

Part III: Low rank matrix estimation
(Lecture 1) From vector to matrix

2014-6-27

Taiji Suzuki (Room W707, post W8-46)
e-mail: suzuki.t.ct@m.titech.ac.jp

Outline of the Lecture

This course introduces several basic concepts of mathematical optimization, probability and statistics, and is intended to provide key knowledge necessary for advanced study in Mathematical and Computing Sciences.

Outline of this part (3rd part)

This part gives basic knowledges of low rank matrix estimation problems. Low rank matrix estimation has various applications such as computer vision, recommendation system, and reduced rank regression. In the series of lectures, problem formulation, methodologies, computational method and statistical properties are shown.

Lecture plan:

1. From vector to matrix: Introduction to sparse estimation and low rank matrix estimation.
2. Estimation method: Statistical methodologies for estimating low rank matrix.
3. Computational method: Optimization method and sampling method.
4. Statistical property: Estimation accuracy, measure concentration of matrix valued random variables.
5. Advanced topics.

Evaluation: report.

References

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1 Linear regression

Before we are going into the low rank matrix estimation, we briefly review the vector estimation problem.

Given fixed covariates $X = \begin{bmatrix} x_1^\top \\ x_2^\top \\ \vdots \\ x_n^\top \end{bmatrix} \in \mathbb{R}^{n \times p}$, we observe

$$Y = X\beta^* + \epsilon, \quad (\text{regression})$$

where $Y = [y_1, \dots, y_n]^\top \in \mathbb{R}^n$ (dependent variable, response) and $\epsilon = [\epsilon_1, \dots, \epsilon_n]^\top \in \mathbb{R}^n$ (noise). We assume that $\{\epsilon_i\}_{i=1}^n$ is i.i.d. random variable with mean 0 and variance σ^2 ($E[\epsilon_i] = 0, E[\epsilon_i^2] = \sigma^2$). We observe $\{(x_i, y_i)\}_{i=1}^n$, and want to estimate β^* (or $X\beta^*$) from the observed data.

There are many methods to estimate β^* , for example

- Least squares estimator.
- Ridge regression.
- Stein's shrinkage estimator.
- Lasso.

2 Least squares estimator

2.1 Definition of least squares estimator

$$\hat{\beta}_{\text{LS}} := \arg \min_{\beta \in \mathbb{R}^p} \|Y - X\beta\|^2 = \arg \min_{\beta \in \mathbb{R}^p} \sum_{i=1}^n (y_i - x_i^\top \beta)^2.$$

For simplicity, we assume that $X^\top X \succ O$. Then $\hat{\beta}_{\text{LS}}$ can be expressed as

$$\hat{\beta}_{\text{LS}} = (X^\top X)^{-1} X^\top Y.$$

(\because) $\hat{\beta}_{\text{LS}}$ satisfies

$$\begin{aligned} \nabla_{\beta} \|Y - X\beta\|^2|_{\beta=\hat{\beta}_{\text{LS}}} &= 0 \\ \Leftrightarrow X^\top (X\hat{\beta}_{\text{LS}} - Y) &= 0 \\ \Leftrightarrow \hat{\beta}_{\text{LS}} &= (X^\top X)^{-1} X^\top Y. \end{aligned}$$

2.2 Statistical properties of least squares estimator

- $\hat{\beta}_{\text{LS}}$ is an unbiased estimator:

$$E_{Y|X}[\hat{\beta}_{\text{LS}}] = \beta^*.$$

$$(\because) E_{Y|X}[\hat{\beta}_{\text{LS}}] = E_{Y|X}[(X^\top X)^{-1} X^\top Y] = (X^\top X)^{-1} X^\top X \beta^* = \beta^*.$$

- Variance (variance and covariance matrix) of $\hat{\beta}_{\text{LS}}$ is given by

$$\text{Var}(\hat{\beta}_{\text{LS}}) = \mathbb{E}_{Y|X}[(\hat{\beta}_{\text{LS}} - \beta^*)(\hat{\beta}_{\text{LS}} - \beta^*)^\top] = (X^\top X)^{-1} \sigma^2.$$

$$\begin{aligned} (\because) \quad & \mathbb{E}_{Y|X}[(\hat{\beta}_{\text{LS}} - \beta^*)(\hat{\beta}_{\text{LS}} - \beta^*)^\top] \\ &= \mathbb{E}_{Y|X}[\{(X^\top X)^{-1} X^\top (X\beta^* + \epsilon) - \beta^*\} \{(X^\top X)^{-1} X^\top (X\beta^* + \epsilon) - \beta^*\}^\top] \\ &= \mathbb{E}_{Y|X}[\{(X^\top X)^{-1} X^\top \epsilon\} \{(X^\top X)^{-1} X^\top \epsilon\}^\top] = (X^\top X)^{-1} X^\top X (X^\top X)^{-1} \sigma^2 \\ &= (X^\top X)^{-1} \sigma^2. \end{aligned}$$

