# 1 Basic Statistical Concepts

Consider a poll with two answers, A and B, regarding political parties. Let:

- N: total number of voters,
- M: number of voters supporting A,
- n: size of the poll,
- $X_1, X_2, \ldots, X_n$ : responses,
- Each  $X_i \in \{0,1\}$  if  $X_i = 1$  supports A.

Additionally, assume:

- We select n individuals from N at random and record their truthful reply,
- Every person asked replies (no selection bias),
- People can be asked repeatedly.

The aim of the poll is to estimate the fraction of party A supporters, say  $\theta$ .

**Definition 1** (Estimator). An intuitive estimator is:

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

This estimator will be analyzed in the following sections to determine whether it is unbiased, consistent, and optimal.

### 2 Statistical Models

Let  $(X, \mathcal{F})$  be a measurable space, i.e., a set X with a sigma-algebra  $\mathcal{F}$ , in which our statistical observations take values.

**Definition 2** (Statistical Model). Let  $(X, \mathcal{F})$  be some sample space. We call the parameter space  $\Theta$ . A statistical model is a family of probability measures  $\{P_{\theta}\}_{\theta \in \Theta}$ .

**Remark 1.** Often  $(X, \mathcal{F})$  is a product space. For example, if  $X_i \in \{0, 1\}$ , each  $P_{\theta}$  is a product distribution, i.e.,  $X_1, X_2, \ldots, X_n$  are independent and identically distributed (iid). Then we say  $\{P_{\theta} : \theta \in \Theta\}$  is an iid statistical model.

**Remark 2.** If every person could only be asked once, we would have  $P_{\theta}$  as a hypergeometric distribution, which converges to the Bernoulli model as  $N, M \to \infty$ .

### 3 Parameter Estimation

Assume  $(\Omega, \mathcal{F}, P_{\theta})$  is the setting of parametric statistics. Assume  $\Theta$  is measurable.

**Definition 3** (Estimator). An estimator for  $\theta$  is any measurable function  $\hat{\theta}: X \to \Theta$ , i.e., any function that, based on some data X, outputs a guess  $\hat{\theta}(X)$  for  $\theta$ .

### 4 Unbiased and Consistent Estimators

#### 4.1 Unbiased Estimator

**Definition 4** (Unbiased Estimator). Let  $(\Omega, \mathcal{F}, P_{\theta})$  be a measurable space. An estimator  $\hat{\theta}$  is called unbiased if:

$$\mathbb{E}[\hat{\theta}] = \theta \quad \forall \theta \in \Theta$$

where  $\mathbb{E}_{P_{\theta}}$  denotes expectation under the law  $P_{\theta}$ . In more explicit terms, unbiasedness means no systematic error.

*Proof.* For the Bernoulli model, we compute:

$$\mathbb{E}[\hat{\theta}_n] = \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^n X_i\right] = \frac{1}{n}\sum_{i=1}^n \mathbb{E}[X_i] = \frac{1}{n}\sum_{i=1}^n \theta = \theta$$

Thus,  $\hat{\theta}_n$  is an unbiased estimator of  $\theta$ .

### 4.2 Consistent Estimator

**Definition 5** (Consistent Estimator). Let  $\{P_{\theta,n} : n \geq 1\}$  be a sequence of statistical models on the same parameter space. Let  $\hat{\theta}_n$  be a sequence of estimators. The sequence  $\hat{\theta}_n$  is called consistent if for every  $\theta \in \Theta$ :

$$\hat{\theta}_n \to \theta$$
 in probability as  $n \to \infty$ 

or equivalently:

$$P_{\theta} \left( \lim_{n \to \infty} \hat{\theta}_n = \theta \right) = 1$$

*Proof.* For the Bernoulli model:

$$\hat{\theta}_n = \frac{1}{n} \sum_{i=1}^n X_i$$

We know  $\mathbb{E}[\hat{\theta}_n] = \theta$  and  $\operatorname{Var}(\hat{\theta}_n) = \frac{\theta(1-\theta)}{n}$ . Using Chebyshev's inequality, for any  $\epsilon > 0$ :

$$P\left(|\hat{\theta}_n - \theta| > \epsilon\right) \le \frac{\operatorname{Var}(\hat{\theta}_n)}{\epsilon^2} = \frac{\theta(1 - \theta)}{n\epsilon^2}$$

As  $n \to \infty$ , this probability tends to 0, proving that  $\hat{\theta}_n$  is consistent.

