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Topic 15: Sparse Orthogonal Factor Regression

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Key points: Sparcity and dimensionality reduction for Multivariate Linear Regression models.

Disclaimer: *The note is built on Prof. Jinchi Lv's lectures of the course at USC, DSO 607, High-Dimensional Statistics and Big Data Problems.*

15.1 Motivation

Consider a Mutlivariate Linear Regression (MLR) model

$$\underset{n\times q}{\mathbf{Y}} = \underset{n\times p}{\mathbf{X}} \cdot \underset{p\times q}{\mathbf{C}} + \underset{n\times q}{\mathbf{E}}$$

How to apply regularization methods to this model? There are several approaches to consider

- **Shrinkage**: ridge regression to overcome multicollinearity
- **sparsity**: variable selection in multivariate setting
- **Reduced-rank**
  - **Dimension reduction** via reducing rank of $\mathbf{C}$
  - $\min\|\mathbf{Y}-\mathbf{XC}\|_F^2$ s.t. $\text{rank}(\mathbf{C}) \leq r$
- **Combinations**
- **Low-rank** plus **sparse decomposition**: robust PCA, latent variable graphical models, covariance estimation
- **Regularized matrix** or **tensor regression**

Or, we can introduce a very attractive sparsity structure to achieve simultaneous dimension reduction and variable selection. This structure should be characterized by

- Having a few **distinct** channels/pathways relating responses and predictors
- Each of such associations may involve only **a smaller subset**, but not all of the responses and predictors

that is

$$\begin{aligned}
\mathbf{Y} &= \mathbf{XC} + \mathbf{E} \\
&= \mathbf{X} \cdot \begin{pmatrix} c_{11} & c_{12} & \cdots & c_{1q} \\ c_{21} & c_{22} & \cdots & c_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ c_{p1} & c_{p2} & \cdots & c_{pq} \end{pmatrix} + \mathbf{E} \\
&= \mathbf{X} \cdot \begin{pmatrix} 0 & u_{12} & \cdots & u_{1r} \\ u_{21} & 0 & \cdots & c_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ u_{p1} & u_{p2} & \cdots & u_{pr} \end{pmatrix} \cdot \begin{pmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 0 & \cdots & v_{q1} \\ v_{12} & v_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ v_{1r} & v_{2r} & \cdots & v_{qr} \end{pmatrix} + \mathbf{E}
\end{aligned}$$

This way, we can have

- **Sparsity**: selection of both **latent** and **original** variables
- **Low-rank SVD**: different subsets of responses allowed to be associated with different subsets of predictors

Consider an example:

Example 15.1.1: Dimension Reduction and Variable Selection via Sparse SVD

Consider the case where $p = 1000, q = 100$, then C, as a $p \times q$ matrix, contains 100000 coefficients. Meanwhile, for a rank-3 SVD model:

$$\mathbf{C} = d_1\mathbf{u}_1\mathbf{v}_1' + d_2\mathbf{u}_2\mathbf{v}_2' + d_3\mathbf{u}_3\mathbf{v}_3'$$

where $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ are all $p \times 1$, $\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3$ are all $q \times 1$, d_1, d_2, d_3 are all scalars. Hence, there are only $3 \times (1000 + 100 + 1) = 3303$ paramaters to estimate. If futher assume sparcity, the dimension would be even lower.

Now let's develop a scalable procedure for this idea.

15.2 Sparse Orthogonal Factor Regression

Consider the sigular value decomposition of $\mathbf{C}$

$$\mathbf{C} = \mathbf{UDV}' = \sum_{k=1}^{r} d_k\mathbf{u}_k\mathbf{v}_k'$$

where $\mathbf{U}$ and $\mathbf{V}$ are both **orthonormal**: $\mathbf{UU}' = \mathbf{VV}' = \mathbf{I}$. Then we can achieve dimension reduction via **low-dimensional latent model**

$$\tilde{\mathbf{Y}} = \tilde{\mathbf{X}}\mathbf{D} + \tilde{\mathbf{E}}$$

where

- $\tilde{\mathbf{Y}} = \mathbf{YV}$: $\mathbf{V}$ sparsity leads to **response** variable selection
- $\tilde{\mathbf{X}} = \mathbf{XU}$: $\mathbf{U}$ sparsity leads to **predictor** variable selection