This is minimum variance among all unbiased estimator (discussed in the following).

2.3 Least squares estimator as an maximum likelihood estimator

Here assume that ϵ_i is generated from Gaussian distribution ($N(0, \sigma^2)$). Remind that the probability density function of y_i for $\beta^* = \beta$ is given by

$$p(y_i|\beta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - x_i^\top \beta)^2}{2\sigma^2}\right),$$

because of the normality of the noise. Thus the log-likelihood of β is given by

$$\log \prod_{i=1}^n p(y_i|\beta) = -\sum_{i=1}^n \frac{(y_i - x_i^\top \beta)^2}{2\sigma^2} - n \log(\sqrt{2\pi\sigma^2}).$$

Therefore, by maximizing the log-likelihood, we obtain the maximum likelihood estimator $\hat{\beta}_{\text{MLE}} = (X^\top X)^{-1} X^\top Y$. One can observe that

$$\hat{\beta}_{\text{LS}} = \hat{\beta}_{\text{MLE}}.$$

Theorem 1 (Cramer-Rao's Inequality). *For all unbiased estimator $\hat{\beta}$, we have*

$$\text{Var}(\hat{\beta}) = \mathbb{E}_{Y|X}[(\hat{\beta} - \beta^*)(\hat{\beta} - \beta^*)^\top] \succeq \mathbb{E}_{Y|X}[\nabla_\beta \log p(Y|\beta) \nabla_\beta^\top \log p(Y|\beta)]^{-1}|_{\beta=\beta^*} \quad (1)$$

Here, the right hand side of Eq. (1) is the inverse of Fisher information matrix.

Notice that

$$\begin{aligned} \mathbb{E}_{Y|X}[\nabla_\beta \log p(Y|\beta) \nabla_\beta^\top \log p(Y|\beta)]|_{\beta=\beta^*} &= \mathbb{E}_{Y|X} \left[\frac{X^\top (X\beta^* - Y)}{\sigma^2} \frac{(X\beta^* - Y)^\top X}{\sigma^2} \right] \\ &= \mathbb{E}_{Y|X} \left[\frac{X^\top \epsilon \epsilon^\top X}{\sigma^4} \right] = X^\top X \sigma^{-2}. \end{aligned}$$

Thus, $\text{Var}(\hat{\beta}) \succeq (X^\top X)^{-1} \sigma^2$ holds for all unbiased estimator $\hat{\beta}$. As we have seen, $\text{Var}(\hat{\beta}_{\text{LS}}) = (X^\top X)^{-1} \sigma^2$. Therefore, it holds that

$$\text{Var}(\hat{\beta}) \succeq \text{Var}(\hat{\beta}_{\text{LS}}) \quad \text{for all unbiased estimator } \hat{\beta}.$$

In that sense, the least squares estimator is called Best Unbiased Estimator (BUE).

2.4 Mean Squared Error (MSE) of the least squares estimator

Question: How accurate is the LS estimator?

MSE is defined as

$$\text{MSE} = \mathbb{E}_{Y|X}[\|\hat{\beta}_{\text{LS}} - \beta^*\|^2].$$

MSE can be evaluated as

$$\mathbb{E}_{Y|X}[\|\hat{\beta}_{\text{LS}} - \beta^*\|^2] = \sigma^2 \text{Tr}[(X^\top X)^{-1}],$$

because

$$\mathbb{E}_{Y|X}[\|\hat{\beta}_{\text{LS}} - \beta^*\|^2] = \mathbb{E}_{Y|X}\{\text{Tr}[(\hat{\beta}_{\text{LS}} - \beta^*)(\hat{\beta}_{\text{LS}} - \beta^*)^\top]\} = \sigma^2 \text{Tr}[(X^\top X)^{-1}].$$

