excluded in each model. The “stability” results in Table 4 show how many TFs are selected at least 90 times, between 10 and 90 times, and under 10 times in the 100 runs. The results show that adaptive SRRR selects fewer TFs (60) than regular SRRR (69) and L_2 SVS selects similar number of TFs (59) as adaptive SRRR. RemMap selects 94 out of the 106 TFs and SPLS selects the smallest number 12. The table also reports in parentheses how many of these consistently selected TFs are among the 21 experimentally confirmed TFs that are related to the cell cycle regulation (Wang, Chen, and Li 2007). We can see that SRRR, adaptive SRRR, and L_2 SVS identify similar numbers of confirmed TFs, RemMap identifies slightly more, while SPLS identifies much less.

We remark on the stability of variable selection for each method. Ideally a TF should be either selected or excluded all the time, not affected by random partition in the CV. The more such TFs fall in [90, 100] or [0, 10] categories, the more stable the model is. A higher number in the middle category (10, 90) indicates a less stable selection. We see that L_2 SVS and SPLS are less stable in variable selection. Adaptive SRRR and RemMap have 0 TFs in the middle category and thus are more stable. However, a lower number in the middle category may also be a consequence of over-selection or under-selection indicated by extremely unequal numbers in the other two categories. After taking this into account, we conclude that the adaptive SRRR performs the best in terms of stability of variable selection. Since L_2 SVS can be thought as a special case of SRRR without rank restriction, the fact that SRRR and adaptive SRRR outperform L_2 SVS indicates that efficiency and stability of the variable selection are improved by enforcing a low rank structure on the coefficient matrix.

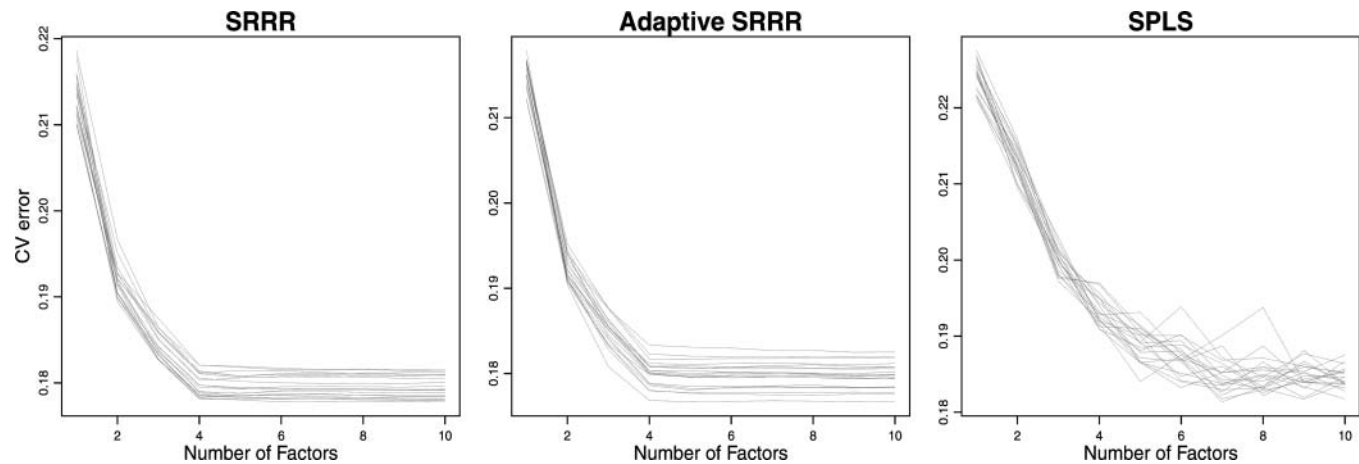


Figure 1. The fivefold CV error at optimal values of tuning parameters when fixing the number of factors.

To further evaluate the variable selection result, we examined the chance of selecting irrelevant variables for each method when we randomly permuted the order of genes for the transcript level data to break the dependence between the transcript level and the TFs. We used fivefold CV for selecting tuning parameters and then fit the entire dataset. We recorded the false positive rate, the ratio of the number of selected TFs to the total number of TFs. The permutation was done 100 times. Table 4 shows the average false positive rates. We see that SRRR methods have the smallest false positive rates.

