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Estimation of Low Rank High-Dimensional Multivariate Linear Models for Multi-Response Data

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ABSTRACT

In this article, we study low rank high-dimensional multivariate linear models (LRMLM) for high-dimensional multi-response data. We propose an intuitively appealing estimation approach and develop an algorithm for implementation purposes. Asymptotic properties are established to justify the estimation procedure theoretically. Intensive simulation studies are also conducted to demonstrate performance when the sample size is finite, and a comparison is made with some popular methods from the literature. The results show the proposed estimator outperforms all of the alternative methods under various circumstances. Finally, using our suggested estimation procedure we apply the LRMLM to analyze an environmental dataset and predict concentrations of PM2.5 at the locations concerned. The results illustrate how the proposed method provides more accurate predictions than the alternative approaches.

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BIC; Cross-validation; High dimensionality; Low rank; Multivariate linear models; Penalized least squares estimation

1. Introduction

It is common to find multi-response data in many real life problems. Component-wise analysis is clearly not a good choice for multi-response data analysis, because it does not fully make use of the information available. For example, the observations of other components may contain the information for the component of interest, and such information would be completely overlooked by component-wise analysis, therefore, the resulting estimators would not be as efficient as we can expect. It is necessary to take multivariate analysis approach for multi-response data analysis. The most commonly used multivariate regression models are the multivariate linear models. The research in the multivariate linear models can be at least traced back to Anderson (1951). There is much literature after Anderson (1951) about the classic multivariate linear models, see the references in Reinsel and Velu (1998) and Anderson (2004).

With the surge in high-dimensional data analysis in the past more than a decade, the multivariate linear models in high-dimensional setting are attracting more and more attention than ever before. Many interesting developments in low rank high-dimensional multivariate linear models have appeared in literature (see, e.g., Yuan et al. 2007; Negahban and Wainwright 2011; Obozinski, Wainwright, and Jordan 2011; Kong et al. 2017; Bing and Wegkamp 2019; Raskutti, Yuan, and Chen 2019; Zheng et al. 2019, and the references therein).

A commonly used approach to deal with the low rank coefficient matrix in a multivariate linear model is based on the idea of decomposing the coefficient matrix, say $\mathbf{A}$ with rank r and size $p \times q$, to $\mathbf{CDQ}$, where $\mathbf{C}$ and $\mathbf{Q}$ are two matrices of size $p \times \hat{r}$ and $\hat{r} \times q$, respectively, and $\mathbf{D}$ is a diagonal matrix of size $\hat{r}$, where $\hat{r}$ is an estimator of r. The estimation of r plays a key role for the success of the approach used. Different approaches may end up with different ways to estimate r (see, e.g., Yuan et al. 2007; Bing and Wegkamp 2019). Although the existing approaches for estimating r enjoy nice asymptotic properties, when implementing them, we often come up against a dilemma: we create a new unknown parameter to estimate an unknown parameter, this is because we have to select a tuning parameter in the estimation of r. In addition to that, as far as the estimation of $\mathbf{A}$ is concerned, which is the ultimate goal for multivariate linear models, even if we knew the rank r, to get the estimator of $\mathbf{A}$ based on the decomposition, we would have to estimate $\mathbf{C}$, $\mathbf{Q}$, and $\mathbf{D}$. Even with the constraints coming with the decomposition, we may have to estimate at least $(p + q)r$ unknown parameters, which is more than the unknown parameters we need to estimate without using the decomposition when $r > pq/(p + q)$. That implies we may end up with a better estimator of $\mathbf{A}$ if we simply apply the standard least squares estimation for multivariate linear models when $r > pq/(p + q)$, which clearly shows the limitation of the decomposition based approach.

In this article, we are going to propose an estimation procedure for the low rank multivariate linear models, in which we only need to estimate $r(p + q) - r^2$ unknown parameters to get the estimator of $\mathbf{A}$. We can easily show $r(p + q) - r^2 \leq pq$, because $r \leq \min(p, q)$. Intuitively speaking, the proposed estimation procedure would be more efficient than either of the standard least squares estimation and the decomposition based approach. This conclusion is confirmed to be true by both the asymptotic theory established in Section 4 and simulation studies in Section 5. As part of the proposed estimation pro-

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cedure, the rank of $\mathbf{A}$ is estimated by the Bayesian information criterion (BIC), which is free of tuning parameter. We will show the resulting estimator enjoys good theoretical properties and performs well in simulation studies.

Another advantage of the proposed estimation procedure is it clearly appreciates the high dimensionality by directly imposing a penalty on those entries of $\mathbf{A}$ in question, which makes the proposed estimation procedure easily accommodate the high-dimensional cases and enjoy the function of feature selection.

In the context of multi-response data analysis, the proposed estimation procedure also comes with a very nice practical implication, which is the impacts of explanatory variables on some responses are linear combinations of the impacts on certain responses when the matrix coefficient is of low rank, this would be very helpful when it comes to interpreting the results for a given real dataset, and may lead to some interesting findings in the discipline which the dataset comes from.

To implement the proposed estimation procedure, we have also developed an algorithm for the estimation. Our simulation studies show the proposed algorithm is fast and accurate.

The rest of this article is organized as follows: we begin with a detailed description of the models we are going to address in Section 2. The proposed estimation procedure and associated computational algorithm are described in Section 3. The asymptotic properties of the estimators obtained by the proposed estimation procedure are presented in Section 4. Section 5 is devoted to simulation studies, in which we will examine how well the proposed estimation works. Finally, in Section 6, we apply the low rank multivariate linear models together with the proposed estimation procedure to analyze an environmental dataset and predict the concentrations of PM2.5 at the locations concerned. The results show the proposed method provides more accurate prediction than other methods. We leave the theoretical proofs of all asymptotic properties in Appendix A.

2. The Low Rank High-Dimensional Multivariate Linear Models

To give a generic description of the models we are going to address, we use Y to denote the vector of all response variables, X the vector of all covariates. Without any confusion, from now on, we call Y the response variable, X the covariate. We assume Y is of q dimension, X is of p dimension. p and q may tend to ∞ when sample size tends to ∞. The low rank high-dimensional multivariate linear models which we are going to address in this article are

$$Y = \mathbf{A}^\top X + \boldsymbol{\epsilon}, \tag{1}$$

where $\mathbf{A}$ is a $p \times q$ unknown matrix of unknown rank r, $r < q < p$, $\boldsymbol{\epsilon} = (\epsilon_1, \ldots, \epsilon_q)^\top$ is a q dimensional random error, and

$$\mathbb{E}(\boldsymbol{\epsilon}|X) = \mathbf{0}, \quad \text{cov}(\boldsymbol{\epsilon}|X) = \boldsymbol{\Sigma}.$$

Like Yuan et al. (2007), Bing and Wegkamp (2019), and Raskutti, Yuan, and Chen (2019), we assume $\boldsymbol{\Sigma} = \sigma^2 \mathbf{I}_q$, and σ^2 is unknown.

Suppose we have a sample $(X_i^\top, Y_i^\top)$, $i = 1, \ldots, n$, from $(X^\top, Y^\top)$, the model for the sample can be written as

$$\mathbf{Y} = \mathbf{X}\mathbf{A} + \mathbf{E}, \tag{2}$$

where $\mathbf{Y} = (Y_1, \ldots, Y_n)^\top$, $\mathbf{X} = (X_1, \ldots, X_n)^\top$, and $\mathbf{E} = (\boldsymbol{\epsilon}_1, \ldots, \boldsymbol{\epsilon}_n)^\top$.

3. Estimation Procedure

Throughout this article, for any matrix $\boldsymbol{\Omega} = (w_{ij})$ of size $p \times q$ and any vector $\mathbf{b} = (b_1, \ldots, b_p)$, we define

$$||\boldsymbol{\Omega}||_1 = \sum_{i=1}^{p}\sum_{j=1}^{q} |w_{ij}|, \quad ||\boldsymbol{\Omega}|| = \left(\sum_{i=1}^{p}\sum_{j=1}^{q} w_{ij}^2\right)^{1/2},$$

$$||\mathbf{b}||_2 = (\mathbf{b}^\top \mathbf{b})^{1/2}, \quad ||\mathbf{b}||_1 = \sum_{i=1}^{p} |b_i|.$$

For any integers $1 \le j_1 < j_2 < \cdots < j_r \le q$, the complement set of set $\mathcal{D}_r$, $\mathcal{D}_r = \{j_1, \ldots, j_r\}$, is denoted by $\mathcal{D}_r^c$, that is $\mathcal{D}_r^c = \{1, 2, \ldots, q\} \setminus \mathcal{D}_r$. Let $\mathbf{Y}^i$ be the ith column of $\mathbf{Y}$,

$$\mathbf{Y}_{\mathcal{D}_r} = (\mathbf{Y}^{j_1}, \ldots, \mathbf{Y}^{j_r}), \quad \mathbb{H}_k(r) = \{\mathcal{D}_k : \text{rank}(\mathbf{A}_{\mathcal{D}_k}) = r\},$$

$$\bar{\mathbb{H}}_k(r) = \{\mathcal{D}_k : \text{rank}(\mathbf{A}_{\mathcal{D}_k}) < r\},$$

$$\mathbb{G}(k) = \{\mathbf{B} \in \mathbb{R}^{p\times k} : \text{rank}(\mathbf{B}) = k\},$$

and $\lambda_{\min}(\mathbf{B})$ and $\lambda_{\max}(\mathbf{B})$ be the smallest and largest eigenvalues of a square matrix $\mathbf{B}$.

Suppose we have an independent and identically distributed sample $(Y_i^\top, X_i^\top)$, $i = 1, \ldots, n$, from $(Y^\top, X^\top)$. A standard penalized least squares estimation would provide us with an estimator $\tilde{\mathbf{A}}$ of $\mathbf{A}$, which is the minimizer of

$$\sum_{i=1}^{n} ||Y_i - \mathbf{A}^\top X_i||^2 + P_\lambda(||\mathbf{A}||_1), \tag{3}$$

where $P_\lambda(\cdot)$ is a penalty function. However, this estimation does not take into account the information that $\mathbf{A}$ is of low rank, which would result in an estimator not as efficient as we could expect. In fact, it is easy to see this estimation is equivalent to componentwise penalized least squares estimation for (1).

The proposed estimation procedure will fully make use of the low rank information of $\mathbf{A}$, and the resulting estimator will be more efficient.

3.1. Estimation Method

The idea, based on which the proposed estimation is constructed, is that each column of $\mathbf{A}$ is a linear combination of r linearly independent columns of $\mathbf{A}$. Based on this idea, we propose the following estimation procedure for $\mathbf{A}$. We start with the case when the rank r of $\mathbf{A}$ is known, then propose an estimation for r.

