Robust reduced-rank regression

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Abstract

In high-dimensional multivariate regression problems, enforcing low rank in the coefficient matrix offers effective dimension reduction, which greatly facilitates parameter estimation and model interpretation. However, commonly-used reduced-rank methods are sensitive to data corruption, as the low-rank dependence structure between response variables and predictors is easily distorted by outliers. We propose a robust reduced-rank regression approach for joint modeling and outlier detection. The problem is formulated as a regularized multivariate regression with a sparse mean-shift parametrization, which generalizes and unifies some popular robust multivariate methods. An efficient thresholding-based iterative procedure is developed for optimization. We show that the algorithm is guaranteed to converge, and the coordinatewise minimum point produced is statistically accurate under regularity conditions. Our theoretical investigations focus on nonasymptotic robust analysis, which demonstrates that joint rank reduction and outlier detection leads to improved prediction accuracy. In particular, we show that redescending $\psi$-functions can essentially attain the minimax optimal error rate, and in some less challenging problems convex regularization guarantees the same low error rate. The performance of the proposed method is examined by simulation studies and real data examples.

Keywords: low-rank matrix approximation; nonasymptotic analysis; robust estimation; sparsity.
1 Introduction

Given $n$ observations of $m$ response variables and $p$ predictors, denoted by $y_i \in \mathbb{R}^m$ and $x_i \in \mathbb{R}^p$ for $i = 1, \ldots, n$, we consider the multivariate regression model

$$Y = XB^* + \mathcal{E},$$

(1)

where $Y = (y_1, \ldots, y_n)^T$, $X = (x_1, \ldots, x_n)^T$, $B^* \in \mathbb{R}^{p \times m}$ is an unknown coefficient matrix, and $\mathcal{E} = (e_1, \ldots, e_n)^T \in \mathbb{R}^{n \times m}$ is a random error matrix. Such a high-dimensional multivariate problem, in which both $p$ and $m$ may be comparable to or even exceed the sample size $n$, has drawn increasing attention in both applied and theoretical statistics.

Conventional least squares linear regression ignores the multivariate nature of the problem and may fail when $p$ is large relative to $n$. Dimension reduction holds the key to characterizing the dependence between responses and predictors in a parsimonious way. Reduced-rank regression (Anderson, 1951; Izenman, 1975) achieves this by restricting the rank of the coefficient matrix, i.e., by solving the problem

$$\min_{B \in \mathbb{R}^{p \times m}} \text{tr}\{ (Y - XB)\Gamma(Y - XB)^T \} \quad \text{subject to } r(B) \leq r,$$

(2)

where $\text{tr}(\cdot)$ and $r(\cdot)$ denote trace and rank, and $\Gamma$ is a pre-specified positive definite weighting matrix (Reinsel and Velu, 1998). The ranks are typically much smaller than $m$ and $p$. A global solution to (2) can be obtained explicitly. See Reinsel and Velu (1998) for a comprehensive account of reduced-rank regression under the classical large-$n$ asymptotic regime. Finite-sample theories on rank selection and estimation accuracy of the penalized form of reduced-rank regression were developed by Bunea et al. (2011). The nuclear norm and Schatten $p$-norms can also be used to promote sparsity of the singular values of $B$ or $XB$; see Yuan et al. (2007), Koltchinskii et al. (2011), Rohde and Tsybakov (2011), Agarwal et al. (2012), Foygel et al. (2012), Chen et al. (2013), among others. Reduced-rank regression is closely connected with principal component analysis, canonical correlation analysis, partial least squares, matrix completion, and many other multivariate methods (Izenman, 2008).

Although reduced-rank regression can substantially reduce the number of free parameters in multivariate problems, it is extremely sensitive to outliers, which are bound to occur, and thus in real-world data analysis, the low-rank structure could easily be masked or distorted. This is even more serious in high-dimensional or big-data applications. For example, in cancer genetics, multivariate regression...
is commonly used to explore the associations between genotypical and pheno-
typical characteristics (Vounou et al., 2010), where employing rank regularization
can help to reveal latent regulatory pathways linking the two sets of variables. But
pathway recovery should not be distorted by abnormal samples or subjects. As an-
other example, financial time series, even after stationarity transformation, often
contain anomalies or demonstrate heavier tails than those of a normal distribution,
which may jeopardize the recovery of common market behaviors and asset return
forecasting.

Consider the 52 weekly stock log-return data for nine of the ten largest Amer-
ican corporations in 2004 available from the R package MRCE (Rothman et al.,
2010), with $y_t \in \mathbb{R}^9$ ($t = 1, \ldots, T$) and $T = 52$. Chevron was excluded
due to its drastic changes (Yuan et al., 2007). The nine time series are shown
in Figure 1. For the purpose of constructing market factors that drive general
stock movements, a reduced-rank vector autoregressive model can be used, i.e.,
$y_t = B^*y_{t-1} + e_t$, with $B^*$ of low rank. By conditioning on the initial state $y_0$
and assuming the normality of $e_t$, the conditional likelihood leads to a least squares
criterion, so the estimation of $B^*$ can be formulated as a reduced-rank regression
problem (Reinsel, 1997; Lütkepohl, 2007). However, as shown in the figure, sev-
eral stock returns experienced short-term changes, and the autoregressive structure
makes any outlier in the time series also a leverage point in the covariates.

Using the weekly log-returns in the first 26 weeks for training and those in
the last 26 weeks for forecast, we analyzed the data with the reduced-rank re-
gression and the proposed robust reduced-rank regression approach. While both
methods resulted in unit-rank models, the robust reduced-rank regression auto-
matically detected three outliers, i.e., the log-returns of Ford at weeks 5 and 17
and the log-return of General Motors at week 5. These correspond to two real ma-
jor market disturbances attributed to the auto industry. Our robust method au-
tomatically took the outlying samples into account and led to a more reliable
model. Table 1 displays the factor coefficients indicating how the stock returns
are related to the estimated factors, and the $p$-values for testing the associations
between the estimated factors and the individual stock return series using the data
in the last 26 weeks. The stock factor estimated robustly has positive influence
over all nine companies, and overall, it correlates with the series better according
to the reported $p$-values. The out-of-sample prediction errors for least squares,
reduced-rank regression and robust reduced-rank regression are 9.97, 8.85 and
6.72, respectively, when measured by mean square error, and are 5.44, 4.52 and
3.58, respectively, when measured by 40% trimmed mean square error. The ro-
bstification of rank reduction resulted in about 20% improvement in prediction.
Figure 1: Stock return example: scaled weekly log-returns of stocks in 2004. The log-returns of Ford at weeks 5 and 17 and the log-return of General Motors at week 5 are captured as outliers by fitting robust reduced-rank regression with data in the first 26 weeks; the corresponding points are indicated by the circles. The dashed line in each panel separates the series to two parts, i.e., the first 26 weeks for training and the last 26 weeks for testing. The horizontal line in each panel is drawn at zero height.

In this work, we deem explicit outlier detection to be as important as robust low-rank estimation. Indeed, the reduced-rank component may not be of direct interest in some applications, as it often represents common background information shared across the response variables, while capturing unusual changes or jumps is helpful. The robustification of low-rank matrix estimation is non-trivial. A straightforward idea might be to use a robust loss function $\rho$ in place of the squared error loss in (2), leading to

$$\min_B \sum_{i=1}^n \rho(\|\Gamma^{1/2}(y_i - B^T x_i)\|_2) \quad \text{subject to } r(B) \leq r,$$  

but such an estimator may be difficult to compute. To the best of our knowledge, even when $\rho$ is Huber’s loss function (Huber, 1981), there is no algorithm for
Table 1: Stock return example: the factor coefficients showing how the stock returns load on the estimated factors, and the \( p \)-values for testing the associations between the estimated factors and the stock returns using the data in the last 26 weeks

| Stock          | Reduced-rank regression coefficient | Reduced-rank regression \( p \)-value | Robust reduced-rank regression coefficient | Robust reduced-rank regression \( p \)-value |
|----------------|-------------------------------------|-------------------------------------|------------------------------------------|------------------------------------------|
| Walmart        | 0.46                                | 0.44                                | 0.36                                     | 0.23                                     |
| Exxon          | -0.15                               | 0.32                                | 0.14                                     | 0.84                                     |
| General Motors | 0.96                                | 0.42                                | 0.90                                     | 0.02                                     |
| Ford           | 1.20                                | 0.64                                | 0.59                                     | 0.18                                     |
| General Electric | 0.24                           | 0.67                                | 0.32                                     | 0.06                                     |
| Conoco Phillips | -0.04                              | 0.19                                | 0.36                                     | 0.08                                     |
| Citi Group     | 0.27                                | 0.93                                | 0.45                                     | 0.00                                     |
| International Business Machines | 0.36                         | 0.42                                | 0.57                                     | 0.13                                     |
| American International Group | 0.19                         | 0.01                                | 0.58                                     | 0.00                                     |

solving (3), let alone those nonconvex losses which are known to be more effective in dealing with multiple gross outliers with possibly high leverage values. Another motivation is that nonasymptotic theory on the topic is limited. Classical robust analysis, ignoring the low-rank constraint, falls in either deterministic worst-cases studies, or large-\( n \) asymptotics with \( p \) and \( m \) held fixed, which may not meet modern needs.

We propose a novel robust reduced-rank regression method for concurrent robust modeling and outlier identification. We explicitly introduce a sparse mean-shift outlier component and formulate a shrinkage multivariate regression in place of (3), where \( p \) and/or \( m \) can be much larger than \( n \). The robust reduced-rank regression provides a general framework and includes M-estimation and principal component pursuit (Huber, 1981; Hampel et al., 2005; Zhou et al., 2010; Candès et al., 2011). It is worth mentioning that all the techniques developed in this work apply to high-dimensional sparse regression with a single response. In Section 2 we show that low-rank estimation can be ruined by a single rogue point, and propose a robust reduced-rank estimation framework. A universal connection between the proposed robustification and conventional M-estimation is established, regardless of the size of \( p, m \) or \( n \). Section 3 performs finite-sample theoretical studies of the proposed robust estimators, with the intention of pushing classical robust analysis to multivariate data with possible large \( p \) and/or \( m \). A computational algorithm developed in Section 4 is easy to implement and leads to a coordinatewise minimum point with theoretical guarantees. Section 5 shows some real applications. All proofs and simulation studies are given in the Appen-
dices.

The following notation and symbols will be used throughout the paper. We denote by \( \mathbb{N} \) the set of natural numbers. We use \( a \land b \) to denote \( \min(a, b) \) and \( e \) to denote the Euler constant. Let \( [n] = \{1, \ldots, n\} \). Given any matrix \( A \), \( \mathcal{P}_A \) denotes the orthogonal projection matrix onto the range of \( A \), i.e., \( A(A^tA)^{-1}A^t \), where \( ^{-1} \) stands for the Moore–Penrose pseudoinverse. When there is no ambiguity, we also use \( \mathcal{P}_A \) to denote the column space of \( A \). Let \( \| A \|_F \) denote the Frobenius norm, \( \| A \|_2 \) denote the spectral norm, \( \| A \|_0 = \| \text{vec}(A) \|_0 = |\{(i, j) : A(i, j) \neq 0\}| \) with \( | \cdot | \) denoting the cardinality of the enclosed set. For \( A = (a_1 \ldots a_n)^T \in \mathbb{R}^{n \times m}, \| A \|_{2,1} = \sum_{i=1}^n \| a_i \|_2 \), and \( \| A \|_{2,0} = \sum_{i=1}^n 1_{\| a_i \| \neq 0} \) which gives the number of non-zero rows of \( A \). Given \( J \subset [n] \), we often denote \( \sum_{i \in J} \| a_i \|_2 \) by \( \| A_J \|_{2,1} \).

Threshold functions are defined as follows.

**Definition 1** (Threshold function). A threshold function is a real-valued function \( \Theta(t; \lambda) \) defined for \( -\infty < t < \infty \) and \( 0 \leq \lambda < \infty \) such that (i) \( \Theta(-t; \lambda) = -\Theta(t; \lambda) \); (ii) \( \Theta(t; \lambda) \leq \Theta(t'; \lambda) \) for \( t \leq t' \); (iii) \( \lim_{t \to \infty} \Theta(t; \lambda) = \infty \); (iv) \( 0 \leq \Theta(t; \lambda) \leq t \) for \( 0 \leq t < \infty \).

**Definition 2** (Multivariate Threshold function). Given any \( \Theta \), \( \tilde{\Theta} \) is defined for any vector \( a \in \mathbb{R}^m \) such that \( \tilde{\Theta}(a; \lambda) = a \Theta(\| a \|_2; \lambda) / \| a \|_2 \) for \( a \neq 0 \) and 0 otherwise. For any matrix \( A = (a_1 \ldots a_n)^T \in \mathbb{R}^{n \times m}, \tilde{\Theta}(A; \lambda) = \{ \tilde{\Theta}(a_1; \lambda) \ldots \tilde{\Theta}(a_n; \lambda) \}^T \).

## 2 Robust Reduced-Rank Regression

### 2.1 Motivation

Although reduced-rank regression is associated with a highly nonconvex problem \( (2) \), a global minimizer \( \hat{B} \) can be obtained in explicit form. Given any \( r \) \( (1 \leq r \leq \min(m, q)) \) with \( q = r(X) \),

\[
\hat{B}(r) = \mathcal{R}(X, Y, \Gamma, r) = (X^TX)^{-1}X^TY\Gamma^{1/2}\mathcal{P}_{V(X,Y,\Gamma,r)}\Gamma^{-1/2}, \tag{4}
\]

where \( V(X, Y, \Gamma, r) \) is formed by the leading \( r \) eigenvectors of \( \Gamma^{1/2}Y^T\mathcal{P}_X Y \Gamma^{1/2} \). See, e.g., Reinsel and Velu (1998) for a detailed justification. When \( \Gamma = I \), we abbreviate \( \mathcal{R}(X, Y, I, r) \) to \( \mathcal{R}(X, Y, r) \). The reduced-rank regression estimator is denoted by \( \hat{B}(r) \) to emphasize its dependence on the regularization parameter.