# 5 Maximum Likelihood Estimation (MLE)

**Definition 6** (Maximum Likelihood Estimator). The maximum likelihood estimator (MLE) is the parameter that maximizes the likelihood function:

$$L(\theta) = \prod_{i=1}^{n} P_{\theta}(X_i)$$

### 5.1 Proof: MLE for Bernoulli Model

*Proof.* For the Bernoulli model,  $P_{\theta}(X_i) = \theta^{X_i}(1-\theta)^{1-X_i}$ , so the likelihood function is:

$$L(\theta) = \prod_{i=1}^{n} \theta^{X_i} (1 - \theta)^{1 - X_i} = \theta^{\sum X_i} (1 - \theta)^{n - \sum X_i}$$

Taking the logarithm:

$$\log L(\theta) = \sum X_i \log \theta + (n - \sum X_i) \log(1 - \theta)$$

Setting the derivative with respect to  $\theta$  equal to 0 gives:

$$\frac{d}{d\theta}\log L(\theta) = \frac{\sum X_i}{\theta} - \frac{n - \sum X_i}{1 - \theta} = 0$$

Solving for  $\theta$ , we get:

$$\hat{\theta}_n = \frac{1}{n} \sum_{i=1}^n X_i$$

which is the MLE.

# 6 Bayesian Methods

**Definition 7** (Posterior Distribution in Bayesian Inference). In Bayesian statistics, a key element is the prior distribution, denoted by  $\pi(\theta)$ , which reflects our beliefs about the parameter  $\theta$  before observing data. The posterior distribution is given by:

$$\pi(\theta|X) \propto P_{\theta}(X)\pi(\theta)$$

### 6.1 Example: Posterior for Bernoulli Model

**Example 1.** Suppose we have a Beta prior for  $\theta$ ,  $\pi(\theta) \sim Beta(\alpha, \beta)$ , and observe  $X_1, \ldots, X_n$  as Bernoulli trials. The likelihood is:

$$P(X|\theta) = \theta^{\sum X_i} (1 - \theta)^{n - \sum X_i}$$

The posterior is proportional to the product of the prior and likelihood:

$$\pi(\theta|X) \propto \theta^{\sum X_i + \alpha - 1} (1 - \theta)^{n - \sum X_i + \beta - 1}$$

Thus, 
$$\pi(\theta|X) \sim Beta(\sum X_i + \alpha, n - \sum X_i + \beta)$$
.

# Notes on Bayes and Posterior

 $\mathbf{Posterior} = \mathrm{prior} \times \mathrm{likelihood}$ 

**Normalizing Constant** 

$$\int Posterior \, dx = 1$$

So,

$$\int Posterior \, dx = 1$$

 $\mathbf{Prior} \to \mathbf{Posterior}$  via Bayes.

Let  $\mathcal{F}_0$  be a  $\sigma$ -algebra on  $\Omega$  and suppose  $(\Omega, \mathcal{F}_0, P_\theta)$  is a dominated statistical model with densities  $p(x|\theta)$ . Assume

$$x, \theta \in \Omega \implies p(x|\theta)$$

is jointly measurable with respect to  $\mathcal{F}_0 \times \mathcal{F}_1$ .

Let  $\pi$  be a prior distribution on  $\Omega$  with density  $\pi(\theta)$  with respect to measure  $\nu$ . Define posterior density

$$\pi(\theta|x) = \frac{p(x|\theta)\pi(\theta)}{\int p(x|\theta)\pi(\theta) d\theta}$$

The corresponding probability measure is called the **posterior distribution**.

Think of  $p(x|\theta)$  as a Lebesgue measure. Let  $\nu$  be a Lebesgue density.

**Exception**: If  $\Omega = \{0, 1\}$ , then we take  $\nu$  to be the counting measure.

From the posterior, we can derive several estimators. For example,  $E[\theta|X=x]$  is convex:

$$\int \theta p(x|\theta) d\theta = E[\theta|X = x]$$

**Example:** Binomial model  $X|\theta \sim \text{Binomial}(n,\theta)$  with prior  $\theta \sim \text{Unif}(0,1)$ .

For a uniform prior, we know the MAP and MLE.