Now, we evaluate how MSE is dependent on the dimension p . To do so, we assume that x_i is i.i.d. random variable generated from a distribution that satisfies $\mathbb{E}_x[xx^\top] = S (\in \mathbb{R}^{p \times p})$. By the law of large numbers, we have that

$$\frac{X^\top X}{n} \rightarrow S \quad (\text{in probability}).$$

This implies that

$$\mathbb{E}_{Y|X}[\|\hat{\beta}_{\text{LS}} - \beta^*\|^2] = \frac{\sigma^2}{n} \text{Tr}[(X^\top X/n)^{-1}] \rightarrow \frac{\sigma^2}{n} \text{Tr}[S^{-1}] \quad (\text{in probability}),$$

by the continuity of the inverse operation of a matrix (Slutsky's lemma).

If $S \succeq \lambda_{\min} I_p \succ O$ for some $\lambda_{\min} > 0$, then

$$\frac{\sigma^2}{n} \text{Tr}[S^{-1}] \leq \frac{\sigma^2}{n} \text{Tr}[(\lambda_{\min} I_p)^{-1}] \leq \frac{p}{n} \frac{\sigma^2}{\lambda_{\min}}.$$

This is linear to p (the dimension of the parameter).

Predictive accuracy is also an important performance measure. That (more precisely the in-sample predictive accuracy) is defined as

$$\text{Predictive accuracy} = \mathbb{E}_{Y|X} \left[\frac{1}{n} \sum_{i=1}^n (x_i^\top \beta^* - x_i^\top \hat{\beta}_{\text{LS}}) \right].$$

(Check that $\frac{1}{n} \sum_{i=1}^n (x_i^\top \beta^* - x_i^\top \hat{\beta}_{\text{LS}})$ is equivalent to $\mathbb{E}_{\tilde{Y}|X}[\frac{1}{n} \|\tilde{Y} - X \hat{\beta}_{\text{LS}}\|^2]$ up to constant where \tilde{Y} is an independent copy of Y). The predictive accuracy is evaluated as

$$\begin{aligned} \mathbb{E}_{Y|X} \left[\frac{1}{n} \sum_{i=1}^n (x_i^\top \beta^* - x_i^\top \hat{\beta}_{\text{LS}}) \right] &= \mathbb{E}_{Y|X} \left[\frac{1}{n} \|X \beta^* - X \hat{\beta}_{\text{LS}}\|^2 \right] \\ &= \frac{1}{n} \text{Tr}[X \text{Var}(\hat{\beta}_{\text{LS}}) X^\top] = \frac{\sigma^2}{n} \text{Tr}[I_p] = \sigma^2 \frac{p}{n}. \end{aligned}$$

The predictive accuracy is also linear to p . Therefore, if p is large compared to n , we don't have favorable estimation accuracy.

Question: What happens if β^* is **sparse**? Can we improve the accuracy?

\Rightarrow Yes. Model selection.

3 Model Selection: AIC

AIC (Akaike's Information Criterion) invented by **Hirotsugu Akaike** is a criterion to minimize the predictive accuracy. AIC is originally developed to specify the order of AR model. It can be applied to not only linear regression but also other statistical models.

Suppose that the number of non-zero component of β^* is small (the explanatory variable contains a lot of redundant information). We want to estimate the index set of the non-zero components ($J := \{j | \beta_j^* \neq 0\}$).

Note: Just choosing the index set that minimizes the empirical risk is not a good idea. \rightarrow **Overfitting**.

Let $\hat{\beta}_{\hat{J}}$ be the least squares estimator on the submodel \hat{J} :

$$\hat{\beta}_{\hat{J}} := \arg \min_{\beta \in \mathbb{R}^p: \beta_{\hat{J}^c} = \mathbf{0}} \|Y - X\beta\|^2.$$

Ideally if we know the true non-zero components, i.e. $\hat{J} = J$, then

$$\text{predictive accuracy of } \hat{\beta}_{\hat{J}} = \sigma^2 \frac{|J|}{n} \ll \sigma^2 \frac{p}{n},$$

under a sparse setting $|J| \ll p$. However, in practice, we don't know J . Thus we need to estimate that.

$$\text{AIC}(\hat{J}) = \|Y - X\hat{\beta}_{\hat{J}}\|^2 + 2\sigma^2|\hat{J}|.$$

Choose $\hat{J} \subseteq \{1, \dots, n\}$ that minimizes AIC.