Outliers are unavoidable in real data. We define the finite-sample breakdown point for an arbitrary estimator \( \hat{B} \), in the spirit of Donoho and Huber (1983): given
finite data \((X, Y, \Gamma)\) and an estimator \(\hat{B}(X, Y, \Gamma)\), its breakdown point is

\[
e^\star(\hat{B}) = \frac{1}{n} \min \left\{ k \in \mathbb{N} \cup \{0\} : \sup_{\tilde{Y} \in \mathbb{R}^{n \times m} : \|\tilde{Y} - Y\|_0 \leq k} \|X \hat{B}(X, \tilde{Y}, \Gamma)\|_F = +\infty \right\}.
\]

In addition to the reduced-rank regression estimator \(\hat{B}(r)\), we take into account a general low-rank estimator obtained by imposing a singular value penalty

\[
\hat{B}(\lambda) \in \arg\min_B \frac{1}{2} \text{tr}\{(Y - XB)\Gamma(Y - XB)^T\} + \sum_{s=1}^{p \wedge m} P(\sigma_s^{B\Gamma^{1/2}}; \lambda).
\]  

(5)

Here, \(\lambda\) is a regularization parameter, and \(\sigma_s^{B\Gamma^{1/2}}\) denote the singular values of \(B\Gamma^{1/2}\). The penalty \(P\) is constructed from an arbitrary thresholding rule \(\Theta(\cdot; \lambda)\) by

\[
P(t; \lambda) - P(0; \lambda) = P_\Theta(t; \lambda) + q(t; \lambda), \quad P_\Theta(t; \lambda) = \int_0^{[t]} \left[\sup\{s : \Theta(s; \lambda) \leq u\} - u\right] du,
\]  

(6)

for some nonnegative \(q(\cdot; \lambda)\) satisfying \(q(\Theta(s; \lambda); \lambda) = 0, \text{ for all } s \in \mathbb{R}\).

**Theorem 1.** Given any finite \((X, Y, \Gamma)\) and \(r \geq 1\) with \(\Gamma\) positive definite and \(X \neq 0\), let \(\hat{B}(r)\) be a reduced-rank regression estimator which solves (2). Then its finite-sample breakdown point is exactly \(1/n\). Furthermore, for any \(\hat{B}(\lambda)\) given by (5), \(e^\star\{\hat{B}(\lambda)\} = 1/n\) still holds for any finite value of \(\lambda\).

The result indicates that a single outlier can completely ruin low-rank matrix estimation, whether one applies a rank constraint or, say, a Schatten \(p\)-norm penalty. The conclusion limits the use of ordinary rank reduction in big data applications. Because with the low-rank constraint, directly applying a robust loss function, as in (3), may result in nontrivial computational and theoretical challenges, we will apply a novel additive robustification, motivated by She and Owen (2011).

### 2.2 The additive framework

We introduce a multivariate mean-shift regression model to explicitly encompass outliers,

\[
Y = XB^* + C^* + \mathcal{E},
\]  

(7)
where \( B^* \in \mathbb{R}^{p \times m} \) gives the matrix of coefficients, \( C^* \in \mathbb{R}^{n \times m} \) describes the outlying effects on \( Y \), and \( E \in \mathbb{R}^{n \times m} \) has independently and identically distributed rows following \( N(0, \Sigma) \). Obviously, this leads to an over-parameterized model, so we must regularize the unknown matrices appropriately. We assume that \( B^* \) has low rank and \( C^* \) is a sparse matrix with only a few nonzeros because outliers are inconsistent with the majority of the data. Given a positive definite weighting matrix \( \Gamma \), we propose the robust reduced-rank regression problem

\[
\min_{B,C} \frac{1}{2} \text{tr}\{(Y - XB - C)\Gamma(Y - XB - C)^T\} + P(C; \lambda) \quad \text{subject to } r(B) \leq r.
\]

(8)

Here, \( P(\cdot; \lambda) \) is a sparsity-promoting penalty function with \( \lambda \) to adjust the amount of shrinkage, but it can also be a constraint, such as (14). The following form of \( P \) can handle element-wise outliers

\[
P(C; \lambda) = \sum_{i=1}^{n} \sum_{k=1}^{m} P(|c_{i,k}|; \lambda),
\]

(9)

which was used in the stock return analysis. It is more common in robust statistics to assume outlying samples, or outlying rows in \( (Y, X) \), which corresponds to

\[
P(C; \lambda) = \sum_{i=1}^{n} P(\|c_i\|_2; \lambda),
\]

(10)

where \( c_i^T \) is the \( i \)th row vector of \( C \). Unless otherwise specified, we consider row-wise outliers. But all our algorithms and analyses after simple modification can handle element-wise outliers.

In the literature on reduced-rank regression, it is common to regard the weighting matrix \( \Gamma \) as known (Reinsel and Velu, 1998; Yuan et al., 2007; Izenman, 2008). The choice of \( \Gamma \) is flexible and is usually based on a pilot covariance estimate \( \hat{\Sigma} \). For example, it can be \( \hat{\Sigma}^{-1} \) when \( \hat{\Sigma} \) is nonsingular, or a regularized version \( (\hat{\Sigma} + \delta I)^{-1} \) for some \( \delta > 0 \). Although it sounds intriguing to consider jointly estimating the high-dimensional mean and the even higher-dimensional covariance matrix in the presence of outliers, this is beyond the scope of this paper. When a reliable estimate of \( \Sigma \) is unavailable, a standard practice in finance and econometric forecasting is to reduce \( \Gamma \) to a diagonal matrix, or equivalently, an identity matrix after robustly scaling the response variables. For ease of presentation, we
take $\Gamma$ as the identity matrix unless otherwise noted, and mainly focus on the following robust reduced-rank regression criterion,

$$\min_{B,C} \frac{1}{2} \|Y - XB - C\|_F^2 + P(C; \lambda) \quad \text{subject to } r(B) \leq r. \quad (11)$$

We show that the proposed additive outlier characterization indeed comes with a robust guarantee, and interestingly, it generalizes M-estimation to the multivariate rank-deficient setting. We write $Y = (y_1, \ldots, y_n)^T$ and $C = (c_1, \ldots, c_n)^T$.

**Theorem 2.** (i) Suppose $\Theta(\cdot; \lambda)$ is an arbitrary thresholding rule satisfying Definition[7] and let $P$ be any penalty associated with $\Theta$ through [6]. Consider

$$\min_{B,C} \frac{1}{2} \|Y - XB - C\|_F^2 + \sum_{i=1}^n P(\|c_i\|_2; \lambda) \quad \text{subject to } r(B) \leq r. \quad (12)$$

For any fixed $B$, a globally optimal solution for $C$ is $C(B) = \hat{\Theta}(Y - XB; \lambda)$. By profiling out $C$ with $C(B)$, (12) can be expressed as an optimization problem with respect to $B$ only, and it is equivalent to the robust M-estimation problem

$$\min_B \sum_{i=1}^n \rho(\|y_i - B^T x_i\|_2; \lambda) \quad \text{subject to } r(B) \leq r, \quad (13)$$

where the robust loss function $\rho$ is given by

$$\rho(t; \lambda) = \int_0^{|t|} \psi(u; \lambda) \, du, \quad \psi(t; \lambda) = t - \Theta(t; \lambda).$$

(ii) Given $\varrho \in \{0, 1, \ldots, n\}$, consider

$$\min_{B,C} \frac{1}{2} \|Y - XB - C\|_F^2 \quad \text{subject to } r(B) \leq r, \|C\|_{2,0} \leq \varrho. \quad (14)$$

Similarly, (14), after profiling out $C$, can be expressed as an optimization problem with respect to $B$ only, and is equivalent to the rank-constrained trimmed least squares problem

$$\min_B \frac{1}{2} \sum_{i=1}^{n-\varrho} r_i \quad \text{subject to } r(B) \leq r, r_i = \|y_i - B^T x_i\|_2, \quad (15)$$

where $r_1, \ldots, r_n$ are the order statistics of $r_1, \ldots, r_n$ satisfying $|r_1| \leq \cdots \leq |r_n|$.
Remark 1. Theorem 2 connects $P$ to $\rho$ through $\Theta$. As is well known, changing the squared error loss to a robust loss amounts to designing a set of multiplicative weights for $y_i - B^T x_i$ ($i = 1, \ldots, n$). Our additive robustification achieves the same robustness, but leaves the original loss function untouched. The connection is also valid in the case of element-wise outliers, with $P$ and $\rho$ applied in an element-wise manner. In fact, the identity built in Lemma 2 in the Appendices,

$$\frac{1}{2} \{ r - \Theta(r; \lambda) \}^2 + P \{ \Theta(r; \lambda); \lambda \} = \int_0^{|r|} \psi(t; \lambda) \, dt, \quad r \in \mathbb{R},$$

implies that the equivalence holds much more generally, with $B$ subject to an arbitrary constraint or penalty, and regardless of the number of response variables and the number of predictors. This extends the main result in She and Owen (2011) to multiple-response models with $p$ possibly larger than $n$.

Remark 2. Theorem 2 holds for all thresholding rules, and popularly-used convex and nonconvex penalties are all covered by (6). For example, the convex group $\ell_1$ penalty $\lambda \sum ||c_i||_2$ is associated with the soft-thresholding $\Theta_S(s; \lambda) = \text{sgn}(s)(|s| - \lambda)_+$. The group $\ell_0$ penalty $(\lambda^2/2) \sum_{i=1}^n 1_{||c_i||_2 \neq 0}^2$ can be obtained from (6) with the hard-thresholding $\Theta_H(s; \lambda) = s 1_{|s| > \lambda}$, and $q(t; \lambda) = 0.5(\lambda - |t|)21_{0 < |t| < \lambda}$. Our $\Theta$-$P$ coupling framework also covers $\ell_p$ ($0 < p < 1$), the smoothly clipped absolute deviation penalty (Fan and Li, 2001), the minimax concave penalty (Zhang, 2010a), and the capped $\ell_1$ (Zhang, 2010b) as particular instances; see She (2012).

Remark 3. The universal link between (12) and (13) provides insight into the choice of regularization. It is easy to verify that the $\ell_1$-norm penalty as commonly used in variable selection leads to Huber’s loss, which is prone to masking and swamping and may fail with even moderately leveraged outliers occurring. To handle gross outliers, redescending $\psi$ functions are often advocated, which amounts to using nonconvex penalties in (12). For example, Hampel’s three-part $\psi$ (Hampel et al., 2005) can be shown to give Fan and Li’s smoothly clipped absolute deviation penalty, the skipped mean $\psi$ corresponds to the exact $\ell_0$ penalty, and rank constrained least trimmed squares can be rephrased as the $\ell_0$-constrained form as in (14). Our approach not only provides a unified way to robustify low-rank matrix estimation, but facilitates theoretical analysis and computation of reduced-rank M-estimators in high dimensions.
2.3 Connections and extensions

Before we dive into theoretical study, it is worth pointing out some connections and extensions of the proposed framework. First, one can set $\Gamma$ equal to the inverse covariance matrix of the response variables to perform robust canonical correlation analysis; see Reinsel and Velu (1998). Although we mainly focus on the rank-constrained form, there is no difficulty in extending our discussion to

\[
\min_{B,C} \frac{1}{2} \| Y - XB - C \|_F^2 + \sum_{s=1}^{p \land m} P_B(\sigma_s^B; \lambda_B) + P_C(C; \lambda_C),
\]

where $\sigma_s^B$ denote the singular values of $B$, and $P_B$ and $P_C$ are sparsity-inducing penalties.

Our robust reduced-rank regression subsumes a special but important case, $Y = B + C + \mathcal{E}$. This problem is perhaps less challenging than its supervised counterpart, but has wide applications in computer vision and machine learning (Wright et al., 2009; Candès et al., 2011).

Finally, our method can be extended to reduced-rank generalized linear models; see, e.g., Yee and Hastie (2003) and She (2013) for some computational details. In these scenarios, directly robustifying the loss can be messy, but a sparse outlier term can always be introduced without altering the form of the given loss, so that many algorithms designed for fitting ordinary generalized linear models can be seamlessly applied.

3 Nonasymptotic Robust Analysis

Theorem 2 provides robustness and some helpful intuition for the proposed method, but it might not be enough from a theoretical point of view. For example, can one justify the need for robustification in estimating a matrix of low rank? Is using redescending $\psi$ functions still preferable in rank-deficient settings? Different from traditional robust analysis, we cannot assume an infinite sample size and a fixed number of predictors or response variables, because $p$ and/or $m$ can be much larger than $n$ in modern applications. Conducting nonasymptotic robust analysis would be desirable. The finite-sample results in this section contribute to this type of robust analysis.

For simplicity we assume that the model is given by $Y = XB^* + C^* + \mathcal{E}$, where $\mathcal{E}$ has independent and identically distributed $N(0, \sigma^2)$ entries, and consider the robust reduced-rank regression problem defined in (11). The noise distribution
can be more general. For example, in all the following theorems except Theorem 5, \( E \) can be sub-Gaussian. Given an estimator \((\hat{B}, \hat{C})\), we focus on its prediction accuracy measured by \( M(\hat{B} - B^*, \hat{C} - C^*) \), where

\[
M(B, C) = \|XB + C\|_2^2. \tag{17}
\]

This predictive learning perspective is always legitimate in evaluating the performance of an estimator, and requires no signal strength or model uniqueness assumptions. The \( \ell_2 \)-recovery of \( M(\hat{B} - B^*, \hat{C} - C^*) \) is fundamental, and such a bound, together with additional regularity assumptions, can be easily adapted to obtain estimation error bounds in different norms as well as selection consistency (Ye and Zhang, 2010; Lounici et al., 2011); see Theorem 10 in the Appendices for instance. Given a penalty function \( P \), or equivalently, a robust loss \( \rho \), we will study the performance of the set of global minimizers to show the ultimate power of the associated method. But our proof techniques apply more generally; see, e.g., Theorem 7.

For any \( C = (c_1, \ldots, c_n)^T \), define

\[
J(C) = \{i : c_i \neq 0\}, \quad J(C) = |J(C)| = \|C\|_{2,0}. \tag{18}
\]

We use \( r^* = r(B^*) \) to denote the rank of the true coefficient matrix, and \( J^* = J(C^*) \) to denote the number of nonzero rows in \( C^* \), i.e., the number of outliers. Let \( q = r(X) \).