Posterior mean:

$$\theta_{\text{MAP}} = \frac{k+1}{n+2}$$

In the case of coin flips,  $X \sim \text{Binomial}(n, \theta)$ , where k is the number of heads, we conclude  $\theta | X \sim \text{Beta}(k+1, n-k+1)$ .

$$\theta | X \sim \text{Beta}(k+1, n-k+1)$$

Conjugate Bayes Models: Let  $P_{\theta} \in \mathcal{P}$  be a statistical model. Then some family of priors is called conjugate if

$$P_{\theta} \in \mathcal{P} \Rightarrow \theta | X \in \mathcal{P}$$

for all  $X \in \mathcal{X}$ , where  $\mathcal{X}$  is the sample space.

$$\theta | X \sim \text{Beta}(a, b), \quad X \sim \text{Bernoulli}(p)$$

# Loss Functions and Risk

**Loss Function**: A function  $L: \Theta \times \mathcal{X} \to [0, \infty)$  is a basis function if for every  $\theta \in \Theta$ ,  $L(\theta, \cdot)$  is measurable.

Given an estimator  $\delta$ , the expected loss is

$$R(\theta, \delta) = E_{\theta}[L(\theta, \delta)]$$

Mean Squared Error (MSE):

$$L(x,y) = (x-y)^2 \Rightarrow R(\theta,\delta) = E_{\theta}[(\delta-\theta)^2]$$

**Bias-Variance Decomposition:** 

$$L(x,y) = (x-y)^2$$

Proof: Let  $\delta(x) = E[\theta|X = x]$ .

$$R(\theta, \delta) = E_{\theta}[(\delta(X) - \theta)^2]$$

Bias-variance decomposition:

$$E[(\delta(X) - \theta)^2] = Var(\delta(X)) + (Bias)^2$$

# Minimax and Bayes Risk

**Minimax Risk**: Given an estimator  $\delta$  in a model  $P_{\theta} \in \mathcal{P}$ , the maximal risk of it is

$$\sup_{\theta \in \Theta} R(\theta, \delta)$$

The minimax of a model  $P_{\theta}$  is given as  $\inf_{\delta} \sup_{\theta} R(\theta, \delta)$ , where the inf is over all estimators. An estimator is called minimax if

$$\sup_{\theta} R(\theta, \delta) = \inf_{\delta} \sup_{\theta} R(\theta, \delta)$$

**Bayes Risk**: Given an estimator  $\delta$  and prior  $\pi$  on  $\Theta$ , the Bayes risk of  $\delta$  is defined as

$$R_{\pi}(\delta) = \int R(\theta, \delta) d\pi(\theta)$$

The posterior risk of an estimator  $\delta(X)$  is defined by

$$R(\delta|X=x) = E[L(\theta,\delta(X))|X=x]$$

Suppose  $\delta^*$  is an estimator that minimizes the posterior risk,  $\delta^*(x) = E[\theta|X=x]$ . Then it also minimizes the Bayes risk. ec If  $L(x,y) = (x-y)^2$ , the Bayes optimal estimator  $\delta(x)$  is the posterior mean.

We want to construct C(x) s.t.  $P_{\theta}(\theta \in C(x)) \ge 1 - \alpha, \forall \theta \in [0, 1]$ 

$$x^{(1)}$$
 ( )  $C(x^{(1)})$ 

$$x^{(k)} \qquad (\quad) \quad C(x^{(k)})$$

 $\theta \rightarrow \rightarrow \rightarrow$  contains true param 3/4 times

# Example cont.:

Best guess:  $C(x) = \left[\frac{\bar{X}_n - a}{n}, \frac{\bar{X}_n + b}{n}\right]$ 

$$P_{\theta}^{n}(\theta \in C(x)) = P_{\theta}^{n} \left( \frac{\bar{X}_{n}}{n} - \theta \in [-b, a] \right)$$
$$= F_{\theta}^{n}(a) - F_{\theta}^{n}(-b) + \rho_{n}$$

where  $F_{\theta}^{n}: \mathbb{R} \to [0,1], F_{\theta}^{n}(t) = P_{\theta}^{n}\left(\frac{\bar{X}_{n}-\theta}{n} \leq t\right)$  is the CDF of  $\frac{\bar{X}_{n}-\theta}{n}$  under  $P_{\theta}$  and  $\rho_{n} = P_{\theta}^{n}\left(\frac{\bar{X}_{n}}{n} - \theta = -b\right)$ .

