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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

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

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 C
 - $\min \|\mathbf{Y} \mathbf{XC}\|_F^2$ s.t. $\operatorname{rank}(\mathbf{C}) \le r$
- 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

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

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 C

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

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

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

where

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

How consider

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

where

- $\rho_a(\cdot)$, $\rho_b(\cdot)$ are penalty functions with regularization parameters λ_d , λ_a , $\lambda_b \ge 0$. 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 <u>rank reduction</u>
- The orthgonality on U, V allow a flexible form of sparsity-inducing penalties

If we further enrich this model by introducting an adaptive weighting W matrices

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

s.t. $U'U = V'V = I_m$, UD = A, VD = 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

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

Sparse PCA (sparsity in loadings of principla components)

$$(\hat{\mathbf{A}}, \hat{\mathbf{V}}) = \arg\min_{\mathbf{A}, \mathbf{V}} \left\{ \frac{1}{2} \|\mathbf{X} - \mathbf{X}\mathbf{A}\mathbf{V}'\|_F^2 + \lambda_a \rho_a(\mathbf{A}) \right\}$$
 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 **X** is defined as the smallest possible positive integer such that there exists an $n \times \kappa_c$ submatrix of $\frac{1}{\sqrt{n}}$ **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 (C^*, D^*, A^*, B^*) lie in $C \times D \times \mathcal{A} \times \mathcal{B}$, where
 - $C = \{\mathbf{C} \in \mathbb{R}^{p \times q} : \|\mathbf{C}\|_0 < \kappa_{c_2}/2\}$, with κ_{c_2} being the robust spark of \mathbf{X} $\mathcal{D} = \{\mathbf{D} = \text{diag } \{d_j\} \in \mathbb{R}^{q \times q} : d_j = 0 \text{ or } |d_j| \geq \tau\}$ $\mathcal{A} = \{\mathbf{A} = \{a_{ij}\} \in \mathbb{R}^{p \times q} : a_{ij} = 0 \text{ or } |a_{ij}| \geq \tau\}$ $\mathcal{B} = \{\mathbf{B} = \{b_{ij}\} \in \mathbb{R}^{p \times q} : b_{ij} = 0 \text{ or } |b_{ij}| \geq \tau\}$

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

$$\max_{\|\mathbf{u}\|_0 < \frac{\kappa_{c_2}}{2}, \|\mathbf{u}\|_2 = 1} \|\mathbf{X}\mathbf{u}\|_2^2 \le c_3 n, \qquad \max_{1 \le j \le r} \|\mathbf{X}\mathbf{u}_j^*\|_2^2 \le c_3 n$$

where \mathbf{u}_{i}^{*} is the **left singular vector** of \mathbf{C}^{*} corresponding to singular value d_{i}^{*}

- **Error term**: The error term $\mathbf{E} \in \mathbb{R}^{n \times q} \sim \mathcal{N}(\mathbf{0}, \mathbf{I} \otimes \Sigma)$ with the maximum eigenvalue α_{\max} of Σ bounded from above and diagonal entries of Σ being σ_i^2
- **Penalty functions**: For matrices **M** and **M*** of the same size, the penalty functions ρ_h with $h \in \{a, b\}$ satisfies

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

Relative spectral gap: The nonzero singular values of C* satisfy that

$$d_{j-1}^* - d_j^{*2} \ge \sqrt{\delta} d_{j-1}^*, \ 2 \le j \le r$$

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 <u>sparsity-inducing</u> penalties, including entrywise L_1 -norm¹ and row-wise (2, 1)-norm²
- 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:

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

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

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

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

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

and

$$\|\tilde{\mathbf{D}} - \mathbf{D}^*\|_0 + \|\tilde{\mathbf{A}} - \mathbf{A}^*\|_0 + \|\tilde{\mathbf{B}} - \mathbf{B}^*\|_0 \le c(r + s_a + s_b)$$
 (c)

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

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

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 C^*) comes from the first step of Lasso estimation, $r + s_a + s_b$ (total sparsity of D^* , A^* , 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 $s=s_as_b$, 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): $c\sqrt{\frac{s_as_b\log(pq)}{n}}$

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

Implementation with ALM-BCD 15.5

Now consider estimation implementation. The idea is to use the augmented Lagrangian method (ALM) coupled with block coordinate descent (BCD). The implementation procedure uses variable splitting to separate **orthogonality constraints** and **sparsity-inducing penalties** into different subproblems, enabling efficient optimization in a BCD fashion.