To address problems in arbitrary dimensions, we build some finite-sample oracle inequalities (Donoho and Johnstone, 1994). The first theorem considers a general penalty \( P(C; \lambda) = \sum_{i=1}^n P(\|c_i\|_2; \lambda) \). Here, we assume that \( P(\cdot ; \lambda) \) takes \( \lambda \) as the threshold parameter, and satisfies

\[
P(0; \lambda) = 0, \quad P(t; \lambda) \geq P_H(t; \lambda), \tag{19}
\]

where \( P_H(t; \lambda) = (-t^2/2 + \lambda|t|)1_{|t|<\lambda} + (\lambda^2/2)1_{|t|\geq\lambda} \). The latter inequality is natural in view of (6), because a shrinkage estimator with \( \lambda \) as the threshold is always bounded above by the hard-thresholding function \( \Theta_H(\cdot, \lambda) \). From Theorem 2 (19) covers all \( \psi \)-functions bounded below by the skipped mean \( \psi_H(s; \lambda) = s1_{|s|\leq\lambda} \) for any \( s \geq 0 \).

**Theorem 3.** Let \( \lambda = A(\sigma(m + \log n)^{1/2} \) with \( A \) a constant and let \((\hat{B}, \hat{C})\) be a global minimizer of (11). Then, for any sufficiently large \( A \), the following oracle inequality holds for any \((B, C) \in \mathbb{R}^{p \times m} \times \mathbb{R}^{n \times m}\) satisfying \( r(B) \leq r \):

\[
E\{M(\hat{B} - B^*, \hat{C} - C^*)\} \lesssim M(B - B^*, C - C^*) + \sigma^2(q + m)r + P(C; \lambda) + \sigma^2, \tag{20}
\]
where \( \precsim \) means the inequality holds up to a multiplicative constant.

**Corollary 1.** Under the same conditions of Theorem 3, if \( r \geq 1 \) and \( P \) is a bounded nonconvex penalty satisfying \( P(t; \lambda) \precsim \lambda^2 \) for any \( t \in \mathbb{R} \), we have

\[
E\{ M(\hat{B} - B^*, \hat{C} - C^*) \} \precsim \inf_{(B, C): r(B) \leq r} \{ M(B - B^*, C - C^*) + \sigma^2(q + m)r + \sigma^2J(C)m + \sigma^2J(C)\log n \}.
\]

(21)

**Remark 4.** Both (20) and (21) involve a bias term \( M(B - B^*, C - C^*) \). Setting \( r = r^* \), \( B = B^* \) and \( C = C^* \) in, say, (21), we obtain a prediction error bound of the order

\[
\sigma^2(q + m)r^* + \sigma^2J^*(m + \log n).
\]

(22)

On the other hand, the presence of the bias term ensures applicability of robust reduced-rank regression to weakly sparse \( C^* \), and similarly, \( r \) may also deviate from \( r^* \) to some extent, as a benefit from the bias-variance trade-off.

**Remark 5.** Our proof scheme can also be used to show similar conclusions for the doubly penalized form (16) and the doubly constrained form (14), under the general assumption that the noise matrix has sub-Gaussian marginal tails. The following theorem shows the result for (14) which is one of our favorable forms in practical data analysis.

**Theorem 4.** Let \((\hat{B}, \hat{C})\) be a solution to (14). With the convention \( 0 \log 0 = 0 \), we have

\[
E\{ M(\hat{B} - B^*, \hat{C} - C^*) \} \precsim \inf_{r(B) \leq r, J(C) \leq \theta} M(B - B^*, C - C^*) + \sigma^2\{(q + m)r + \varrho m + \varrho \log(en/\varrho)\} + \sigma^2.
\]

Theorem 4 reveals some breakdown point information as a by-product. Specifically, fixing \( \bar{Y} = XB \), we contaminate \( Y \) in the set \( B(\varrho) = \{ Y \in \mathbb{R}^{n \times m} : Y = \bar{Y} + C + \mathcal{E}, \|C\|_{2,0} \leq \varrho \} \), where vec(\( \mathcal{E} \)) is sub-Gaussian and \( \varrho \in \mathbb{N} \cup \{0\} \). Given any estimator \((\hat{B}, \hat{C})\) which implicitly depends on \( Y \), we define its risk-based finite-sample breakdown point by \( \varepsilon^*(\hat{B}, \hat{C}) = (1/n) \times \min\{\varrho : \sup_{Y \in B(\varrho)} E\{ M(\hat{B} - B, \hat{C} - C) \} = +\infty \} \), where the randomness of the estimator is well accounted by taking the expectation. Then, for the estimator defined by (14), it follows from Theorem 4 that \( \varepsilon^* \geq (\varrho + 1)/n \).

We emphasize that neither Theorem 3 nor Theorem 4 places any requirement on \( X \), in contrast to Theorem 6.
Remark 6. The benefit of applying a re-descending $\psi$ is clearly shown by Theorem 3. As an example, for Huber’s $\psi$, which corresponds to the popular convex $\ell_1$ penalty due to Theorem 2, $P(C; \lambda)$ on the right hand side of (20) is unbounded, while Hampel’s three-part $\psi$ gives a finite rate as shown in (21). Furthermore, we show that in a minimax sense, the error rate obtained in Corollary 1 is essentially optimal. Consider the signal class

$$S(r, J) = \{(B^*, C^*) : r(B^*) \leq r, J(C^*) \leq J\}, \quad 1 \leq J \leq n/2, 1 \leq r \leq q \wedge m.$$  

(23)

Let $\ell(\cdot)$ be a nondecreasing loss function with $\ell(0) = 0, \ell \neq 0$.

Theorem 5. Let $Y = XB^* + C^* + \mathcal{E}$ where $\mathcal{E}$ has independently and identically distributed $N(0, \sigma^2)$ entries. Assume that $n \geq 2, 1 \leq J \leq n/2, 1 \leq r \leq q \wedge m, r(q + m - r) \geq 8$, and $\sigma_{\text{min}}(X)/\sigma_{\text{max}}(X)$ is a positive constant, where $\sigma_{\text{max}}(X)$ and $\sigma_{\text{min}}(X)$ denote the largest and the smallest nonzero singular values of $X$, respectively. Then there exist positive constants $\tilde{c}, c$, depending on $\ell(\cdot)$ only, such that

$$\inf_{(\hat{B}, \hat{C})} \sup_{(B^*, C^*) \in S(r, J)} E(\ell[M(\hat{B} - B^*, \hat{C} - C^*)/\{\tilde{c}P_o(J, r)\}]) \geq c > 0, \quad (24)$$

where $(\hat{B}, \hat{C})$ denotes any estimator of $(B^*, C^*)$ and

$$P_o(J, r) = \sigma^2\{r(q + m) + Jm + J \log(en/J)\}. \quad (25)$$

We give some examples of $\ell$ to illustrate the conclusion. Using the indicator function $\ell(u) = 1_{u \geq 1}$, for any estimator $(\hat{B}, \hat{C}), M(\hat{B} - B^*, \hat{C} - C^*) \geq \sigma^2\{r(q + m) + Jm + J \log(en/J)\}$ holds with positive probability. For $\ell(u) = u$, Theorem 5 shows that the risk $E\{M(\hat{B} - B^*, \hat{C} - C^*)\}$ is bounded from below by $P_o(J, r)$, up to some multiplicative constant. Therefore, (22) attains the minimax optimal rate up to a mild logarithm factor, showing the advantage of utilizing re-descending $\psi$’s in robust low-rank estimation. The analysis is nonasymptotic and applies to any $n, p, \text{ and } m$.

Convex methods are not hopeless, however. In some less challenging problems, where some incoherence regularity condition is satisfied by the augmented design matrix, Huber’s $\psi$ can achieve the same low error rate. The result of the following theorem can be extended to any sub-additive penalties with the associated $\psi$ sandwiched by Huber’s $\psi$ and $\psi_H$. 


**Theorem 6.** Let \((\hat{B}, \hat{C}) = \arg \min_{(B,C)} \|Y - XB - C\|_F^2/2 + \lambda \|C\|_{2,1}\) subject to \(r(B) \leq r\), \(\lambda = A\sigma(m + \log n)^{1/2}\) where \(A\) is a large enough constant. Then
\[
E\{M(\hat{B} - B^*, \hat{C} - C^*)\} \lesssim M(B - B^*, C - C^*) + \sigma^2 + \sigma^2(q + m)r + \sigma^2K^2J(C)(m + \log n) \tag{26}
\]
for any \((B, C)\) with \(\text{rank}(B) \leq r\), if given \(\mathcal{J} = \mathcal{J}(C)\), \(X\) satisfies \((1 + \vartheta)|C'_{\mathcal{J}}|_{2,1} \leq \|C'_{\mathcal{J}}\|_{2,1} + K|\mathcal{J}|^{1/2}\|I - P_{r}\|_F\) for all \(C'\) and \(P_r : P_r \subset P_X, r(P_r) \leq 2r\), where \(K \geq 0\) and \(\vartheta\) is a positive constant.

Compared with (21), (26) has an additional factor of \(K\) on the right-hand side. Under a different regularity condition, an estimation error bound on \(B^*\) can be obtained. See Theorem 10.

**Remark 7.** The results obtained can be used to argue the necessity of robust estimation when outliers occur. Similar to Theorem 3, we can show that the ordinary reduced-rank regression, which sets \(\hat{C} = 0\), satisfies
\[
E\{M(\hat{B} - B^*, \hat{C} - C^*)\} \lesssim \inf_{r(B) \leq r} \|XB - (XB^* + C^*)\|_F^2 + \sigma^2(q + m)r + \sigma^2. \tag{27}
\]

Taking \(r = r^*\), the error bound of the reduced-rank regression, evaluated at the optimal \(B\) satisfying \(XB = XB^* + P_{XB^*}C^*\) and \(r(B) \leq r\), is of order
\[
\sigma^2(q + m)r^* + \|(I - P_{XB^*})C^*\|_F^2. \tag{28}
\]
Because \(XB^*\) has low rank, \(I - P_{XB^*}\) is not null in general. Notable outliers that can affect the projection subspace in performing rank reduction tend to occur in the orthogonal complement of the range of \(XB^*\), and so (28) can be arbitrarily large, which echoes the deterministic breakdown-point conclusion in Theorem 1.

To control the size of the bias term, a better way is to apply a larger rank value in the presence of outliers. Concretely, setting \(B = B^* + (X^TX)^{-1}X^T(C^* - B^*)\) in (27) yields
\[
\sigma^2J^*q + \sigma^2J^*m + \sigma^2(q + m)r^* + \|(I - P_X)C^*\|_F^2, \tag{29}
\]
where we used \(r(B) \leq r^* + J^*\). When \(p > n\), \(P_X = I\), and so (29) offers an improvement over (28) by giving a finite error rate of \(\sigma^2J^*q + \sigma^2J^*m + \sigma^2(q + m)r^*\). But our robust reduced-rank regression guarantees a consistently lower rate at \(\sigma^2J^* \log n + \sigma^2J^*m + \sigma^2(q + m)r^*\), since \(\sigma^2J^*q \gg \sigma^2J^* \log n\). The performance gain can be dramatic in big data applications, where the design matrix is huge and typically multiple outliers are bound to occur.
4 Computation and Tuning

In this section, we show that compared with the M-characterization in Theorem 2 the additive formulation (7) simplifies computation and parameter tuning. Let us consider a penalized form of the robust reduced-rank regression problem

$$\min_{B,C} F(B, C) = \frac{1}{2} \|Y - XB - C\|^2_F + \sum_{i=1}^n P(\|c_i\|_2; \lambda) \text{ subject to } r(B) \leq r.$$  \hfill (30)

The penalties of interest may be nonconvex in light of the theoretical results in Section 3 as stringent incoherence assumptions associated with convex penalties can be much relaxed or even removed. Assuming that $P$ is constructed by (6), a simple algorithm for solving (30) is described as follows, where the two matrices $C$ and $B$ are alternatingly updated with the other held fixed until convergence. Here, the multivariate thresholding, $\tilde{\Theta}$, is defined on basis of $\Theta$, cf. Definition 1 and Definition 2.

Algorithm 1: A robust reduced-rank regression algorithm.

Input $X, Y, C^{(0)}, B^{(0)}, \Theta, t = 0$.
Repeat
(a) $t \leftarrow t + 1$
(b) $C^{(t+1)} \leftarrow \tilde{\Theta}(Y - XB^{(t)}; \lambda)$
(c) $B^{(t+1)} \leftarrow R(X, Y - C^{(t+1)}; r)$, as defined in (4)
Until convergence.

Step (b) performs simple multivariate thresholding operations and Step (c) does reduced-rank regression on the adjusted response matrix $Y - C^{(t+1)}$. We do not really have to explicitly compute $B$ to update $C$ in the iterative process. In fact, only $XB^{(t)}$ is needed, which depends on $X$ through $P_X$, or $I$ when $p \gg n$. The eigenvalue decomposition called in (4) has low computational complexity because the rank values of practical interest are often small. Algorithm 1 is simple to implement and is cost-effective. For example, even for $p = 1200$ and $n = m = 100$, it takes only about 40 seconds to compute a whole solution path for a two-dimensional grid of 100 values of $\lambda$ and 10 rank values.
Theorem 7. Let \( \Theta \) be an arbitrary thresholding rule, and \( F \) be defined in (30), where \( P \) is associated with \( \Theta \) through (5). Then given any \( \lambda \geq 0 \) and \( r \geq 0 \), the proposed algorithm has the property that \( F(B(t), C(t)) \geq F(B(t+1), C(t+1)) \) for all \( t \), and so \( F(B(t), C(t)) \) converges as \( t \to \infty \). Furthermore, under the assumptions that \( \tilde{\Theta}(\cdot; \lambda) \) is continuous in the closure of \( \{Y - XB(t)\} \) and \( \{B(t)\} \) is uniformly bounded, any accumulation point of \( (B(t), C(t)) \) is a coordinatewise minimum point, and a stationary point when \( q(\cdot; \lambda) \equiv 0 \), and hence \( F(B(t), C(t)) \) converges monotonically to \( F(B^*, C^*) \) for some coordinatewise minimum point \((B^*, C^*)\).

The algorithm can be slightly modified to deal with (9), (14), and (16). For example, we can replace \( \tilde{\Theta} \) by \( \Theta \), applied componentwise, to handle element-wise outliers. The \( \ell_0 \)-penalized form with \( P(C; \lambda) = (\lambda^2/2)\|C\|_{2,0} \), as well as the constrained form (14), will be used in data analysis and simulation. In implementation, they correspond to applying hard-thresholding and quantile-thresholding operators (She et al., 2013).

In common with most high breakdown algorithms in robust statistics, we recommend using the multi-sampling iterative strategy (Rousseeuw and van Driessen, 1999). But in many practical applications, we found that the initial values can be made rather freely. Indeed, Theorem 8 shows that if the problem is regular, our algorithm guarantees low statistical error even without the multi-start strategy.