The effect of the 16 confirmed TFs at 18 time points identified by adaptive SRRR is drawn in Figure 2. We see that except for

MET31 and STE12, all TFs show some periodic effect and some of them such as SWI4 and SWI6 show two clear cycles. Lee et al. (2002) identified another 10 TFs that coordinate transcriptional regulation of the cell cycle with other cellular processes (metabolism, environmental responses, and development). The adaptive SRRR can identify 8 of these 10 TFs and their effect is shown in the first two rows of Figure 3. Among the 36 additional TFs identified by adaptive SRRR, we rank them by their overall effect throughout the cell cycle and the last two rows in Figure 3 show the effect of the top 8 TFs. Again most of these TFs show some periodic effect and a lot of them show two clear cycles.

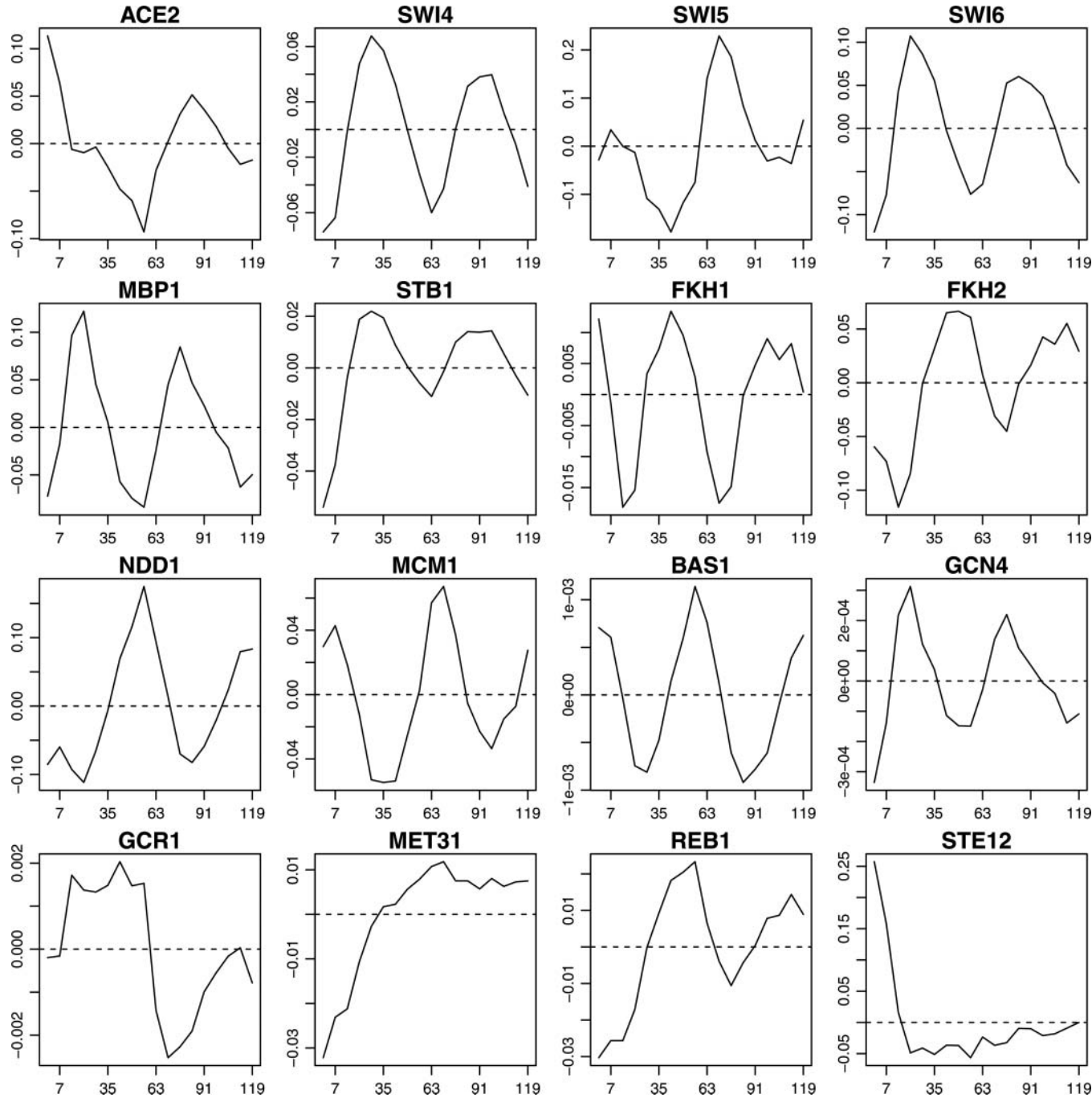


Figure 2. The effect of the 16 confirmed TFs identified by adaptive SRRR. These TFs are confirmed to be related to the cell cycle regulation.

