Lecture 3. Inadmissibility of Maximum Likelihood Estimate and James-Stein Estimator

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Outline

PCA in Noise

- Data: $x_i \in \mathbb{R}^p$, $i = 1, \ldots, n$

- PCA looks for Eigen-Value Decomposition (EVD) of sample covariance matrix:

$$\hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^{n} (x_i - \hat{\mu}_n)(x_i - \hat{\mu}_n)^T$$

  where

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} x_i$$

- Geometric view as the best affine space approximation of data

- What about statistical view when $x_i = \mu + \varepsilon_i$?

Recall: Phase Transitions of PCA

For rank-1 signal-noise model

$$X = \alpha u + \varepsilon, \qquad \alpha \sim \mathcal{N}(0, \sigma_X^2), \quad \varepsilon \sim \mathcal{N}(0, I_p)$$

PCA undergoes a phase transition if $p/n \to \gamma$:

- The primary eigenvalue of sample covariance matrix satisfies

$$\lambda_{\max}(\widehat{\Sigma}_n) \to \begin{cases} (1+\sqrt{\gamma})^2 = b, & \sigma_X^2 \leq \sqrt{\gamma} \\ (1+\sigma_X^2)(1+\frac{\gamma}{\sigma_X^2}), & \sigma_X^2 > \sqrt{\gamma} \end{cases} \tag{1}$$

- The primary eigenvector converges to

$$|\langle u, v_{\max}\rangle|^2 \to \begin{cases} 0 & \sigma_X^2 \leq \sqrt{\gamma} \\ \frac{1-\frac{\gamma}{\sigma_X^4}}{1+\frac{\gamma}{\sigma_X^2}}, & \sigma_X^2 > \sqrt{\gamma} \end{cases} \tag{2}$$

Recall: Phase Transitions of PCA

- Here the threshold
$$\gamma = \lim_{n,p\to\infty} \frac{p}{n}$$

- The **law of large numbers** in traditional statistics assumes p fixed and $n \to \infty$:
$$\gamma = \lim_{n\to\infty} p/n = 0.$$
where PCA always works without phase transitions.

- In **high dimensional statistics**, we allow both p and n grow: $p, n \to \infty$, not law of large numbers.

- What might go wrong? Even the sample mean $\hat{\mu}_n$!

In this lecture

- Sample mean $\hat{\mu}_n$ and covariance $\hat{\Sigma}_n$ are both Maximum Likelihood Estimate (MLE) under Gaussian noise models
- In high dimensional scenarios (small n, large p), MLE $\hat{\mu}_n$ is not optimal:
  - Inadmissability: MLE has worse prediction power than James-Stein Estimator (JSE) (Stein, 1956)
  - Many shrinkage estimates are better than MLE and James-Stein Estimator (JSE)
- Therefore, penalized likelihood or regularization is necessary in high dimensional statistics

Outline

Maximum Likelihood Estimate

- Statistical model $f(X|\theta)$ as a conditional probability function on $\mathbb{R}^p$ with parameter space $\theta \in \Theta$

- The likelihood function is defined as the probability of observing the given data $x_i \sim f(X|\theta)$ as a function of θ,

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} f(x_i|\theta)$$

- A Maximum Likelihood Estimator is defined as

$$\begin{aligned} \hat{\theta}_n^{MLE} &\in \arg\max_{\theta \in \Theta} \mathcal{L}(\theta) = \arg\max_{\theta \in \Theta} \prod_{i=1}^{n} f(x_i|\theta) \\ &= \arg\max_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} \log f(x_i|\theta). \end{aligned} \tag{3}$$

Maximum Likelihood Estimate

- For example, consider the normal distribution $\mathcal{N}(\mu, \Sigma)$,

$$f(X|\mu, \Sigma) = \frac{1}{\sqrt{(2\pi)^p|\Sigma|}} \exp\left[-\frac{1}{2}(X-\mu)^T\Sigma^{-1}(X-\mu)\right],$$

  where $|\Sigma|$ is the determinant of covariance matrix Σ.

- Take independent and identically distributed (i.i.d.) samples $x_i \sim \mathcal{N}(\mu, \Sigma)$ $(i = 1, \ldots, n)$

Maximum Likelihood Estimate (continued)

- To get the MLE given $x_i \sim \mathcal{N}(\mu, \Sigma)$ $(i = 1, \ldots, n)$, solve

$$\max_{\mu,\Sigma} \prod_{i=1}^{n} f(x_i|\mu,\Sigma) = \max_{\mu,\Sigma} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi|\Sigma|}} \exp[-(X_i-\mu)^T \Sigma^{-1} (X_i-\mu)]$$