3.1.1. When r Is Known

Let $Y_i = (y_{i1}, \ldots, y_{iq})^\top$, $X_i = (x_{i1}, \ldots, x_{ip})^\top$ for $i = 1, \ldots, n$. Apply the idea of penalized least squares estimation and minimize

$$\sum_{i=1}^{n}\left\{\sum_{l=1}^{r}\left(y_{ij_l} - X_i^\top \mathbf{a}_{j_l}\right)^2 + \sum_{k\notin\{j_1,\ldots,j_r\}}\left(y_{ik} - X_i^\top \sum_{\ell=1}^{r} b_{k\ell}\mathbf{a}_{j_\ell}\right)^2\right\}$$

$$+ \sum_{l=1}^{r} P_\lambda(||\mathbf{a}_{j_l}||_1) \tag{4}$$

with respect to $\mathbf{a}_{jl}$'s, $b_{k\ell}$'s, and $\{j_1,\ldots,j_r\}$, where $1 \le j_1 < \cdots < j_r \le q$, $P_\lambda(\cdot)$ is a penalty function, λ involved is a tuning parameter which can be selected by some criterion, such as BIC.

When r is large, $b_{k\ell}$'s are also likely to have sparsity, in which case, we can add another penalty term into (4) to penalize $b_{k\ell}$'s. However, when r is small, which is the case of main interest, there is no need to penalize $b_{k\ell}$'s, this is because for each component of Y_i, say the kth component, there are only r $b_{k\ell}$'s, which is not many.

Notice that the minimizer of (4) is not unique. We denote a minimizer of (4) by

$$\hat{\mathcal{D}} = \{\hat{j}_1,\ldots,\hat{j}_r\}, \quad \hat{\mathbf{a}}_j,\ j \in \hat{\mathcal{D}}, \quad \hat{b}_{k\ell},\ k \in \hat{\mathcal{D}}^c,\ \ell \in \{1,\ldots,r\}.$$

For any j, $1 \le j \le q$, the jth column of $\mathbf{A}$ is estimated by

$$\begin{cases} \hat{\mathbf{a}}_j, & \text{if } j \in \hat{\mathcal{D}}, \\ \sum_{\ell=1}^{r} \hat{b}_{j\ell}\hat{\mathbf{a}}_{\hat{j}_\ell}, & \text{if } j \in \hat{\mathcal{D}}^c. \end{cases}$$

We use $\hat{\mathbf{A}}(r)$ to denote the estimator of $\mathbf{A}$.

The nonuniqueness of the minimizer of (4) is because that there can be more than one ways to choose r independent columns $\mathcal{D}_r$ so that $\mathbf{A}_{\mathcal{D}_r}$ is full-rank. Theoretically speaking, as long as $\mathbf{A}_{\mathcal{D}_r}$ and r can be well estimated, we can recovery the low-rank structure of $\mathbf{A}$ regardless of the choice of $\mathcal{D}_r$. Our theory shows that the consistency of our proposed estimator holds uniformly in $\mathcal{D}_r$; please refer to Lemmas 1–3 in Appendix A. Hence, this nonunique issue does not affect the performance of the proposed estimation procedure, which is further corroborated via extensive simulations in Section 5.

3.1.2. Estimation of r

The estimation of $\mathbf{A}$ in Section 3.1.1 is built on the assumption that the rank r of $\mathbf{A}$ is known, and this assumption is not realistic in reality. In fact, rank r plays a very important role in the estimation of $\mathbf{A}$. If r is underestimated, a substantial bias would creep into the estimation procedure and make the final estimator of $\mathbf{A}$ very biased. On the other hand, if r is overestimated, we would have to estimate unnecessarily many unknown parameters, which would make the final estimator of $\mathbf{A}$ have big variance. In this article, we use BIC, which is defined as follows, to estimate r

$$\mathrm{BIC}(k) = ||\mathbf{Y} - \mathbf{X}\hat{\mathbf{A}}(k)||^2 + \sqrt{kp\log p}h_n, \tag{5}$$

where h_n is a positive diverging sequence, which can be set to be $\log n$. The estimator of r is given by

$$\hat{r} = \arg\min_{1\le k\le \bar{r}} \mathrm{BIC}(k),$$

where $\bar{r}$ is a prespecified bound for r. The proposed estimator $\hat{\mathbf{A}}(\hat{r})$ of $\mathbf{A}$ is the $\hat{\mathbf{A}}(r)$, obtained in Section 3.1.1, with r being replaced by $\hat{r}$.

We will show in Section 4 the proposed BIC estimator $\hat{r}$ enjoys an excellent asymptotic property, say it tends to identify the true model consistently. If the prediction accuracy is our primary concern, we can consider the multifold cross-validation (CV), which tends to select the model with the optimal prediction performance (Zhang 1993). The data are splitted randomly into M groups of equal sizes (assuming that n/M is an integer for simplicity), $\mathcal{G}_m, m = 1,\ldots,M$. For each k, $1 \le k \le q$, let $\hat{\mathbf{A}}_{-m}(k)$ be the estimator of $\mathbf{A}$, obtained by the method in Section 3.1.1 when the rank of $\mathbf{A}$ is k, without using the observations of the mth group. The CV sum is defined as

$$\mathrm{CV}(k) = \sum_{m=1}^{M}\sum_{i\in\mathcal{G}_m} ||Y_i - \hat{\mathbf{A}}_{-m}^\top(k)X_i||^2. \tag{6}$$

The CV estimator of r is taken to be the minimizer of $\mathrm{CV}(k)$.

3.2. Computational Algorithm

The minimization of (4) can be difficult. We propose an iterative algorithm to solve this problem. The route of our algorithm is: we first minimize (4), for given $\{j_1,\ldots,j_r\}$, with respect to $\mathbf{a}_{jl}$'s, $b_{k\ell}$'s, and denote the resulting minimum of (4) by $F(j_1,\ldots,j_r)$, then minimize $F(j_1,\ldots,j_r)$, with respect to $j_1,\ldots,j_r$. The details of our algorithm are described as follows.

For any given $\{j_1,\ldots,j_r\}$, we minimize (4) with respect to $\mathbf{a}_{jl}$'s and $b_{k\ell}$'s by the following iterative approach

1. We minimize
$$\sum_{i=1}^{n}\sum_{l=1}^{r}\left(y_{ijl} - X_i^\top\mathbf{a}_{jl}\right)^2 + \sum_{l=1}^{r}P_\lambda(||\mathbf{a}_{jl}||_1)$$
with respect to $\mathbf{a}_{jl}$'s, and denote the minimizer by $\mathbf{a}_{jl}^{(0)}$'s. There are many existing methods to do the minimization in this step, because this is the minimization for standard penalized least squares estimation.
2. Minimize
$$\sum_{i=1}^{n}\sum_{k\notin\{j_1,\ldots,j_r\}}\left(y_{ik} - X_i^\top\sum_{\ell=1}^{r}b_{k\ell}\mathbf{a}_{j_\ell}^{(0)}\right)^2$$
with respect to $b_{k\ell}$'s, and denote the minimizer by $b_{k\ell}^{(0)}$'s. Clearly, $b_{k\ell}^{(0)}$ enjoys a closed form, therefore, the minimization in this step is very easy.
3. Let $\mathbf{a}_{jl}^{(0)}$'s and $b_{k\ell}^{(0)}$'s be the initial values, and minimize (4) iteratively. Specifically, let $\mathbf{a}_{jl}^{(k)}$s and $b_{k\ell}^{(k)}$'s be the values of $\mathbf{a}_{jl}$'s and $b_{k\ell}$'s in the kth iteration. Replace the $b_{k\ell}$'s in (4) by $b_{k\ell}^{(k)}$s and minimize (4) with respect to $\mathbf{a}_{jl}$'s, $\mathbf{a}_{jl}^{(k+1)}$'s are taken to the resulting minimizer.

   Replace the $\mathbf{a}_{jl}$'s in (4) by $\mathbf{a}_{jl}^{(k+1)}$'s and minimize (4) with respect to $b_{k\ell}$'s, $b_{k\ell}^{(k+1)}$'s are taken to the resulting minimizer.

   Continue the iteration until convergence, the limits of $\mathbf{a}_{jl}^{(k)}$'s and $b_{k\ell}^{(k)}$'s are the minimizer of (4), and the minimum of (4) is denoted by $F(j_1,\ldots,j_r)$.

A naive approach to minimize $F(j_1,\ldots,j_r)$, with respect to $j_1,\ldots,j_r$, would be to compute $F(j_1,\ldots,j_r)$ for each possible $\{j_1,\ldots,j_r\}$, where $1 \le j_1 < \cdots < j_r \le q$, and the $\{j_1,\ldots,j_r\}$ which minimizes the obtained $F(j_1,\ldots,j_r)$'s is the minimizer $\{\hat{j}_1,\ldots,\hat{j}_r\}$ of $F(j_1,\ldots,j_r)$. However, this approach would have to compute $\binom{q}{r}$ $F(j_1,\ldots,j_r)$'s, which is computationally too expensive. We shall borrow the idea of forward selection to minimize $F(j_1,\ldots,j_r)$, which is depicted as follows

(I) Let $F(j_1)$ be $F(j_1,\ldots,j_r)$ when $r=1$, and compute $F(j_1)$ for each possible j_1, $1\le j_1\le q$. Let $\hat{j}_1$ be the one which minimizes $F(j_1)$.

(II) For any $k<r$, when we have $\{\hat{j}_1,\ldots,\hat{j}_k\}$, the way to select a j_{k+1} from $\{\hat{j}_1,\ldots,\hat{j}_k\}^c$, the set $\{1,\ldots,q\}-\{\hat{j}_1,\ldots,\hat{j}_k\}$, to add into the set $\{\hat{j}_1,\ldots,\hat{j}_k\}$ is as follows: for each possible j_{k+1}, we arrange $\hat{j}_1,\ldots,\hat{j}_k$ and j_{k+1} in ascent order, and denote them by $\tilde{j}_1<\cdots<\tilde{j}_{k+1}$. We compute $F(\tilde{j}_1,\ldots,\tilde{j}_{k+1})$. The selected j_{k+1} is the one which minimizes $F(\tilde{j}_1,\ldots,\tilde{j}_{k+1})$. We add the selected j_{k+1} into the set $\{\hat{j}_1,\ldots,\hat{j}_k\}$, and sort the elements in the new set in ascent order. With a little bit abuse of notation, we denote the new set by $\{\hat{j}_1,\ldots,\hat{j}_{k+1}\}$, where $\hat{j}_1<\cdots<\hat{j}_{k+1}$.

(III) Continue (II) until $k=r$. We use the obtained $\{\hat{j}_1,\ldots,\hat{j}_r\}$ to approximate the minimizer of $F(j_1,\ldots,j_r)$.