AIC is an unbiased estimator of the predictive error up to constant (if \hat{J} includes J). Minimizing AIC leads to a good predictive accuracy (indeed it is minimax optimal).

Proof. (Rough proof) Suppose that \hat{J} includes J and let $X_{\hat{J}} = (X_{i,j})_{i=1, \dots, n; j \in \hat{J}}$ (submatrix of X with column indices \hat{J}), then we have

$$\begin{aligned} & \mathbb{E}_{Y|X} \left[\frac{1}{n} \|X\hat{\beta}_{\hat{J}} - X\beta^*\|^2 \right] \\ &= \mathbb{E}_{Y|X} \left[\frac{1}{n} \|X\hat{\beta}_{\hat{J}} - Y - \epsilon\|^2 \right] \\ &= \mathbb{E}_{Y|X} \left[\frac{1}{n} \|X\hat{\beta}_{\hat{J}} - Y\|^2 - \frac{2}{n} \langle X\hat{\beta}_{\hat{J}} - Y, \epsilon \rangle + \frac{1}{n} \|\epsilon\|^2 \right]. \end{aligned}$$

Now, observe that

$$\begin{aligned} & \mathbb{E}_{Y|X} [\langle X\hat{\beta}_{\hat{J}} - Y, \epsilon \rangle] \\ &= \mathbb{E}_{Y|X} [\langle X_{\hat{J}}(X_{\hat{J}}^\top X_{\hat{J}})^{-1} X_{\hat{J}}^\top Y - X\beta^* - \epsilon, \epsilon \rangle] \end{aligned}$$

$$\begin{aligned}
&= \mathbb{E}_{Y|X} [\langle X_{\hat{J}}(X_{\hat{J}}^\top X_{\hat{J}})^{-1} X_{\hat{J}}^\top (X_{\hat{J}} \beta_{\hat{J}}^* + \epsilon) - X_{\hat{J}} \beta_{\hat{J}}^* - \epsilon, \epsilon \rangle] \quad (\because J \subseteq \hat{J}) \\
&= \mathbb{E}_{Y|X} [\|X_{\hat{J}}(X_{\hat{J}}^\top X_{\hat{J}})^{-1} X_{\hat{J}}^\top \epsilon\|^2] - n\sigma^2 = |\hat{J}|\sigma^2 - n\sigma^2.
\end{aligned}$$

Then, we have that

$$\begin{aligned}
\mathbb{E}_{Y|X} \left[\frac{1}{n} \|X \hat{\beta}_{\hat{J}} - X \beta^*\|^2 \right] &= \mathbb{E}_{Y|X} \left[\frac{1}{n} \|X \hat{\beta}_{\hat{J}} - Y\|^2 + \frac{2|\hat{J}|\sigma^2}{n} \right] - \sigma^2 \\
&= \mathbb{E}_{Y|X} \left[\frac{1}{n} \text{AIC}(\hat{J}) \right] - \sigma^2.
\end{aligned}$$

□

Minimizing AIC is computationally much demanding ($O(2^p)$).

⇒ NP-hard (submodular function maximization).

⇒ L_1 -regularization (Lasso) [7]: Convex optimization, statistically nice properties.

4 Estimation of low rank matrix: From vector to matrix

Model:

$$y_i = \langle X_i, A^* \rangle + \epsilon_i, \quad (i = 1, \dots, n),$$

where $\langle X, A \rangle = \text{Tr}[X^\top A]$, $X_i \in \text{Real}^{M \times N}$ is an explanatory variable, $A^* \in \text{Real}^{M \times N}$ is the true matrix (supposed to be low rank), and ϵ_i is i.i.d. noise.

Basic idea:

$$\begin{aligned}
&\min_{A \in \mathbb{R}^{M \times N}} \sum_{i=1}^n (y_i - \langle X_i, A \rangle) \\
&\text{s.t.} \quad \text{rank}(A) \leq d.
\end{aligned}$$

Analogous to AIC minimization. The cardinality of non-zero components is replaced by rank. Note that this is non-convex.

Applications:

- Computer vision
- Recommendation system [6] (NetFlix prize [3])
- Reduced rank regression [1, 4, 5]
- Multi-task learning [2]

References

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