- Equivalently, consider the logarithmic likelihood

$$\begin{aligned} J(\mu,\Sigma) &= \log \prod_{i=1}^{n} f(x_i|\mu,\Sigma) \\ &= -\frac{1}{2} \sum_{i=1}^{n} (X_i-\mu)^T \Sigma^{-1} (X_i-\mu) - \frac{n}{2} \log|\Sigma| + C \end{aligned}$$

where C is a constant independent to parameters

MLE: sample mean $\hat{\mu}_n$

- To solve μ, the log-likelihood is a quadratic function of μ,

$$0 = \frac{\partial J}{\partial \mu}\bigg|_{\mu=\mu^*} = -\sum_{i=1}^{n} \Sigma^{-1}(x_i - \mu^*)$$

$$\Rightarrow \mu^* = \frac{1}{n}\sum_{i=1}^{n} x_i =: \hat{\mu}_n$$

MLE: sample covariance $\hat{\Sigma}_n$

- To solve Σ, the first term in (4)

$$
\begin{aligned}
& -\frac{1}{2}\sum_{i=1}^{n}\mathbf{Tr}(x_i-\mu)^T\Sigma^{-1}(x_i-\mu) \\
= & -\frac{1}{2}\sum_{i=1}^{n}\mathbf{Tr}[\Sigma^{-1}(x_i-\mu)(x_i-\mu)^T], \quad \mathbf{Tr}(ABC)=\mathbf{Tr}(BCA) \\
= & -\frac{n}{2}(\mathbf{Tr}\,\Sigma^{-1}\hat{\Sigma}_n), \quad \hat{\Sigma}_n := \frac{1}{n}\sum_{i=1}^{n}(x_i-\hat{\mu}_n)(x_i-\hat{\mu}_n)^T, \\
= & -\frac{n}{2}\,\mathbf{Tr}(\Sigma^{-1}\hat{\Sigma}_n^{\frac{1}{2}}\hat{\Sigma}_n^{\frac{1}{2}}) \\
= & -\frac{n}{2}\,\mathbf{Tr}(\hat{\Sigma}_n^{\frac{1}{2}}\Sigma^{-1}\hat{\Sigma}_n^{\frac{1}{2}}), \quad \mathbf{Tr}(ABC)=\mathbf{Tr}(BCA) \\
= & -\frac{n}{2}\,\mathbf{Tr}(S), \quad S := \hat{\Sigma}_n^{\frac{1}{2}}\Sigma^{-1}\hat{\Sigma}_n^{\frac{1}{2}}
\end{aligned}
$$

MLE: sample covariance $\hat{\Sigma}_n$

Use S to represent Σ:

- Notice that

$$\Sigma = \hat{\Sigma}_n^{\frac{1}{2}} S^{-1} \hat{\Sigma}_n^{\frac{1}{2}}$$

$$\Rightarrow -\frac{n}{2} \log |\Sigma| = \frac{n}{2} \log |S| - \frac{n}{2} \log |\hat{\Sigma}_n| = f(\hat{\Sigma}_n)$$

  where we use for determinant of squared matrices of equal size, $\det(AB) = |AB| = \det(A)\det(B) = |A| \cdot |B|$.

- Therefore,

$$\max_{\Sigma} J(\Sigma) \Leftrightarrow \min_{S} \frac{n}{2} \mathbf{Tr}(S) - \frac{n}{2} \log |S| + Const(\hat{\Sigma}_n, 1)$$

MLE: sample covariance $\hat{\Sigma}_n$

- Since $S = \hat{\Sigma}_n^{\frac{1}{2}} \Sigma^{-1} \hat{\Sigma}_n^{\frac{1}{2}}$ is symmetric and positive semidefinite, let $S = U \Lambda U^T$ be its eigenvalue decomposition, $\Lambda = \mathbf{diag}(\lambda_i)$ with $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \geq 0$. Then we have

$$J(\lambda_i) = \frac{n}{2} \sum_{i=1}^{p} \lambda_i - \frac{n}{2} \sum_{i=1}^{p} \log(\lambda_i) + Const$$

$$\Rightarrow 0 = \left. \frac{\partial J}{\partial \lambda_i} \right|_{\lambda_i^*} = \frac{n}{2} - \frac{n}{2} \frac{1}{\lambda_i^*} \Rightarrow \lambda_i^* = 1$$

$$\Rightarrow S^* = I_p$$

- Hence the MLE solution

$$\Sigma^* = \hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^{n} (X_i - \hat{\mu}_n)(X_i - \hat{\mu}_n)^T,$$

Note

- In statistics, it is often defined

$$\hat{\Sigma}_n = \frac{1}{n-1} \sum_{i=1}^{n} (X_i - \hat{\mu}_n)(X_i - \hat{\mu}_n)^T,$$

  where the denominator is $(n-1)$ instead of n. This is because that for sample covariance matrix, a single sample $n = 1$ leads to no variance at all.

Model Assumptions of LDA

Input X is p-dimensional. Output $Y = 1, ..., K$, totally K classes. Assume, for $k = 1, ..., K$,

$$X|Y = k \sim \mathcal{N}(\mu_k, \Sigma),$$

where μ_k is p-vector and Σ is p-by-p covariance matrix, i.e. class density

$$f_k(x) = \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\Big(-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)\Big)$$

Note that we assumed the same Σ for all classes $k = 1, ..., K$.

The Bayes Theorem

- Suppose there are K, denoted as $1, 2, ..., K$, for the output Y.
- X is the input of p-dimension. Both Y and X are random variables.
- Let $\pi_k = P(Y = k)$.
- Let $f_k(x) = f(x|Y = k)$ be the conditional density function of X given $Y = k$.
- Then, Bayes theorem[1] implies

$$p_k(x) = P(Y = k|X = x) = \frac{\pi_k f_k(x)}{\sum_{j=1}^{K} \pi_j f_j(x)}$$

- We classify a subject with input x into class k, if its $p_k(x)$ is the largest, for $k = 1, ..., K$.