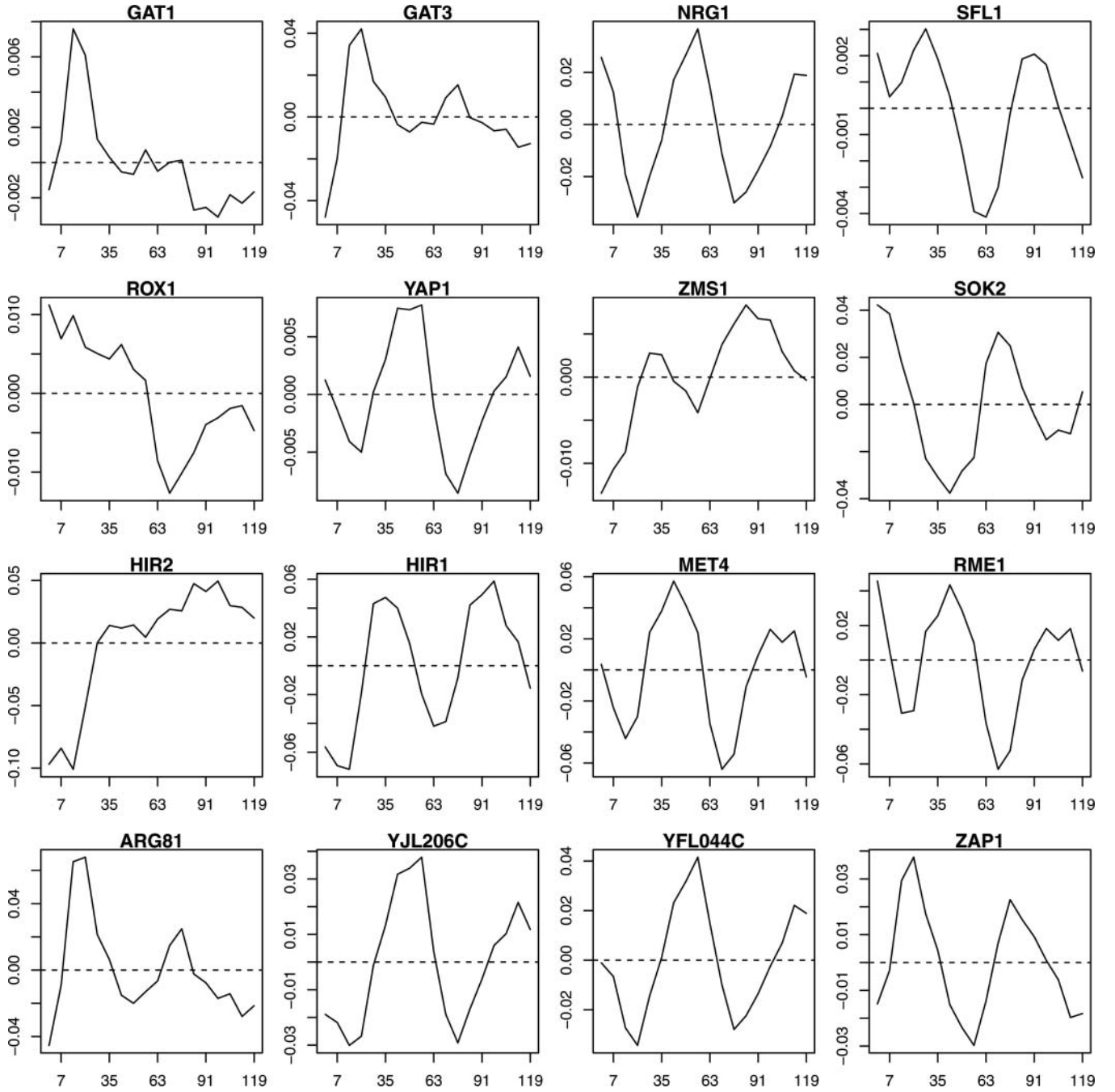


Figure 3. The effect of 16 of the additional 44 TFs identified adaptive SRRR. The first 8 TFs are confirmed TFs with the function of coordinating transcriptional regulation of the cell cycle with other cellular processes. The last 8 TFs have larger overall effect throughout the cell cycle among the rest TFs.

APPENDIX

Proof of Lemma 4. Writing $\mathbf{U} = \mathbf{U}_* + \Delta_u$ and similarly for \mathbf{D} and \mathbf{V} , we obtain the following expansion

$$\begin{aligned}
 \mathbf{U}\mathbf{D}\mathbf{V}^T - \mathbf{U}_*\mathbf{D}_*\mathbf{V}_*^T &= (\mathbf{U}_* + \Delta_u)(\mathbf{D}_* + \Delta_d)(\mathbf{V}_* + \Delta_v)^T - \mathbf{U}_*\mathbf{D}_*\mathbf{V}_*^T \\
 &= \mathbf{U}_*\mathbf{D}_*\Delta_v^T + \mathbf{U}_*\Delta_d\mathbf{V}_*^T + \Delta_u\mathbf{D}_*\mathbf{V}_*^T + \Delta_u\Delta_d\mathbf{V}_*^T + \Delta_u\mathbf{D}_*\Delta_v^T \\
 &\quad + \mathbf{U}_*\Delta_d\Delta_v^T + \Delta_u\Delta_d\Delta_v^T. \tag{A.1}
 \end{aligned}$$

It follows from (17) that $\|\Delta_u\| = \|\mathbf{U}_*\mathbf{G}_u + \mathbf{H}_u\| + O(\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2) = O((\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2)^{1/2})$. Similarly, $\|\Delta_v\| = O((\|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2)^{1/2})$ and $\|\Delta_d\| = O(\|\mathbf{K}\|)$. Note that $\|\mathbf{U}_*\|$, $\|\mathbf{D}_*\|$ and $\|\mathbf{V}_*\|$ are all bounded. Thus,