### How to choose a and b:

CDF CDF 
$$\leftarrow$$
  $-b$   $a \rightarrow t$ 

We'd like to choose  $a = (F_{\theta}^n)^{-1} \left(1 - \frac{\alpha}{2}\right)$  and  $b = (F_{\theta}^n)^{-1} \left(\frac{\alpha}{2}\right)$ , where

$$(F_{\theta}^n)^{-1}(p) := \inf\{t \in \mathbb{R} : F_{\theta}^n(t) \ge x\}$$
 (Quantile Function)

Let's use a normal approximation, for  $\sigma^2 = \theta(1 - \theta)$ :

$$\sqrt{n}\left(\frac{\bar{X}_n}{n} - \theta\right) = \frac{1}{\sqrt{n}} \sum_{k=1}^n \frac{X_k - \theta}{\sigma} \xrightarrow{d} \mathcal{N}(0, 1) \quad [CLT]$$

 $X_k \sim \mathrm{Ber}(\theta)$ 

Then it follows that

$$F_{\theta}^{n}(a_{n}) = P_{\theta}^{n} \left( \frac{\bar{X}_{n}}{n} - \theta \leq a_{n} \right)$$

$$= P_{\theta}^{n} \left( \frac{\sqrt{n}}{\sigma} \left( \frac{\bar{X}_{n} - \theta}{n} \right) \leq \sqrt{n} a_{n} \right)$$

$$= \Phi \left( \frac{\sqrt{n}}{\sigma} a_{n} \right),$$

where the convergence is valid if  $a_n := \text{const.} \frac{1}{\sqrt{n}}$ .

Now, let us choose

$$a := \frac{\sigma}{\sqrt{n}} z_{1 - \frac{\alpha}{2}}$$

where  $z_{1-\frac{\alpha}{2}} = \Phi^{-1}\left(1-\frac{\alpha}{2}\right)$  is the  $1-\frac{\alpha}{2}$  quantile of  $\mathcal{N}(0,1)$  and b=a. Then

$$C(x) = \left[ \frac{\bar{X}_n}{n} - \frac{\sigma}{\sqrt{n}} z_{1-\frac{\alpha}{2}}, \frac{\bar{X}_n}{n} + \frac{\sigma}{\sqrt{n}} z_{1-\frac{\alpha}{2}} \right]$$

It follows

$$P_{\theta}^{n}(\theta \in C(x)) = F_{\theta}^{n}(a_{n}) - F_{\theta}^{n}(b) + \rho_{n} = 1 - \frac{\alpha}{2} + o(1) + o(1)$$
$$= 1 - \alpha + o(1) \text{ as } n \to \infty$$

⇒ Asymptotically valid confidence set

One more problem:  $\sigma$  depends on  $\theta$ 

- Upper bound:  $\sup_{\theta \in [0,1]} \theta(1-\theta) = \frac{1}{4}$  (maximized at  $\theta = \frac{1}{2})$
- Empirical Variance:  $\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^n (X_i \frac{1}{n} \sum_{i=1}^n X_i)^2$

$$\frac{\hat{\sigma}^2}{\sigma^2} \stackrel{P_{\theta}}{\to} 1$$

# Slutsky's Theorem:

$$X_n \xrightarrow{d} X$$
,  $Y_n \xrightarrow{d} \text{const.} \Rightarrow X_n Y_n \xrightarrow{d} CX$ 

Exercise: Use this to deduce that  $a_n = \frac{\hat{\sigma}}{\sqrt{n}} z_{1-\frac{\alpha}{2}}$  is also valid

### Remark:

# Hypothesis Testing

**Definition:** Let  $(P_{\theta}: \theta \in \Theta)$  be a statistical model and let  $\Theta = \Theta_0 \cup \Theta_1$  be a partition. Then:

- A statistical test is a measurable function of the data  $\varphi: (\mathcal{X}, \mathcal{F}) \to [0, 1]$
- If  $\forall x \in \mathcal{X}, \varphi(x) \in \{0,1\}$ , then  $\varphi$  is a non-randomized test
- Else  $\varphi$  is randomized