[1] General Bayes theorem: for $A_i \cap A_j = \emptyset, P(\cup_i A_i) = 1$,

$$P(A_k|B) = \frac{P(B|A_k)P(A_k)}{\sum_{j=1}^{K} P(B|A_j)P(A_j)}.$$

Computing $p_k(x)$ for LDA

- We aim to maximize over k the following

$$p_k(x) = \frac{\pi_k \exp[(-1/2)(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)]}{\sum_{l=1}^K \pi_l \exp[(-1/2)(x-\mu_l)^T\Sigma^{-1}(x-\mu_l)]}$$

- Maximizing conditional likelihood $p_k(x)$ is the same as maximizing the k-th score, which is linear in x,

$$\delta_k(x) = \mu_k^{-1}\Sigma^{-1}x - \frac{1}{2}\mu_k^T\Sigma^{-1}\mu_k + \log \pi_k.$$

  where the Bayesian classifier is the k with the largest δ_k.
- A practical problem: parameter Σ and μ_j and π_j, $j = 1, ..., K$ are usually unknown?

Fisher's Linear Discriminant Analysis

Choose the class to maximize the following *linear* score function:

$$\max_k \hat{\delta}_k(x) = \hat{\mu}_k^T \hat{\Sigma}^{-1} x - \frac{1}{2} \hat{\mu}_k^T \hat{\Sigma}^{-1} \hat{\mu}_k + \log \hat{\pi}_k, \tag{4}$$

where given data $(x_i, y_i), i = 1, ..., n$,

- $\hat{\mu}_k$ is the sample mean of class k

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i:y_i=k} x_i;$$

- $\hat{\Sigma}$ is the pooled (overall) sample covariance

$$\hat{\Sigma} = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i:y_i=k} (x_i - \hat{\mu}_k)(x_i - \hat{\mu}_k)^T,$$

- $\hat{\pi}_k = n_k/n$ is the sample proportion of class k where n_k is the number of subjects in class k

Consistency of MLE

Under some regularity conditions, the maximum likelihood estimator $\hat{\theta}_n^{MLE}$ has the following nice *limit* properties for fixed p and $n \to \infty$:

A. (Consistency) $\hat{\theta}_n^{MLE} \to \theta_0$, in probability and almost surely.

B. (Asymptotic Normality) $\sqrt{n}(\hat{\theta}_n^{MLE} - \theta_0) \to \mathcal{N}(0, I_0^{-1})$ in distribution, where I_0 is the Fisher Information matrix

$$I(\theta_0) := \mathbf{E}[(\frac{\partial}{\partial\theta} \log f(X|\theta_0))^2] = -\mathbf{E}[\frac{\partial^2}{\partial\theta^2} \log f(X|\theta_0)].$$

C. (Asymptotic Efficiency) $\lim_{n\to\infty} \mathrm{cov}(\hat{\theta}_n^{MLE}) = I^{-1}(\theta_0)$. Hence $\hat{\theta}_n^{MLE}$ is the **Uniformly Minimum-Variance Unbiased Estimator**, i.e. the estimator with the least variance among the class of unbiased estimators, for any unbiased estimator $\hat{\theta}_n$, $\lim_{n\to\infty} \mathrm{var}(\hat{\theta}_n^{MLE}) \leq \lim_{n\to\infty} \mathrm{var}(\hat{\theta}_n)$.

However, large p small n?

- The asymptotic results all hold under the assumption by fixing p and taking $n \to \infty$, where MLE satisfies $\hat{\mu}_n \to \mu$ and $\hat{\Sigma}_n \to \Sigma$.
- However, when p becomes large compared to finite n, $\hat{\mu}_n$ is not the best estimator for *prediction* measured by expected mean squared error from the truth, to to shown below.

Outline

Prediction Error and Risk

- To measure the *prediction* performance of an estimator $\hat{\mu}_n$, it is natural to consider the expected squared loss in regression, i.e. given a response $y = \mu + \epsilon$ with zero mean noise $\mathbf{E}[\epsilon] = 0$,

$$\mathbf{E}\,\|y - \hat{\mu}_n\|^2 = \mathbf{E}\,\|\mu - \hat{\mu} + \epsilon\|^2 = \mathbf{E}\,\|\mu - \hat{\mu}\|^2 + \mathbf{Var}(\epsilon), \quad \mathbf{Var}(\epsilon) = \mathbf{E}(\epsilon^T \epsilon).$$

- Since $\mathbf{Var}(\epsilon)$ is a constant for all estimators $\hat{\mu}$, one may simply look at the first part which is often called as *risk* in literature,

$$\mathcal{R}(\hat{\mu}, \mu) = \mathbf{E}\,\|\mu - \hat{\mu}\|^2$$

It is the *mean square error* (MSE) between μ and its estimator $\hat{\mu}$, that measures the expected prediction error.