Substitute $\{\hat{j}_1,\ldots,\hat{j}_r\}$ for $\{j_1,\ldots,j_r\}$ in (4), and minimize (4) with respect to $\mathbf{a}_{\hat{j}_l}$'s and $b_{k\ell}$'s. Denote the resulting minimizer by $\hat{\mathbf{a}}_{\hat{j}_l}$'s and $\hat{b}_{k\ell}$'s. We take

$$\{\hat{j}_1,\ldots,\hat{j}_r\},\quad \hat{\mathbf{a}}_{\hat{j}_l},\ l=1,\ldots,r,\quad \hat{b}_{k\ell},\ k\notin\{\hat{j}_1,\ldots,\hat{j}_r\},\ \ell=1,\ldots,r$$

as a minimizer of (4) with respect to $\{j_1,\ldots,j_r\}$, $\mathbf{a}_{j_l}$'s and $b_{k\ell}$'s.

4. Asymptotic Properties

In this section, we are going to investigate the asymptotic behavior of the proposed estimator of $\mathbf{A}$.

Throughout this article, $A_n\sim B_n$ means that there is a constant $C>1$ such that $B_n/C\le A_n\le B_nC$ with probability tending to 1. "$\gtrsim$" and "$\lesssim$" are similarly defined.

To make the theoretical derivation more neat, we write the minimization of (4) in matrix form. Specifically, for any given integer $k\in[1,\ q)$, when $r=k$, the minimization of (4) can be written to the minimization of the following objective function

$$\mathcal{L}(\mathbf{U},\mathbf{V},\mathcal{D}_k;k)=||\mathbf{Y}_{\mathcal{D}_k}-\mathbf{X}\mathbf{U}||^2+||\mathbf{Y}_{\mathcal{D}_k^c}-\mathbf{X}\mathbf{U}\mathbf{V}^\top||^2+\sum_{\ell=1}^{k}P_{\boldsymbol{\lambda}_n}(||\mathbf{U}_\ell||_1) \tag{7}$$

with respect to $\{\mathcal{D}_k,\ \mathbf{U}\in\mathbb{G}(k),\ \mathbf{V}\in\mathbb{R}^{(q-k)\times k}\}$.

Without loss of generality, we use the (adaptive) lasso type penalty

$$P_{\boldsymbol{\lambda}_n}(||\mathbf{U}_\ell||_1)=n\sum_{j=1}^{p}\lambda_{j\ell}|u_{j\ell}|,$$

see Zou (2006), where $\lambda_{j\ell}>0$ and $u_{j\ell}$ are the (j,ℓ)th element of $\mathbf{U}$.

Throughout this section, we assume that each column of $\mathbf{X}$ has been normalized to have L_2-norm of n. Furthermore, we denote

$$\gamma_{0n}=\min\{\lambda_{j\ell}:a_{j\ell}=0\},\quad \gamma_{1n}=\max\{\lambda_{j\ell}:a_{j\ell}\ne0\},$$

where $a_{j\ell}$ is the (j,ℓ)th entry of $\mathbf{A}$.

To establish the asymptotic properties of the proposed methods, we impose the following technical conditions:

Condition 1. There exist positive constants $\bar{\kappa}$ and $\underline{\kappa}$ such that with probability one $\underline{\kappa}\le\lambda_{\min}(n^{-1}\mathbf{X}^\top\mathbf{X})<\lambda_{\max}(n^{-1}\mathbf{X}^\top\mathbf{X})\le\bar{\kappa}$.

Condition 2. For some positive constants C and K, $\mathbb{E}\{\exp(C\epsilon_j^2)\}<K$ for $j=1,\ldots,q$.

Condition 3. The elements of $\mathbf{A}$ and $\mathbf{X}\mathbf{A}$ are bounded. The matrix $\mathbf{A}$ is s_n-sparse in the sense that $\max_{1\le\ell\le q}\sum_{j=1}^{p}\mathbb{I}(a_{j\ell}\ne0)\le s_n$.

Condition 4. $rp\log p/n\to0$ when $n\to\infty$.

Condition 5. For any given $k\in[1,q)$,

$$\liminf_{n\to\infty}\frac{\min_{\mathcal{D}\in\bar{\mathbb{H}}_k(r),\mathbf{U}\in\mathbb{G}(k)}\left[||\mathbf{X}\mathbf{U}-\mathbf{X}\mathbf{A}_{\mathcal{D}}||^2+\mathrm{tr}\left\{(\mathbf{X}\mathbf{A}_{\mathcal{D}^c})^\top(\mathbf{I}-\mathbf{H}_{\mathbf{U}})\mathbf{X}\mathbf{A}_{\mathcal{D}^c}\right\}\right]}{\max(\sqrt{nrp\log p},nrs_n\gamma_{1n})}\to\infty,$$

where $\mathbf{H}_{\mathbf{U}}=\mathbf{Z}_{\mathbf{U}}(\mathbf{Z}_{\mathbf{U}}^\top\mathbf{Z}_{\mathbf{U}})^{-1}\mathbf{Z}_{\mathbf{U}}^\top$ and $\mathbf{Z}_{\mathbf{U}}=n^{-1/2}\mathbf{X}\mathbf{U}$.

Remark 1. Condition 1 implies that the predictor matrix has a reasonably good behavior; this is a type of restricted eigenvalue assumption and is commonly used in the literature (e.g., Fan and Peng 2004). Condition 2 requires that each entry of $\mathbf{E}$ is sub-Gaussian, which ensures its tail probability decays exponentially. Condition 3 facilitates our derivation but can be much relaxed so that the true signal strength depends on n as well. Condition 4 imposes requirement on the diverging rate to obtain consistent estimation when p, r diverges with n. Condition 5 is an identifiability assumption, ensuring that a true low-rank structure can be recognized.

We start with the establishment of the asymptotic property of the minimizer $\hat{\mathbf{A}}(r)=(\hat{\mathbf{U}},\hat{\mathbf{V}})$ of (7) when $k=r$. As far as the asymptotic properties are concerned, p, q, and r are allowed to depend on n and diverge as $n\to\infty$. The reason for us to suppress the subscript n of p, q, and r is to make notations neat.

We define an index set

$$\mathcal{M}(\mathcal{D})=\{1\le j\le p,\ \ell\in\mathcal{D}:a_{j\ell}\ne0\},$$

and its complement set is denoted by $\mathcal{M}^c(\mathcal{D})$. We have the following theorem:

Theorem 1. Under Conditions 1–5, if $\gamma_{0n}/\sqrt{rp\log p/n}\to\infty$ and $rs_n\gamma_{1n}^2\to0$ as $n\to\infty$, there exists, with probability tending to one, a local minimizer $\{\hat{\mathcal{D}}_r,\hat{\mathbf{A}}(r)\}$ of $\mathcal{L}(\mathbf{U},\mathbf{V},\mathcal{D}_r;r)$ satisfying: $\mathbf{A}_{\hat{\mathcal{D}}_r}$ is full-rank, and

$$\hat{\mathbf{A}}_{\mathcal{M}^c(\hat{\mathcal{D}}_r)}=0,\quad ||\hat{\mathbf{A}}(r)-\mathbf{A}||=O_p(\{r(s_n+q)(\log p/n+\gamma_{1n}^2)\}^{1/2}).$$

Theorem 1 implies that we can identify a "correct" $\hat{\mathcal{D}}_r$ in the sense that $\mathbf{A}_{\hat{\mathcal{D}}_r}$ is full rank with an overwhelming probability when n is large. The penalized estimators of the zero coefficients are exactly zero under some conditions on γ_{0n}. The condition $rs_n\gamma_{1n}^2\to0$ together with Condition 4 ensures that the proposed estimator is consistent. From the proof of this theorem in Appendix A, we can see, as a special case, that $||\hat{\mathbf{A}}(r)-\mathbf{A}||=$

$O_p(\sqrt{r(p+q)\log p/n})$ when $\gamma_{0n} = \gamma_{1n} = 0$. This is in line with the relevant existing results (see, e.g., Negahban and Wainwright 2011).

When the coefficient matrix is sparse, under properly selected tuning parameters, the proposed penalized estimator would enjoy the "oracle property." Specifically, if the adaptive lasso penalty with tuning parameter $\lambda_{j\ell} = \lambda_n \tilde{a}_{j\ell}^{-1}$ is used, where $\tilde{\mathbf{A}} = (\tilde{a}_{jl})_{p\times q}$ is the standard least-squares estimator of $\mathbf{A}$, we can verify that $||\hat{\mathbf{A}}(r) - \mathbf{A}|| = O_p(\{r(s_n+q)(\log p/n)\}^{1/2})$, provided that $rqp^2 \log p/n \to 0$ as $n \to \infty$, by setting $\lambda_n \sim \sqrt{\log p/n}$ and using the fact that $\tilde{a}_{j\ell} = O_p(1)$ for $a_{j\ell} \neq 0$ and $\tilde{a}_{j\ell} = O_p(\sqrt{pq\log p/n})$ for $a_{j\ell} = 0$.

As mentioned before, the estimation of the rank r of $\mathbf{A}$ plays a very important role in the estimation procedure of $\mathbf{A}$. Theorem 2 shows that the proposed BIC estimator $\hat{r}$, defined by (5), is consistent.

Theorem 2. Under the conditions in Theorem 1, if $\bar{r}/h_n \to 0$ as $n \to \infty$, we have $\Pr(\hat{r} = r) \to 1$ as $n \to \infty$.

It is very easy to see Theorem 1 together with Theorem 2 imply the proposed estimator of $\mathbf{A}$ is consistent.

5. Simulation Studies

In this section, we use two simulated examples, low- and high-dimensional ones, to assess the coefficient matrix estimation, the prediction, and the rank recovery performance of the proposed method. We assess the proposed method and consider the rank being estimated by either 5-fold CV (OUR-CV; Equation (6)) or BIC (OUR-BIC; Equation (5)). Throughout this section, OUR-CV and OUR-BIC are implemented by the algorithm introduced in Section 3.2 with $P_\lambda(\cdot)$ being the L_1 penalty function. The tuning parameter λ is selected by 5-fold CV.

