1 Warm-up

Let X be a random vector in \mathbb{R}^d with mean $\mu \in \mathbb{R}^d$ and covariance matrix $\Sigma \in \mathbb{R}^{d \times d}$ and A a symmetric matrix in $\mathbb{R}^{d \times d}$. Then,

$$\mathbb{E}[X^{\top}AX] = \mu^{\top}A\mu + \operatorname{Trace}(A\Sigma).$$

As $X^{\top}AX$ is a real number, $\mathbb{E}[X^{\top}AX] = \mathbb{E}[\operatorname{Trace}(X^{\top}AX)] = \mathbb{E}[\operatorname{Trace}(AXX^{\top})]$. By linearity, $\mathbb{E}[X^{\top}AX] = \operatorname{Trace}(A\mathbb{E}[XX^{\top}])$ which yields,

$$\mathbb{E}[X^{\top}AX] = \operatorname{Trace}(A\{\mathbb{V}[X] + \mathbb{E}[X]\mathbb{E}[X]^{\top}\}) = \mu^{\top}A\mu + \operatorname{Trace}(A\Sigma).$$

2 Student's t-statistics

We assume that for all $1 \leqslant i \leqslant n$, $Y_i = X_i^\top \theta_\star + \varepsilon_i$ for some unknown $\theta_\star \in \mathbb{R}^d$ where the $(\varepsilon_i)_{1 \leqslant i \leqslant n}$ are i.i.d. random variables with distribution $\mathcal{N}(0,\sigma_\star^2)$. Let $\varepsilon \in \mathbb{R}^n$ be the random vector such that for all $1 \leqslant i \leqslant n$, the i-th component of ε is ε_i . The model is then written $Y = X\theta_\star + \varepsilon$. Assume that X has full rank and that $\widehat{\theta}_n = (X^\top X)^{-1} X^\top Y$ and $\widehat{\sigma}_n^2 = \|Y - X\widehat{\theta}_n\|^2/(n-d)$.

1. For all $1 \leq j \leq d$, show that

$$\frac{\widehat{\theta}_{n,j} - \theta_{\star,j}}{\widehat{\sigma}_n \sqrt{(X^T X)_{j,j}^{-1}}} \sim \mathcal{S}(n-d),$$

where S(n-d) is the Student's t-distribution with n-d degrees of freedom, i.e. the law of $X/\sqrt{Y/(n-d)}$ where $X \sim \mathcal{N}(0,1)$ is independent of $Y \sim \chi^2(n-d)$.

By definition, for all $1 \leq j \leq d$,

$$\frac{\widehat{\theta}_{n,j} - \theta_{\star,j}}{\widehat{\sigma}_n \sqrt{(X^\top X)_{j,j}^{-1}}} = \frac{\sigma_{\star}^{-1}(\widehat{\theta}_{n,j} - \theta_{\star,j})}{\sigma_{\star}^{-1}\widehat{\sigma}_n \sqrt{(X^\top X)_{j,j}^{-1}}} = \frac{e_j^\top (\sigma_{\star}^{-1}(\widehat{\theta}_n - \theta_{\star}))}{\sigma_{\star}^{-1}\widehat{\sigma}_n \sqrt{(X^\top X)_{j,j}^{-1}}}.$$

Note that $\sigma_{\star}^{-1}(\widehat{\theta}_n - \theta_{\star}) \sim \mathcal{N}(0, (X^{\top}X)^{-1})$ so that $e_j^{\top}(\sigma_{\star}^{-1}(\widehat{\theta}_n - \theta_{\star})) \sim \mathcal{N}(0, e_j^{\top}(X^{\top}X)^{-1}e_j)$ and

$$\frac{e_j^{\top}(\sigma_{\star}^{-1}(\widehat{\theta}_n - \theta_{\star}))}{\sqrt{(X^{\top}X)_{j,j}^{-1}}} \sim \mathcal{N}(0,1).$$

In addition,

$$\sigma_{\star}^{-1}\widehat{\sigma}_n = \sqrt{\sigma_{\star}^{-2}\widehat{\sigma}_n^2} = \sqrt{\|\sigma_{\star}^{-1}(I_n - X(X^{\top}X)^{-1}X^{\top})\varepsilon\|_2^2/(n-d)}$$

where $(n-d)\sigma_{\star}^{-2}\widehat{\sigma}_n^2 = \|\sigma_{\star}^{-1}(I_n - X(X^{\top}X)^{-1}X^{\top})\varepsilon\|_2^2 \sim \chi^2(n-d)$. The proof is concluded by noting that $\widehat{\theta}_n$ and $\widehat{\sigma}_n^2$ are independent.