Bias-Variance Decomposition

- The risk or MSE enjoy the following important *bias-variance decomposition*, as a result of the Pythagorean theorem.

$$\begin{aligned}\mathcal{R}(\hat{\mu}_n, \mu) &= \mathbf{E}\,\|\hat{\mu}_n - \mathbf{E}[\hat{\mu}_n] + \mathbf{E}[\hat{\mu}_n] - \mu\|^2 \\ &= \mathbf{E}\,\|\hat{\mu}_n - \mathbf{E}[\hat{\mu}_n]\|^2 + \|\,\mathbf{E}[\hat{\mu}_n] - \mu\|^2 \\ &=: \mathbf{Var}(\hat{\mu}_n) + \mathbf{Bias}(\hat{\mu}_n)^2\end{aligned}$$

- Consider multivariate Gaussian model, $x_1, \ldots, x_n \sim \mathcal{N}(\mu, \sigma^2 I_p)$ $(i = 1, \ldots, n)$, and the maximum likelihood estimators (MLE) of the parameters (μ and $\Sigma = \sigma^2 I_p$)

Example: Bias-Variance Decomposition of MLE

- Consider multivariate Gaussian model, $Y_1, \ldots, Y_n \sim \mathcal{N}(\mu, \sigma^2 I_p)$ $(i = 1, \ldots, n)$, and the maximum likelihood estimators (MLE) of the parameters (μ and $\Sigma = \sigma^2 I_p$)

- The MLE estimator satisfies

$$\mathbf{Bias}(\hat{\mu}_n^{MLE}) = 0$$

  and

$$\mathbf{Var}(\hat{\mu}_n^{MLE}) = \frac{p}{n}\sigma^2$$

  In particular for $n = 1$, $\mathbf{Var}(\hat{\mu}^{MLE}) = \sigma^2 p$ for $\hat{\mu}^{MLE} = Y$.

Example: Bias-Variance Decomposition of Linear Estimators

- Consider $Y \sim \mathcal{N}(\mu, \sigma^2 I_p)$ and linear estimator $\hat{\mu}_C = CY$
- Then we have

$$\mathbf{Bias}(\hat{\mu}_C) = \|(I - C)\mu\|^2$$

and

$$\begin{aligned} \mathbf{Var}(\hat{\mu}_C) &= \mathbf{E}[(CY - C\mu)^T (CY - C\mu)] \\ &= \mathbf{E}[\mathrm{tr}((Y - \mu)^T C^T C (Y - \mu))] \\ &= \sigma^2 \, \mathrm{tr}(C^T C). \end{aligned}$$

- Linear estimator includes an important case, the *Ridge regression* (a.k.a. Tikhonov regularization) with $C = X(X^T X + \lambda I)^{-1} X^T$,

$$\min_\beta \frac{1}{2}\|Y - X\beta\|^2 + \frac{\lambda}{2}\|\beta\|^2, \quad \lambda > 0.$$

Example: Bias-Variance Decomposition of Diagonal Estimators

- For simplicity, one may restrict our discussions on the diagonal linear estimators $C = \mathbf{diag}(c_i)$ (up to an change of orthonormal basis for Ridge regression), whose risk is

$$\mathcal{R}(\hat{\mu}_C, \mu) = \sigma^2 \sum_{i=1}^{p} c_i^2 + \sum_{i=1}^{p} (1 - c_i)^2 \mu_i^2.$$

- For hyper-rectangular model class $|\mu_i| \leq \tau_i$, the minimax risk is

$$\inf_{c_i} \sup_{|\mu_i| \leq \tau_i} \mathcal{R}(\hat{\mu}_C, \mu) = \sum_{i=1}^{p} \frac{\sigma^2 \tau_i^2}{\sigma^2 + \tau_i^2}.$$

  For sparse models such that $\#\{i : \tau_i = O(\sigma)\} = k \ll p$, it is possible to trade bias with variance toward a **smaller risk using linear estimators than MLE!**

Note

$$\mathcal{R}(\hat{\mu}_C, \mu) = \sigma^2 \sum_{i=1}^{p} c_i^2 + \sum_{i=1}^{p} (1 - c_i)^2 \mu_i^2.$$

- For the supreme over $|\mu_i| \leq \tau_i$,

$$\Rightarrow \sup_{|\mu_i| \leq \tau_i} \mathcal{R}(\hat{\mu}_C, \mu) = \sigma^2 \sum_{i=1}^{p} c_i^2 + \sum_{i=1}^{p} (1 - c_i)^2 \tau_i^2 =: J(c).$$

- To see the infimum over c_i,

$$0 = \frac{\partial J(c)}{\partial c_i} = 2\sigma^2 c_i - 2\tau_i^2 (1 - c_i) \Rightarrow c_i = \frac{\tau_i^2}{\sigma^2 + \tau_i^2}$$

- The minimax risk is thus

$$\inf_{c_i} \sup_{|\mu_i| \leq \tau_i} \mathcal{R}(\hat{\mu}_C, \mu) = \sum_{i=1}^{p} \frac{\sigma^2 \tau_i^2}{\sigma^2 + \tau_i^2}.$$

Formality: Inadmissibility

Definition (Inadmissible, Charles Stein (1956))

An estimator $\hat{\mu}_n$ of the parameter μ is called **inadmissible** on $\mathbb{R}^p$ with respect to the squared risk if there exists another estimator μ_n^* such that

$$\mathbf{E}\left\|\mu_n^* - \mu\right\|^2 \leq \mathbf{E}\left\|\hat{\mu}_n - \mu\right\|^2 \qquad \text{for all } \mu \in \mathbb{R}^p,$$

and there exist $\mu_0 \in \mathbb{R}^p$ such that

$$\mathbf{E}\left\|\mu_n^* - \mu_0\right\|^2 < \mathbf{E}\left\|\hat{\mu}_n - \mu_0\right\|^2.$$

In this case, we also call that μ_n^* **dominates** $\hat{\mu}_n$. Otherwise, the estimator $\hat{\mu}_n$ is called **admissible**.