How consider

$$\left(\hat{\mathbf{D}}, \hat{\mathbf{U}}, \hat{\mathbf{V}}\right) = \arg\min_{\mathbf{D},\mathbf{U},\mathbf{V}} \left\{\frac{1}{2}\|\mathbf{Y} - \mathbf{XUDV}'\|_F^2 + \lambda_d\|\mathbf{D}\|_1 + \lambda_a\rho_a(\mathbf{UD}) + \lambda_b\rho_b(\mathbf{VD})\right\} \quad \text{s.t. } \mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m \tag{15.1}$$

where

- $\rho_a(\cdot), \rho_b(\cdot)$ are penalty functions with regularization parameters $\lambda_d, \lambda_a, \lambda_b \geq 0$. These sparsity penalizations on **UD** and **VD** can be thought as **importance weighting**
- $\|\cdot\|_F$ is the nuclear norm, defined as the **sum** of its singular values $\|\mathbf{A}\|_F = \sum_i \sigma_i(\mathbf{A})$. It encourages sparsity among singular values and achieve **rank reduction**
- The orthgonality on $\mathbf{U}, \mathbf{V}$ allow a flexible form of sparsity-inducing penalties

If we further enrich this model by introducting an adaptive weighting $\mathbf{W}$ matrices

$$\left(\hat{\mathbf{\Theta}}, \hat{\mathbf{\Omega}}\right) = \arg\min_{\mathbf{\Theta},\mathbf{\Omega}} \left\{\frac{1}{2}\|\mathbf{Y} - \mathbf{XUDV}'\|_F^2 + \lambda_d\|\mathbf{W}_d \circ \mathbf{D}\|_1 + \lambda_a\rho_a(\mathbf{W}_a \circ \mathbf{A}) + \lambda_b\rho_b(\mathbf{W}_b \circ \mathbf{B})\right\}$$

s.t. $\mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m$, $\mathbf{UD} = \mathbf{A}$, $\mathbf{VD} = \mathbf{B}$. But why? Singular values and singular vectors of **larger magnitude** should be **less penalized** to reduce bias and improve efficiency.

Two applications are

- Biclustering with sparse SVD

$$\left(\hat{\mathbf{D}}, \hat{\mathbf{U}}, \hat{\mathbf{V}}\right) = \arg\min_{\mathbf{D},\mathbf{U},\mathbf{V}} \left\{\frac{1}{2}\|\mathbf{X} - \mathbf{UDV}'\|_F^2 + \lambda_d\|\mathbf{D}\|_1 + \lambda_a\rho_a(\mathbf{UD}) + \lambda_b\rho_b(\mathbf{VD})\right\} \quad \text{s.t. } \mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m$$

- Sparse PCA (sparsity in loadings of principla components)

$$\left(\hat{\mathbf{A}}, \hat{\mathbf{V}}\right) = \arg\min_{\mathbf{A},\mathbf{V}} \left\{\frac{1}{2}\|\mathbf{X} - \mathbf{XAV}'\|_F^2 + \lambda_a\rho_a(\mathbf{A})\right\} \qquad \text{s.t. } \mathbf{V}'\mathbf{V} = \mathbf{I}_m$$

15.3 Nonasymptotic Properties of SOFAR

First, define the robust spark for the regularity conditions

Definition 15.3.1: The robust spark κ_c

The robust spark κ_c of the $n \times p$ design matrix $\mathbf{X}$ is defined as the smallest possible positive integer such that there exists an $n \times \kappa_c$ submatrix of $\frac{1}{\sqrt{n}}\mathbf{X}$ having a **singular value** **less than** a given positive constant c

The robust spark κ_c here can be at least of order $O\left(\frac{n}{\log p}\right)$ with large probability for Gaussian design with dependency. With this definition, we characterize the following 5 conditions

- **Parameter space**: True parameters $(\mathbf{C}^*, \mathbf{D}^*, \mathbf{A}^*, \mathbf{B}^*)$ lie in $\mathcal{C} \times \mathcal{D} \times \mathcal{A} \times \mathcal{B}$, where
  - $\mathcal{C} = \{\mathbf{C} \in \mathbb{R}^{p\times q} : \|\mathbf{C}\|_0 < \kappa_{c_2}/2\}$, with κ_{c_2} being the robust spark of $\mathbf{X}$
  - $\mathcal{D} = \left\{\mathbf{D} = \operatorname{diag}\left\{d_j\right\} \in \mathbb{R}^{q\times q} : d_j = 0 \text{ or } |d_j| \geq \tau\right\}$
  - $\mathcal{A} = \left\{\mathbf{A} = \left\{a_{ij}\right\} \in \mathbb{R}^{p\times q} : a_{ij} = 0 \text{ or } |a_{ij}| \geq \tau\right\}$
  - $\mathcal{B} = \left\{\mathbf{B} = \left\{b_{ij}\right\} \in \mathbb{R}^{p\times q} : b_{ij} = 0 \text{ or } |b_{ij}| \geq \tau\right\}$