In the following theorem, given \( \Theta \), define \( L_\Theta = 1 - \text{ess inf} \{ d\Theta^{-1}(u; \lambda)/du : u \geq 0 \} \), where \( \text{ess inf} \) is the essential infimum. By definition, \( L_\Theta \leq 1 \). We use \( P_{2,\Theta}(C; \lambda) \) to denote \( \sum_{i=1}^n P_\Theta(||c_i||_2; \lambda) \) for short and set \( r = (1 + \alpha)r^* \) with \( \alpha \geq 0 \) and \( r^* \geq 1 \).

Theorem 8. Let \( (\hat{B}, \hat{C}) \) be any solution satisfying \( \hat{B} = \mathcal{R}(X, Y - \hat{C}, r) \) and \( \hat{C} = \tilde{\Theta}(Y - XB; \lambda) \) with \( \hat{B} \) of rank \( r \) and \( \tilde{\Theta} \) continuous at \( Y - XB \). Let \( \Theta \) be associated with a bounded nonconvex penalty as described in Corollary 7 and \( \lambda = A\sigma(m + \log n)^{1/2} \) with \( A \) a large enough constant. Assume that \( (1 + \alpha)^{-1/2}||XB - XB^*||_F^2 + L_\Theta||C - C^*||_F^2 + \vartheta P_{2,H}(C - C^*; \lambda) \leq (2 - \delta)M(B - B^*, C - C^*) + 2P_{2,\Theta}(C; \lambda) + \zeta P_{2,0}(C^*; \lambda) \) holds for all \( (B, C) \) satisfying \( r(B) \leq r \), where \( \zeta \geq 0 \), \( \delta > 0 \) and \( \vartheta > 0 \) are constants. Then \( E\{M(\hat{B} - B^*, \hat{C} - C^*)\} \lesssim \sigma^2(1 + \alpha)(q + m) + \sigma^2J^*m + \sigma^2J^* \log n \).

To choose an optimal rank for \( B \) and an optimal row support for \( C \) jointly, cross-validation appears to be an option. However, it lacks theoretical support in the robust low-rank setting, and for large-scale problems, cross-validation can be
quite expensive. Motivated by Theorem 5, we propose the predictive information criterion

\[ \log \| Y - XB - C \|_F^2 + \frac{1}{mn} [A_1 \{ Jm + (m + q - r)r \} + A_2 J \log(en/J)], \tag{31} \]

where \( \| Y - XB - C \|_F^2 \) is the residual sum of squared errors, \( r = r(B) \), \( J = \| C \|_{2,0} \), and recall that \( e \) denotes the Euler constant. The term \( Jm + (m + q - r)r \) counts the degrees of freedom of the obtained model, and \( J \log(en/J) \) characterizes the risk inflation. The benefits of the criterion include no noise scale parameter needs to be estimated, and minimizing (31) achieves the minimax optimal error rate when the true model is parsimonious, as is shown below.

**Theorem 9.** Let \( P(B, C) = Jm + (m + q - r)r + J \log(en/J) \), where \( r = r(B) \) and \( J = \| C \|_{2,0} \). Suppose that the true model is parsimonious in the sense that \( P(B^*, C^*) < mn/A_0 \) for some constant \( A_0 > 0 \). Let \( \delta(B, C) = AP(B, C)/(mn) \) where \( A \) is a positive constant satisfying \( A < A_0 \), and so \( \delta(B^*, C^*) < 1 \). Then for sufficiently large values of \( A_0 \) and \( A \), any \((\hat{B}, \hat{C})\) that minimizes \( \log \| Y - XB - C \|_F^2 + \delta(B, C) \) subject to \( \delta(B, C) < 1 \) satisfies \( M(\hat{B} - B^*, \hat{C} - C^*) \lesssim \sigma^2 \{ J^*m + (m + q - r^*)r^* + J^* \log(en/J^*) \} \) with probability at least \( 1 - c_1n^{-c_1} - c_2 \exp(-c_2mn) \) for some constants \( c_1, c_1', c_2, c_2' > 0 \).

Based on computer experiments, we set \( A_1 = 7, A_2 = 2 \).

## 5 Arabidopsis Thaliana Data

We performed extensive simulation studies to compare our method with some classical robust multivariate regression approaches and several reduced-rank methods (Tatsuoka and Tyler, 2000; Aelst and Willems, 2005; Roelant et al., 2009; Reinsel and Velu, 1998; Bunea et al., 2011; Mukherjee and Zhu, 2011) in both low and high dimensions. The results are reported in the Appendices and show the excellent performance of the proposed method.

Isoprenoids are abundant and diverse in plants, and they serve many important biochemical functions and have roles in respiration, photosynthesis and regulation of growth and development in plants. To examine the regulatory control mechanisms in the gene network for isoprenoid in Arabidopsis thaliana, a genetic association study was conducted, and with \( n = 118 \) GeneChip microarray experiments performed to monitor gene expression levels under various experimental conditions (Wille et al., 2004). It was experimentally verified that there
exist strong connections between some downstream pathways and two isoprenoid biosynthesis pathways. We thus considered a multivariate regression setup, with the expression levels of \( p = 39 \) genes from the two isoprenoid biosynthesis pathways serving as predictors, and the expression levels of \( m = 62 \) genes from four downstream pathways, namely plastoquinone, carotenoid, phytosterol and chlorophyll, serving as the responses.

Because of the small sample size relative to the number of unknowns, we applied robust reduced-rank regression with the predictive information criterion for parameter tuning. The final model has rank five, which reduces the effective number of unknowns by about 80% compared with the least squares model. Interestingly, our method also identified two outliers, samples 3 and 52. Figure 2 shows the detection paths by plotting the \( \ell_2 \) norm of each row in the \( C \)-estimates for a sequence of values of \( \lambda \). The two unusual samples are distinctive. The outlyingness might be caused by different experimental conditions. In particular, sample 3 was the only sample with Arabidopsis tissue culture in a baseline experiment. The two outliers have a surprisingly big impact on both coefficient estimation and model prediction. This can be seen from \( \| \hat{B} - \tilde{B} \|_F / \| \tilde{B} \|_F \approx 50\% \), and \( \| X \hat{B} - X \tilde{B} \|_F / \| X \tilde{B} \|_F \approx 26\% \), where \( \hat{B} \) and \( \tilde{B} \) denote the robust reduced-rank regression and the plain reduced-rank regression estimates, respectively. In addition, Figure 2 reveals that sample 27 could be a potential outlier which merits further investigation.

![Figure 2: Arabidopsis thaliana data: outlier detection paths by the robust reduced-rank regression. Sample 3 and sample 52 are captured as outliers, whose paths are shown as a dotted line and a dashed line, respectively. The path plot also suggests sample 27 as a potential outlier.](image-url)
The low-rank model obtained reveals robust score variables, or factors, constructed from isoprenoid biosynthesis pathways, in response to the 62 genes on the four downstream pathways. Let \( \hat{X} \) denote the design matrix after removing the two detected outliers, and \( \hat{U} \hat{D} \hat{V}^T \) be the singular value decomposition of \( \hat{X} \hat{B} \). Then \( \hat{U} \) delivers five orthogonal factors, and \( \hat{V} \hat{D} \) gives the associated factor coefficients. Figure 3 plots the coefficients of the first three leading factors for all 62 response variables. Given the \( s \)th factor \( (s = 1, 2, 3) \), the genes are grouped into the four pathways separated by vertical lines, and two horizontal lines are placed at heights \( \pm \sigma_s \hat{X} \hat{B} m^{-1/2} \). Therefore, the genes located beyond the two horizontal lines have relatively large coefficients on the corresponding factor in magnitude.

Figure 3: Arabidopsis thaliana data: factor coefficients of the 62 response genes from plastoquinone, carotenoid, phytosterol, and chlorophyll pathways. The panels from left to right correspond to the top three factors estimated by the robust reduced-rank regression. For the \( s \)th factor \( (s = 1, 2, 3) \), two horizontal lines are plotted at heights \( \pm \sigma_s \hat{X} \hat{B} m^{-1/2} \), and three vertical lines separate the genes into different pathways.

We also tested the significance of the factors in response to each of the 62 genes; see Table 2. Plastoquinone was excluded since it has only two genes and its behavior couples with that of carotenoid most of the time. Even with the family-wise error rate controlled at 0.01, the factors obtained are overall predictive according to the significance percentages, although they play very different roles.
Table 2: Arabidopsis thaliana data: percentage of genes on each response pathway that show significance of a given factor, with the family-wise error rate controlled at level 0.01

| Pathway    | Number of genes | Factor 1 | Factor 2 | Factor 3 |
|------------|-----------------|----------|----------|----------|
| Carotenoid | 11              | 55%      | 73%      | 9%       |
| Phytosterol| 25              | 20%      | 48%      | 32%      |
| Chlorophyl | 24              | 75%      | 21%      | 0%       |

in different pathways. In fact, according to Figure 3 and Table 2, the genes that are correlated with the first factor are mainly from carotenoid and chlorophyll, and almost all the coefficients there are negative. It seems that the first factor interprets some joint characteristics of carotenoid and chlorophyll. The second factor differentiates phytosterol genes from carotenoid genes, and the third factor seems to mainly contribute to the phytosterol pathway. Therefore, by projecting the data onto a proper low-dimensional subspace in a supervised and robust manner, distinct behaviors of the downstream pathways and their potential subgroup structures can be revealed. More biological insights could be gained by closely examining the experimental and background conditions.

Appendices

A Proofs

A.1 Notation and definitions

Given $\mathcal{I} \subset [n], \mathcal{J} \subset [p]$, $X(\mathcal{I}, \mathcal{J})$ denotes a submatrix of $X$ by extracting the rows and columns indexed by $\mathcal{I}$ and $\mathcal{J}$, respectively. We use $c, L$ to denote constants. They are not necessarily the same at each occurrence. Denote by $CS(A)$ the column space of $A$. Given $P_A$, denote by $P_A^\perp$ the projection onto its orthogonal complement. In addition to the definitions of thresholding function $\Theta$ and the multivariate thresholding function $\vec{\Theta}$, we will use a matrix threshold function.

**Definition 3** (Matrix threshold function). Given any threshold function $\Theta(\cdot; \lambda)$, its matrix version $\Theta^\sigma$ is defined for $B \in \mathbb{R}^{n \times m}$ as follows

$$\Theta^\sigma(B; \lambda) = U \text{diag} \{ \Theta(\sigma^B_i; \lambda) \} V^T,$$

where $U, V,$ and $\sigma^B_i$ are obtained from the SVD of $B$: $B = U \text{diag}(\sigma^B_i)V^T$. 

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Finally, we describe a quantile thresholding \( \Theta^\#(\cdot; \varrho, \eta) \) which is convenient in analyzing the constraint-type problems. It can be seen as a vector variant of the hard-ridge thresholding \( \Theta_{HR}(t; \lambda, \eta) = t / (1 + \eta)^{1/2} \) \( |t| > \lambda \) \cite{She2009}. Given \( 1 \leq \varrho \leq n \) and \( \eta \geq 0 \), \( \Theta^\#(a; \varrho, \lambda) : \mathbb{R}^n \rightarrow \mathbb{R}^n \) is defined for any \( a \in \mathbb{R}^n \) such that the \( \varrho \) largest components of \( a \), in absolute value, are shrunk by a factor of \( (1 + \lambda) \) and the remaining components are all set to be zero. In the case of ties, a random tie breaking rule is used. We abbreviate \( \Theta^\#(a; \varrho, 0) \) to \( \Theta^\#(a; \varrho) \).

### A.2 Proof of Theorem 1

We show the proof detail for the penalized estimators. First, the loss term in the objective can be decomposed into

\[
\text{tr}\{(Y - XB)\Gamma(Y - XB)^T\} = \|Y\Gamma^{1/2} - X\Gamma^{1/2}\|_F^2 = \|P_XY\Gamma^{1/2} - X\Gamma^{1/2}\|_F^2 + \|P_X^\perp Y\Gamma^{1/2}\|_F^2.
\]

Let \( Z = P_XY\Gamma^{1/2} \). Clearly, \( P_X \subset P_Z \). Consider the following optimization problem

\[
\min_A \frac{1}{2}\|Z - A\|_F^2 + \sum_{s=1}^{p\land m} P(\sigma_A^s; \lambda) . \tag{33}
\]

From the proof of Proposition 2.1 in \cite{She2013}, the following results can be obtained: (i) any optimal solution \( \hat{A} \) to (33) must satisfy \( \hat{A} \in P_Z \); (ii) \( A_o = \Theta^\sigma(Z; \lambda) \) gives a particular minimizer of (33), and \( \|\hat{A} - A_o\|_* \leq C(\lambda) \) holds for any \( \hat{A} \), where \( \|\cdot\|_* \) represents the nuclear norm and \( C(\lambda) \) is a function dependent on the regularization parameter only. From (i), \( X\hat{B}\Gamma^{1/2} \) is always a solution to (33). It suffices to study the breakdown point of \( A_o \).

Because \( X \neq 0 \), there must exist \( i \in [n] \) such that the \( i \)th column of \( P_X \) is not 0. Let \( \tilde{Y} = Y + Me_i e_i^T \), where \( e_i \) is the unit vector with the \( i \)th entry being 1. Due to the construction of \( \tilde{Y} \) and the positive-definiteness of \( \Gamma \),

\[
\|P_X\tilde{Y}\Gamma^{1/2}\|_F^2 = M^2\|P_X e_i e_i^T\Gamma^{1/2}\|_F^2 + 2M\langle P_X Y, e_i e_i^T \Gamma \rangle + \|P_X Y\Gamma^{1/2}\|_F^2 \rightarrow +\infty
\]

as \( M \rightarrow \infty \). That is, given \( \lambda \), \( \Theta^\sigma(\mathcal{P}_X\tilde{Y}\Gamma^{1/2}; \lambda) \) thresholds the singular values of \( \mathcal{P}_X\tilde{Y}\Gamma^{1/2} \) the sum of which can be made arbitrarily large as \( M \) increases. It follows from the definition of \( \Theta \) that \( \sup_M \|\Theta^\sigma(\mathcal{P}_X\tilde{Y}\Gamma^{1/2}; \lambda)\|_F = \infty \).

The proof for the reduced-rank regression estimator follows similar lines and is omitted.
A.3 Proof of Theorem 2

Part (i): The proof of this part is based on the following two lemmas.