2. Provide a confidence interval with confidence level $1 - \alpha$ for $\theta_{\star,j}$.

For $\alpha \in (0,1)$, if $s_{1-\alpha/2}^{n-d}$ denotes the quantile of order $1-\alpha/2$ of the law S(n-d), then

$$\mathbb{P}\left(\left|\frac{\widehat{\theta}_{n,j} - \theta_{\star,j}}{\widehat{\sigma}_n \sqrt{(X^T X)_{i,j}^{-1}}}\right| \leqslant s_{1-\alpha/2}^{n-d}\right) = 1 - \alpha.$$

Therefore,

$$I_{n,j}^{n-d}(\theta_{\star}) = \left[\widehat{\theta}_{n,j} - \widehat{\sigma}_{n} s_{1-\alpha/2}^{n-d} \sqrt{(X^{\top} X)_{j,j}^{-1}} \, ; \, \widehat{\theta}_{n,j} + \widehat{\sigma}_{n} s_{1-\alpha/2}^{n-d} \sqrt{(X^{\top} X)_{j,j}^{-1}} \right]$$

is a confidence interval for $\theta_{\star,j}$ with confidence level $1-\alpha$.

3 Random design

Consider the regression model given by

$$Y = X\theta_{\star} + \varepsilon \,,$$

where $X \in \mathbb{R}^{n \times d}$, the $(\varepsilon_i)_{1 \le i \le n}$ are i.i.d. centered Gaussian random variables with variance σ_{\star}^2 and independent of $(X_i)_{1 \le i \le n}$ which are assumed to be random. Assume that $X^{\top}X$ has full rank and that θ_{\star} is estimated by

$$\widehat{\theta}_n = (X^\top X)^{-1} X^\top Y$$
.

1. Compute the excess risk $R(\theta) - R(\theta_{\star})$, where $R(\theta) = n^{-1} \mathbb{E}[\|Y - X\theta\|_2^2]$.

By definition, using that $\mathbb{E}[\varepsilon] = 0$,

$$\begin{split} \mathsf{R}(\theta) &= n^{-1} \mathbb{E}[\|Y - X\theta\|_2^2] = n^{-1} \mathbb{E}[\|X\theta_\star + \varepsilon - X\theta\|_2^2] \,, \\ &= n^{-1} \mathbb{E}[\|X\theta_\star - X\theta\|_2^2] + n^{-1} \mathbb{E}[\|\varepsilon\|_2^2] \,, \\ &= (\theta_\star - \theta)^\top n^{-1} \mathbb{E}[X^\top X] (\theta_\star - \theta) + \sigma_\star^2 \,. \end{split}$$

Therefore,
$$R(\theta) - R(\theta_{\star}) = (\theta_{\star} - \theta)^{\top} n^{-1} \mathbb{E}[X^{\top} X] (\theta_{\star} - \theta)$$
.

2. Compute then the excess risk $\mathbb{E}[\mathsf{R}(\widehat{\theta}_n) - \mathsf{R}(\theta_{\star})]$.

By the previous question,

$$\mathbb{E}[\mathsf{R}(\widehat{\theta}_n) - \mathsf{R}(\theta_\star)] = n^{-1} \mathbb{E}[(\theta_\star - \widehat{\theta}_n)^\top \mathbb{E}[X^\top X](\theta_\star - \widehat{\theta}_n)].$$

Since $\widehat{\theta}_n$ is an unbiased estimate of θ_{\star} ,

$$\begin{split} \mathbb{E}[\mathsf{R}(\widehat{\theta}_n) - \mathsf{R}(\theta_\star)] &= n^{-1} \mathbb{E}[(\theta_\star - \mathbb{E}[\widehat{\theta}_n])^\top \mathbb{E}[X^\top X] (\theta_\star - \mathbb{E}[\widehat{\theta}_n])] \,, \\ &= n^{-1} \mathrm{Trace}\left(\mathbb{E}[X^\top X] \mathbb{V}[\widehat{\theta}_n]\right) \,, \\ &= \frac{\sigma_\star}{n} \mathrm{Trace}\left(\mathbb{E}[X^\top X] \mathbb{E}\left[(X^\top X)^{-1}\right]\right) \,. \end{split}$$

4 Fisher statistics (bonus)

Consider the regression model given by

$$Y = X\theta_{\star} + \varepsilon$$
,

where $X \in \mathbb{R}^{n \times d}$ and the $(\varepsilon_i)_{1 \leqslant i \leqslant n}$ are i.i.d. centered Gaussian random variables with variance σ_{\star}^2 . Assume that $X^{\top}X$ has full rank and that θ_{\star} and σ_{\star}^2 are estimated by

$$\widehat{\theta}_n = (X^\top X)^{-1} X^\top Y$$
 and $\widehat{\sigma}_n^2 = \frac{\|Y - X \widehat{\theta}_n\|^2}{n - d}$.