$$\begin{aligned}
 \|\Delta_u\Delta_d\mathbf{V}_*^T + \Delta_u\mathbf{D}_*\Delta_v^T + \mathbf{U}_*\Delta_d\Delta_v^T + \Delta_u\Delta_d\Delta_v^T\| \\
 = O(\|\mathbf{G}_u\|^2 + \|\mathbf{H}_u\|^2 + \|\mathbf{G}_v\|^2 + \|\mathbf{H}_v\|^2 + \|\mathbf{K}\|^2).
 \end{aligned}$$

Plugging (17)–(19) into (A.1) and using the antisymmetry property $\mathbf{G}_v^T = -\mathbf{G}_v$, we obtain the desired result. \square

Proof of Lemma 5. Since \mathbf{G}_u and \mathbf{G}_v are antisymmetric, we can write $\mathbf{G}_u = \mathbf{A} - \mathbf{A}^T$ and $\mathbf{G}_v = \mathbf{\Gamma} - \mathbf{\Gamma}^T$, where \mathbf{A} and $\mathbf{\Gamma}$ are lower triangular square matrices whose diagonal elements are 0's. Therefore,

$$\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v = (\mathbf{A} \mathbf{D}_* - \mathbf{D}_* \mathbf{\Gamma}) - (\mathbf{A}^T \mathbf{D}_* - \mathbf{D}_* \mathbf{\Gamma}^T).$$

Since the two terms on the above right-hand side are, respectively, lower triangular and upper triangular, taking the Frobenius norm yields

$$f \equiv \|\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v\|^2 = \|\mathbf{A} \mathbf{D}_* - \mathbf{D}_* \mathbf{\Gamma}\|^2 + \|\mathbf{A}^T \mathbf{D}_* - \mathbf{D}_* \mathbf{\Gamma}^T\|^2.$$