**Lemma 1.** Given an arbitrary thresholding rule \( \Theta \) satisfying Definition 1 in the paper, let \( P \) be any function associated with \( \Theta \) through

\[
P(t; \lambda) - P(0; \lambda) = P_\Theta(t; \lambda) + q(t; \lambda), \quad P_\Theta(t; \lambda) = \int_0^{t|} \sup \{s : \Theta(s; \lambda) \leq u\} - u\, du,
\]

for some nonnegative \( q(\theta; \lambda) \) satisfying \( q(\Theta(t; \lambda)) = 0 \) for all \( t \). Then, \( \hat{\beta} = \vec{\Theta}(y; \lambda) \) gives a globally optimal solution to

\[
\min_{\beta \in \mathbb{R}^n} \frac{1}{2} \|y - \beta\|_2^2 + P(\|\beta\|_2; \lambda).
\]

This result is implied by Lemma 1 of [She (2012)](#). It is worth mentioning that \( \vec{\Theta}(y; \lambda) \) is not necessarily unique when \( \Theta \) has discontinuities. Next we prove an identity.

**Lemma 2.** Given any thresholding rule \( \Theta(t; \lambda) \), define \( P_\Theta(t; \lambda) = \int_0^{t|} \Theta^{-1}(u; \lambda) - u\, du \) where \( \Theta^{-1}(u; \lambda) = \sup \{t : \Theta(t; \lambda) \leq u\} \). Then the following identity holds for any \( r \in \mathbb{R} \)

\[
\frac{1}{2} \{r - \Theta(r; \lambda)\}^2 + P_\Theta(\Theta(r; \lambda); \lambda) = \int_0^{|r|} \psi(t; \lambda) \, dt, \tag{34}
\]

where \( \psi(t; \lambda) = t - \Theta(t; \lambda) \).

**Proof.** Without loss of generality, assume \( r \geq 0 \). By definition, \( \int_0^r \psi(t; \lambda) \, dt = r^2/2 - \int_0^r \Theta(t; \lambda) \, dt \) and \( P_\Theta(\Theta(r; \lambda); \lambda) = \int_0^{\Theta(r; \lambda)} \Theta^{-1}(t; \lambda) \, dt - r^2/2 \). It suffices to show that

\[
\int_0^{\Theta(r; \lambda)} \Theta^{-1}(t; \lambda) \, dt + \int_0^r \Theta(t; \lambda) \, dt = r \Theta(r; \lambda).
\]

In fact, changing the order of integration, and using the monotone property of \( \Theta \), we get

\[
\int_0^r \Theta(t; \lambda) \, dt - r \Theta(r; \lambda) = \int_0^r dt \int_0^{\Theta(t; \lambda)} ds - \int_0^{\Theta(r; \lambda)} r \, dt
\]

\[
= \int_0^{\Theta(r; \lambda)} ds \int_0^{\Theta^{-1}(s; \lambda)} dt - \int_0^{\Theta(r; \lambda)} r \, dt
\]

\[
= - \int_0^{\Theta(r; \lambda)} \Theta^{-1}(t; \lambda) \, dt.
\]
The conclusion thus follows. □

We have the pieces in place to prove part (i) of the theorem. Without loss of generality, assume $\Gamma = I$. Let $f(B, C) = \text{tr}\{(Y - XB - C)(Y - XB - C)^T\}/2 + \sum_{i=1}^{n} P(\|\Gamma^{1/2}c_i\|_2; \lambda)$, and $g(B) = \sum_{i=1}^{n} \rho(\|y_i - B^Tx_i\|_2; \lambda)$. By Lemma [1] fixing $B$, $\hat{C} = (c_1 \ldots c_n)^T$ with $\hat{c}_i = \hat{\Theta}(y_i - B^Tx_i; \lambda)$ gives an optimal solution to $\min_C f(B, C)$. For this $\hat{C}$, $f(B, \hat{C}) = g(B)$ holds by Lemma [2].

Part (ii): The proof follows similar lines of that of Part (i), based on the quantile thresholding and Lemma C.1 in [She et al., 2013]. The details are omitted.

### A.4 Proofs of Theorem 3 & Theorem 6

Recall that $P_1(t; \lambda) = \lambda|t|$, $P_0(t; \lambda) = (\lambda^2/2)1_{t\neq 0}$, $P_H(t; \lambda) = (-t^2/2+\lambda|t|)1_{|t|<\lambda} + (\lambda^2/2)1_{|t|\geq \lambda}$. For convenience, $P_2(1; \lambda)$ is used to denote $\lambda\|C\|_{2,1}$, and $P_{2,0}$ and $P_{2,H}$ are used similarly.

By definition, $(\hat{B}, \hat{C})$ satisfies the following inequality for any $(B, C)$ with $r(B) \leq r$,

$$\frac{1}{2} M(\hat{B} - B^*, \hat{C} - C^*) \leq \frac{1}{2} M(B - B^*, C - C^*) + P(C; \lambda) - P(\hat{C}; \lambda) + \langle \mathcal{E}, X\Delta B + \Delta C \rangle.$$

(35)

Here, $\Delta B = \hat{B} - B$, $\Delta C = \hat{C} - C$ and so $r(\Delta B) \leq 2r$.

**Lemma 3.** For any given $1 \leq J \leq n$, $1 \leq r \leq m \land p$, define $\Gamma_{r,J} = \{(B, C) \in \mathbb{R}^{p \times m} \times \mathbb{R}^{n \times m} : r(B) \leq r, J(C) = J\}$. Then there exist universal constants $A_0, C, c > 0$ such that for any $a \geq 2b > 0$, the following event

$$\sup_{(B, C) \in \Gamma_{r,J}} \left\{ 2\langle \mathcal{E}, XB + C \rangle - \frac{1}{a}\|XB + C\|_F^2 - \frac{1}{b}P_{2,H}(C; \lambda) - aA_0\sigma^2 r(m + q) \right\} \geq a\sigma^2 t$$

(36)

occurs with probability at most $c' \exp(-ct)$, where $\lambda = A\lambda^0$, $\lambda^0 = \sigma(m + \log n)^{1/2}$, $A = (abA_1)^{1/2}$, $A_1 \geq A_0$, and $t \geq 0$.

Let $l_H(B, C, r) = 2\langle \mathcal{E}, XB + C \rangle - \|XB + C\|_F^2/a - P_{2,H}(C; \lambda)/b - aA_0\sigma^2 r(m + q)$. Define

$$R = \sup_{1 \leq J \leq n, 1 \leq r \leq m \land p} \sup_{(B, C) \in \Gamma_{r,J}} l_H(B, C, r).$$
From Lemma 3, it is easy to see $ER \leq aco^2$. Substituting the bound below into (35),

$$2\langle E, X \Delta B + \Delta C \rangle \leq \frac{1}{a} \|X \Delta B + \Delta C\|_F^2 + \frac{1}{b} P_{2,H}(\Delta^C; \lambda) + 2aA_0\sigma^2 r(m + q) + R$$

\begin{align*}
&\leq \frac{2}{a} M(B - B^*, C - C^*) + \frac{2}{a} M(\hat{B} - B^*, \hat{C} - C^*) \\
&\quad + 2aA_0\sigma^2 r(m + q) + R + \frac{1}{b} P_{2,H}(\Delta^C; \lambda),
\end{align*}

we have

$$(1 - \frac{2}{a})M(\hat{B} - B^*, \hat{C} - C^*) \leq (1 + \frac{2}{a})M(B - B^*, C - C^*) + 2aA_0\sigma^2 r(m + q) + R$$

\begin{align*}
&\quad + 2P(C; \lambda) - 2P(\hat{C}; \lambda) + \frac{1}{b} P_{2,H}(\Delta^C; \lambda).
\end{align*}

It remains to deal with $2P(C; \lambda) - 2P(\hat{C}; \lambda) + P_{2,H}(\Delta^C; \lambda)/b$ which is denoted by $I$ below.

(i) Due to the sub-additivity of the function $P_H$ that is concave on $[0, \infty)$,

\begin{align*}
I &\leq 2P(C; \lambda) - 2P_{2,H}(\hat{C}; \lambda) + \frac{1}{b} P_{2,H}(\Delta^C; \lambda) \\
&\leq 2P(C; \lambda) + \frac{1}{b} P_{2,H}(C; \lambda) + \frac{1}{b} P_{2,H}(\hat{C}; \lambda) - 2P_{2,H}(\hat{C}; \lambda) \\
&\leq (2 + \frac{1}{b})P(C; \lambda),
\end{align*}

if $b \geq 1/2$. Theorem 3 can be obtained by choosing $a = 4$, $b = 1/2$, and $\lambda = \lambda^o$ with $A \geq (2A_0)^{1/2}$.

(ii) When $P$ is the group $\ell_1$ penalty as in Theorem 6, by the sub-additivity of $P$, we have

\begin{align*}
I &\leq 2P_{2,1}(C; \lambda) - 2P_{2,1}(\hat{C}; \lambda) + \frac{1}{b} P_{2,1}(\Delta^C; \lambda) \\
&\leq 2A\lambda^o \{(1 + \theta)\|\Delta^C_j\|_{2,1} - (1 - \theta)\|\Delta_{J^c}^C\|_{2,1}\} \\
&\leq 2A(1 - \theta)\lambda^o \{(1 + \vartheta)\|\Delta^C_J\|_{2,1} - \|\Delta_{J^c}^C\|_{2,1}\},
\end{align*}

where $\mathcal{J}(C)$ and $J(C)$ are abbreviated to $\mathcal{J}$, $J$, respectively, and we set $b = 1/(2\theta), \theta = \vartheta/(2 + \vartheta)$. From the regularity condition, $(1 + \vartheta)\|\Delta^C_{\mathcal{J}}\|_{2,1} - \|\Delta_{J^c}^C\|_{2,1} \leq$
KJ^{1/2}||I - P_{XΔ^B})Δ^C||_F ≤ KJ^{1/2}||XΔ^B + Δ^C||_F, and so

I ≤ 2A(1 - θ)νKJ^{1/2}||XΔ^B + Δ^C||_F

≤ \frac{2}{a}M(B - B^*, C - C^*) + \frac{2}{a}M(\hat{B} - B^*, \hat{C} - C^*) + aA^2(1 - θ)^2K^2(ν)^2J.

Taking a = 4 + 1/θ, b = 1/(2θ), and A ≥ (abA_0)^{1/2} gives the conclusion in Theorem 6.

**Proof of Lemma 3**

Proof. Define

\[ l_H(B, C, r) = 2\langle \mathcal{E}, XB + C \rangle - \frac{1}{a}||XB + C||^2_F - \frac{1}{b}P_{2,H}(C; λ) - aA_0σ^2r(m + q). \]

Similarly, define \( l_0(B, C, r) \) with \( P_{2,0} \) in place of \( P_{2,H} \) in the above. Let \( \mathcal{A}_H = \{\sup_{(B, C)\in\Gamma_{r,j}} l_H(B, C, r) ≥ atσ^2\} \), and \( \mathcal{A}_0 = \{\sup_{(B, C)\in\Gamma_{r,j}} l_0(B, C, r) ≥ atσ^2\} \).

Since \( \mathcal{A}_H \subset \{\sup_{(B, C)\in\Gamma_{r,j}} l_H(B, C, r) ≥ atσ^2\} \), the occurrence of \( \mathcal{A}_H \) implies that

\[ l_H(B^o, C^o, r) ≥ atσ^2, \quad (37) \]

for any \((B^o, C^o)\) that solves

\[ \min_{B: r(B) ≤ r, C} \frac{1}{a}||XB + C||^2_F - 2\langle \mathcal{E}, XB + C \rangle + \frac{1}{b}P_{2,H}(C; λ). \quad (38) \]

**Lemma 4.** Given any \( θ ≥ 1 \), there exists a globally optimal solution \( C^o \) to min\( C \) \( ||Y - C||^2_F/2 + θP_{2,H}(C; λ) \) such that for any \( i : 1 ≤ i ≤ n \), either \( c^o_i = 0 \) or \( ||c^o_i||_2 ≥ λθ^{1/2} ≥ λ \).

See She (2012) for its proof. From Lemma 4 and \( a ≥ 2b \), (37) further indicates that there exists an optimal solution \((B^o, C^o)\) such that \( l_0(B^o, C^o, r) ≥ atσ^2 \). Hence \( \mathcal{A}_H \subset \mathcal{A}_0 \) and it suffices to show \( \Pr(\mathcal{A}_0) ≤ C\exp(-ct) \).

Let \( \mathcal{J} = \mathcal{J}(C) \) for short. Denote by \( I_{\mathcal{J}} \) the submatrix of \( I_{n×n} \) formed by the columns indexed by \( \mathcal{J} \). We write the stochastic term into

\[ 2\langle \mathcal{E}, XB + C \rangle = 2\langle \mathcal{E}, \mathcal{P}_{I_{\mathcal{J}}^c}XB \rangle + 2\langle \mathcal{E}, \mathcal{P}_{I_{\mathcal{J}}}XB + C \rangle \]

\[ ≡ 2\langle \mathcal{E}, A_1 \rangle + 2\langle \mathcal{E}, A_2 \rangle, \quad (39) \]

and \( ||A_1||^2_F + ||A_2||^2_F = ||XB + C||^2_F \).
Lemma 5. Given $X \in \mathbb{R}^{n \times p}$, $1 \leq J \leq n$, $1 \leq r \leq m \wedge p$, define $\Gamma_{r,J}^1 = \{ A \in \mathbb{R}^{n \times m} : \| A \|_F \leq 1, r(A) \leq r, CS(A) \subset CS\{ X(J^c,;) \} \}$ for some $J : |J| = J$.

Let

$$P_o^1(J, r) = \sigma^2 \left[ \{ q \wedge (n - J) \} r + (m - r)r + \log \left( \frac{n}{J} \right) \right].$$

Then for any $t \geq 0$,

$$\text{pr} \left[ \sup_{A \in \Gamma_{r,J}^1} \langle E, A \rangle \geq t\sigma + \{ LP_o^1(J, r) \}^{1/2} \right] \leq c' \exp(-ct^2), \quad (40)$$

where $L, c, c' > 0$ are universal constants.

