REGRESSION: INTRODUCTION

1 Gaussian vectors

1. Let Σ be a symmetric positive definite matrix of $\mathbb{R}^{n \times n}$. Provide a solution to sample a Gaussian vector with covariance matrix Σ based on i.i.d. standard Gaussian variables.

It is enough to remark that $X = \mu + \Sigma^{1/2} \varepsilon \sim \mathcal{N}(\mu, \Sigma)$ where $\mu \in \mathbb{R}^d$ and $\varepsilon \sim \mathcal{N}(0, I_d)$.

- 2. Let ε be a random variable in $\{-1,1\}$ such that $\mathbb{P}(\varepsilon=1)=1/2$. If $(X,Y)^{\top} \sim \mathcal{N}(0,I_2)$ explain why the following vectors are or are not Gaussian vectors.
 - (a) $(X, \varepsilon X)$.

Not Gaussian since the probability that $X + \varepsilon X = 0$ is 1/2.

(b) $(X, \varepsilon Y)$.

Gaussian since coordinates are independent Gaussian random variables.

(c) $(X, \varepsilon X + Y)$.

Not Gaussian since the characteristic function of $(1 + \varepsilon)X + Y$ is not the Gaussian characteristic function.

(d) $(X, X + \varepsilon Y)$.

Gaussian as a linear transform of (b). Indeed,

$$\begin{pmatrix} X \\ X + \varepsilon Y \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} X \\ \varepsilon Y \end{pmatrix}.$$

3. Let X be a Gaussian vector in \mathbb{R}^n with mean $\mu \in \mathbb{R}^n$ and covariance matrix $\sigma^2 I_n$. Prove that the random variables \bar{X}_n and $\hat{\sigma}_n^2$ defined as

$$\bar{X}_n = \frac{1}{n} \sum_{i=1}^n X_i$$
 and $\hat{\sigma}_n^2 = \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X}_n)^2$

are independent.

Let $\mathbb{1}_n$ the vector of \mathbb{R}^n with all entries equal to 1. Then, $\bar{X}_n = n^{-1} \mathbb{1}_n^\top X$ and $(n-1)\sigma_n^2 = \|X - \bar{X}_n \mathbb{1}_n\|_2^2 = \|X - n^{-1} \mathbb{1}_n \mathbb{1}_n^\top X\|_2^2 = \|(I_n - (n^{-1/2} \mathbb{1}_n)(n^{-1/2} \mathbb{1}_n)^\top) X\|_2^2$. Note that $(n^{-1/2} \mathbb{1}_n)(n^{-1/2} \mathbb{1}_n)^\top$ is the orthogonal projection onto $\operatorname{span}(\mathbb{1}_n)$ and $I_n - (n^{-1/2} \mathbb{1}_n)(n^{-1/2} \mathbb{1}_n)^\top$ onto its orthogonal. The proof is completed by using Cochran's theorem.

2 Regression: prediction of a new observation

Consider the regression model given by

$$Y = X\beta_{\star} + \mathcal{E}$$
.

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

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

Let $x_{\star} \in \mathbb{R}^d$ and assume that its associated observation $Y_{\star} = x_{\star}^{\top} \beta_{\star} + \varepsilon_{\star}$ is predicted by $\widehat{Y}_{\star} = x_{\star}^{\top} \widehat{\beta}_{n}$.

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1. Provide the expression of $\mathbb{E}[(\widehat{Y}_{\star} - x_{\star}^{\top} \beta_{\star})^2]$.

By definition of $\widehat{\beta}_n$,

$$\widehat{Y}_{\star} - x_{\star}^{\top} \beta_{\star} = x_{\star}^{\top} (\widehat{\beta}_n - \beta_{\star}),$$

so that $\mathbb{E}[\widehat{Y}_{\star}] = x_{\star}^{\top} \beta_{\star}$ and

$$\mathbb{E}[(\widehat{Y}_{\star} - x_{\star}^{\top} \beta_{\star})^{2}] = \mathbb{V}[\widehat{Y}_{\star}] = x_{\star}^{\top} \mathbb{V}[\widehat{\beta}_{n}] x_{\star}.$$

On the other hand,

$$\mathbb{V}[\widehat{\beta}_n] = (X^{\top} X)^{-1} X^{\top} \mathbb{V}[Y] X (X^T X)^{-1} = \sigma^2 (X^{\top} X)^{-1}.$$

Therefore,

$$\mathbb{E}[(\widehat{Y}_{\star} - x_{\star}^{\top} \beta_{\star})^{2}] = \sigma^{2} x_{\star}^{\top} (X^{\top} X)^{-1} x_{\star}.$$

2. Provide a confidence interval for $x_{\star}^{\top}\beta_{\star}$ with statistical significance $1-\alpha$ for $\alpha \in (0,1)$.