### **Definitions:**

- $H_0: \theta \in \Theta_0$  is called the null hypothesis
- $H_1: \theta \in \Theta_1$  is called the alternative hypothesis
- The map  $\theta \to \beta_{\varphi}(\theta) = P_{\theta}[\varphi = 1]$  is called the power function of a test  $\varphi$

$$1 \quad \beta_{\varphi}(\theta) \quad 0 \quad \Theta_0 \quad \Theta_1 \quad \Theta$$

- For  $\theta \in \Theta_0$ ,  $\beta_{\varphi}(\theta)$  is the type-I-error under  $\theta$  [Wrongly rejecting the null]
- For  $\theta \in \Theta_1$ ,  $1 \beta_{\varphi}(\theta)$  is the type-II-error

#### Note:

$$1 - P_{\theta}(\varphi = 1) = P_{\theta}(\varphi = 0) = P_{\theta}$$
 (wrongly accepting the null)

### Definition: [Level]

$$\varphi: \mathcal{X} \to [0,1]$$
 has level  $\alpha \in [0,1]$  if

$$\sup_{\theta \in \Theta_0} \beta_{\varphi}(\theta) \le \alpha$$

#### Definition: [Uniformly most powerful test]

Given a level  $\alpha \in (0,1)$ ,  $\varphi : \mathcal{X} \to [0,1]$  is called UMP if for every other test  $\varphi'$  of level  $\alpha$  and all  $\theta \in \Theta_1$ ,

$$\beta_{\varphi}(\theta) \ge \beta_{\varphi'}(\theta)$$

$$1 \quad \alpha \quad 0 \qquad \beta_{\varphi}(\theta) \qquad \beta_{\varphi'}(\theta) \qquad \Theta_0 \qquad \Theta_1$$

#### Remark:

In general, it is very hard to find UMP tests. But: for simple hypotheses, i.e.  $\Theta_0 = \{\theta_0\}, \Theta_1 = \{\theta_1\}$ , it is possible. Here, likelihood ratio tests are UMP.

# Theorem: [Neyman-Pearson Lemma]

Let  $\Theta_0 = \{\theta_0\}, \Theta_1 = \{\theta_1\}$  be simple:

1. **Existence:** There exists a test  $\varphi$  and a constant  $k \in [0, \infty)$ , s.t.  $P_{\theta_0}(\varphi = 1) = \alpha$ , of the form

$$\varphi(x) = \begin{cases} 1, & \text{if } \frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} > k \\ 0, & \text{if } \frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} < k \end{cases} (*)$$

Here  $p_{\theta_1}, p_{\theta_0}$  are densities w.r.t. some dominated measure  $\mu$ , e.g.  $\mu = p_{\theta_0} + p_{\theta_1}$ . Finite  $\Theta$  implies measure is always dominated (likelihood always exists).

- 2. Sufficiency: If  $\varphi$  satisfies  $P_{\theta_0}(\varphi = 1) = \alpha$  and (\*) then  $\varphi$  is a UMP level  $\alpha$  test.
- 3. Necessity: If  $\varphi_k$  is UMP for level  $\alpha$ , then it must be of the form (\*), and it also satisfies  $P_{\theta_0}(\varphi_k = 1) = \alpha$ , or else it must satisfy  $P_{\theta_1}(\varphi_k = 1) = 1$ .

### **Proof:**

1. Define  $r(x) = \frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} \in [0, \infty) \cup \{\pm \infty\}$ . Let  $F_0$  be the CDF of r(x) under  $P_{\theta_0}$ .

$$F_0(t) = P_{\theta_0}(r(x) \le t)$$

Then define also  $\alpha(t) = 1 - F_0(t) = P_{\theta_0}(r(x) > t)$ 

•  $\alpha$  is right-continuous:

$$\lim_{\epsilon \to 0} \alpha(t+\epsilon) = \lim_{\epsilon \to 0} P_{\theta_0}(r(x) > t+\epsilon) = P_{\theta_0}(r(x) > t) = \alpha(t)$$