The proof follows similar lines of the proof of Lemma 4 in She (2017) and is omitted. Now, we can bound the the first term on the right hand side of (39) as follows

$$2\langle E, A_1 \rangle - \frac{1}{a} \| A_1 \|_F^2 - 2aLP_o^1(J, r)$$

$$\leq 2\langle E, A_1/\| A_1 \|_F \rangle \| A_1 \|_F - 2\| A_1 \|_F \{ LP_o^1(J, r) \}^{1/2} - \frac{1}{2a} \| A_1 \|_F^2$$

$$\leq 2a \left[ \langle E, A_1/\| A_1 \|_F \rangle - \{ LP_o^1(J, r) \}^{1/2} \right]_+ + \frac{1}{2a} \| A_1 \|_F^2 - \frac{1}{2a} \| A_1 \|_F^2$$

$$= 2a \left[ \langle E, A_1/\| A_1 \|_F \rangle - \{ LP_o^1(J, r) \}^{1/2} \right]_+.$$

By Lemma 5, for $L$ large enough,

$$\text{pr} \left\{ 2\langle E, A_1 \rangle - \frac{1}{a} \| A_1 \|_F^2 - 2aLP_o^1(J, r) > \frac{1}{2}at\sigma^2 \right\} \leq c' \exp(-ct).$$

Similarly, for the second term on the right hand side of (39),

$$\text{pr} \left\{ 2\langle E, A_2 \rangle - \frac{1}{a} \| A_2 \|_F^2 - 2aLP_o^2(J, r) > \frac{1}{2}at\sigma^2 \right\} \leq c' \exp(-ct),$$

where

$$P_o^2(J, r) = \sigma^2 \left\{ Jm + \log \left( \frac{n}{J} \right) \right\},$$

and $L$ is a large constant. Applying the union bound gives

$$\text{pr} \left[ 2\langle E, XB + C \rangle - \frac{1}{a} \| XB + C \|_F^2 - 2aL\sigma^2 \{ (q + m - r)r + Jm + J \log(en/J) \} > at\sigma^2 \right]$$

$$\leq c' \exp(-ct). \quad (41)$$

The conclusion follows.
A.5 Proof of Theorem 4

Similar to Section A.4, we have
\[ \frac{1}{2} M(\hat{B} - B^*, \hat{C} - C^*) \leq \frac{1}{2} M(B - B^*, \hat{C} - C^*) + \langle \mathcal{E}, X \Delta B + \Delta C \rangle, \]
where \( \Delta B = \hat{B} - B, \Delta C = \hat{C} - C \). Let \( \tilde{r} = r(\Delta B) \) and \( \tilde{J} = J(\Delta C) \). Then from (41) in the proof of Lemma 3,
\[ 2\langle \mathcal{E}, X \Delta B + \Delta C \rangle \leq \frac{1}{a} \|X \Delta B + \Delta C\|_F^2 - 2aL\sigma^2 \left\{ (q+m)\tilde{r} + \tilde{J}m + \tilde{J} \log(en/\tilde{J}) \right\} + R, \]
where \( ER \leq a \sigma^2 \). The oracle inequality can be shown following the lines of Section A.4, noticing that \( \tilde{r} \leq 2r, \tilde{J} \leq 2\tilde{\kappa} \) and \( \tilde{J} \log(2en/\tilde{J}) \leq 2\tilde{\kappa} \log(2en) \).

A.6 Proof of Theorem 5

The proof is based on the general reduction scheme in Chapter 2 of Tsybakov (2009). We consider two cases.

Case (i) \((q+m)r \geq Jm + J \log(en/J)\). Suppose the SVD of \( X \) is \( X = UD\hat{V}^T \) with \( D \) of size \( q \times q \). Given an arbitrary estimator \( (\hat{B}, \hat{C}) \), let \( \hat{A} = V^T\hat{B} \) and \( \tilde{S}(r, J) = \{(A, C) \in \mathbb{R}^{q \times m} \times \mathbb{R}^{n \times m} : r(A) \leq r, J(C) \leq J \} \). Then
\[ \sup_{(B^*, C^*) \in \tilde{S}(r, J)} \text{pr} \{ \|XB^* - X\hat{B} + C^* - \hat{C}\|_F^2 \geq cP_o(J, r) \} \]
\[ \geq \sup_{(A^*, C^*) \in \tilde{S}(r, J)} \text{pr} \{ \|UDA^* - U\hat{D}\hat{A} + C^* - \hat{C}\|_F^2 \geq cP_o(J, r) \}, \]
because for any \( A : r(A) \leq r, B = VA \) satisfies \( r(B) \leq r \). The new design matrix \( UD \) has \( q \) columns, and it is easy to see that for any \( A \in \mathbb{R}^{q \times m} \),
\[ \underline{\kappa} \|A\|_F^2 \leq \|UDA\|_F^2 \leq \bar{\sigma} \|A\|_F^2, \]
(42)
where \( \underline{\kappa} = \sigma_{\min}^2 (X) \) and \( \bar{\sigma} = \sigma_{\max}^2 (X) \) as defined in the theorem. Therefore, without any loss of generality we assume \( X \in \mathbb{R}^{n \times q} \) and \( B \in \mathbb{R}^{q \times m} \) in the rest of the proof.

Consider a signal subclass
\[ B^1(r) = \{ B = (b_{jk}), C = 0 : b_{jk} \in \{0, \gamma R\} \text{ if } (j, k) \in [q] \times [r/2] \cup [r/2] \times [m] \}
\[ b_{jk} = 0 \text{ otherwise} \}. \]
where \( R = \sigma/(\kappa^{3/2}) \), and \( \gamma > 0 \) is a small constant to be chosen later. Clearly, 
\(|B^1(r)| = 2^{(q+m-r/2)r/2} \), \( B^1(r) \subset S(r, J) \), and \( r(B_1 - B_2) \leq r \), for any \( B_1, B_2 \in B^1(r) \). Also, since \( r \leq q \wedge m \), \( (q + m - r/2)r/2 \geq c(q + m)r \) for some constant \( c \).

Let \( \rho(B_1, B_2) = \| \text{vec}(B_1) - \text{vec}(B_2) \|_0 \), the Hamming distance between \( \text{vec}(B_1) \) and \( \text{vec}(B_2) \). By the Varshamov-Gilbert bound, cf. Lemma 2.9 in [Tsybakov (2009)], there exists a subset \( B^{10}(r) \subset B^1(r) \) such that
\[
 \log |B^{10}(r)| \geq c_1 r(q + m), \quad \rho(B_1, B_2) \geq c_2 r(q + m), B_1, B_2 \in B^{10}(r), B_1 \neq B_2
\]
for some universal constants \( c_1, c_2 > 0 \). Then
\[
\| B_1 - B_2 \|_F^2 = \gamma^2 R^2 \rho(B_1, B_2) \geq c_2 \gamma^2 R^2(q + m)r.
\]
It follows from (42) that
\[
\| XB_1 - XB_2 \|_F^2 \geq c_2 \kappa \gamma^2 R^2(q + m)r \tag{43}
\]
for any \( B_1, B_2 \in B^{10}(r), B_1 \neq B_2 \), where \( \kappa/\kappa \) is a positive constant.

For Gaussian models, the Kullback-Leibler divergence of \( MN(XB_2, \sigma^2 I \otimes I) \), denoted by \( P_{B_2} \), from \( MN(XB_1, \sigma^2 I \otimes I) \), denoted by \( P_{B_1} \), is
\[
\mathcal{K}(P_{B_1}, P_{B_2}) = \frac{1}{2\sigma^2} \| XB_1 - XB_2 \|_F^2.
\]
Let \( P_0 \) be \( MN(0, \sigma^2 I \otimes I) \). By (42) again, for any \( B : r(B) \leq r \), we have
\[
\mathcal{K}(P_0, P_B) \leq \frac{1}{2\sigma^2} \kappa \gamma^2 R^2 \rho(0, B) \leq \frac{\gamma^2}{\sigma^2} R^2(q + m)r,
\]
where we used \( \rho(B_1, B_2) \leq r(q + m) \). Therefore,
\[
\frac{1}{|B^{10}|} \sum_{B \in B^{10}} \mathcal{K}(P_0, P_B) \leq \gamma^2 r(q + m). \tag{44}
\]
Combining (43) and (44) and choosing a sufficiently small value for \( \gamma \), we can apply Theorem 2.7 of [Tsybakov (2009)] to get the desired lower bound.

Case (ii) \((q + m)r < Jm + J \log(en/J)\). Define a signal subclass
\[
B^2(J) = \{ B, C = (c_1, \ldots, c_n)^T : B = 0, c_i = 0 \text{ or } \gamma R(1^T, b^T)^T \}
\]
with \( 1 = (1 \ldots 1)^T \in \mathbb{R}^{m-[m/2]}, b \in \{0, 1\}^{[m/2]}, J(C) \leq J \).

where
\[
R = \frac{\sigma}{\kappa^{3/2}} \left( \left. \frac{1 + \frac{\log(en/J)}{m} \right. \right)^{1/2}.
\]

and $\gamma > 0$ is a small constant. Clearly, $B^2(J) \subset S(r, J)$. By Stirling’s approximation,

$$\log |B^2(J)| \geq \log \binom{n}{J} + \log 2^{jm/2} \geq J \log(n/J) + Jm \log 2 / 2 \geq c\{J \log(en/J) + Jm\}$$

for some universal constant $c$. Applying Lemma 8.3 in Rigollet and Tsybakov (2011) and the Varshamov-Gilbert bound, there exists a subset $B^{20}(J) \subset B^2(J)$ such that

$$\log |B^{20}(J)| \geq c_1\{J \log(en/J) + Jm\}$$

and $\rho(B_1, B_2) \geq c_2 Jm$, $\forall B_1, B_2 \in B^{20}, B_1 \neq B_2$ for some universal constants $c_1, c_2 > 0$. The afterward treatment follows the same lines as in (i) and the details are omitted.

### A.7 Proof of Theorem 7

The first conclusion follows from the block coordinate descent design and the optimality of the multivariate thresholding for solving the $C$-optimization problem (She, 2012).

When the continuity condition holds, $\tilde{\Theta}(Y - XB; \lambda)$ is the unique minimizer of $\min_B F(B, C)$; see Lemma 1 of She (2012). But in general, the problem of $\min_B F(B, C)$ subject to $r(B) \leq r$ may not have a unique solution. The accumulation point result is an application of Zangwill’s Global Convergence Theorem (Luenberger and Ye, 2008), and the proof proceeds along similar lines of the proof of Theorem 7 of Bunea et al. (2012). The details are omitted.

To get the stationarity guarantee when $q(\cdot; \lambda) \equiv 0$, we can write the problem as $\min ||Y - XSV^T - C||^2_F / 2 + \sum_{i=1}^{n} P_{\Theta}(||c_i||_2; \lambda)$ subject to $(S, V, C) \in \mathbb{R}^{p \times r} \times O^{m \times r} \times \mathbb{R}^{n \times m}$, where $O^{m \times r} = \{V \in \mathbb{R}^{m \times r} : V^T V = I\}$. Then one can view the problem as an unconstrained one on the manifold $\mathbb{R}^{p \times r} \times O^{m \times r} \times \mathbb{R}^{n \times m}$, and define the Riemannian gradient with respect to $V$; see Theorem 6 of Bunea et al. (2012) for more detail.

### A.8 Proof of Theorem 8

First, by a bit of algebra we have the following result.

**Lemma 6.** For any $(\hat{B}, \hat{C})$ defined in the theorem, we have

$$\hat{B}, \hat{C} \in \arg \min_{(B, C)} g(B, C; B^-, C^-)|_{B^- = \hat{B}, C^- = \hat{C}} \text{ s.t. } r(B) \leq r,$$
where \( g \) is constructed by \( g(B; C; B^-, C^-) = l(B^-, C^-) + P_{2,\Theta}(C; \lambda) + \langle XB^- + C^- - Y, XB - XB^- + C - C^- \rangle + \|XB - XB^-\|_F^2/2 + \|C - C^-\|_F^2/2 \), with \( l(B, C) = \|XB + C - Y\|_F^2/2 \) and \( P_{2,\Theta}(C; \lambda) = \sum_{i=1}^n P_{\alpha}(\|c_i\|_2; \lambda) \).

The following result can be obtained from Lemma 2 in She (2012).

**Lemma 7.** Let \( Q(C) = \|C - Y\|_F^2/2 + P_{2,\Theta}(C; \lambda) \) and \( C^o = \hat{\Theta}(Y; \lambda) \). Assume that \( \hat{\Theta} \) is continuous at \( Y \). Then for any \( C \), \( Q(C) - Q(C^o) \geq (1 - \mathcal{L}_\Theta)\|C - C^o\|_F^2/2 \).

**Lemma 8.** Let \( Q(B) = \|XB - Y\|_F^2/2 \) and \( B^o = \mathcal{R}(X, Y, r) \) which is of rank \( r \). Then for any \( B : r(B) \leq r/(1 + \alpha) \) with \( \alpha \geq 0 \), \( Q(B) - Q(B^o) \geq (1 - (1 + \alpha)^{-1/2})\|XB - XB^o\|_F^2/2 \).

The lemma follows from Proposition 2.2 of She (2013) and Lemma 9 below.

**Lemma 9.** The optimization problem \( \min_{\beta \in \mathbb{R}^p} l(\beta) = \|y - \beta\|_2^2/2 \) s.t. \( \|\beta\|_0 \leq q \) has \( \hat{\beta} = \Theta^\#(y; q) \) as a globally optimal solution. Assume that \( J(\hat{\beta}) = q \), where \( J(\cdot) = \| \cdot \|_0 \). Then for any \( \beta \) with \( J(\beta) \leq s = q/\theta \) and \( \theta \geq 1 \), we have \( l(\beta) - l(\hat{\beta}) \geq \{1 - \mathcal{L}(J, \hat{J})\}\|\hat{\beta} - \beta\|_2^2/2 \) where \( \mathcal{L}(J, \hat{J}) = (|J \setminus \hat{J}|/|\hat{J} \setminus J|)^{1/2} \leq (s/q)^{1/2} = \theta^{-1/2} \), \( \hat{J} = \mathcal{J}(\hat{\beta}) \) and \( J = \mathcal{J}(\beta) \).

With Lemmas 6, 7 and 8 available, the conclusion results from Theorem 2 of She (2016).