Let δ_{ij} and γ_{ij} be the (i, j) entry of \mathbf{A} and $\mathbf{\Gamma}$, respectively. By the definition of the Frobenius norm and using the lower/upper triangular property of relevant matrices, we obtain that

$$\begin{aligned} f &= \sum_{i>j} (\delta_{ij} d_j - d_i \gamma_{ij})^2 + \sum_{i>j} (d_i \delta_{ij} - \gamma_{ij} d_j)^2 \\ &= \sum_{i>j} (d_j^2 \delta_{ij}^2 + d_i^2 \gamma_{ij}^2 + d_i^2 \delta_{ij}^2 + d_j^2 \gamma_{ij}^2 - 2d_i d_j \delta_{ij} \gamma_{ij} \\ &\quad - 2d_i d_j \delta_{ij} \gamma_{ij}). \end{aligned}$$

For a lower bound of f , we use the inequality $2\delta_{ij}\gamma_{ij} \leq \delta_{ij}^2 + \gamma_{ij}^2$ and complete the squares $d_i^2 + d_j^2 - 2d_i d_j = (d_i - d_j)^2$ to get

$$\begin{aligned} f &\geq \sum_{i>j} \{(d_i - d_j)^2 (\delta_{ij}^2 + \gamma_{ij}^2)\} \geq \min_{i>j} (d_i - d_j)^2 \sum_{i>j} (\delta_{ij}^2 + \gamma_{ij}^2) \\ &= \frac{1}{2} \min_{i>j} (d_i - d_j)^2 (\|\mathbf{G}_u\|^2 + \|\mathbf{G}_v\|^2). \end{aligned}$$

For an upper bound, we use the inequality $(a - b)^2 \leq 2(a^2 + b^2)$ to obtain

$$\begin{aligned} f &\leq 2 \sum_{i>j} (d_i^2 + d_j^2) (\delta_{ij}^2 + \gamma_{ij}^2) \leq 2 \max_{i>j} (d_i^2 + d_j^2) \sum_{i>j} (\delta_{ij}^2 + \gamma_{ij}^2) \\ &= 2 \max_i d_i^2 (\|\mathbf{G}_u\|^2 + \|\mathbf{G}_v\|^2). \end{aligned}$$

The proof of the lemma is complete. \square

Proof of Theorem 1. We first prove part (i). We only need to show that (23) holds. Without loss of generality, we assume that $\mathbf{X} \mathbf{X}^T / n \rightarrow \mathbf{I}$, because if $\mathbf{X} \mathbf{X}^T / n \rightarrow \mathbf{\Sigma}$, then the argument below goes through when \mathbf{X} is replaced by $\mathbf{\Sigma}^{-1/2} \mathbf{X}$. Set $\alpha_n = \alpha / \sqrt{n}$. We need to find a uniform lower bound of $Q(\boldsymbol{\Theta}) - Q(\boldsymbol{\Theta}_*)$ for all $\boldsymbol{\Theta}$ with $\|\boldsymbol{\Theta}\| = \alpha_n$. Denote $\mathbf{E} = \mathbf{Y} - \mathbf{X} \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T$. We have that

$$\begin{aligned} Q(\boldsymbol{\Theta}) - Q(\boldsymbol{\Theta}_*) &= \|\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}^T\|^2 - \|\mathbf{E}\|^2 + \sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}^i \mathbf{D}\| \\ &\quad - \sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}_*^i \mathbf{D}_*\|. \end{aligned} \quad (\text{A.2})$$

We first consider the terms that involve penalty functions. Using $\|\mathbf{U}_*^i \mathbf{D}_*\| = 0$ for $i > p_0$ and the inequality $\|\mathbf{a}\| - \|\mathbf{b}\| \geq -\|\mathbf{a} - \mathbf{b}\|$, we obtain that

$$\begin{aligned} &\sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}^i \mathbf{D}\| - \sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}_*^i \mathbf{D}_*\| \\ &\geq \sum_{i=1}^{p_0} \lambda_{n,i} \|\mathbf{U}^i \mathbf{D}\| - \sum_{i=1}^{p_0} \lambda_{n,i} \|\mathbf{U}_*^i \mathbf{D}_*\| \\ &\geq - \sum_{i=1}^{p_0} \lambda_{n,i} \|\mathbf{U}^i \mathbf{D} - \mathbf{U}_*^i \mathbf{D}_*\|. \end{aligned} \quad (\text{A.3})$$