In the low-dimensional example, we compare OUR-CV and OUR-BIC with the factor estimation and selection method (FES) proposed in Yuan et al. (2007), the rank selection criterion (RSC) proposed in Bunea, She, and Wegkamp (2011), and the self-tuning rank selection (STRS) proposed in Bing and Wegkamp (2019). Besides, we also consider the ordinary least squares estimator (OLS) and a low-rank matrix decomposition estimator (LMD) as two benchmarks. Denote $\hat{\mathbf{A}}_{\text{OLS}}$ the OLS estimator of $\mathbf{A}$, the LMD estimator of $\mathbf{A}$ is obtained from a rank $\hat{r}$ truncated singular value decomposition of $\hat{\mathbf{A}}_{\text{OLS}}$ as

$$\hat{\mathbf{A}}_{\text{LMD}} = \mathbf{U}\mathbf{D}\mathbf{V}^\top = \sum_{l=1}^{\hat{r}} \sigma_l \mathbf{u}_l \mathbf{v}_l^\top,$$

where $\mathbf{D} = \text{diag}\{\sigma_1, \ldots, \sigma_{\hat{r}}\}$ is a diagonal matrix of $\hat{r}$ largest positive singular values of $\hat{\mathbf{A}}_{\text{OLS}}$, and $\mathbf{U} = (\mathbf{u}_1, \ldots, \mathbf{u}_{\hat{r}})$ and $\mathbf{V} = (\mathbf{v}_1, \ldots, \mathbf{v}_{\hat{r}})$ are corresponding left and right singular vectors of $\hat{\mathbf{A}}_{\text{OLS}}$, respectively. Further, $\hat{r}$ is estimated by the eigen-ratio method (see, e.g., Ahn and Horenstein 2013 and references therein). In the high-dimensional example, we only compare OUR-CV and OUR-BIC with RSC and STRS as FES, OLS, and LMD are not applicable.

Table 1. Summary of parameters in data generating process.

Parameter	Description
n	Training sample size
n^*	Testing sample size
p	Dimension of covariate variables
q	Dimension of response variables
r	Rank of coefficient matrix
b	Signal strength parameter
η	Correlation level among covariates

5.1. Simulation Settings

Consider the multivariate linear regression model (2). Similar to Bunea, She, and Wegkamp (2011) and Bing and Wegkamp (2019), we consider a data generating process as follows.

1. Coefficient matrix $\mathbf{A}$: Let $\mathbf{A} = b\Gamma_0\Gamma_1$, with $b > 0$, $\Gamma_0 \in \mathbb{R}^{p\times r}$, $\Gamma_1 \in \mathbb{R}^{r\times q}$ and $r \le \min(p, q)$. The entries of Γ_0 and Γ_1 are independently drawn from $N(0, 1)$. The parameter r controls the rank of $\mathbf{A}$. The parameters b and r together control the signal-to-noise ratio in (2).
2. Error matrix $\mathbf{E}$: The entries of $\mathbf{E}$ are independently drawn from $N(0, 1)$.

The design matrix $\mathbf{X}$ is generated with the following two settings to cover the low- and high-dimensional cases, respectively.

3(a) Design matrix $\mathbf{X}$ when $n > p$ (low-dimensional case): X_i, $i = 1, \ldots, n$ are independently drawn from multivariate normal distribution $N_p(\mathbf{0}, \Sigma)$. For $i, j = 1, \ldots, p$, the (i, j)th entry of Σ is defined as $\Sigma_{ij} = \eta^{|i-j|}$ for some $\eta \in (0, 1)$.

3(b) Design matrix $\mathbf{X}$ when $p > n > q$ (high-dimensional case): Let $\mathbf{X} = \Lambda_0\Lambda_1\Sigma^{1/2}$, with $\Lambda_0 \in \mathbb{R}^{n\times q}$, and $\Lambda_1 \in \mathbb{R}^{q\times p}$. The entries of Λ_0 and Λ_1 are independently drawn from $N(0, 1)$. The covariance matrix Σ is defined as in 3(a).

For each case, we generate a testing sample $\{\mathbf{Y}^*, \mathbf{X}^*\}$ of size n^* independent of $\{\mathbf{Y}, \mathbf{X}\}$ to assess the prediction performance of each method. To sum up, the parameters that control the data generating process are listed in Table 1.

5.2. Low-Dimensional Example

In the first example, we examine the performance of OUR-CV, OUR-BIC, RSC, STRS, FES, OLS, and LMD in the low-dimensional case. We set $n = 100$, $n^* = 50$, $p = 25$, and $q = 20$. Then, we vary the rank $r = 5, 10, 15$, the signal strength parameter $b = 0.2, 0.4$, and the correlation level $\eta = 0.5, 0.9$. We simulate 200 replications for each scenario.

For each replication, we calculate two rescaled Frobenius norms as

$$\Delta_k = \frac{1}{pq}||\hat{\mathbf{A}}_k - \mathbf{A}||^2 \quad \text{and} \tag{8}$$
$$\Gamma_k = \frac{1}{n^*q}||\mathbf{Y}^* - \mathbf{X}^*\hat{\mathbf{A}}_k||^2, \quad k = 1, \ldots, 200,$$

where $\hat{\mathbf{A}}_k$ is the estimate of $\mathbf{A}$ in the kth replication, and $\{\mathbf{Y}^*, \mathbf{X}^*\}$ is a testing sample of size n^*. Then, we calculate the sample

Table 2. Results for the low-dimensional example with $b = 0.2$.

Rank	Method	$\eta = 0.5$			$\eta = 0.9$		
		Δ	Γ	R	Δ	Γ	R
5	OUR-CV	0.013(0.005)	1.121(0.052)	1.00	0.040(0.006)	1.130(0.053)	1.00
	OUR-BIC	0.013(0.005)	1.124(0.054)	1.00	0.041(0.006)	1.132(0.053)	0.99
	RSC	0.017(0.011)	1.130(0.074)	0.87	0.062(0.018)	1.249(0.071)	0.59
	STRS	0.013(0.010)	1.128(0.053)	1.00	0.052(0.013)	1.133(0.055)	0.97
	FES	0.018(0.015)	1.132(0.045)	NA	0.073(0.022)	1.221(0.048)	NA
	OLS	0.022(0.026)	1.332(0.066)	NA	0.125(0.027)	1.335(0.069)	NA
	LMD	0.014(0.008)	1.253(0.195)	0.76	0.046(0.015)	1.247(0.075)	0.68
10	OUR-CV	0.015(0.006)	1.235(0.058)	0.98	0.087(0.010)	1.254(0.060)	0.95
	OUR-BIC	0.015(0.006)	1.236(0.058)	0.96	0.089(0.009)	1.257(0.061)	0.92
	RSC	0.018(0.017)	1.290(0.087)	0.81	0.097(0.019)	1.278(0.068)	0.40
	STRS	0.016(0.013)	1.244(0.061)	0.90	0.093(0.016)	1.254(0.059)	0.65
	FES	0.019(0.016)	1.267(0.049)	NA	0.106(0.022)	1.276(0.051)	NA
	OLS	0.022(0.028)	1.341(0.067)	NA	0.124(0.035)	1.341(0.067)	NA
	LMD	0.020(0.032)	1.391(0.230)	0.38	0.135(0.048)	1.505(0.187)	0.27
15	OUR-CV	0.020(0.009)	1.312(0.061)	0.96	0.095(0.012)	1.321(0.064)	0.88
	OUR-BIC	0.020(0.009)	1.314(0.063)	0.92	0.097(0.012)	1.322(0.064)	0.86
	RSC	0.022(0.019)	1.338(0.069)	0.44	0.117(0.015)	1.329(0.067)	0.28
	STRS	0.021(0.012)	1.323(0.067)	0.65	0.104(0.013)	1.325(0.064)	0.42
	FES	0.022(0.015)	1.326(0.058)	NA	0.117(0.018)	1.332(0.059)	NA
	OLS	0.024(0.029)	1.337(0.065)	NA	0.124(0.032)	1.338(0.041)	NA
	LMD	0.029(0.033)	1.373(0.292)	0.15	0.136(0.041)	2.012(0.403)	0.12

NOTE: The columns Δ and Γ report the sample mean and sample standard deviation (in parentheses) of Δ_k and Γ_k, which are defined in (8), over 200 replications. The column R reports the rank recovery rate, which is defined in (9), over 200 replications.

Table 3. Results for the low-dimensional example with $b = 0.4$.

Rank	Method	$\eta = 0.5$			$\eta = 0.9$		
		Δ	Γ	R	Δ	Γ	R
5	OUR-CV	0.010(0.003)	1.125(0.052)	1.00	0.037(0.005)	1.125(0.052)	1.00
	OUR-BIC	0.011(0.003)	1.125(0.052)	0.99	0.037(0.005)	1.126(0.052)	0.98
	RSC	0.015(0.005)	1.168(0.069)	0.32	0.051(0.007)	1.135(0.056)	0.82
	STRS	0.011(0.003)	1.126(0.052)	1.00	0.037(0.006)	1.125(0.052)	1.00
	FES	0.015(0.008)	1.154(0.026)	NA	0.054(0.013)	1.139(0.051)	NA
	OLS	0.023(0.015)	1.332(0.066)	NA	0.125(0.027)	1.332(0.066)	NA
	LMD	0.011(0.004)	1.171(0.095)	0.99	0.041(0.017)	1.280(0.085)	0.86
10	OUR-CV	0.014(0.006)	1.231(0.057)	1.00	0.078(0.009)	1.238(0.059)	0.97
	OUR-BIC	0.014(0.006)	1.231(0.057)	0.99	0.080(0.009)	1.240(0.059)	0.95
	RSC	0.019(0.017)	1.309(0.069)	0.86	0.093(0.017)	1.292(0.078)	0.66
	STRS	0.015(0.013)	1.233(0.057)	0.98	0.082(0.011)	1.245(0.061)	0.73
	FES	0.017(0.016)	1.312(0.055)	NA	0.096(0.012)	1.258(0.060)	NA
	OLS	0.024(0.021)	1.340(0.027)	NA	0.124(0.025)	1.341(0.067)	NA
	LMD	0.018(0.016)	1.322(0.067)	0.90	0.108(0.035)	1.506(0.109)	0.45
15	OUR-CV	0.019(0.009)	1.301(0.061)	0.97	0.103(0.011)	1.314(0.065)	0.91
	OUR-BIC	0.020(0.009)	1.303(0.062)	0.95	0.104(0.011)	1.315(0.065)	0.88
	RSC	0.021(0.019)	1.331(0.071)	0.63	0.119(0.014)	1.339(0.071)	0.35
	STRS	0.021(0.012)	1.322(0.069)	0.81	0.107(0.011)	1.323(0.067)	0.54
	FES	0.021(0.015)	1.327(0.063)	NA	0.110(0.013)	1.327(0.066)	NA
	OLS	0.022(0.023)	1.335(0.065)	NA	0.125(0.025)	1.342(0.065)	NA
	LMD	0.028(0.037)	1.414(0.165)	0.36	0.175(0.097)	1.949(0.269)	0.17

NOTE: The columns Δ and Γ report the sample mean and sample standard deviation (in parentheses) of Δ_k and Γ_k, which are defined in (8), over 200 replications. The column R reports the rank recovery rate, which is defined in (9), over 200 replications.

mean and sample standard deviation of Δ_k and Γ_k over 200 replications.