**Proof of Lemma 9**

**Proof.** Let \( \mathcal{J}_1 = J \cap \hat{J}, \mathcal{J}_2 = \hat{J} \setminus J \) and \( \mathcal{J}_3 = J \setminus \hat{J} \). Then \( \beta = \beta_{\mathcal{J}_1} + \beta_{\mathcal{J}_3} \) and \( \hat{\beta} = \beta_{\mathcal{J}_1} + \beta_{\mathcal{J}_2} \). By writing \( \beta_{\mathcal{J}_1} = y_{\mathcal{J}_1} + \delta_{\mathcal{J}_1} \) and \( \beta_{\mathcal{J}_3} = y_{\mathcal{J}_3} + \delta_{\mathcal{J}_3} \), we have

\[
l(\beta) - l(\hat{\beta}) = \frac{1}{2}\|\delta_{\mathcal{J}_1}\|_2^2 + \frac{1}{2}\|y_{\mathcal{J}_2}\|_2^2 + \frac{1}{2}\|\delta_{\mathcal{J}_1}\|_2^2 - \frac{1}{2}\|y_{\mathcal{J}_3}\|_2^2
\]

\[
\frac{1}{2}\|\hat{\beta} - \beta\|_2^2 = \frac{1}{2}\|\delta_{\mathcal{J}_1}\|_2^2 + \frac{1}{2}\|y_{\mathcal{J}_2}\|_2^2 + \frac{1}{2}\|y_{\mathcal{J}_3} + \delta_{\mathcal{J}_3}\|_2^2.
\]

The key lies in the comparison between \( \|y_{\mathcal{J}_2}\|_2^2 + \|\delta_{\mathcal{J}_3}\|_2^2 - \|y_{\mathcal{J}_3}\|_2^2 \) and \( \|y_{\mathcal{J}_3}\|_2^2 + \|y_{\mathcal{J}_3} + \delta_{\mathcal{J}_3}\|_2^2 \). Let \( K \leq 1 \) satisfy

\[
\frac{1}{2}\|y_{\mathcal{J}_2}\|_2^2 + \frac{1}{2}\|\delta_{\mathcal{J}_3}\|_2^2 - \frac{1}{2}\|y_{\mathcal{J}_3}\|_2^2 \geq \frac{K}{2}\|y_{\mathcal{J}_2}\|_2^2 + \frac{K}{2}\|y_{\mathcal{J}_3} + \delta_{\mathcal{J}_3}\|_2^2.
\]
which is equivalent to
\[(1 - K)\|y_{\mathcal{J}_3}\|^2 + \|\delta_{\mathcal{J}_3}\|^2 \geq K\|y_{\mathcal{J}_3}\|^2 + \|\delta_{\mathcal{J}_3}\|^2 + \|y_{\mathcal{J}_3}\|^2. \quad (45)\]

By construction, \(|y_i| \geq |y_j|\) for any \(i \in \mathcal{J}_2\) and \(j \in \mathcal{J}_3\). Thus \(\|y_{\mathcal{J}_3}\|^2/J_2 \geq \|y_{\mathcal{J}_3}\|^2/J_3\), from which it follows that (45) is implied by
\[(1 - K)\frac{J_2}{J_3}\|y_{\mathcal{J}_3}\|^2 + \|\delta_{\mathcal{J}_3}\|^2 \geq (1 + K)\|y_{\mathcal{J}_3}\|^2 + K\|\delta_{\mathcal{J}_3}\|^2 + 2K\langle y_{\mathcal{J}_3}, \delta_{\mathcal{J}_3}\rangle,\]
or
\[\frac{(1 - K)(J_2/J_3) - (1 + K)}{K}\|y_{\mathcal{J}_3}\|^2 + \frac{1 - K}{K}\|\delta_{\mathcal{J}_3}\|^2 \geq 2\langle y_{\mathcal{J}_3}, \delta_{\mathcal{J}_3}\rangle.\]

Therefore, the largest possible \(K\) satisfies
\[\frac{(1 - K)(J_2/J_3) - (1 + K)}{K} \times \frac{1 - K}{K} = 1\]
or \((1 - K)^2 = J_3/J_2\). This gives
\[\mathcal{L} = 1 - K = (J_3/J_2)^{1/2} \leq \{(J_3 + J_1)/(J_2 + J_1)\}^{1/2} = (J/J)^{1/2} \leq \theta^{-1/2}.\]
The proof is complete. \(\square\)

### A.9 Proof of Theorem 9

Let \(h(B, C; A) = 1/\{mn - AP(B, C)\}\). It follows from \(1/(1 - \delta) \geq \exp(\delta)\) for any \(0 \leq \delta < 1\) and \(\exp(\delta) \geq 1/(1 - \delta/2)\) for any \(0 \geq \delta \leq 2\) that
\[mn\|Y - X\hat{B} - \hat{C}\|^2_{\mathcal{F}} h(\hat{B}, \hat{C}; A/2) \leq \|Y - X\hat{B} - \hat{C}\|^2_{\mathcal{F}} \exp\{\delta(\hat{B}, \hat{C})\}\]
\[\leq \|Y - XB^* - C^*\|^2_{\mathcal{F}} \exp\{\delta(B^*, C^*)\}\]
\[\leq \|Y - XB^* - C^*\|^2_{\mathcal{F}} h(B^*, C^*; A)mn.\]

Since \(h(\hat{B}, \hat{C}; A/2) > 0\), we have
\[\|Y - X\hat{B} - \hat{C}\|^2 \leq \|Y - XB^* - C^*\|^2_{\mathcal{F}} h(B^*, C^*; A)/h(\hat{B}, \hat{C}; A/2).\]

With a bit of algebra, we get
\[M(\hat{B} - B^*, \hat{C} - C^*) \leq \|\mathcal{E}\|_{\mathcal{F}}^2 \{h(B^*, C^*; A)/h(\hat{B}, \hat{C}; 0.5A) - 1\}
+ 2\langle \mathcal{E}, X\hat{B} - XB^* + \hat{C} - C^* \rangle
\leq \frac{A\|\mathcal{E}\|_{\mathcal{F}}^2}{mn\sigma^2 - A\sigma^2 P(B^*, C^*)^2 P(B^*, C^*) - \frac{0.5A\|\mathcal{E}\|_{\mathcal{F}}^2}{0.5A\|\mathcal{E}\|_{\mathcal{F}}^2} \sigma^2 P(\hat{B}, \hat{C})}
+ 2\langle \mathcal{E}, X\hat{B} - XB^* + \hat{C} - C^* \rangle.\]
We give a finer treatment of the last stochastic term than that in the proof of Lemma 3 to show that \( \langle \mathcal{E}, X\hat{B} - XB^* + \hat{C} - C^* \rangle \) can be bounded by \( P(B^*, C^*) + P(\hat{B}, \hat{C}) \) up to a multiplicative constant with high probability. Let \( \Delta^B = \hat{B} - B^* \), \( \Delta^C = \hat{C} - C^* \), \( \hat{J} = \hat{J}(\hat{C}) \), \( J^* = J(C^*) \), \( \hat{r} = r(\hat{B}) \), \( r^* = r(C^*) \). In the following, given any index set \( J \subset [n] \), we denote by \( I_J \) the submatrix of \( I_{n \times n} \) formed by the columns indexed by \( J \), and abbreviate \( P_{I_J} \) to \( P_J \). Let \( P_1 = P_{J^*} \), \( P_2 = P_{(J^*)^c \cap \hat{J}} \), \( P_3 = P_{(J^* \cup \hat{J})^c} \), and \( P_{rs} \) be the orthogonal projection onto the row space of \( XB^* \) which is of rank \( \leq r^* \). Then

\[
X\Delta^B - \Delta^C = P_1(X\Delta^B - \Delta^C) + P_2(X\Delta^B - \Delta^C) + P_3(X\Delta^B - \Delta^C)P_{rs} + P_3(X\Delta^B - \Delta^C)P_{rs}^\perp
\]

\[
\equiv \Delta_1 + \Delta_2 + \Delta_3 + \Delta_4,
\]

and \( \sum_{i=1}^4 \| \Delta_i \|_F^2 = \| X\Delta^B - \Delta^C \|_F^2 \). Then \( CS(\Delta_1) \subset P_{J^*} \), \( CS(\Delta_2) \subset P_{\hat{J}} \), \( r(\Delta_3) \leq r^* \), and \( r(\Delta_4) = r(P_3X\Delta^B P_{rs}) = r(P_3X\hat{B} P_{rs}^\perp) \leq \hat{r} \). The stochastic term can then be handled in a way similar to that in Lemma 3. For example, we can use the following result to handle \( \langle \mathcal{E}, \Delta_4 \rangle \).

**Lemma 10.** Given \( X \in \mathbb{R}^{n \times p} \), \( 1 \leq J_1, J_2 \leq n \), \( 1 \leq r \leq m \wedge p \), define \( \Gamma_{r, J_1, J_2} = \{ A \in \mathbb{R}^{n \times m} : \| A \|_F \leq 1, r(A) \leq r, CS(A) \subset CS[X((J_1 \cup J_2)^c, :)\} \} \). Then for any \( t \geq 0 \),

\[
\text{pr}\left[ \sup_{A \in \Gamma_{r, J_1, J_2}} \langle \mathcal{E}, A \rangle \geq t\sigma + \{ LP_\sigma(J_1 J_2, r)\}^{1/2} \right] \leq c' \exp(-ct^2), \quad (46)
\]

where \( L, c, c' > 0 \) are universal constants.

Following the lines of the proof of Theorem 2 in She (2017), we can show that for any constants \( a, b, a' > 0 \) satisfying \( 4b > a \), the following event

\[
2\langle \mathcal{E}, X\Delta^B - \Delta^C \rangle \leq 2(1/a + 1/a')M(\hat{B} - B^*, \hat{C} - C^*) + 8bL\sigma^2 \{ P(\hat{B}, \hat{C}) + P(B^*, C^*) \}
\]

occurs with probability at least \( 1 - c'_1 n^{-c_1} \) for some \( c_1, c'_1 > 0 \), where \( L \) is a sufficiently large constant.
Let \( \gamma \) and \( \gamma' \) be constants satisfying \( 0 < \gamma < 1, \gamma' > 0 \). On \( \mathcal{A} = \{(1 - \gamma)mn\sigma^2 \leq \|E\|_F^2 \leq (1 + \gamma)mn\sigma^2 \} \), we have
\[
\frac{A\|E\|_F^2}{mn\sigma^2 - A\sigma^2 P(B^*, C^*)} = P(B^*, C^*) - 0.5A\|E\|_F^2 \leq \frac{(1 + \gamma')AA_0 - A}{A_0 - A} \sigma^2 P(B^*, C^*) - 0.5(1 - \gamma)A\sigma^2 P(\hat{B}, \hat{C}).
\]
From [Laurent and Massart (2000)](#), the complement of \( \mathcal{A} \) occurs with probability at most \( c_2' \exp(-c_2 mn) \), where \( c_2, c_2' \) are dependent on constants \( \gamma, \gamma' \). With \( A_0 \) large enough, we can choose \( a, a', b, A \) such that \( (1/a + 1/a') < 1/2, 4b > a, \) and \( 16bL \leq (1 - \gamma)A \). The conclusion results.

### A.10 Theorem 10

**Theorem 10.** Let \( (\hat{B}, \hat{C}) = \arg\min_{(B, C)} \|Y - XB - C\|_F^2/2 + \lambda\|C\|_{2,1} \) subject to \( r(B) \leq r, \lambda = A\sigma(m + \log n)^{1/2} \) where \( r \geq r^* \geq 1 \) and \( A \) is a large enough constant. Assume that \( X \) satisfies \( (1 + \vartheta)\lambda\|C'\|_{2,1} \leq \lambda\|C'\|_{2,1} + c\|X\|_{2,1} + \sigma\zeta\|X\|_{2,1} \) for all \( B' \) and \( C' \) with \( r(B') \leq 2r, \) where \( \vartheta > 0 \) is a constant and \( \zeta \geq 0 \). Then, we have
\[
E(\|\hat{B} - B^*\|_F^2) \lesssim \sigma^2(1 + \zeta^2)(m + q)r.
\]

**Proof.** A careful examination of the proof of Theorem 3 shows that for any \( a \geq 2b > 0 \),
\[
(1 - \frac{1}{a})M(\hat{B} - B^*, \hat{C} - C^*) \leq 2aA_0\sigma^2 r(m + q) + R + 2P(C^*; \lambda) - 2P(\hat{C}; \lambda) + \frac{1}{b}P_{2,1}(\hat{C} - C^*; \lambda),
\]
where \( \lambda = A\lambda^o, \lambda^o = \sigma(m + \log n)^{1/2}, A = (abA_1)^{1/2}, A_1 \geq A_0 \) with \( A_0 \) a universal constant, and \( ER \leq ac\sigma^2 \).

Set \( b = 1/(2\vartheta), \theta = \vartheta/(2 + \vartheta) \). Then
\[
(1 - \frac{1}{a})M(\hat{B} - B^*, \hat{C} - C^*) \leq 2(1 - \theta)\lambda\{(1 + \vartheta)\|\hat{C} - C^*\|_{2,1} - \|\hat{C} - C^*\|_{2,1}\} + 2aA_0\sigma^2 r(m + q) + R
\]
\[
\leq 2(1 - \theta)\{\sigma\zeta\{(m + q)r\}^{1/2}M(\hat{B} - B^*, \hat{C} - C^*)\}^{1/2}
\]
\[
- n\|\hat{B} - B^*\|_F^2 + 2aA_0\sigma^2 r(m + q) + R.
\]

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The conclusion follows by applying Hölder’s inequality and setting, say, $a = 2 + 1/\theta$, $b = 1/2\theta$ and $A \geq (abA_0)^{1/2}$.

\section{Simulations}

\subsection{Simulation setups}

We consider three model setups. In Models I and II, we set $n = 100$, $p = 12$, $m = 8$, and $r^* = 3$. The design matrix $X$ is generated by sampling its $n$ rows from $N(0, \Delta_0)$, where $\Delta_0$ is with diagonal elements 1 and off-diagonal elements 0.5. This brings in wide-range predictor correlation. The rows of the error matrix $E$ are generated as independently and identically distributed samples from $N(0, \sigma^2 \Sigma_0)$. Models I and II differ in their error structures. In Model I, we set $\Sigma_0 = I$, whereas in Model II, $\Sigma_0$ has the same compound symmetry structure as $\Delta_0$. In each simulation, $\sigma^2$ is computed to control the signal to noise ratio, defined as the ratio between the $r^*$th singular value of $XB^*$ and $\|E\|_F$.

Model III is a high-dimensional setup with $n = 100$, $p = 500$, $m = 50$, $r^* = 3$ and $q = 10$. As such, there are 25,000 unknown parameters in the coefficient matrix, posing a challenging high-dimensional problem. The design is generated as $X = X_1 X_2 \Delta_0^{1/2}$, where $X_1 \in \mathbb{R}^{n \times q}$, $X_2 \in \mathbb{R}^{q \times p}$, and all entries of $X_1$ and $X_2$ are independently and identically distributed samples from $N(0, 1)$. The error structure is the same as in Model II.