It follows from Cauchy-Schwarz inequality and a simpler version of Lemma 4 that

$$\begin{aligned} &\sum_{i=1}^{p_0} \lambda_{n,i} \|\mathbf{U}^i \mathbf{D} - \mathbf{U}_*^i \mathbf{D}_*\| \\ &\leq \left(\max_{1 \leq i \leq p_0} \lambda_{n,i} \right) \sqrt{p_0} \|\mathbf{U} \mathbf{D} - \mathbf{U}_* \mathbf{D}_*\| \\ &\leq \left(\max_{1 \leq i \leq p_0} \frac{\lambda_{n,i}}{\sqrt{n}} \right) \sqrt{n} O(\|\mathbf{G}_u\| + \|\mathbf{H}_u\| + \|\mathbf{K}\|) \leq O(\sqrt{n} \alpha_n). \end{aligned} \quad (\text{A.4})$$

Next, consider the first two terms on the right side of (A.2). Since $\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}^T = \mathbf{Y} - \mathbf{X} \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T - \mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T) = \mathbf{E} - \mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T)$, we have that

$$\begin{aligned} \|\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}^T\|^2 &= \|\mathbf{E}\|^2 - 2\langle \mathbf{E}, \mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T) \rangle \\ &\quad + \|\mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T)\|^2. \end{aligned} \quad (\text{A.5})$$

According to Lemma 4, we can write $\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T = \mathbf{F} + \mathbf{T}$, where

$$\begin{aligned} \mathbf{F} &= \mathbf{U}_* (\mathbf{G}_u \mathbf{D}_* - \mathbf{D}_* \mathbf{G}_v) \mathbf{V}_*^T + \mathbf{U}_* \mathbf{D}_* \mathbf{H}_v^T + \mathbf{H}_u \mathbf{D}_* \mathbf{V}_*^T \\ &\quad + \mathbf{U}_* \mathbf{D}_* \mathbf{K} \mathbf{V}_*^T, \end{aligned}$$

and $\|\mathbf{T}\| = O(\alpha_n^2)$. Lemma 5 and (21) imply that $\|\mathbf{F}\| = O(\alpha_n)$. By expanding the norm squared and using the Cauchy-Schwarz inequality, we obtain that

$$\|\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T\|^2 = \|\mathbf{F} + \mathbf{T}\|^2 = \|\mathbf{F}\|^2 + O(\alpha_n^3).$$

Since $\mathbf{X} \mathbf{X}^T / n \rightarrow \mathbf{I}$, it follows that

$$\frac{1}{n} \|\mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T)\|^2 = \|\mathbf{F}\|^2 + O(\alpha_n^3). \quad (\text{A.6})$$

Note that

$$\langle \mathbf{E}, \mathbf{X} (\mathbf{U} \mathbf{D} \mathbf{V}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T) \rangle = \langle \mathbf{E}, \mathbf{X} \mathbf{F} \rangle + \langle \mathbf{E}, \mathbf{X} \mathbf{T} \rangle. \quad (\text{A.7})$$

Since $\|\mathbf{X}\|^2 / n = \text{tr}(\mathbf{X}^T \mathbf{X}) / n \rightarrow p$, we have that $\|\mathbf{X}\| = O(\sqrt{n})$. Simple calculation yields that, for any matrix \mathbf{S} with compatible dimensions, $\text{var}(\langle \mathbf{E}, \mathbf{X} \mathbf{S} \rangle) = O(\|\mathbf{X}\|^2 \|\mathbf{S}\|^2)$, and thus $|\langle \mathbf{E}, \mathbf{X} \mathbf{S} \rangle| = O_P(\|\mathbf{X}\| \|\mathbf{S}\|) = O_P(\sqrt{n}) \|\mathbf{S}\|$. Using this result, we obtain that

$$\langle \mathbf{E}, \mathbf{X} \mathbf{T} \rangle = O_P(\sqrt{n}) \|\mathbf{T}\| = O_P(\sqrt{n} \alpha_n^2). \quad (\text{A.8})$$