We use $\hat{r}_k$ to denote the estimated rank of $\mathbf{A}$ in the kth replication, $k = 1, \ldots, 200$. The estimation accuracy of the rank r is assessed by the correct rank recovery rate which is defined as

$$R = \frac{1}{200} \sum_{k=1}^{200} I(\hat{r}_k = r), \tag{9}$$

where $I(\cdot)$ is the indicator function.

The simulation results of the low-dimensional example with $b = 0.2$ and 0.4 are presented in Tables 2 and 3, respectively. In most scenarios, OUR-CV performs slightly better than OUR-BIC but pays a price on the computational cost. When the rank is small (e.g., $r = 5$), OUR-CV, OUR-BIC, and STRS can recovery the correct rank with a rate close to 1 and have small estimation and prediction errors. RSC struggles when η is large and results in low correct recovery rates. LMD suffers when the signal-to-noise ratio is small. When the rank is moderate or large (e.g., $r = 10$ or 15), the correct rank recovery rates of RSC, STRS, and LMD drop. As a result, the estimation and prediction errors of

Table 4. Results for the high-dimensional example with $b = 0.2$

Rank	Method	$\eta = 0.5$			$\eta = 0.9$		
		Δ	Γ	R	Δ	Γ	R
10	OUR-CV	0.225(0.030)	1.468(0.142)	1.00	0.273(0.034)	1.508(0.146)	0.96
	OUR-BIC	0.226(0.031)	1.471(0.146)	0.99	0.273(0.034)	1.511(0.146)	0.96
	RSC	0.299(0.036)	2.165(0.185)	0.85	0.351(0.085)	2.392(0.203)	0.38
	STRS	0.226(0.031)	1.470(0.144)	0.97	0.2857(0.039)	1.522(0.151)	0.94
20	OUR-CV	0.402(0.047)	1.679(0.183)	0.93	0.502(0.046)	1.790(0.208)	0.85
	OUR-BIC	0.406(0.049)	1.685(0.184)	0.91	0.508(0.048)	1.794(0.210)	0.84
	RSC	0.618(0.072)	2.602(0.471)	0.15	0.758(0.091)	2.627(0.616)	0.06
	STRS	0.449(0.058)	2.052(0.235)	0.62	0.561(0.062)	2.156(0.273)	0.51

NOTE: The columns Δ and Γ report the sample mean and sample standard deviation (in parentheses) of Δ_k and Γ_k, which are defined in (8), over 200 replications. The column R reports the rank recovery rate, which is defined in (9), over 200 replications.

Table 5. Results for the high-dimensional example with $b = 0.4$.

Rank	Method	$\eta = 0.5$			$\eta = 0.9$		
		Δ	Γ	R	Δ	Γ	R
10	OUR-CV	0.949(0.102)	1.526(0.148)	1.00	0.977(0.122)	1.560(0.151)	0.99
	OUR-BIC	0.951(0.104)	1.527(0.148)	0.98	0.979(0.123)	1.568(0.153)	0.98
	RSC	1.198(0.124)	2.392(0.188)	0.74	1.201(0.159)	2.548(0.195)	0.50
	STRS	0.954(0.107)	1.528(0.150)	1.00	0.982(0.126)	1.570(0.156)	0.98
20	OUR-CV	1.021(0.152)	1.770(0.201)	0.95	1.181(0.184)	1.838(0.211)	0.88
	OUR-BIC	1.025(0.155)	1.774(0.202)	0.92	1.183(0.188)	1.841(0.214)	0.87
	RSC	1.808(0.406)	2.656(0.482)	0.35	2.059(0.685)	2.744(0.658)	0.13
	STRS	1.457(0.189)	2.104(0.262)	0.78	1.513(0.197)	2.210(0.285)	0.67

NOTE: The columns Δ and Γ report the sample mean and sample standard deviation (in parentheses) of Δ_k and Γ_k, which are defined in (8), over 200 replications. The column R reports the rank recovery rate, which is defined in (9), over 200 replications.

RSC, STRS, and LMD are also inflated. Compared with the other methods, OUR-CV and OUR-BIC are less sensitive to rank, correlation level and the signal-to-noise ratio. In general, FES performs similar as RSC in terms of estimation and prediction, and OLS performs unsatisfactory as it ignores the low rank structure in $\mathbf{A}$.

5.3. High-Dimensional Example

In the high-dimensional example, we examine the performance of OUR-CV and OUR-BIC and compare them with RSC and STRS. We set $n = 40$, $n^* = 40$, $p = 100$, and $q = 25$. Then, we vary the rank $r = 10, 20$, the signal strength parameter $b = 0.2, 0.4$, and the correlation level $\eta = 0.5, 0.9$. We simulate 200 replications for each scenario. The estimation and prediction errors are still measured by the sample mean and sample standard deviation of the rescaled Frobenius norms defined in (8). The estimation accuracy of rank r is measured by the correct rank recovery rate defined in (9).

The simulation results of the high-dimensional example with $b = 0.2$ and 0.4 are presented in Tables 4 and 5, respectively. Similar to the low-dimensional case, OUR-CV outperforms OUR-BIC in most scenarios. When both η and r are large, OUR-CV and OUR-BIC maintain reasonable correct rank recovery rates while RSC and STRS fail to recovery the correct rank in most replications.

6. Real Data Analysis

Particulate matter up to 2.5 μm (PM2.5) is a complex mixture of solid particles, chemicals (e.g., sulfates, nitrates) and liquid droplets in the air, which include inhalable particles that are small enough to penetrate the thoracic region of the respiratory system. Short term (days) exposure to inhalable PM2.5 can cause an increase in hospital admissions related to respiratory and cardiovascular morbidity, such as aggravation of asthma, respiratory symptoms, and cardiovascular disorders. Long term (years) exposure to inhalable PM2.5 may lead to an increase in mortality from cardiovascular and respiratory diseases, like lung cancer. The hazardous effects of inhalable PM2.5 on human health have been well-documented (see, e.g., Riediker et al. 2004; Polichetti et al. 2009; Franck et al. 2011; Xing et al. 2016; Pun et al. 2017, and references therein).

In this section, we investigate the relationship between concentration of PM2.5 and four air pollutants: ozone, sulfur dioxide (SO_2), carbon monoxide (CO), and nitrogen dioxide (NO_2). The dataset for us to study is available at *https://www.epa.gov/outdoor-air-quality-data*, it was collected from 37 outdoor monitoring sites across the United States. Specifically, the concentration of each of the four pollutants was measured and collected daily from the 37 sites between January 2017 to April 2019, and it has 729 observations in total. The concentration of PM2.5 was collected in the same manner.

What we are interested in is the association between the concentrations of PM2.5 and the concentrations of the four air pollutants at the 37 monitor sites. As the concentrations of the four air pollutants at one site may also contribute the concentrations of PM2.5 at other sites, we include the concentrations of the four air pollutants at all 37 sites in the explanatory variables for the concentration of PM2.5 at each site of the 37 sites, this gives us 148 explanatory variables for the concentration of PM2.5 at each site. In Figure 1, we plot the sample means of the concentrations of PM2.5 and of the four air pollutants against the geological locations where they were collected.

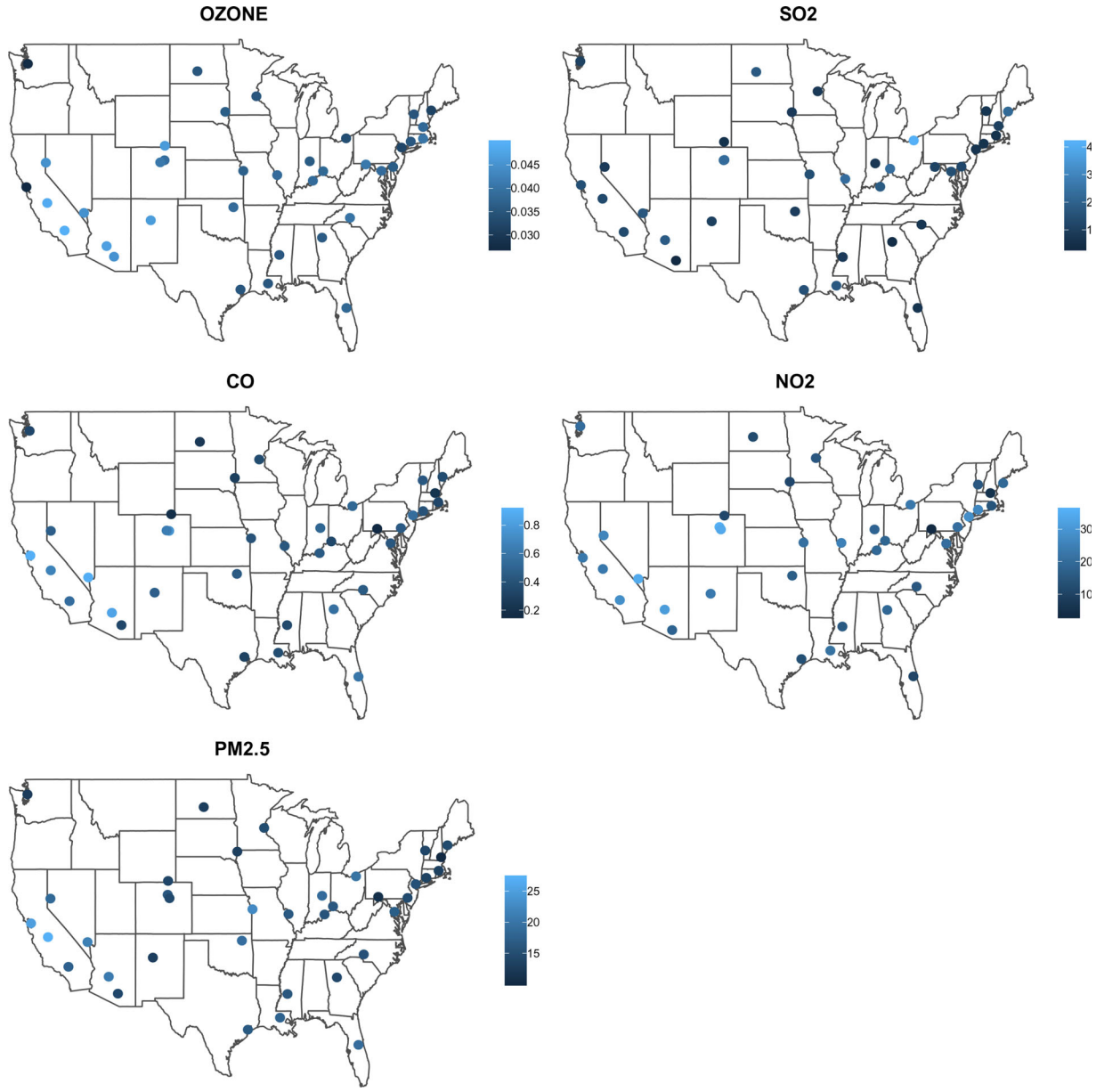

Figure 1. Sample means of the concentrations of PM2.5 and of the four air pollutants.