Stein's Phenomenon

- (Charles Stein (1956)) For $p \geq 3$, there exists $\hat{\mu}$ such that $\forall \mu \in \mathbb{R}^p$,

  $$\mathcal{R}(\hat{\mu}, \mu) < \mathcal{R}(\hat{\mu}^{\mathsf{MLE}}, \mu)$$

  which makes MLE inadmissible.

- What are such estimators?

Example (James-Stein Estimator)

$$\hat{\mu}^{JS} = \left(1 - \frac{\sigma^2(p-2)}{\|\hat{\mu}^{MLE}\|^2}\right)\hat{\mu}^{MLE}. \tag{5}$$

Such an estimator shrinks each component of $\hat{\mu}^{MLE}$ toward 0.

- Charles Stein shows in 1956 that MLE is inadmissible, while the following original form of James-Stein estimator is demonstrated by his student Willard James in 1961.
- Bradley Efron summarizes the history and gives a simple derivation of these estimators from an *Empirical Bayes* point of view, while we shall give a *ridge regression* derivation.

James-Stein Estimator with Shrinkage toward Mean

- A varied form of James-Stein estimator can shrink MLE toward other points such as the component mean of $\hat{\mu}^{MLE}$:

$$\hat{\mu}_i^{JS_1} = \bar{X} + \left(1 - \frac{\sigma^2(p-3)}{S(\hat{\mu}^{MLE})}\right)(\hat{\mu}_i^{MLE} - \bar{X}), \tag{6}$$

where $\bar{X} = \sum_{i=1}^{p} X_i/p$ and $S(X) = \sum_i (X_i - \bar{X})^2$,

- *Positive part James-Stein estimator*:

$$\tilde{\mu}^{JS_{1+}} := \bar{X} + \left(1 - \frac{\sigma^2(p-3)}{S(\hat{\mu}^{MLE})}\right)_+ (\hat{\mu}_i^{MLE} - \bar{X}), \quad (x)_+ := \min(0, x)$$

- Both dominate MLE if $p > 3$ and can be derived from ridge regression.

James-Stein Estimator as Multi-task Ridge Regression

James-Stein estimators can be written as a *multi-task ridge regression*:

$$(\widehat{\mu}_i, \widehat{\mu}) := \arg\min_{\mu_i, \mu} \sum_{i=1}^{p} [(\mu_i - X_i)^2 + \lambda(\mu_i - \mu)^2]. \tag{7}$$

- Denote $\bar{X} = \sum_{i=1}^{p} X_i/p$ and $S(X) = \sum_i (X_i - \bar{X})^2$
- Taking $\lambda = \sigma^2(p-3)/(S - \sigma^2(p-3))$, $\widehat{\mu}_i$ gives $\widehat{\mu}^{JS_1}$;
- Taking $\lambda = \min(S, \sigma^2(p-3))/(S - \min(S, \sigma^2(p-3)))$ with $1/0 = \infty$, it gives $\widehat{\mu}^{JS_{1+}}$.

Proof sketch

Consider

$$J(\mu_i, \mu) = \sum_{i=1}^{p} [(\mu_i - X_i)^2 + \lambda(\mu_i - \mu)^2$$

- $\partial J / \partial \mu = 0$ we get

$$2\lambda \sum_{i=1}^{p} (\widehat{\mu} - \widehat{\mu}_i) = 0 \Rightarrow \widehat{\mu} = \frac{1}{p} \sum_{i=1}^{p} \widehat{\mu}_i$$

- $0 = \partial J / \partial \mu_i = 2(\widehat{\mu}_i - X_i) + 2\lambda(\widehat{\mu}_i - \widehat{\mu}) = 0$

$$\Rightarrow \widehat{\mu}_i = \frac{1}{1+\lambda}(X_i + \lambda\widehat{\mu}) = \widehat{\mu} + \frac{1}{1+\lambda}(X_i - \widehat{\mu})$$

whose average over i gives

$$\frac{1}{p} \sum_{i=1}^{p} \widehat{\mu}_i = \widehat{\mu} = \widehat{\mu} + \frac{1}{(1+\lambda)} \left(\frac{1}{p} \sum_{i=1}^{p} X_i - \widehat{\mu} \right) \Rightarrow \widehat{\mu} = \frac{1}{p} \sum_{i=1}^{p} X_i = \bar{X}$$

Proof sketch

Now

$$\widehat{\mu}_i = \bar{X} + \frac{1}{1+\lambda}\left(X_i - \bar{X}\right) = \bar{X} + \left(1 - \frac{\lambda}{1+\lambda}\right)\left(X_i - \bar{X}\right)$$

- Taking $\lambda = \sigma^2(p-3)/(S - \sigma^2(p-3))$, $\frac{\lambda}{1+\lambda} = \frac{\sigma^2(p-3)}{S}$ $(\widehat{\mu}_{JS_1})$
- Taking $\lambda = \min(S, \sigma^2(p-3))/(S - \min(S, \sigma^2(p-3)))$,
  - if $S > \sigma^2(p-3)$, the same as above
  - if $S \leq \sigma^2(p-3)$, $\lambda = S/(S-S)$ and $\frac{\lambda}{1+\lambda} = \frac{S}{S-S+S} = 1$ $(\widehat{\mu}_{JS_{1+}})$
- Note: taking $\widehat{\mu} = \bar{X} = 0$ and $\lambda = \sigma^2(p-2)/(S - \sigma^2(p-2))$, it gives James-Stein shrinkage toward 0 $(\widehat{\mu}_{JS_0})$. $\square$