Combining (A.5)–(A.8) yields

$$\begin{aligned} \|\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}^T\|^2 &= \|\mathbf{E}\|^2 - 2\langle \mathbf{E}, \mathbf{X} \mathbf{F} \rangle + n \|\mathbf{F}\|^2 + O(n \alpha_n^3) \\ &\quad + O_P(\sqrt{n} \alpha_n^2). \end{aligned} \quad (\text{A.9})$$

Applying the same argument for (A.8) gives

$$|\langle \mathbf{E}, \mathbf{X} \mathbf{F} \rangle| = O_P(\sqrt{n}) \|\mathbf{F}\|. \quad (\text{A.10})$$

Consequently,

$$\begin{aligned} \|\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}^T\|^2 - \|\mathbf{E}\|^2 &\geq -O_P(\sqrt{n}) \|\mathbf{F}\| + n \|\mathbf{F}\|^2 \\ &\quad + O(n \alpha_n^3) + O_P(\sqrt{n} \alpha_n^2). \end{aligned} \quad (\text{A.11})$$

Combining (A.2)–(A.4) and (A.11), we obtain that

$$\begin{aligned} Q(\boldsymbol{\Theta}) - Q(\boldsymbol{\Theta}_*) &\geq -O_P(\sqrt{n}) \|\mathbf{F}\| + n \|\mathbf{F}\|^2 - O(\sqrt{n} \alpha_n) \\ &\quad + O(n \alpha_n^3) + O_P(\sqrt{n} \alpha_n^2). \end{aligned}$$

Lemma 5 and (21) together imply that $M_1 \|\boldsymbol{\Theta}\| \leq \|\mathbf{F}\| \leq M_2 \|\boldsymbol{\Theta}\|$ for some positive constants M_1 and M_2 . Thus, if $\|\boldsymbol{\Theta}\| = \alpha_n = \alpha / \sqrt{n}$,

$$\begin{aligned} Q(\boldsymbol{\Theta}) - Q(\boldsymbol{\Theta}_*) &\geq -O_P(\alpha) + M_1 \alpha^2 + O(\alpha^3 / \sqrt{n}) \\ &\quad + O_P(\alpha^2 / \sqrt{n}). \end{aligned}$$

Therefore, for any $\epsilon > 0$, we can choose a large α such that, $\inf_{\Theta: \|\Theta\|=\alpha_n} Q(\Theta) - Q(\Theta_*) > 0$ with probability larger than $1 - \epsilon$. The proof of part (i) is complete.

To prove part (ii), note that part (i) implies that $\|\hat{\Theta}\| = O_p(n^{-1/2})$. Since $\|\hat{\Theta}\|^2 = \|\hat{\mathbf{G}}_u\|^2 + \|\hat{\mathbf{H}}_u\|^2 + \|\hat{\mathbf{G}}_v\|^2 + \|\hat{\mathbf{H}}_v\|^2 + \|\hat{\mathbf{K}}\|^2$, we obtain that $(\|\hat{\mathbf{G}}_u\|^2 + \|\hat{\mathbf{H}}_u\|^2)^{1/2} = O_p(n^{-1/2})$, $(\|\hat{\mathbf{G}}_v\|^2 + \|\hat{\mathbf{H}}_v\|^2)^{1/2} = O_p(n^{-1/2})$, and $\|\hat{\mathbf{K}}\| = O_p(n^{-1/2})$. The desired result then follows from Lemma 3. \square

Proof of Theorem 2. Denote the diagonal elements of \mathbf{D}_* as \mathbf{D}_{*kk} , $1 \leq k \leq r$, and similarly for $\hat{\mathbf{D}}$. Because $\mathbf{D}_{*kk} > 0$ and $\hat{\mathbf{D}}$ is consistent in estimating \mathbf{D}_* , we have that $\hat{\mathbf{D}}_{kk} > 0$ for all k . The optimizing objective function can be written as

$$\begin{aligned} \|\mathbf{Y} - \mathbf{XUDV}^T\|^2 + \sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}^i \mathbf{D}\| &= \text{tr}(\mathbf{Y}^T \mathbf{Y}) \\ &+ \text{tr}(\mathbf{DU}^T \mathbf{X}^T \mathbf{XUD} - 2\mathbf{V}^T \mathbf{Y}^T \mathbf{XUD}) + \sum_{i=1}^p \lambda_{n,i} \|\mathbf{U}^i \mathbf{D}\|. \end{aligned}$$