We take the first-order difference for each column of the dataset to remove the nonstationarity, and standardize it to make it have mean 0 and variance 1. Let $\mathbf{Y} = (\mathbf{Y}^1, \ldots, \mathbf{Y}^{37}) \in \mathbb{R}^{728\times 37}$ be the matrix of the 728 observations of the response variable which contains the concentrations of PM2.5 collected by the 37 sites, and $\mathbf{X} = (\mathbf{X}^1, \ldots, \mathbf{X}^{148}) \in \mathbb{R}^{728\times 148}$ be matrix of the 728 observations of predictor which contains the 148 explanatory variables. We apply the multivariate linear regression model (2) to fit the dataset, where $\mathbf{E} \in \mathbb{R}^{728\times 37}$ is the matrix of random errors, and $\mathbf{A} \in \mathbb{R}^{148\times 37}$ is the coefficient matrix of interest.

We compare the prediction performance of our method with rank estimated by the 5-fold CV (OUR-CV), the self-tuning rank selection (STRS) proposed in Bing and Wegkamp (2019), and the ordinary least squares estimator (OLS). For each method, we use the first 600 observations as the training set and predict the remaining 128 observations (the test set). Let $\mathbf{Y}_{\text{test}}$ and $\hat{\mathbf{Y}}_{\text{test}}$ be the matrices, respectively, of true and predicted values (obtained by one of the three methods listed above) of the response variable in the test set. The prediction accuracy is measured by the mean squared Frobenius norm of the difference between $\hat{\mathbf{Y}}_{\text{test}}$ and $\mathbf{Y}_{\text{test}}$, which is defined as

$$\text{Prediction error} = \frac{1}{n_t q}||\hat{\mathbf{Y}}_{\text{test}} - \mathbf{Y}_{\text{test}}||^2,$$

where $q = 37$ and $n_t = 128$, which are the number of columns and the number of rows of $\mathbf{Y}_{\text{test}}$, respectively.

Table 6. Prediction error and estimated rank of the coefficient matrix.

Methods	OUR-CV	STRS	OLS
Prediction error	0.7692	0.8551	1.0394
Estimated rank	3	10	NA

We report in Table 6 the prediction error as well as the estimated rank of the coefficient matrix for each method concerned. According to Table 6, OUR-CV achieves the smallest prediction error among the three competitors. Besides, the rank estimated

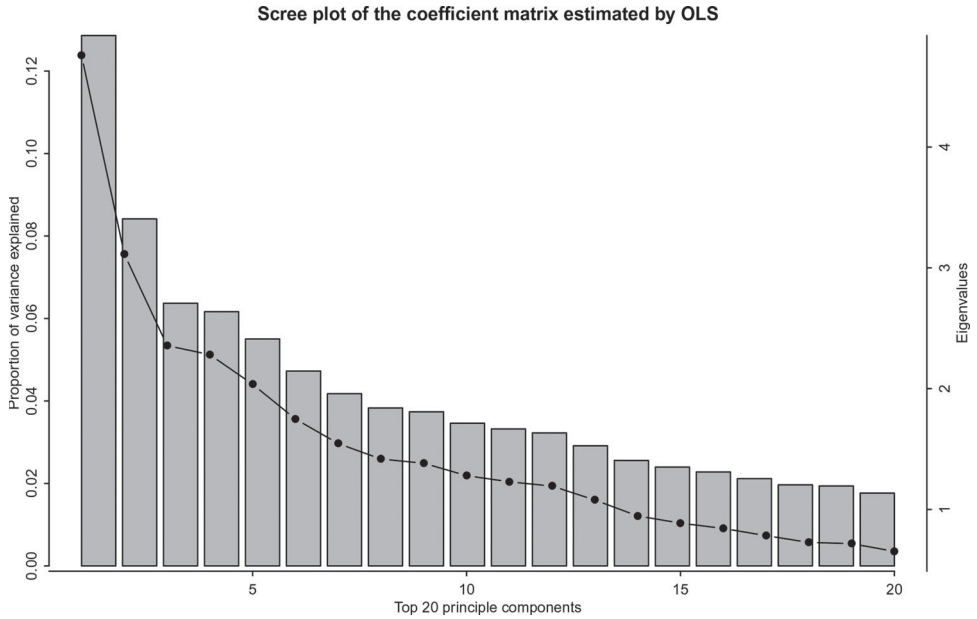

Figure 2. Scree plot of the coefficient matrix estimated by the OLS method. The solid dotted line denotes the leading eigenvalues in descending order. The gray bars denote the proporation of variance explained by each eigenvector.

by OUR-CV is 3 which is more parsimonious than the one estimated by STRS. To justify the rank estimation results, we apply eigen-decomposition to the coefficient matrix estimated by the OLS method, and draw the scree plot with the top 20 eigenvalues in Figure 2. The scree plot shows a clear elbow shape at the third eigenvalue.

The coefficient matrix estimated by OUR-CV unveils a parsimonious yet interpretable relationship between PM2.5 and the other four air pollutants. Among the four pollutants, CO has the largest positive contribution to the concentration of PM2.5. As we know, CO is usually produced in the incomplete combustion of carbon-containing fuels, such as gasoline, natural gas, coal, and wood. Two major anthropogenic sources of CO in the United States are vehicle emissions and heating. We find that monitors located in California and around New York City have high CO coefficients which are caused by the dense vehicle population. Also, we notice that the monitors with higher latitudes have higher CO coefficients which may reflect the impact of heating. Further, the attributes of each pollutant tend to cluster into three geological areas in the United States: west coast, central coast, and east coast.

Appendix A: Proofs

Given $\mathcal{D}_k$, the objective function (with respect to $(\mathbf{U}, \mathbf{V})$) is

$$\mathcal{L}(\mathbf{U}, \mathbf{V}; \mathcal{D}_k) = ||\mathbf{Y}_{\mathcal{D}_k} - \mathbf{X}\mathbf{U}||^2 + ||\mathbf{Y}_{\mathcal{D}_k^c} - \mathbf{X}\mathbf{U}\mathbf{V}^\top||^2 + n\sum_{\ell=1}^{k}\sum_{j=1}^{p}\lambda_{j\ell}|u_{j\ell}|$$

$$:= \mathcal{L}_1(\mathbf{U}; \mathcal{D}_k) + \mathcal{L}_2(\mathbf{U}, \mathbf{V}; \mathcal{D}_k) + n\sum_{\ell=1}^{k}\sum_{j=1}^{p}\lambda_{j\ell}|u_{j\ell}|.$$

We present three useful lemmas.

Lemma 1. Suppose Conditions 1–4 are satisfied. The following result holds uniformly for $\mathcal{D}_r$ such that $\mathbf{A}_{\mathcal{D}_r}$ is full-rank: with probability tending to one, there exists a local minimizer $\hat{\mathbf{A}}(r)$ of $\mathcal{L}(\mathbf{U}, \mathbf{V}; \mathcal{D}_r)$ such that $||\hat{\mathbf{A}}(r) - \mathbf{A}|| = O_p(\alpha_n)$, where $\alpha_n = \sqrt{r(p+q)\log p/n} + \sqrt{rs_n}\gamma_{1n}$.

Proof. For notational simplicity, in what follows we suppress the dependence of $\mathcal{D}$ on r and write $\mathcal{L}(\mathbf{U}, \mathbf{V}; \mathcal{D}_r)$ as $\mathcal{L}(\mathbf{U})$. It is easy to verify that for a given $\mathbf{U}$, by minimizing the function $\mathcal{L}_2(\mathbf{U}, \mathbf{V}; \mathcal{D}_r)$ with respect to $\mathbf{V}$, we obtain that

$$\mathcal{L}_2(\mathbf{U}) := \mathcal{L}_2(\mathbf{U}, \hat{\mathbf{V}}; \mathcal{D}_r) = \mathrm{tr}\left\{\mathbf{Y}_{\mathcal{D}^c}^\top(\mathbf{I} - \mathbf{H}_\mathbf{U})\mathbf{Y}_{\mathcal{D}^c}\right\}. \tag{A.1}$$

We will show that there exists a large constant $C > 0$ such that

$$\Pr\left\{\inf_{\mathbf{w}\in\mathbb{R}^{p\times r}; ||\mathbf{w}||=C} \mathcal{L}(\mathbf{A}_\mathcal{D} + \alpha_n\mathbf{w}) < \mathcal{L}(\mathbf{A}_\mathcal{D}),\ \forall\mathcal{D} \in \mathbb{H}_r(r)\right\} \to 0, \tag{A.2}$$

which implies with probability tending to one that there exists a local minimum in the ball $\{\mathbf{A}_\mathcal{D} + \alpha_n\mathbf{w} : ||\mathbf{w}|| \le C\}$ uniformly in $\mathcal{D}$. Hence, there exists a local minimizer of $\mathcal{L}(\mathbf{U})$ such that $||\hat{\mathbf{U}} - \mathbf{A}_\mathcal{D}|| = O_p(\alpha_n)$.

Write

$$\begin{aligned}
&\mathcal{L}(\mathbf{A}_\mathcal{D} + \alpha_n\mathbf{w}) - \mathcal{L}(\mathbf{A}_\mathcal{D})\\
=&\{\mathcal{L}_1(\mathbf{A}_\mathcal{D} + \alpha_n\mathbf{w}) - \mathcal{L}_1(\mathbf{A}_\mathcal{D})\} + \{\mathcal{L}_2(\mathbf{A}_\mathcal{D} + \alpha_n\mathbf{w}) - \mathcal{L}_2(\mathbf{A}_\mathcal{D})\}\\
&+ n\sum_{\ell\in\mathcal{D}}\sum_{j=1}^{p}\lambda_{j\ell}(|a_{j\ell} + \alpha_n w_{j\ell}| - |a_{j\ell}|)\\
:=&\Delta_1 + \Delta_2 + \Delta_3.
\end{aligned}$$

Observe that $\Delta_1 = n\alpha_n^2\mathrm{tr}\{\mathbf{w}^\top(n^{-1}\mathbf{X}^\top\mathbf{X})\mathbf{w}\} - 2\alpha_n\mathrm{tr}(\mathbf{E}_\mathcal{D}^\top\mathbf{X}\mathbf{w})$. By Condition 1, we have $\mathrm{tr}\{\mathbf{w}^\top(n^{-1}\mathbf{X}^\top\mathbf{X})\mathbf{w}\} \ge \underline{\kappa}||\mathbf{w}||^2$. It follows then, that the first term of Δ_1 is uniformly larger than $C^2\underline{\kappa}n\alpha_n^2$, which is quadratic in C.