Example

- Let's look at an example of James-Stein Estimator
  - R: `https://github.com/yuany-pku/2017_CSIC5011/blob/master/slides/JSE.R`

Illustration that JSE dominates MLE

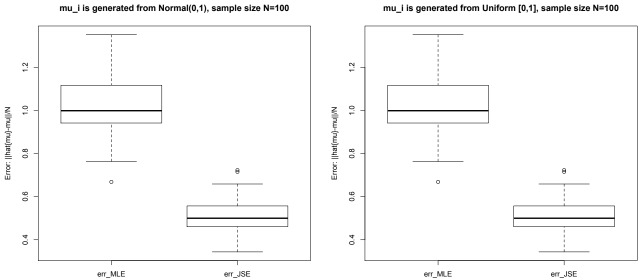

Figure: Comparison of risks between Maximum Likelihood Estimators and James-Stein Estimators with $X_i \sim \mathcal{N}(0, I_p)$ (left) and $X_{ij} \sim \mathcal{U}[0,1]$ (right) for $i = 1, \ldots, N$ and $j = 1, \ldots, p$ where $p = N = 100$.

Efron's Batting Example in 1970

Table: Efron's Batting example. $\hat{\mu}^{MLE}$ is obtained from the mean hits in these early games, while μ is obtained by averages over the remainder of the season.

Players	hits/AB	$\hat{\mu}_i^{(MLE)}$	μ_i	$\hat{\mu}_i^{(JS)}$	$\hat{\mu}_i^{(JS_1)}$
Clemente	18/45	0.4	**0.346**	0.378	0.294
F.Robinson	17/45	0.378	**0.298**	0.357	0.289
F.Howard	16/45	0.356	**0.276**	0.336	0.285
Johnstone	15/45	0.333	**0.222**	0.315	0.28
Berry	14/45	0.311	**0.273**	0.294	0.275
Spencer	14/45	0.311	**0.27**	0.294	0.275
Kessinger	13/45	0.289	**0.263**	0.273	0.27
L.Alvarado	12/45	0.267	**0.21**	0.252	0.266
Santo	11/45	0.244	**0.269**	0.231	0.261
Swoboda	11/45	0.244	**0.23**	0.231	0.261
Unser	10/45	0.222	**0.264**	0.21	0.256
Williams	10/45	0.222	**0.256**	0.21	0.256
Scott	10/45	0.222	**0.303**	0.21	0.256
Petrocelli	10/45	0.222	**0.264**	0.21	0.256
E.Rodriguez	10/45	0.222	**0.226**	0.21	0.256
Campaneris	9/45	0.2	**0.286**	0.189	0.252
Munson	8/45	0.178	**0.316**	0.168	0.247
Alvis	7/45	0.156	**0.2**	0.147	0.242
Mean Square Error	-	0.075545	-	0.072055	0.021387

James-Stein Estimator Dominates MLE

Theorem (James-Stein (1956, 1961))

Suppose $Y \sim \mathcal{N}_p(\mu, I)$. Then $\hat{\mu}^{\mathsf{MLE}} = Y$. $\mathcal{R}(\hat{\mu}, \mu) = \mathbf{E}_\mu \|\hat{\mu} - \mu\|^2$, and define

$$\hat{\mu}^{JS} = \left(1 - \frac{p-2}{\|Y\|^2}\right) Y$$

Then if $p \geq 3$ and for all $\mu \in \mathbb{R}^p$

$$\mathcal{R}(\hat{\mu}^{JS}, \mu) < \mathcal{R}(\hat{\mu}^{\mathsf{MLE}}, \mu)$$

More Estimators Dominates MLE

- *Stein estimator*: $a = 0, b = \sigma^2 p$,

$$\tilde{\mu}_S := \left(1 - \frac{\sigma^2 p}{\|y\|^2}\right) y$$

- *James-Stein estimator*: $c \in (0, 2(p-2))$

$$\tilde{\mu}_{JS}^{c} := \left(1 - \frac{\sigma^2 c}{\|y\|^2}\right) y$$

- *Positive part James-Stein estimator*:

$$\tilde{\mu}_{JS+} := \left(1 - \frac{\sigma^2 (p-2)}{\|y\|^2}\right)_+ y, \quad (x)_+ := \min(0, x)$$

- *Positive part Stein estimator*:

$$\tilde{\mu}_{S+} := \left(1 - \frac{\sigma^2 p}{\|y\|^2}\right)_+ y$$

$$\mathcal{R}(\tilde{\mu}_{JS+}) < \mathcal{R}(\tilde{\mu}_{JS}) < \mathcal{R}(\hat{\mu}_n), \qquad \mathcal{R}(\tilde{\mu}_{S+}) < \mathcal{R}(\tilde{\mu}_S) < \mathcal{R}(\hat{\mu}_n)$$

Stein's Unbiased Risk Estimates

Lemma (Stein's Unbiased Risk Estimates (SURE))

Suppose $Y \sim \mathcal{N}_p(\mu, I)$ and $\hat{\mu} = Y + g(Y)$. If g satisfies

1. g is weakly differentiable.
2. $\sum_{i=1}^{p} \int |\partial_i g_i(x)| \mathrm{d}x < \infty$

Denote

$$U(Y) := p + 2\nabla^T g(Y) + \|g(Y)\|^2 \tag{8}$$

Then

$$\mathcal{R}(\hat{\mu}, \mu) = \mathbf{E}\, U(Y) = \mathbf{E}(p + 2\nabla^T g(Y) + \|g(Y)\|^2) \tag{9}$$

where $\nabla^T g(Y) := \sum_{i=1}^{p} \frac{\partial}{\partial y_i} g_i(Y)$.