1. Let L be a $\mathbb{R}^{q \times d}$ matrix with rank $q \leqslant d$. Show that

$$\frac{(\widehat{\theta}_n - \theta_\star)^\top L^\top (L(X^\top X)^{-1} L^\top)^{-1} L(\widehat{\theta}_n - \theta_\star)}{q\widehat{\sigma}_n^2} \sim \mathcal{F}(q, n - d),$$

where $\mathcal{F}(q, n-d)$ is the Fisher distribution with q and n-d degrees of freedom, i.e. the law of (X/q)/(Y/(n-d)) where $X \sim \chi^2(q)$ is independent of $Y \sim \chi^2(n-d)$.

Note that $\operatorname{rank}(L(X^{\top}X)^{-1}L^{\top}) = \operatorname{rank}(LL^{\top}) = q$. The matrix $L(X^{\top}X)^{-1}L^{\top}$ is therefore positive definite. There exists a diagonal matrix $D \in \mathbb{R}^{q \times q}$ with positive diagonal terms and an orthogonal matrix $Q \in \mathbb{R}^{q \times q}$ such that $L(X^{\top}X)^{-1}L^{\top} = QDQ^{-1}$. The matrix $(L(X^{\top}X)^{-1}L^{\top})^{-1/2}$ may be defined as $(L(X^{\top}X)^{-1}L^{\top})^{-1/2} = QD^{-1/2}Q^{-1}$.

It is then enough to note that $(L(X^{\top}X)^{-1}L^{\top})^{-1/2}L(\widehat{\theta}_n - \theta_{\star})/\sigma_{\star} \sim \mathcal{N}(0, I_q)$. Therefore,

$$\begin{split} \sigma_{\star}^{-2} \| (L(X^{\top}X)^{-1}L^{\top})^{-1/2} L(\widehat{\theta}_{n} - \theta_{\star}) \|^{2} \\ &= (\widehat{\theta}_{n} - \theta_{\star})^{\top} L^{\top} (L(X^{\top}X)^{-1}L^{\top})^{-1} L(\widehat{\theta}_{n} - \theta_{\star}) / \sigma_{\star}^{2} \sim \chi^{2}(q) \,. \end{split}$$

On the other hand, we know that

$$(n-d)\sigma_{\star}^{-2}\widehat{\sigma}_{n}^{2} \sim \chi^{2}(n-d)$$
.

The proof is concluded by noting that $\widehat{\theta}_n$ and $\widehat{\sigma}_n^2$ are independent.

2. Using the previous question, build a confidence region with confidence level $1 - \alpha \in (0,1)$ for θ_{\star} .

By the previous question, for $\alpha \in (0,1)$, if $f_{1-\alpha}^{q,n-d}$ denotes the quantile of order $1-\alpha$ of the law $\mathcal{F}(q,n-p)$, then

$$\mathbb{P}\left(\theta_{\star} \in \left\{\theta \in \mathbb{R}^{d} ; (\widehat{\theta}_{n} - \theta)^{\top} L^{\top} (L(X^{\top}X)^{-1}L^{\top})^{-1} L(\widehat{\theta}_{n} - \theta) \leqslant q\widehat{\sigma}_{n}^{2} f_{1-\alpha}^{q,n-d}\right\}\right) = 1 - \alpha.$$

Therefore,

$$I_n^{q,n-d}(\theta_\star) = \left\{ \theta \in \mathbb{R}^d \; ; \; (\widehat{\theta}_n - \theta)^\top L^\top (L(X^\top X)^{-1} L^\top)^{-1} L(\widehat{\theta}_n - \theta) \leqslant q \widehat{\sigma}_n^2 f_{1-\alpha}^{q,n-d} \right\}$$

is a confidence region for θ_{\star} with confidence level $1-\alpha$.