For the second term of Δ_1, using Cauchy–Schwartz inequality, we have

$$2\alpha_n\mathrm{tr}(\mathbf{E}_\mathcal{D}^\top\mathbf{X}\mathbf{w}) \le 2\alpha_n C\left(\sum_{\ell\in\mathcal{D}}\sum_{j=1}^{p}(\mathbf{X}_j^\top\mathbf{E}^\ell)^2\right)^{1/2}.$$

By Condition 2 and tail probability of sub-Gaussian variables, we have

$$pq\Pr\left(|\mathbf{X}_j^\top \mathbf{E}^\ell| > c\sqrt{n\log p}\right) \to 0 \tag{A.3}$$

for a sufficiently large $c > 0$, and thus $\mathbf{X}_j^\top \mathbf{E}^\ell = O_p(\sqrt{n\log p})$ uniformly in j and ℓ. Consequently, the second term is uniformly of order $O_p(\sqrt{rnp\log p}\alpha_n C)$, which is linear in C. Therefore, by the definition of α_n, as long as the constant C is sufficiently large, the first term dominates the second term with arbitrarily large probability.

Next, we deal with Δ_2. To facilitate the presentation, denote $\tilde{\mathbf{A}}_\mathcal{D} = \mathbf{A}_\mathcal{D} + \alpha_n \mathbf{w}$, $\tilde{\mathbf{Z}} = n^{-1/2}\mathbf{X}\tilde{\mathbf{A}}_\mathcal{D}$, $\mathbf{H}_{\mathbf{A}_\mathcal{D}} = \mathbf{H}$ and $\tilde{\mathbf{H}}_{\tilde{\mathbf{A}}_\mathcal{D}} = \tilde{\mathbf{H}}$.

By $\mathbf{Y}_{\mathcal{D}^c} = \mathbf{X}\mathbf{A}_\mathcal{D}\mathbf{V}^{*\top} + \mathbf{E}_{\mathcal{D}^c}$ and $\mathbf{Z}(\mathbf{I}-\mathbf{H}) = \mathbf{0}$, simple algebra yields that

$$\begin{aligned}\Delta_2 = {} & \alpha_n^2 \mathrm{tr}\left\{(\mathbf{X}\mathbf{w}\mathbf{V}^{*\top})^\top(\mathbf{I}-\tilde{\mathbf{H}})(\mathbf{X}\mathbf{w}\mathbf{V}^{*\top})\right\} \\ & + 2\alpha_n \mathrm{tr}\left\{\mathbf{E}_{\mathcal{D}^c}^\top(\mathbf{I}-\tilde{\mathbf{H}})(\mathbf{X}\mathbf{w}\mathbf{V}^{*\top})\right\} \\ & + \mathrm{tr}\left\{\mathbf{E}_{\mathcal{D}^c}^\top(\mathbf{H}-\tilde{\mathbf{H}})\mathbf{E}_{\mathcal{D}^c}\right\}, \end{aligned} \tag{A.4}$$

where $\mathbf{V}^* \in \mathbb{R}^{(q-r)\times r}$ such that $\mathbf{A}_\mathcal{D}\mathbf{V}^{*\top} = \mathbf{A}_{\mathcal{D}^c}$.

Following the same arguments as in Δ_1, it can be shown that as long as the constant C is sufficiently large, the first term on the right side of (A.4) will always dominate the second term with arbitrarily large probability. Consider the third term on the right side of (A.4). By Condition 1 again, we get

$$\begin{aligned} ||\tilde{\mathbf{Z}} - \mathbf{Z}|| &\le \bar{\kappa}||\tilde{\mathbf{A}}_\mathcal{D} - \mathbf{A}_\mathcal{D}|| = O(\alpha_n C), \\ ||\tilde{\mathbf{Z}}^\top\tilde{\mathbf{Z}} - \mathbf{Z}^\top\mathbf{Z}|| &= O(\alpha_n C), \\ ||(\tilde{\mathbf{Z}}^\top\tilde{\mathbf{Z}})^{-1} - (\mathbf{Z}^\top\mathbf{Z})^{-1}|| &= O(\alpha_n C), \end{aligned}$$

and accordingly $||\tilde{\mathbf{H}} - \mathbf{H}|| = O(\alpha_n C)$. By (A.3), we have that

$$\begin{aligned} & \mathrm{tr}\left\{\mathbf{E}_{\mathcal{D}^c}^\top(\mathbf{H}-\tilde{\mathbf{H}})\mathbf{E}_{\mathcal{D}^c}\right\} \\ & = \mathrm{tr}\left[n^{-1}\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{X}\left\{\mathbf{A}_\mathcal{D}(\mathbf{Z}^\top\mathbf{Z})^{-1}(\mathbf{A}_\mathcal{D})^\top - \tilde{\mathbf{A}}_\mathcal{D}(\tilde{\mathbf{Z}}^\top\tilde{\mathbf{Z}})^{-1}\tilde{\mathbf{A}}_\mathcal{D}^\top\right\}\mathbf{X}^\top\mathbf{E}_{\mathcal{D}^c}\right] \\ & = \mathrm{tr}\Bigg[n^{-1/2}\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{X}\Big\{\mathbf{A}_\mathcal{D}(\mathbf{Z}^\top\mathbf{Z})^{-1}(\mathbf{A}_\mathcal{D})^\top \\ & \quad - \tilde{\mathbf{A}}_\mathcal{D}(\tilde{\mathbf{Z}}^\top\tilde{\mathbf{Z}})^{-1}\tilde{\mathbf{A}}_\mathcal{D}^\top\Big\}n^{-1/2}\mathbf{X}^\top\mathbf{E}_{\mathcal{D}^c}\Bigg] \\ & \le O(\alpha_n C)||n^{-1/2}\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{X}||^2 \\ & = O_p(\alpha_n C r p\log p) \end{aligned}$$

holds uniformly in $\mathcal{D}$, which is of smaller order of Δ_1.

For Δ_3, observe that

$$\begin{aligned}\Delta_3 &:= \Delta_{31} + \Delta_{32} \\ &= n\sum_{j,\ell\in\mathcal{M}(\mathcal{D})}\sum \lambda_{j\ell}\left(|a_{j\ell} + \alpha_n w_{j\ell}| - |a_{j\ell}|\right) + \Delta_{32},\end{aligned}$$

where $\Delta_{32} \ge 0$. By the definition of α_n and s_n, $|\Delta_{31}| \le \sqrt{rs_n}n\alpha_n\gamma_{1n}||\mathbf{w}||$ which is dominated by the Δ_1. Hence, by choosing a sufficiently large C, (A.2) holds.

By similar arguments, we can verify that $||\hat{\mathbf{V}} - \mathbf{V}^*|| = O_p(\alpha_n)$, and accordingly $||\hat{\mathbf{A}}(r) - \mathbf{A}|| = O_p(\alpha_n)$ follows. □

The next lemma establishes the sparsity property of $\hat{\mathbf{A}}(r)$.

Lemma 2. Suppose the conditions given in Lemma 1 all hold. If $n^{1/2}\gamma_{0n}/\sqrt{rp\log p} \to \infty$, then the following result holds uniformly for $\mathcal{D}_r$ such that $\mathbf{A}_{\mathcal{D}_r}$ is full-rank: For any $\hat{\mathbf{A}}_{\mathcal{D}_r}$ satisfying $||\hat{\mathbf{A}}_{\mathcal{D}_r} - \mathbf{A}_{\mathcal{D}_r}|| = O_p(\alpha_n)$, $\Pr(\hat{a}_{j\ell} = 0, \forall j, \ell \in \mathcal{M}^c(\mathcal{D}_r)) \to 1$, where $\hat{\mathbf{A}} = (\hat{a}_{j\ell})_{p\times q}$.

Proof. The objective function can be written as

$$\begin{aligned}\mathcal{L}(\mathbf{U}) = {} & \mathrm{tr}(\mathbf{Y}_\mathcal{D}^\top\mathbf{Y}_\mathcal{D} + \mathbf{Y}_{\mathcal{D}^c}^\top\mathbf{Y}_{\mathcal{D}^c}) - 2\mathrm{tr}(\mathbf{Y}_\mathcal{D}^\top\mathbf{X}\mathbf{U} + \mathbf{Y}_{\mathcal{D}^c}^\top\mathbf{X}\mathbf{U}\mathbf{V}^\top) \\ & + \mathrm{tr}(\mathbf{U}^\top\mathbf{X}^\top\mathbf{X}\mathbf{U} + \mathbf{U}^\top\mathbf{X}^\top\mathbf{X}\mathbf{U}\mathbf{V}^\top\mathbf{V}) + n\sum_{\ell=1}^r\sum_{j=1}^p \lambda_{j\ell}|u_{j\ell}|.\end{aligned}$$

The $\hat{\mathbf{U}}^\ell$, the ℓth column of $\hat{\mathbf{U}}$, satisfies the KKT optimality condition

$$\begin{aligned}\frac{\partial\mathcal{L}(\mathbf{U})}{\partial u_{j\ell}}_{|\hat{\mathbf{A}}_\mathcal{D}} = {} & 2(\mathbf{X}^\top)_j(\mathbf{X}\hat{\mathbf{A}}_\mathcal{D} - \mathbf{Y}_\mathcal{D})^\ell + 2(\mathbf{X}^\top)_j(\mathbf{X}\hat{\mathbf{A}}_\mathcal{D}\mathbf{V}^\top - \mathbf{Y}_{\mathcal{D}^c})\mathbf{V}^\ell \\ & + n\lambda_{j\ell}\mathrm{sgn}(\hat{a}_{j\ell}) = 0.\end{aligned} \tag{A.5}$$

First, consider the first term of (A.5). Note that

$$n^{-1/2}(\mathbf{X}^\top)_j(\mathbf{X}\mathbf{A}_\mathcal{D} - \mathbf{Y}_\mathcal{D})^\ell = -n^{-1/2}(\mathbf{X}^\top)_j\mathbf{E}_\mathcal{D}^\ell = O_p(\sqrt{\log p})$$

holds uniformly in j and $\mathcal{D}$. By $||\hat{\mathbf{A}}_\mathcal{D} - \mathbf{A}_\mathcal{D}|| = O_p(\alpha_n)$, we have

$$\begin{aligned} & n^{-1/2}(\mathbf{X}^\top)_j(\mathbf{X}\hat{\mathbf{A}}_\mathcal{D} - \mathbf{Y}_\mathcal{D})^\ell \\ & = n^{-1/2}(\mathbf{X}^\top)_j(\mathbf{X}\mathbf{A}_\mathcal{D} - \mathbf{Y}_\mathcal{D})^\ell + n^{-1/2}(\mathbf{X}^\top)_j\mathbf{X}(\hat{\mathbf{A}}_\mathcal{D} - \mathbf{A}_\mathcal{D})^\ell \\ & = O_p(\sqrt{\log p}) + n^{-1/2}(\mathbf{X}^\top)_j\mathbf{X}O_p(\alpha_n) \\ & = O_p(\sqrt{n}\alpha_n). \end{aligned} \tag{A.6}$$

Next, for the second term of (A.5), observe that

$$\begin{aligned} & n^{-1/2}(\mathbf{X}^\top)_j(\mathbf{X}\hat{\mathbf{A}}_\mathcal{D}\mathbf{V}^\top - \mathbf{Y}_{\mathcal{D}^c}) \\ & = -n^{-1/2}(\mathbf{X}^\top)_j\mathbf{E}_{\mathcal{D}^c} + n^{-1/2}(\mathbf{X}^\top)_j\mathbf{X}(\hat{\mathbf{A}}_\mathcal{D}\mathbf{V}^\top - \mathbf{A}_\mathcal{D}\mathbf{V}^{*\top}) \end{aligned}$$

and consequently,

$$n^{-1/2}(\mathbf{X}^\top)_j(\mathbf{X}\hat{\mathbf{A}}_\mathcal{D}\mathbf{V}^\top - \mathbf{Y}_{\mathcal{D}^c})\mathbf{V}^\ell = O_p(\sqrt{n}\alpha_n) \tag{A.7}$$

holds uniformly in j and $\mathcal{D}$.