In each of the three models, $B^*$ is randomly generated as $B^* = B_1 B_2^T$ in each simulation, where $B_1 \in \mathbb{R}^{p \times r^*}$, $B_2 \in \mathbb{R}^{m \times r^*}$ and all entries in $B_1$ and $B_2$ are independently and identically distributed samples from $N(0, 1)$. Outliers are then added by setting the first $n \times O\%$ rows of $C^*$ to be nonzero, where $O\% \in \{5\%, 10\%, 15\%\}$. Concretely, the $j$th entry in any outlier row of $C^*$ is $\alpha$ times the standard deviation of the $j$th column of $XB^*$, where $1 \leq j \leq m$ and $\alpha = 2, 4$. To make the problem even more challenging, we modify all entries of the first two rows of the design to 10. This yields some outliers with high leverage values. Finally, the response $Y$ is generated as $Y = XB^* + C^* + E$. Overall, the signal is contaminated by both random errors and gross outliers. Under each setting, the entire data generation process described above is replicated 200 times.
B.2 Methods and evaluation metrics

We compare the proposed robust reduced-rank regression with several robust regression approaches and rank reduction methods. There exist many robust multivariate regression methods in the traditional large-$n$ setting. We mainly consider the MM-estimator by Tatsuoka and Tyler (2000), using its implementation provided by the R package FRB and the default settings therein. Other robust estimators including the S-estimator (Aelst and Willems, 2005) and the GS-estimator (Roelant et al., 2009) were also examined; we omit their results here, as they were similar to or slightly worse than those of the MM-estimator. None of these classical methods is applicable in high dimensions, and so they were only used on the datasets generated according to Models I and II.

For reduced-rank methods, we consider the plain reduced-rank regression (Bunea et al., 2011) and the reduced-rank ridge regression (Mukherjee and Zhu, 2011; She, 2013), both tuned by 10-fold cross validation. The latter method combines rank reduction and shrinkage estimation, which can potentially improve the predictive performance of the former when the predictors exhibit strong correlation.

We also consider a three-step fitting-detection-refitting procedure. Specifically, the first step is to fit a plain reduced-rank regression using all data; in the second step, the value of the residual sum of squares is computed for each of the $n$ observation rows, and exactly $n \times O\%$ observations with the largest residual sum of squares are labeled as outliers and discarded; at the third step, the plain reduced-rank regression is refitted with the rest of the observations. This method can be regarded as a naive oracle procedure, as it relies on the knowledge of the true number of outliers.

As for the proposed robust reduced-rank regression, we used the $\ell_0$ penalized form and the predictive information criterion for tuning. Our method allows the incorporation of the error structure through setting the weighting matrix $\Gamma$; see Equation (8) of the paper. To investigate the impact of weighting, we considered both $\Gamma = I$ and $\Gamma = \hat{\Sigma}^{-1}$ in the setting of Model II, where $\hat{\Sigma}$ is a robust estimate of $\Sigma = \sigma^2 \Sigma_0$ from MM-estimation. Since it is in general difficult to estimate $\Sigma$ in high dimensional settings, for the data generated in Model III we just set $\Gamma = I$. For each rank value $r = 1, \ldots, \min(n, q)$, we compute the solutions over a grid of 100 $\lambda$ values equally spaced on the log scale, corresponding to a proper interval of the proportion of outliers given by $[v_L, v_U]$. We take $v_L = 0$ and $v_U \approx 0.4$, as in practice the proportion of outliers is usually under 40%. All the methods are implemented in a user-friendly R package.

To characterize estimation accuracy robustly, we report the 10% trimmed mean
of the mean squared error from all runs,
\[
\text{Err}(\hat{B}) = \|XB^* - X\hat{B}\|_F^2 / (mn).
\]
In Model II, we additionally report the 10\% trimmed mean of the weighted mean squared errors from all runs, defined as
\[
\text{Err}(\hat{B}; \Sigma) = \text{tr}\{(XB^* - X\hat{B})\Sigma^{-1}(XB^* - X\hat{B})^T\} / (mn),
\]
where \(\Sigma = \sigma^2\Sigma_0\) is the true error covariance matrix. Similarly, the prediction error is defined as
\[
\text{Err}(\hat{B}, \hat{C}) = \|XB^* + C^* - X\hat{B} - \hat{C}\|_F^2 / (mn).
\]

While the robust reduced-rank regression explicitly estimates \(C^*\), this is not the case for the other approaches. In the plain reduced-rank regression and the reduced-rank ridge regression, \(\hat{C}\) is set as a zero matrix, while in the MM estimation and the three-step procedure, the rows in \(\hat{C}\) corresponding to the identified outliers are filled with model residuals in \(Y - X\hat{B}\). The leverage points, if exists, are removed from \(X\) in the above calculations.

To evaluate the rank selection performance, we report the average of rank estimates from all runs. To examine the outlier detection performance, we report the average masking rate, i.e., the fraction of undetected outliers, the average swamping rate, i.e., the fraction of good points labeled as outliers, and the frequency of correct joint outlier detection, i.e., the fraction of simulations with no masking and no swamping.

### B.3 Simulation results

Tables 3–5 summarize the simulation results of Models I–III, respectively, for \(\alpha = 2\) and signal to noise ratio 0.75. We omit the results in other settings since they deliver similar messages.

In Models I and II, the MM-estimates achieved better predictive performance than both reduced-rank regression and reduced-rank ridge regression. This demonstrates that when severe outliers are present, it is pivotal to perform robust estimation. Even in these low-dimensional settings, the proposed robust reduced-rank regression outperforms all other methods, and perfectly detects all outliers jointly. MM-estimation can also achieve pretty low masking rates, but this comes at the cost of increasing false positives, which translates to efficiency loss. In particular, when the errors become correlated, our robust reduced-rank regression still
showed impressive performance in both prediction and outlier detection. Additionally, the inverse covariance weighting did show some improvements over the identity weighting, but the gain was small.

Both reduced-rank regression and reduced-rank ridge regression tended to overestimated the rank in the presence of highly leveraged outliers. This complies with the theoretical results, cf. Remark 7 following Theorem 6. In contrast, robust reduced-rank regression achieved nearly perfect rank selection in all the experiments. The three-step procedure relies on the accuracy of the estimated model residuals, and often fails in the presence of leverage points. In practice, making a judgement of the number of outliers is critical. One merit of the proposed method is that the theoretically justified predictive information criterion can choose suitable parameters regardless of the size of $n$, $m$, or $p$, leading to an automatic identification of the right amount of outlyingness from a predictive learning perspective.

Similar conclusions can be drawn from the comparison in the high-dimensional model. Indeed, according to Table 5, the robust reduced-rank regression showed comparable or better performance than the other methods in almost all categories.
Table 3: Simulation results of Model I with $\alpha = 2$ and signal to noise ratio 0.75. The errors are reported with their standard errors in parentheses.

|      | $\text{Err}(\hat{B})$ | $\text{Err}(\hat{B}, \hat{C})$ | Rank | Mask | Swamp | Detection |
|------|------------------------|-------------------------------|------|------|--------|-----------|
| MM   | 0.4 (0.2)              | 4.2 (1.7)                     | 8.0  | 0%   | 3.7%   | 0%        |
| RRR  | 2.9 (3.7)              | 6.1 (4.4)                     | 3.6  | 100% | 0%     | 0%        |
| RRS  | 1.8 (0.8)              | 4.7 (1.7)                     | 4.0  | 100% | 0%     | 0%        |
| RRO  | 0.3 (0.3)              | 1.2 (1)                       | 3.1  | 18.1%| 1%     | 28.5%     |
| R$^4$| 0.2 (0.1)              | 0.3 (0.1)                     | 3.0  | 0%   | 0%     | 100%      |
| MM   | 0.4 (0.2)              | 12.3 (6)                      | 8.0  | 0%   | 2.6%   | 1.5%      |
| RRR  | 5.4 (5)                | 15.9 (8.5)                    | 3.5  | 100% | 0%     | 0%        |
| RRS  | 3.5 (2.4)              | 14.3 (9.7)                    | 4.1  | 100% | 0%     | 0%        |
| RRO  | 0.3 (0.2)              | 2.1 (1.3)                     | 3.0  | 13.3%| 1.5%   | 20.5%     |
| R$^4$| 0.2 (0.1)              | 0.4 (0.2)                     | 3.0  | 0%   | 0%     | 100%      |
| MM   | 0.5 (0.4)              | 17.8 (6.6)                    | 8.0  | 0.1% | 1.4%   | 24%       |
| RRR  | 4.4 (2.1)              | 17.9 (5.5)                    | 3.8  | 100% | 0%     | 0%        |
| RRS  | 4.2 (2.5)              | 18.4 (6.1)                    | 3.9  | 100% | 0%     | 0%        |
| RRO  | 0.5 (0.3)              | 2.3 (1.5)                     | 3.0  | 8.9% | 1.6%   | 27.5%     |
| R$^4$| 0.3 (0.2)              | 0.8 (0.5)                     | 2.9  | 0%   | 0%     | 100%      |
Table 4: Simulation results of Model II with $\alpha = 2$ and signal to noise ratio 0.75. The layout of the table is similar to that of Table 3.

|          | Err($\hat{B}$) | Err($\hat{B}; \Sigma$) | Err($\hat{B}, \hat{C}$) | Rank | Mask | Swamp | Detection |
|----------|----------------|-------------------------|--------------------------|------|------|-------|-----------|
|          | 5%             | 10%                     | 15%                       |      |      |       |           |
| MM       | 0.4 (0.3)      | 0.4 (0.3)               | 6.9 (2.9)                | 8.0  | 0%   | 3.3%  | 0%        |
| RRR      | 2.6 (2.4)      | 4.6 (4.3)               | 9.8 (6.2)                | 4.0  | 100% | 0%    | 0%        |
| RRS      | 1.9 (1.4)      | 3.3 (2.5)               | 8.5 (4.4)                | 4.3  | 100% | 0%    | 0%        |
| RRO      | 0.4 (0.3)      | 0.5 (0.3)               | 2.7 (1.8)                | 3.0  | 25.7%| 1.4%  | 17%       |
| $R^d$    | 0.2 (0.2)      | 0.2 (0.2)               | 0.3 (0.2)                | 3.0  | 0%   | 0%    | 0%        |
| $R^d_w$  | 0.2 (0.1)      | 0.2 (0.2)               | 0.3 (0.2)                | 3.0  | 0%   | 0%    | 100%      |
| MM       | 0.5 (0.3)      | 0.5 (0.4)               | 21.2 (9.7)               | 8.0  | 0%   | 1.9%  | 12.5%     |
| RRR      | 3.6 (1.1)      | 6.5 (2.3)               | 21.7 (9.1)               | 4.1  | 100% | 0%    | 0%        |
| RRS      | 4 (1.8)        | 7.4 (3.7)               | 24.6 (10.6)              | 4.0  | 100% | 0%    | 0%        |
| RRO      | 0.4 (0.2)      | 0.6 (0.3)               | 4.3 (2.1)                | 3.0  | 16.4%| 1.8%  | 4.5%      |
| $R^d$    | 0.3 (0.2)      | 0.4 (0.3)               | 0.7 (0.6)                | 3.0  | 0%   | 0%    | 99.5%     |
| $R^d_w$  | 0.2 (0.1)      | 0.3 (0.2)               | 0.6 (0.4)                | 3.0  | 0%   | 0%    | 100%      |
| MM       | 0.4 (0.2)      | 0.4 (0.2)               | 31.3 (12.4)              | 8.0  | 0%   | 1.1%  | 46.5%     |
| RRR      | 4.5 (2.7)      | 7.9 (5.2)               | 33.4 (13.4)              | 4.3  | 100% | 0%    | 0%        |
| RRS      | 4.8 (3.4)      | 8.7 (6.8)               | 36.5 (16.1)              | 4.0  | 100% | 0%    | 0%        |
| RRO      | 0.4 (0.2)      | 0.6 (0.2)               | 3.3 (1.4)                | 3.0  | 9.4% | 1.7%  | 10%       |
| $R^d$    | 0.2 (0.2)      | 0.3 (0.2)               | 0.6 (0.3)                | 3.0  | 0.3% | 0%    | 95.5%     |
| $R^d_w$  | 0.2 (0.1)      | 0.2 (0.1)               | 0.5 (0.2)                | 3.0  | 0%   | 0%    | 100%      |
Table 5: Simulation results of Model III with $\alpha = 2$ and signal to noise ratio 0.75. The values of actual $\text{Err}(\hat{B})$ and $\text{Err}(\hat{B}, \hat{C})$ are divided by 100 for better presentation. The layout of the table is similar to that of Table 3.

| Err($\hat{B}$) | Err($\hat{B}, \hat{C}$) | Rank | Mask   | Swamp | Detection |
|----------------|-------------------------|------|--------|-------|-----------|
| RRR 2.5 (0.9)  | 15.5 (6.3)              | 4.0  | 100%   | 0%    | 0%        |
| RRS 2.4 (0.9)  | 15.6 (6.3)              | 4.0  | 100%   | 0%    | 0%        |
| RRO 1 (0.6)    | 3.9 (3.9)               | 3.0  | 11.3%  | 0.6%  | 67.5%     |
| $R_i^1$ 0.9 (0.5) | 1.6 (0.9)          | 3.0  | 1.6%   | 0%    | 96%       |
| RRR 5.4 (2.3)  | 47.5 (18)               | 4.0  | 100%   | 0%    | 0%        |
| RRS 5.1 (2.1)  | 47.8 (18)               | 4.0  | 100%   | 0%    | 0%        |
| RRO 0.8 (0.4)  | 5.1 (4.6)               | 3.0  | 4.9%   | 0.5%  | 68.5%     |
| $R_i^1$ 0.7 (0.3) | 2.2 (0.9)          | 3.0  | 0%     | 0%    | 100%      |
| RRR 8.7 (4.2)  | 77.9 (39.9)             | 4.0  | 100%   | 0%    | 0%        |
| RRS 8 (3.6)    | 77.4 (40)               | 4.0  | 100%   | 0%    | 0%        |
| RRO 1.4 (0.8)  | 11.9 (8.5)              | 3.0  | 9.7%   | 1.7%  | 24%       |
| $R_i^1$ 0.8 (0.3) | 3.1 (1.1)          | 3.2  | 3.2%   | 0%    | 75.5%     |
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