Examples of weakly differentiable g

- For linear estimator $\hat{\mu} = CY$,

$$g(Y) = (C - I)Y$$

- For James-Stein estimator

$$g(Y) = -\frac{p-2}{\|Y\|^2}Y$$

Soft-Threshholding

- Soft-Thresholding solves LASSO (ℓ_1-regularized MLE)

$$\hat{\mu} = \arg\min_{\mu} J_1(\mu) = \arg\min_{\mu} \frac{1}{2}\|Y - \mu\|^2 + \lambda\|\mu\|_1$$

- Subgradients of objective function leads to

$$0 \in \partial_{\mu_j} J_1(\mu) = (\mu_j - y_j) + \lambda\, \mathbf{sign}(\mu_j)$$

$$\Rightarrow \hat{\mu}_j(y_j) = \mathbf{sign}(y_j)(|y_j| - \lambda)_+$$

  where the set-valued map $\mathbf{sign}(x) = 1$ if $x > 0$, $\mathbf{sign}(x) = -1$ if $x < 0$, and $\mathbf{sign}(x) = [-1, 1]$ if $x = 0$, is the subgradient of absolute function $|x|$.

- Then

$$g_i(x) = \begin{cases} -\lambda & x_i > \lambda \\ -x_i & |x_i| \leq \lambda \\ \lambda & x_i < -\lambda \end{cases}$$

  which is weakly differentiable

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Hard-Thresholding, a Counter Example

- Hard-Thresholding solves the ℓ_0-regularized MLE where $\|x\|_0 := \#\{x_i \neq 0\}$
$$\hat{\mu} = \arg\min_{\mu} J_0(\mu) = \arg\min_{\mu} \frac{1}{2}\|Y-\mu\|^2 + \lambda\|\mu\|_0$$
that is NP-hard

- Closed-form solution
$$\hat{\mu}_i(y_i) = \begin{cases} y_i & y_i > \lambda \\ 0 & |y_i| \leq \lambda \\ y_i & y_i < -\lambda \end{cases}$$

- Then
$$g_i(x) = \begin{cases} 0 & |x_i| > \lambda \\ -x_i & |x_i| \leq \lambda \end{cases}$$
which is **NOT** weakly differentiable!

Sketchy Proof of SURE Lemma

Proof.

Assume that $\sigma = 1$. Let $\phi(y)$ be the density function of Gaussian distribution $\mathcal{N}_p(0, I)$.

$$\begin{aligned}\mathcal{R}(\hat{\mu}, \mu) &= \mathop{\mathbf{E}}_{\mu} \|Y + g(Y) - \mu\|^2 \\ &= \mathbf{E}\left(p + 2(Y-\mu)^T g(Y) + \|g(Y)\|^2\right)\end{aligned}$$

$$\begin{aligned}\mathbf{E}(Y-\mu)^T g(Y) &= \sum_{i=1}^{p} \int_{-\infty}^{\infty} (y_i - \mu_i) g_i(Y) \phi(Y-\mu) \mathrm{d}Y \\ &= \sum_{i=1}^{p} \int_{-\infty}^{\infty} -g_i(Y) \frac{\partial}{\partial y_i} \phi(Y-\mu_i) \mathrm{d}Y, \quad \text{derivative of } \phi \\ &= \sum_{i=1}^{p} \int_{-\infty}^{\infty} \frac{\partial}{\partial y_i} g_i(Y) \phi(Y-\mu_i) \mathrm{d}Y, \quad \text{Integration by parts} \\ &= \mathbf{E}\, \nabla^T g(Y)\end{aligned}$$

$\square$

Risk of Linear Estimator

Suppose $Y \sim \mathcal{N}(\mu, I_p)$

$$\hat{\mu}_C(Y) = Cy$$

$$\Rightarrow g(Y) = (C - I)Y$$

$$\Rightarrow \nabla^T g(Y) = -\sum_i \frac{\partial}{\partial y_i}\left((C - I)Y\right) = \operatorname{tr}(C) - p$$

$$\begin{aligned}
\Rightarrow U(Y) &= p + 2\nabla^T g(Y) + \|g(Y)\|^2 \\
&= p + 2(\operatorname{tr}(C) - p) + \|(I - C)Y\|^2 \\
&= -p + 2\operatorname{tr}(C) + \|(I - C)Y\|^2
\end{aligned}$$

In general, if $Y \sim \mathcal{N}(\mu, \sigma^2 I)$,

$$\mathcal{R}(\hat{\mu}_C, \mu) = \|(I - C(\lambda))Y\|^2 - p\sigma^2 + 2\sigma^2 \operatorname{tr}(C(\lambda)).$$

When Linear Estimator is Admissible?