Finally, notice that if $\hat{a}_{j\ell} \ne 0$ for $j, \ell \in \mathcal{M}^c(\mathcal{D}_r)$, then $\mathrm{sgn}(\hat{a}_{j\ell}) \ne 0$. Combining (A.6) and (A.7), and the assumption that $n^{1/2}\gamma_{0n}/\sqrt{rp\log p} \to \infty$, then (A.5) will not hold for any $j, \ell \in \mathcal{M}^c(\mathcal{D}_r)$. This is a contradiction, which yields the assertion of this lemma. □

Lemma 3. Suppose Conditions 1–4 are satisfied. The following result holds uniformly for $\mathcal{D}_r$ such that $\mathbf{A}_{\mathcal{D}_r}$ is full-rank: With probability tending to one, there exists a local minimizer $\hat{\mathbf{A}}$ of $\mathcal{L}(\mathbf{U}, \mathbf{V}; \mathcal{D}_r)$ such that $\hat{\mathbf{A}}_{\mathcal{M}^c(\mathcal{D}_r)} = 0$, and $||\hat{\mathbf{A}} - \mathbf{A}|| = O_p(\beta_{n,k})$, where $\beta_{n,k} = \sqrt{r(s_n+q)(\log p/n + \gamma_{1n}^2)}$.

Proof. By Lemma 2, with probability tending to one, $\hat{\mathbf{A}}_{\mathcal{M}^c(\mathcal{D}_r)} = 0$. Hence, it suffices to show that there exists a large constant $C > 0$ such that

$$\Pr\left\{\inf_{||\mathbf{w}||=C}\mathcal{L}(\mathbf{A}_\mathcal{D} + \beta_{n,k}\mathbf{w}) < \mathcal{L}(\mathbf{A}_\mathcal{D}),\ \forall\mathcal{D} \in \mathbb{H}_r(r)\right\} \to 0, \tag{A.8}$$

where $\mathbf{w}_{\mathcal{M}^c(\mathcal{D})} = 0$. The proof of (A.8) follows similarly from the arguments in the proof of Lemma 1, except for the second term of Δ_1. Notice that

$$2\beta_{n,k}\mathrm{tr}(\mathbf{E}_\mathcal{D}^\top\mathbf{X}\mathbf{w}) = O_p(C\beta_{n,k}\sqrt{rns_n\log p}),$$

where we use (A.3) again. Therefore, all the other arguments in the proof of Lemma 1 follows with α_n replaced with β_n. □

Lemma 4. Suppose Conditions 1-5 are satisfied. With probability tending to one, $\mathbf{A}_{\hat{\mathcal{D}}_r}$ is full-rank, where $(\hat{\mathcal{D}}_r, \hat{\mathbf{U}}, \hat{\mathbf{V}})$ is the minimizer of $\mathcal{L}(\mathbf{U}, \mathbf{V}, \mathcal{D}_r; r)$.

Proof. It suffices to show that there exists some $\mathcal{K}_r \in \mathbb{H}_r$,

$$\Pr\left\{\min_{\mathcal{D}_r\in\bar{\mathbb{H}}_r}\min_{\mathbf{U}}\mathcal{L}(\mathbf{U};\mathcal{D}_r) < \mathcal{L}(\mathbf{A}_{\mathcal{K}_r};\mathcal{K}_r)\right\} \to 0. \tag{A.9}$$

Consider $\mathcal{D} \in \bar{\mathbb{H}}_r$. Firstly, by the proof of Lemma 1, we see that

$$\mathcal{L}(\mathbf{U}) = \mathrm{tr}(\mathbf{Y}_{\mathcal{D}}^\top\mathbf{Y}_{\mathcal{D}}) - 2\mathrm{tr}(\mathbf{Y}_{\mathcal{D}}^\top\mathbf{X}\mathbf{U}) + \mathrm{tr}(\mathbf{U}^\top\mathbf{X}^\top\mathbf{X}\mathbf{U}) + \mathcal{L}_2(\mathbf{U}) + n\sum_{\ell\in\mathcal{D}}\sum_{j=1}^{p}\lambda_{j\ell}|u_{j\ell}|.$$

Accordingly,

$$\begin{aligned}
&\min_{\mathbf{U}}\mathcal{L}(\mathbf{U}) - \mathcal{L}(\mathbf{A}_{\mathcal{K}})\\
&\geq \min_{\mathbf{U}}\left[||\mathbf{X}\mathbf{U} - \mathbf{X}\mathbf{A}_{\mathcal{D}}||^2 + \mathrm{tr}\left\{(\mathbf{X}\mathbf{A}_{\mathcal{D}^c})^\top(\mathbf{I}-\mathbf{H}_{\mathbf{U}})\mathbf{X}\mathbf{A}_{\mathcal{D}^c}\right\}\right]\\
&- \max_{\mathbf{U}}\left(2||\mathbf{X}^\top\mathbf{E}_{\mathcal{D}}||||\mathbf{A}_{\mathcal{D}}-\mathbf{U}|| + 2||\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{H}_{\mathbf{U}}\mathbf{X}\mathbf{A}_{\mathcal{D}^c}|| + rns_n\gamma_{1n}C\right)\\
&- \left\{2||\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{X}\mathbf{A}_{\mathcal{D}^c}|| + \mathrm{tr}\left(\mathbf{E}_{\mathcal{K}^c}^\top\mathbf{H}_{\mathbf{A}_{\mathcal{K}}}\mathbf{E}_{\mathcal{K}^c}\right)\right\} := \Delta_1+\Delta_2+\Delta_3,
\end{aligned}$$

where $C > 0$ is a constant.

Denote $c_n = \sqrt{nrp\log p}$. Observe that $||\mathbf{X}^\top\mathbf{E}_{\mathcal{D}}|| = O_p(c_n)$, $||\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{X}\mathbf{A}_{\mathcal{D}^c}|| = O_p(c_n)$, $||\mathbf{E}_{\mathcal{D}^c}^\top\mathbf{H}_{\mathbf{U}}\mathbf{X}\mathbf{A}_{\mathcal{D}^c}|| = O_p(c_n)$ and $\mathrm{tr}(\mathbf{E}_{\mathcal{K}^c}^\top\mathbf{H}_{\mathbf{A}_{\mathcal{K}}}\mathbf{E}_{\mathcal{K}^c}) = O_p(rp\log p)$.

By Condition 5, we know that

$$c_n^{-1}\min_{\mathbf{U}}\left[||\mathbf{X}\mathbf{U} - \mathbf{X}\mathbf{A}_{\mathcal{D}}||^2 + \mathrm{tr}\left\{(\mathbf{X}\mathbf{A}_{\mathcal{D}^c})^\top(\mathbf{I}-\mathbf{H}_{\mathbf{U}})\mathbf{X}\mathbf{A}_{\mathcal{D}^c}\right\}\right] \to \infty,$$

we have either $c_n^{-1}||\mathbf{X}\mathbf{U} - \mathbf{X}\mathbf{A}_{\mathcal{D}}||^2 \to \infty$ or $c_n^{-1}\mathrm{tr}\left\{(\mathbf{X}\mathbf{A}_{\mathcal{D}^c})^\top(\mathbf{I}-\mathbf{H}_{\mathbf{U}})\mathbf{X}\mathbf{A}_{\mathcal{D}^c}\right\} \to \infty$.

Consider the former one. Note that $||\mathbf{X}\mathbf{U} - \mathbf{X}\mathbf{A}_{\mathcal{D}}||^2 \lesssim n\bar{\kappa}||\mathbf{A}_{\mathcal{D}} - \mathbf{U}||^2$ and thus $||\mathbf{A}_{\mathcal{D}} - \mathbf{U}||/\sqrt{c_n/n} \to \infty$. In this case, the $\Delta_1 \geq \min_{\mathbf{U}}||\mathbf{X}\mathbf{U}-\mathbf{X}\mathbf{A}_{\mathcal{D}}||^2$ which dominates Δ_2 and Δ_3. Under the situation that the later one holds, it can be similarly shown that the Δ_1 will dominate the other terms. □

Proof of Theorem 1. Theorem 1 follows immediately from Lemmas 3 and 4. □

Proof of Theorem 2. Consider $k < r$ first. Using the same arguments in the proof of Lemma 4, it can be seen that

$$\min_k \mathrm{BIC}(k) - \mathrm{BIC}(r) \gtrsim \sqrt{nrp\log p} - \sqrt{rp\log p}h_n.$$

It follows immediately that $\Pr(\min_k \mathrm{BIC}(k) > \mathrm{BIC}(r)) \to 1$ as $n \to \infty$, provided that $h_n/\sqrt{n} \to 0$.

For the case $k > r$, we firstly notice that using the same procedure in the proof of Lemma 1, it can be shown that $||\hat{\mathbf{A}}(k) - \mathbf{A}|| = O_p(\beta_{n,k})$. Accordingly,

$$\begin{aligned}
\min_k \mathrm{BIC}(k) - \mathrm{BIC}(r) &\gtrsim O_p(\sqrt{kp\log p}) + (\sqrt{k}-\sqrt{k-1})\sqrt{p\log p}h_n\\
&\geq O_p(\sqrt{kp\log p}) + \frac{1}{2}k^{-1/2}\sqrt{p\log p}h_n,
\end{aligned}$$

which implies that with probability tending to one the case of $k > r$ would not happen as long as $k/h_n \to 0$.

Combining the two cases together implies that any k failing to identify the true low-rank structure cannot be selected as the optimal rank. That is to say, the model associated with the optimal k must be the true one. This completes the proof. □

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