Consider $\Theta = (D, U, V)$, $\Omega = (A, B)$ in the optimization problem

$$\min_{\mathbf{\Theta}, \mathbf{\Omega}} \left\{ \frac{1}{2} \| \mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}' \|_F^2 + \lambda_d \| \mathbf{D} \|_1 + \lambda_a \rho_a(\mathbf{A}) + \lambda_b \rho_b(\mathbf{B}) \right\}$$

s.t. $U'U = V'V = I_m$, UD = A, VD = B. Then the **augmented Lagrangian** is

$$\mathcal{L}_{\mu}(\boldsymbol{\Theta}, \boldsymbol{\Omega}, \boldsymbol{\Gamma}) = \frac{1}{2} \|\mathbf{Y} - \mathbf{X}\mathbf{U}\mathbf{D}\mathbf{V}'\|_{F}^{2} + \lambda_{d} \|\mathbf{D}\|_{1} + \lambda_{a}\rho_{a}(\mathbf{A}) + \lambda_{b}\rho_{b}(\mathbf{B})$$
$$+ \langle \Gamma_{a}\mathbf{U}\mathbf{D} - \mathbf{A} \rangle + \langle \Gamma_{b}\mathbf{V}\mathbf{D} - \mathbf{B} \rangle + \frac{\mu}{2} \|\mathbf{U}\mathbf{D} - \mathbf{A}\|_{F}^{2} + \frac{\mu}{2} \|\mathbf{V}\mathbf{D} - \mathbf{B}\|_{F}^{2}$$

where $\Gamma = (\Gamma_a, \Gamma_b)$. The procedure has 2 components

(Θ, Ω)-step

$$\left(\mathbf{\Theta}^{k+1}, \mathbf{\Omega}^{k+1}\right) \leftarrow \arg\min_{\mathbf{\Theta}, \mathbf{\Omega}} \mathcal{L}_{\mu}(\mathbf{\Theta}, \mathbf{\Omega}, \mathbf{\Gamma}^{k})$$

- s.t. $U'U = V'V = I_m$. This step embodies
- block coordinate descent
- orthogonal Procrustes problem
- entrywise or block shoft thresholding
- Γ-step

$$\Gamma_a^{k+1} \leftarrow \Gamma_a^k + \mu \left(\mathbf{U}^{k+1} \mathbf{D}^{k+1} - \mathbf{A}^{k+1} \right)$$

$$\Gamma_b^{k+1} \leftarrow \Gamma_b^k + \mu \left(\mathbf{V}^{k+1} \mathbf{D}^{k+1} - \mathbf{B}^{k+1} \right)$$

where

- The penalty parameter μ increases by a ratio $\gamma > 1$ at the end of each iteration

Then the algorithm can be established as the following

Algorithm 15.5.1: SOFAR algorithm with ALM-BCD

- *Parameters*: λ_d , λ_a , λ_b and $\gamma > 1$
- Initialize \mathbf{U}^0 , \mathbf{V}^0 , \mathbf{D}^0 , \mathbf{A}^0 , \mathbf{B}^0 , Γ_a^0 , Γ_b^0 , μ^0
- For $k = 0, 1, \dots, do$
 - update U, V, D, A, B:

$$\mathbf{U}^{k+1} \leftarrow \arg\min_{\mathbf{U}'\mathbf{U} = \mathbf{I}_m} \frac{1}{2} \left\| \mathbf{Y} - \mathbf{X}\mathbf{U}\mathbf{D}^k\mathbf{V}^{k'} \right\|_F^2 + \frac{\mu^k}{2} \left\| \mathbf{U}\mathbf{D}^k - \mathbf{A}^k + \frac{\mathbf{\Gamma}_a^k}{\mu^k} \right\|_F^2$$
 (i)