- $\alpha$  is non-increasing
- $\alpha$  has left limits

$$\lim_{\epsilon \to 0} \alpha(t - \epsilon) = P_{\theta_0}(r(x) > t - \epsilon) = \alpha(t^-)$$

 $\alpha$  is cadlag:

- Continuous from the right
- Limit from the left

There exists some  $k \in [0, \infty)$  s.t.  $\alpha \leq \alpha(k^-)$  and  $\alpha \geq \alpha(k)$ 

We define our test

$$\varphi(x) = \begin{cases} 1 & \text{if } r(x) > k \\ \gamma & \text{if } r(x) = k \\ 0 & \text{if } r(x) < k \end{cases} \text{ [reject null w.p. } \gamma \text{]}$$

We set

$$\gamma = \frac{\alpha - \alpha(k)}{\alpha(k^-) - \alpha(k)}$$

The level of  $\varphi$  is

$$E_{\theta_0}[\varphi(x)] = P_{\theta_0}(\varphi(x) = 1)$$

$$= P_{\theta_0}(r(x) > k) + P_{\theta_0}(r(x) = k) \cdot \gamma$$

$$= \alpha(k) + \left[\alpha(k^-) - \alpha(k)\right] \cdot \frac{\alpha - \alpha(k)}{\alpha(k^-) - \alpha(k)} = \alpha$$
(randomizing the test)

## Lecture 6

### Neyman-Pearson

Power of a test:

$$E_{\theta_1}[\varphi] = P_{\theta_1}(\varphi = 1)$$

Likelihood ratio test:

$$\frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} = r(x)$$

LR test

$$\varphi(x) = \begin{cases} 1 & \text{if } r(x) > k \\ \gamma & \text{if } r(x) = k \\ 0 & \text{if } r(x) < k \end{cases}$$

for some  $k \in [0, \infty), \gamma \in [0, 1]$ .

Note: LR tests are UMP for simple hypothesis testing:

- Given some  $\alpha$ , if LR satisfies  $E_{\theta_0}[\varphi] = \alpha$ , it represents a Type I error.
- $\varphi$  minimizes the Type II error

$$E_{\theta_1}[\varphi] \ge E_{\theta_1}[\varphi'] \quad \forall \varphi'$$

## Cont. of proof (part of UMP)

Let  $\varphi'$  be another level  $\alpha$  test,  $E_{\theta_0}[\varphi'] \leq \alpha$ .

Goal:  $E_{\theta_1}[\varphi] \geq E_{\theta_1}[\varphi']$ . Let  $\mu$  be the dominating measure.

Consider

$$\int (\varphi(x) - \varphi'(x))(p_{\theta_1}(x) - kp_{\theta_0}(x)) d\mu(x) = 0$$

Claim:  $p \geq 0$ .

Observe:

- If  $p_{\theta_1}(x) kp_{\theta_0}(x) > 0 \Rightarrow \frac{p_{\theta_1}(x)}{p_{\theta_0}(x)} > k \Rightarrow \varphi(x) = 1$ .
- If  $p_{\theta_1}(x) kp_{\theta_0}(x) < 0 \Rightarrow \varphi(x) = 0$ .
- If  $p_{\theta_1}(x) kp_{\theta_0}(x) = 0 \Rightarrow \text{integrand} = 0$ .

$$\Rightarrow p = 0$$

$$\Rightarrow \int (\varphi - \varphi') p_{\theta_1} d\mu = \int (\varphi - \varphi') p_{\theta_0} d\mu = k \left[ E_{\theta_0}[\varphi] - E_{\theta_0}[\varphi'] \right] \ge 0$$

$$\Rightarrow E_{\theta_1}[\varphi] \geq E_{\theta_1}[\varphi']$$

**Part (3) UMP**  $\Rightarrow$  (LR): Take  $\varphi^*$  a UMP test,  $E_{\theta_0}[\varphi^*] = \alpha$ , and let  $\varphi$  be the LR test with  $E_{\theta_0}[\varphi] = \alpha$  with (\*).

Goal:  $\varphi = \varphi^*$  a.e. except on  $\{r(x) = k\}$ .

Define

$$x^+ = \{x : \varphi(x) > \varphi^*(x)\}$$

$$x^- = \{x : \varphi(x) < \varphi^*(x)\}$$

$$x^0 = \{x : \varphi(x) = \varphi^*(x)\}\$$

$$\tilde{x} = (x^+ \cup x^-) \cap \{x : p_{\theta_1}(x) \neq kp_{\theta_0}(x)\}$$

It suffices to show  $\mu(\tilde{x}) = 0$ .

