

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

Yuan Yao

Hong Kong University of Science and Technology

March 4, 2020

Outline

Recall: PCA in Noise

Maximum Likelihood Estimate

Example: Multivariate Normal Distribution

James-Stein Estimator

Risk and Bias-Variance Decomposition

Inadmissability

James-Stein Estimators

Stein's Unbiased Risk Estimates (SURE)

Proof of SURE Lemma

PCA in Noise

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

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

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

- ▶ The primary eigenvalue of sample covariance matrix satisfies

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

- ▶ The primary eigenvector converges to

$$|\langle u, v_{\max} \rangle|^2 \rightarrow \begin{cases} 0 & \sigma_X^2 \leq \sqrt{\gamma} \\ \frac{1 - \frac{\gamma}{\sigma_X^2}}{1 + \frac{\gamma}{\sigma_X^2}}, & \sigma_X^2 > \sqrt{\gamma} \end{cases} \quad (2)$$

Recall: Phase Transitions of PCA

- ▶ Here the threshold

$$\gamma = \lim_{n,p \rightarrow \infty} \frac{p}{n}$$

- ▶ The **law of large numbers** in traditional statistics assumes p fixed and $n \rightarrow \infty$:

$$\gamma = \lim_{n \rightarrow \infty} p/n = 0.$$

where PCA always works without phase transitions.

- ▶ In **high dimensional statistics**, we allow both p and n grow: $p, n \rightarrow \infty$, 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

Recall: PCA in Noise

Maximum Likelihood Estimate

Example: Multivariate Normal Distribution

James-Stein Estimator

Risk and Bias-Variance Decomposition

Inadmissability

James-Stein Estimators

Stein's Unbiased Risk Estimates (SURE)

Proof of SURE Lemma

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

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

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 $x_i \sim \mathcal{N}(\mu, \Sigma)$ ($i = 1, \dots, n$)

Maximum Likelihood Estimate (continued)

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

$$\begin{aligned} J(\mu, \Sigma) &= \log \prod_{i=1}^n f(x_i | \mu, \Sigma) \\ &= -\frac{1}{2} \sum_{i=1}^n (X_i - \mu)^T \Sigma^{-1} (X_i - \mu) - \frac{n}{2} \log |\Sigma| + C \quad (4) \end{aligned}$$

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 ,

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

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

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,

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

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 $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$. 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.

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 $n \rightarrow \infty$:

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

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

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

C. (Asymptotic Efficiency) $\lim_{n \rightarrow \infty} \text{cov}(\hat{\theta}_n^{MLE}) = I^{-1}(\theta_0)$. 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 $\hat{\theta}_n$,
 $\lim_{n \rightarrow \infty} \text{var}(\hat{\theta}_n^{MLE}) \leq \lim_{n \rightarrow \infty} \text{var}(\hat{\theta}_n)$.

However, large p small n ?

- ▶ The asymptotic results all hold under the assumption by **fixing p and taking $n \rightarrow \infty$** , where MLE satisfies $\hat{\mu}_n \rightarrow \mu$ and $\hat{\Sigma}_n \rightarrow \Sigma$.
- ▶ 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 be shown below.

Outline

Recall: PCA in Noise

Maximum Likelihood Estimate

Example: Multivariate Normal Distribution

James-Stein Estimator

Risk and Bias-Variance Decomposition

Inadmissability

James-Stein Estimators

Stein's Unbiased Risk Estimates (SURE)

Proof of SURE Lemma

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, $x_1, \dots, x_n \sim \mathcal{N}(\mu, \sigma^2 I_p)$ ($i = 1, \dots, n$), 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, $Y_1, \dots, Y_n \sim \mathcal{N}(\mu, \sigma^2 I_p)$ ($i = 1, \dots, n$), 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

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

- ▶ 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

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

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

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

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 $\forall \mu \in \mathbb{R}^p$,

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

which makes MLE inadmissible.

- ▶ What are such estimators?

James-Stein Estimator

Example (James-Stein Estimator)

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

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.

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 $\hat{\mu}^{MLE}$:

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

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

- ▶ It dominates the MLE if $p \geq 4$.

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

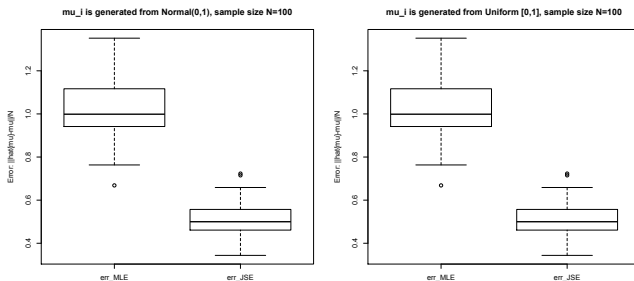


Figure: Comparison of risks between Maximum Likelihood Estimators and James-Stein Estimators with $X_i \sim \mathcal{N}(0, I_p)$ (left) and $X_{ij} \sim \mathcal{U}[0, 1]$ (right) for $i = 1, \dots, N$ and $j = 1, \dots, p$ where $p = N = 100$.

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	$\hat{\mu}_i^{(JS)}$	$\hat{\mu}_i^{(JS1)}$
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 $\hat{\mu}^{\text{MLE}} = Y$. $\mathcal{R}(\hat{\mu}, \mu) = \mathbf{E}_\mu \|\hat{\mu} - \mu\|^2$, and define

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

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

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

More Estimators Dominates MLE

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

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

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

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

- ▶ *Positive part James-Stein estimator*:

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

- ▶ *Positive part Stein estimator*:

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

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

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. $\sum_{i=1}^p \int |\partial_i g_i(x)| dx < \infty$

Denote

$$U(Y) := p + 2\nabla^T g(Y) + \|g(Y)\|^2 \quad (7)$$

Then

$$\mathcal{R}(\hat{\mu}, \mu) = \mathbf{E}U(Y) = \mathbf{E}(p + 2\nabla^T g(Y) + \|g(Y)\|^2) \quad (8)$$

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 $\hat{\mu} = CY$,

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

- ▶ For James-Stein estimator

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

Soft-Thresholding

- ▶ 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



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 $\mathcal{N}_p(0, I)$.

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

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



Risk of Linear Estimator

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

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

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

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

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

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

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

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

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

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 ¹

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

we have

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

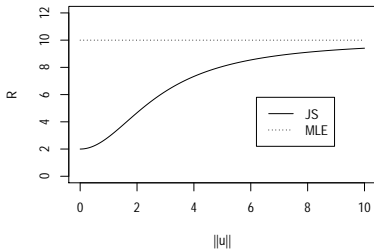
¹This is a homework.

Upper Bound for JSE

Proposition (Upper bound of MSE for JSE)

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

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



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)

- ▶ Using the inequality

$$\frac{1}{2}a \wedge b \leq \frac{ab}{a+b} \leq a \wedge b$$

the upper bound of James-Stein estimator can be converted to RHS below and compared with Soft-Thresholding

$$1 + (2 \log p + 1) \sum_{i=1}^p (\mu_i^2 \wedge 1) \leq 2 + c \left(\left(\sum_{i=1}^p \mu_i^2 \right) \wedge p \right) \quad c \in (1/2, 1)$$

- ▶ 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 $\text{LHS} = O(s \log p) < O(p) = \text{RHS}^2$.

²for details cf. p43 of Gaussian Estimation, by I. Johnstone.

Summary

The following results are about mean estimation under noise:

- ▶ Sample mean as the maximum likelihood estimator is consistent as $n \rightarrow \infty$ 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