  $\tau > 0$ asymptotically vanishing.
- **Constrained eigenvalue**: It holds that for some constant $c_3 > 0$

$$\max_{\|\mathbf{u}\|_0 < \frac{\kappa_{c2}}{2}, \|\mathbf{u}\|_2 = 1} \|\mathbf{Xu}\|_2^2 \leq c_3 n, \qquad \max_{1\leq j\leq r}\|\mathbf{Xu}_j^*\|_2^2 \leq c_3 n$$

  where $\mathbf{u}_j^*$ is the **left singular vector** of $\mathbf{C}^*$ corresponding to singular value d_j^*
- **Error term**: The error term $\mathbf{E} \in \mathbb{R}^{n\times q} \sim \mathcal{N}(\mathbf{0}, \mathbf{I} \otimes \mathbf{\Sigma})$ with the maximum eigenvalue $\alpha_{\max}$ of $\mathbf{\Sigma}$ bounded from above and diagonal entries of $\mathbf{\Sigma}$ being σ_j^2
- **Penalty functions**: For matrices $\mathbf{M}$ and $\mathbf{M}^*$ of the same size, the penalty functions ρ_h with $h \in \{a, b\}$ satisfies

$$|\rho_h(\mathbf{M}) - \rho_h(\mathbf{M}^*)| \leq \|\mathbf{M} - \mathbf{M}^*\|_1$$

- **Relative spectral gap**: The nonzero singular values of $\mathbf{C}^*$ satisfy that

$${d_{j-1}^*}^2 - d_j^{*2} \geq \sqrt{\delta}{d_{j-1}^*}^2, \;\; 2 \leq j \leq r$$

  with a constant $\delta > 0$, both r and $\sum_{j=1}^r \left(\frac{d_1^*}{d_j^*}\right)^2$ can diverge as $n \to \infty$

How to understand the 5 conditions?

- **Parameter space** and **constrained eigenvalue** are essential for investigating computable solution to non-convex SOFAR optimization problem
- Gaussianity of error term can be relaxed
- **Penalty functions** can be many kinds of sparsity-inducing penalties, including entrywise L_1-norm[1] and row-wise $(2,1)$-norm[2]
- **Relative spectral gap** rules out non-identifiable case where some non-zero singular values are tied with each other and associated singular vectors in matrices $\mathbf{U}^*, \mathbf{V}^*$ are identifiable only up to some **orthogonal transformation**

15.4 Estimation: Convexity-Assisted Nonconvex Optimization

Non-convexity of SOFAR objective function poses important algorithmic and theoretical challenges, hence consider a **two-step** approach exploiting the framework of **convexity-assisted nonconvex optimization** (CANO) to obtain SOFAR estimator:

Step 1 minimize **L_1-penalized squared loss** for multivariate regression to obtain an initial estimator

Theorem 15.4.1: Error Bounds for the Initial Estimator

Under some regularity conditions, with large probability the initial estimator satisfies the following error bounds simultaneously:

$$\left\|\tilde{\mathbf{C}} - \mathbf{C}^*\right\|_F \le R_n \equiv c\sqrt{\frac{s\log(pq)}{n}} \tag{A}$$

$$\left\|\tilde{\mathbf{D}} - \mathbf{D}^*\right\|_F \le c\sqrt{\frac{s\log(pq)}{n}} \tag{B}$$

$$\left\|\tilde{\mathbf{A}} - \mathbf{A}^*\right\|_F + \left\|\tilde{\mathbf{B}} - \mathbf{B}^*\right\|_F \le c\eta_n\sqrt{\frac{s\log(pq)}{n}} \tag{C}$$

where $c = \|\mathbf{C}^*\|_0$ and $\eta_n = 1 + \sqrt{\frac{\sum_{j=1}^r (d_1^*/d_j^*)^2}{\delta}}$

When $q = 1$, bound (A) is consistent with the oracle inequality for Lasso. In this step, finer sparse SVD structure of coefficient matrix $\mathbf{C}^*$ is completely ignored, so intuitively, the second step should be able to improve error bounds.