Suppose $\|\hat{\mathbf{U}}^i\| > 0$. The first-order condition for $\hat{\mathbf{U}}^i$ is

$$2\mathbf{X}_i^T \mathbf{X} \hat{\mathbf{U}} \hat{\mathbf{D}}^2 - 2\mathbf{X}_i^T \mathbf{Y} \hat{\mathbf{V}} \hat{\mathbf{D}} + \lambda_{n,i} \frac{\hat{\mathbf{U}}^i \hat{\mathbf{D}}^2}{\|\hat{\mathbf{U}}^i \hat{\mathbf{D}}\|} = \mathbf{0},$$

or equivalently,

$$\frac{2}{\sqrt{n}} \mathbf{X}_i^T (\mathbf{X} \hat{\mathbf{U}} \hat{\mathbf{D}} \hat{\mathbf{V}}^T - \mathbf{Y}) \hat{\mathbf{V}} + \frac{\lambda_{n,i}}{\sqrt{n}} \frac{\hat{\mathbf{U}}^i \hat{\mathbf{D}}}{\|\hat{\mathbf{U}}^i \hat{\mathbf{D}}\|} = \mathbf{0}. \quad (\text{A.12})$$

Note that $(1/\sqrt{n})\mathbf{X}_i^T (\mathbf{XU}_* \mathbf{D}_* \mathbf{V}_*^T - \mathbf{Y}) = -(1/\sqrt{n})\mathbf{X}_i^T \mathbf{E} = O_p(1)$, $\hat{\mathbf{U}} \hat{\mathbf{D}} \hat{\mathbf{V}}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T = O_p(1/\sqrt{n})$, and $\mathbf{X}^T \mathbf{X}/n = O_p(1)$. Therefore,

$$\begin{aligned} &\frac{1}{\sqrt{n}} \mathbf{X}_i^T (\mathbf{X} \hat{\mathbf{U}} \hat{\mathbf{D}} \hat{\mathbf{V}}^T - \mathbf{Y}) \\ &= \frac{1}{\sqrt{n}} \mathbf{X}_i^T (\mathbf{XU}_* \mathbf{D}_* \mathbf{V}_*^T - \mathbf{Y}) + \frac{1}{\sqrt{n}} \mathbf{X}_i^T \mathbf{X} (\hat{\mathbf{U}} \hat{\mathbf{D}} \hat{\mathbf{V}}^T - \mathbf{U}_* \mathbf{D}_* \mathbf{V}_*^T) \\ &= O_p(1) + \frac{1}{\sqrt{n}} \mathbf{X}_i^T \mathbf{X} O_p\left(\frac{1}{\sqrt{n}}\right) = O_p(1). \end{aligned}$$

This implies that

$$\frac{1}{\sqrt{n}} \mathbf{X}_i^T (\hat{\mathbf{U}} \hat{\mathbf{D}} \hat{\mathbf{V}}^T - \mathbf{Y}) \mathbf{V} = O_p(1). \quad (\text{A.13})$$

If $\|\hat{\mathbf{U}}^i\| > 0$ for some $i > p_0$, letting

$$k^* = \arg \max_{1 \leq k \leq r} |\hat{\mathbf{U}}_k^i \hat{\mathbf{D}}_{kk}|,$$

we have that

$$\frac{|\hat{\mathbf{U}}_{k^*}^i \hat{\mathbf{D}}_{k^*k^*}|}{\|\hat{\mathbf{U}}^i \hat{\mathbf{D}}\|} > \frac{1}{\sqrt{r}}. \quad (\text{A.14})$$

Considering (A.13), (A.14), and the assumption that $\lambda_{n,i}/\sqrt{n} \rightarrow \infty$, for $i > p_0$, we obtain that the first-order condition (A.12) will not hold for $i > p_0$. This is a contradiction. Consequently, $\|\hat{\mathbf{U}}^i\| = 0$ for all $i > p_0$ with probability tending to one. \square

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