$$\mathbf{V}^{k+1} \leftarrow \arg\min_{\mathbf{V}'\mathbf{V} = \mathbf{I}_m} \frac{1}{2} \left\| \mathbf{Y} - \mathbf{X}\mathbf{U}^{k+1}\mathbf{D}^k\mathbf{V}' \right\|_F^2 + \frac{\mu^k}{2} \left\| \mathbf{V}\mathbf{D}^k - \mathbf{B}^k + \frac{\mathbf{\Gamma}_b^k}{\mu^k} \right\|_F^2$$
 (ii)

$$\mathbf{D}^{k+1} \leftarrow \arg\min_{\mathbf{D} \geq 0} \frac{1}{2} \left\| \mathbf{Y} - \mathbf{X} \mathbf{U}^{k+1} \mathbf{D} \mathbf{V}^{k+1'} \right\|_F^2 + \frac{\mu^k}{2} \left\| \mathbf{U}^{k+1} \mathbf{D} - \mathbf{A}^k + \frac{\Gamma_a^k}{\mu^k} \right\|_F^2$$

$$+ \frac{\mu^k}{2} \left\| \mathbf{V}^{k+1} \mathbf{D} - \mathbf{B}^k + \frac{\mathbf{\Gamma}_b^k}{\mu^k} \right\|_{\Gamma}^2 + \lambda_d \|\mathbf{D}\|_1$$
 (c)

$$\mathbf{A}^{k+1} \leftarrow \arg\min_{\mathbf{A}} \frac{\mu^k}{2} \left\| \mathbf{U}^{k+1} \mathbf{D}^{k+1} - \mathbf{A} + \frac{\mathbf{\Gamma}_a^k}{\mu^k} \right\|_F^2 + \lambda_a \rho_a(\mathbf{A})$$
 (d)

$$\mathbf{B}^{k+1} \leftarrow \arg\min_{\mathbf{B}} \frac{\mu^k}{2} \left\| \mathbf{V}^{k+1} \mathbf{D}^{k+1} - \mathbf{B} + \frac{\Gamma_b^k}{\mu^k} \right\|_F^2 + \lambda_b \rho_b(\mathbf{B})$$
 (e)

- update Γ_a , Γ_b :

$$\boldsymbol{\Gamma}_a^{k+1} \leftarrow \boldsymbol{\Gamma}_a^k + \boldsymbol{\mu}^k \left(\mathbf{U}^{k+1} \mathbf{D}^{k+1} - \mathbf{A}^{k+1} \right) \qquad \qquad \boldsymbol{\Gamma}_b^{k+1} \leftarrow \boldsymbol{\Gamma}_b^k + \boldsymbol{\mu}^k \left(\mathbf{V}^{k+1} \mathbf{D}^{k+1} - \mathbf{B}^{k+1} \right)$$

where μ is updated by $\mu^{k+1} \leftarrow \gamma \mu^k$

This algorithm has strong convergence properties

Theorem 15.5.2: Convergence of SOFAR algorithm

Assume

- $\sum_{k=1}^{\infty} \left\{ \left[\Delta \mathcal{L}_{\mu}(\mathbf{U}^{k}) \right]^{1/2} + \left[\Delta \mathcal{L}_{\mu}(\mathbf{V}^{k}) \right]^{1/2} + \left[\Delta \mathcal{L}_{\mu}(\mathbf{D}^{k}) \right]^{1/2} \right\} < \infty$ where $\Delta \mathcal{L}_{\mu}(\cdot)$ denotes the decrease in $\mathcal{L}_{\mu}(\cdot)$ by a block update
- the penalty functions $\rho_a(\cdot)$, $\rho_b(\cdot)$ are **convex** Then the sequence generated by the SOFAR algorithm coverges to a **local** solution of the augmented Lagrangian for SOFAR problem.

Both matrix norm penalties $\|\cdot\|_1$ and $\|\cdot\|_{2,1}$ satisfy the assumption.