Step 2 minimize SOFAR objective function in an **asymptotically shrinking neighborhood** of initial estimator

[1] Entrywise L_1-norm encourages sparsity among predictor/response effects specific to each rank-1 SVD layer

[2] $(2,1)$-norm is defined as the summation of absolute values of all components of a matrix. It promotes predictor/response-wise sparsity **regardless** of specific layer

Theorem 15.4.2: Nonasymptotic Error Bounds for SOFAR Estimator

Under some regularity conditions, with large probability the SOFAR estimator satisfies the following error bounds simultaneously:

$$\left\|\tilde{\mathbf{C}} - \mathbf{C}^*\right\|_F \leq c\sqrt{\min\left\{s, (r + s_a + s_b)\eta_n^2\right\} \cdot \frac{\log(pq)}{n}} \quad \text{(a)}$$

$$\left\|\tilde{\mathbf{D}} - \mathbf{D}^*\right\|_F + \left\|\tilde{\mathbf{A}} - \mathbf{A}^*\right\|_F + \left\|\tilde{\mathbf{B}} - \mathbf{B}^*\right\|_F \leq c\eta_n\sqrt{\min\left\{s, (r + s_a + s_b)\eta_n^2\right\} \cdot \frac{\log(pq)}{n}} \quad \text{(b)}$$

and

$$\left\|\tilde{\mathbf{D}} - \mathbf{D}^*\right\|_0 + \left\|\tilde{\mathbf{A}} - \mathbf{A}^*\right\|_0 + \left\|\tilde{\mathbf{B}} - \mathbf{B}^*\right\|_0 \leq c(r + s_a + s_b) \quad \text{(c)}$$

$$\left\|\tilde{\mathbf{D}} - \mathbf{D}^*\right\|_1 + \left\|\tilde{\mathbf{A}} - \mathbf{A}^*\right\|_1 + \left\|\tilde{\mathbf{B}} - \mathbf{B}^*\right\|_1 \leq c(r + s_a + s_b)\eta_n^2\lambda_{\max} \quad \text{(d)}$$

$$\frac{1}{n}\left\|\mathbf{X}\left(\hat{\mathbf{C}} - \mathbf{C}^*\right)\right\|_F^2 \leq c(r + s_a + s_b)\eta_n^2\lambda_{\max}^2 \quad \text{(e)}$$

where $r = \|\mathbf{D}^*\|_0$, $s_a = \|\mathbf{A}^*\|_0$, $s_b = \|\mathbf{B}^*\|_0$ and still $c = \|\mathbf{C}^*\|_0$ and $\eta_n = 1 + \sqrt{\frac{\sum_{j=1}^r (d_1^*/d_j^*)^2}{\delta}}$

here

- Bound (d) and (e) are the minimum of 2 rates
- s (the sparsity of matrix $\mathbf{C}^*$) comes from the first step of Lasso estimation, $r + s_a + s_b$ (total sparsity of $\mathbf{D}^*, \mathbf{A}^*, \mathbf{B}^*$) comes from the second step of SOFAR refinement
- Under Frobenius norm, $s > (r + s_a + s_b)\eta_n^2$ gives that the two-step procedure enhances error rates

also,

- In the case of univariate response with $q = 1$, $\eta_n = 1 + \delta$, $r = 1$, $s_a = s$, $s_b = 1$, the upper bounds are then reduced to those for high-dimensional univariate response regressions
- In the case of rank-one $r = 1$, $\eta_n = 1 + \frac{1}{\sqrt{\delta}}$ and $s = s_a s_b$, which leads to
  - SOFAR bounds: $c\sqrt{\frac{(s_a+s_b)\log(pq)}{n}}$, $c\sqrt{\frac{(s_a+s_b)\log(pq)}{n}}$, $c(s_a + s_b)$, $c(s_a + s_b)\sqrt{\frac{\log(pq)}{n}}$ and $\frac{c(s_a+s_b)\log(pq)}{n}$
  - Lasso bound (step 1): $c\sqrt{\frac{s_a s_b \log(pq)}{n}}$

  SOFAR estimator have much improved rates of covergence even in this case.