Theorem (Lemma 2.8 in Johnstone's book (GE))

$Y \sim N(\mu, I)$, $\forall \hat{\mu} = CY$, $\hat{\mu}$ is admissible iff

1. C is symmetric.
2. $0 \leq \rho_i(C) \leq 1$ (eigenvalue).
3. $\rho_i(C) = 1$ for at most two i.

Risk of James-Stein Estimator

- Suppose $Y \sim \mathcal{N}(\mu, I_p)$ and for $p \geq 3$,

$$\hat{\mu}^{JS} = \left(1 - \frac{p-2}{\|Y\|^2}\right) Y \Rightarrow g(Y) = -\frac{p-2}{\|Y\|^2} Y$$

- Now

$$U(Y) = p + 2\nabla^T g(Y) + \|g(Y)\|^2$$

$$\|g(Y)\|^2 = \frac{(p-2)^2}{\|Y\|^2}$$

$$\nabla^T g(Y) = -\sum_i \frac{\partial}{\partial y_i} \left(\frac{p-2}{\|Y\|^2} Y\right) = -\frac{(p-2)^2}{\|Y\|^2}$$

- Finally

$$\Rightarrow \mathcal{R}(\hat{\mu}^{\mathsf{JS}}, \mu) = \mathbf{E}\, U(Y) = p - \mathbf{E}\, \frac{(p-2)^2}{\|Y\|^2} < p = \mathcal{R}(\hat{\mu}^{\mathsf{MLE}}, \mu)$$

Further Analysis of the Risk of James-Stein Estimator

- To find an upper bound of the risk of James-Stein estimator, notice that $\|Y\|^2 \sim \chi^2(\|\mu\|^2, p)$ and [2]

$$\chi^2(\|\mu\|^2, p) \overset{d}{=} \chi^2(0, p+2N), \quad N \sim \text{Poisson}\left(\frac{\|\mu\|^2}{2}\right)$$

we have

$$\begin{aligned}
\mathbf{E}\left(\frac{1}{\|Y\|^2}\right) &= \mathop{\mathbf{E}}_N \mathop{\mathbf{E}}_Y \left[\frac{1}{\|Y\|^2}\Big| N\right] \\
&= \mathbf{E}\,\frac{1}{p+2N-2} \\
&\geq \frac{1}{p+2\,\mathbf{E}\,N-2} \text{ (Jensen's Inequality)} \\
&= \frac{1}{p+\|\mu\|^2-2}
\end{aligned}$$

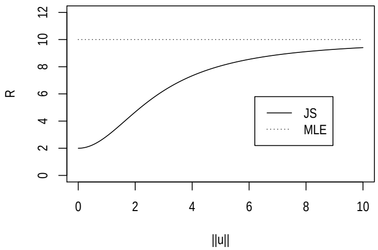
[2] This is a homework.

Upper Bound for JSE

Proposition (Upper bound of MSE for JSE)

Let $Y \sim \mathcal{N}(\mu, I_p)$ for $p \geq 3$,

$$\mathcal{R}(\hat{\mu}^{\mathsf{JS}}, \mu) \leq p - \frac{(p-2)^2}{p-2+\|\mu\|^2} = 2 + \frac{(p-2)\|\mu\|^2}{p-2+\|\mu\|^2}$$



Risk of Soft-Thresholding

- Recall

$$g_i(x) = \begin{cases} -\lambda & x_i > \lambda \\ -x_i & |x_i| \leq \lambda \\ \lambda & x_i < -\lambda \end{cases} \Rightarrow \frac{\partial}{\partial x_i} g_i(x) = -I(|x_i| \leq \lambda)$$

- Then

$$\begin{aligned} \mathcal{R}(\hat{\mu}_\lambda, \mu) &= \mathbf{E}(p + 2\nabla^T g(Y) + \|g(Y)\|^2) \\ &= \mathbf{E}\left(p - 2\sum_{i=1}^{p} I(|y_i| \leq \lambda) + \sum_{i=1}^{p} y_i^2 \wedge \lambda^2\right) \\ &\leq 1 + (2\log p + 1)\sum_{i=1}^{p} \mu_i^2 \wedge 1 \quad \text{if we take } \lambda = \sqrt{2\log p} \end{aligned}$$

Risk of Soft-Thresholding (continued)

- Consider the risk upper bound

$$1 + (2\log p + 1)\sum_{i=1}^{p} \mu_i^2 \wedge 1$$

- The risk of soft-thresholding for each μ_i is bounded by 1: so if μ is sparse ($s = \#\{i : \mu_i \neq 0\}$) but large in magnitudes (s.t. $\|\mu\|_2^2 \geq p$), we may expect the risk of soft-thresholding $\leq O(s\log p) \ll O(p)$, the risk of MLE.

Summary

The following results are about mean estimation under noise:

- Sample mean as the maximum likelihood estimator is consistent as $n \to \infty$ with fixed $p < \infty$, and the minimum variance unbiased estimator.

- For high dimensional statistics, there are many estimators (shrinkage) that dominate MLE in terms of prediction power, e.g.
  - Linear estimator may dominate MLE for sparse targets
  - James-Stein estimator uniformly dominates MLE if $p \geq 3$
  - Soft-thresholding (Lasso) estimator may dominate MLE and even JSE for sparse targets

- Therefore, regularization lies in the core of high dimensional statistics against the noise