By the first question, \widehat{Y}_{\star} is a Gaussian random variable with mean $x_{\star}^{\top}\beta_{\star}$ and variance $\sigma_{\star}^{2}x_{\star}^{\top}(X^{\top}X)^{-1}x_{\star}$. If $z_{1-\alpha/2}$ is the quantile of order $1-\alpha/2$ of the standard Gaussian variable.

$$\mathbb{P}\left(\frac{\left|\widehat{Y}_{\star} - x_{\star}^{\top} \beta_{\star}\right|}{\sigma_{\star}(x_{\star}^{\top}(X^{\top}X)^{-1}x_{\star})^{1/2}} \leqslant z_{1-\alpha/2}\right) \geqslant 1 - \alpha.$$

Therefore, with probability larger than $1 - \alpha$,

$$x_{\star}^{\top} \beta_{\star} \in \left(\widehat{Y}_{\star} - \sigma_{\star} (x_{\star}^{\top} (X^{\top} X)^{-1} x_{\star})^{1/2} z_{1-\alpha/2} \, ; \, \widehat{Y}_{\star} + \sigma_{\star} (x_{\star}^{\top} (X^{\top} X)^{-1} x_{\star})^{1/2} z_{1-\alpha/2} \right) \, .$$

3 Regression: linear estimators

Consider the regression model given, for all $1 \leq i \leq n$, by

$$Y_i = f^*(X_i) + \xi_i,$$

where for all $1 \le i \le n$, $X_i \in X$, and the $(\xi_i)_{1 \le i \le n}$ are i.i.d. centered Gaussian random variables with variance σ^2 . In this exercise, f^* is estimated by a linear estimator of the form

$$\widehat{f}_n: x \mapsto \sum_{i=1}^n w_i(x)Y_i.$$

Prove that

$$\frac{1}{n} \mathbb{E}\left[\sum_{i=1}^{n} (\widehat{f}_n(X_i) - f^*(X_i))^2\right] = \frac{1}{n} \|Wf^*(X) - f^*(X)\|_2^2 + \frac{\sigma^2}{n} \operatorname{Trace}(W^\top W),$$

where $W = (w_i(X_j))_{1 \le i,j \le n}$ and $f^*(X) = (f^*(X_1), \dots, f^*(X_n))^{\top}$.

Note that

$$\frac{1}{n}\mathbb{E}\left[\sum_{i=1}^{n}(\widehat{f}_{n}(X_{i}) - f^{*}(X_{i}))^{2}\right] = \frac{1}{n}\mathbb{E}\left[\|WY - f^{*}(X)\|_{2}^{2}\right],$$

where $Y = (Y_1, \dots, Y_n)^{\top}$. then, write

$$\mathbb{E}\left[\|WY - f^*(X)\|_2^2\right] = \mathbb{E}\left[\|WY - Wf^*(X)\|_2^2\right] + \mathbb{E}\left[\|Wf^*(X) - f^*(X)\|_2^2\right] + 2\mathbb{E}\left[\langle WY - Wf^*(X); Wf^*(X) - f^*(X)\rangle\right].$$

$$As \ \mathbb{E}[Y] = f^*(X), \ this \ yields$$

$$\mathbb{E}\left[\|WY - f^*(X)\|_2^2\right] = \mathbb{E}\left[\|WY - Wf^*(X)\|_2^2\right] + \|Wf^*(X) - f^*(X)\|_2^2.$$

The proof is completed by noting that

$$\mathbb{E}\left[\|WY - Wf^*(X)\|_2^2\right] = \mathbb{E}\left[(Y - f^*(X))^\top W^\top W(Y - f^*(X))\right] = \text{Trace}\left(W^\top W \mathbb{V}[Y - f^*(X)]\right)$$
and $\mathbb{V}[Y - f^*(X)] = \sigma^2 I_n$.