

Topic 15: Sparse Orthogonal Factor Regression

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Key points: Sparsity 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 Multivariate Linear Regression (MLR) model

$$\mathbf{Y} = \mathbf{X} \cdot \mathbf{C} + \mathbf{E}$$

$n \times q \quad n \times p \quad p \times q \quad n \times q$

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 \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:

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

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 $3 \times (1000 + 100 + 1) = 3303$ parameters to estimate. If further assume sparsity, the dimension would be even lower.

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

15.2 Sparse Orthogonal Factor Regression

Consider the singular value decomposition of C

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

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

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

where

- $\tilde{\mathbf{Y}} = \mathbf{Y}\mathbf{V}$: \mathbf{V} sparsity leads to response variable selection
- $\tilde{\mathbf{X}} = \mathbf{X}\mathbf{U}$: \mathbf{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 $\lambda_d, \lambda_a, \lambda_b \geq 0$. These sparsity penalizations on $\mathbf{U}\mathbf{D}$ and $\mathbf{V}\mathbf{D}$ 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 orthogonality on \mathbf{U}, \mathbf{V} allow a flexible form of sparsity-inducing penalties

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

$$(\hat{\mathbf{\Theta}}, \hat{\mathbf{\Omega}}) = \arg \min_{\mathbf{D}, \mathbf{U}, \mathbf{V}} \left\{ \frac{1}{2} \|\mathbf{Y} - \mathbf{X} \mathbf{U} \mathbf{D} \mathbf{V}'\|_F^2 + \lambda_d \|\mathbf{D}\|_1 + \lambda_a \rho_a(\mathbf{U}\mathbf{D}) + \lambda_b \rho_b(\mathbf{V}\mathbf{D}) \right\} \quad \text{s.t. } \mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m \quad (15.2)$$

Two applications are

- Biclustering with sparse SVD

$$(\hat{\mathbf{D}}, \hat{\mathbf{U}}, \hat{\mathbf{V}}) = \arg \min_{\mathbf{D}, \mathbf{U}, \mathbf{V}} \left\{ \frac{1}{2} \|\mathbf{X} - \mathbf{U}\mathbf{D}\mathbf{V}'\|_F^2 + \lambda_d \|\mathbf{D}\|_1 + \lambda_a \rho_a(\mathbf{U}\mathbf{D}) + \lambda_b \rho_b(\mathbf{V}\mathbf{D}) \right\} \quad \text{s.t. } \mathbf{U}'\mathbf{U} = \mathbf{V}'\mathbf{V} = \mathbf{I}_m \quad (15.3)$$

- Sparse PCA (sparsity in loadings of principal components)

$$(\hat{\mathbf{A}}, \hat{\mathbf{V}}) = \arg \min_{\mathbf{A}, \mathbf{V}} \left\{ \frac{1}{2} \|\mathbf{X} - \mathbf{X}\mathbf{A}\mathbf{V}'\|_F^2 + \lambda_a \rho_a(\mathbf{A}) \right\} \quad \text{s.t. } \mathbf{V}'\mathbf{V} = \mathbf{I}_m \quad (15.4)$$