Like before, we have

$$(\varphi - \varphi^*)(p_{\theta_1} - kp_{\theta_0}) > 0 \text{ on } \tilde{x}$$

Thus if  $\mu(\tilde{x}) > 0$ ,

$$\int_{\mathcal{X}} (\varphi - \varphi^*) (p_{\theta_1} - k p_{\theta_0}) \, d\mu \ge 0$$
$$\int_{\tilde{z}} (\varphi - \varphi^*) (p_{\theta_1} - k p_{\theta_0}) \, d\mu \ge 0$$

But also

$$E_{\theta_1}[\varphi] - E_{\theta_1}[\varphi^*] > k \left[ E_{\theta_0}[\varphi] - E_{\theta_0}[\varphi^*] \right] \ge 0$$

$$\Rightarrow \text{Cannot be } \varphi^* \text{ is UMP.}$$

### Example (Gaussian Location Model)

$$X_1, \ldots, X_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$$

$$H_0: \mu = \mu_0, \quad H_1: \mu = \mu_1, \quad \mu_0 < \mu_1$$

Then:

$$\frac{p_1(X_1, \dots, X_n)}{p_0(X_1, \dots, X_n)} = \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (X_i - \mu_1)^2 + \frac{1}{2\sigma^2} \sum_{i=1}^n (X_i - \mu_0)^2\right)$$

$$= \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (\mu_1^2 - \mu_0^2) - \frac{2(\mu_1 - \mu_0)}{\sigma^2} \sum_{i=1}^n X_i\right)$$

$$= \exp\left(-\frac{n}{2\sigma^2} (\mu_1^2 - \mu_0^2) - \frac{2(\mu_1 - \mu_0)}{\sigma^2} \sum_{i=1}^n X_i\right) \ge K_\alpha$$

$$\Rightarrow \frac{1}{n} \sum_{i=1}^n X_i \ge K_\alpha, \text{ some } K_\alpha \in \mathbb{R}$$

To determine  $K_{\alpha}$ :

$$\bar{X}_n := \frac{1}{n} \sum_{i} X_i \overset{H_0}{\sim} \mathcal{N}(\mu_0, \sigma^2/n)$$

$$\Rightarrow \mathbb{L} = P_{H_0} \left( \bar{X}_n \ge K_\alpha \right) = 1 - P_{H_0} \left( \bar{X}_n < K_\alpha \right)$$

$$= 1 - \Phi \left( \frac{\sqrt{n}}{\sigma} (K_\alpha - \mu_0) \right) \quad \text{(CDF for } \mathcal{N}(0, 1))$$

$$\Rightarrow \text{solving for } K_\alpha \text{ gives } K_\alpha = \mu_0 + \frac{\sigma}{\sqrt{n}} \Phi^{-1} (1 - \alpha),$$

$$\varphi(X_1, \dots, X_n) = \begin{cases} 1 & \text{if } \bar{X}_n \ge \mu_0 + \frac{\sigma}{\sqrt{n}} \Phi^{-1} (1 - \alpha) \\ 0 & \text{else} \end{cases}$$

#### Corollary

Consider simple hypothesis testing. Let  $\varphi$  be UMP, for level  $\alpha$ . Then,

$$\alpha = E_{H_0}[\varphi_0] = E_{\theta_0}[\varphi_0] \le E_{\theta_1}[\varphi]$$

Suppose  $E_{\theta_1}[\varphi] = E_{\theta_1}[\varphi_0]$  then  $\varphi_0$  is also UMP,  $\Rightarrow \varphi_0$  is an LR test.

$$\varphi_0 = \begin{cases} 1 & \text{if } \frac{p_{\theta_1}}{p_{\theta_0}} \ge K & \text{a.s., some } K \\ 0 & \text{if } \frac{p_{\theta_1}}{p_{\theta_0}} \end{cases}$$

Also since  $\varphi_0 \in \{\varphi, \beta\}$  we conclude that  $p_{\theta_1} = Kp_{\theta_0}$  a.s.

But

$$L = \int p_{\theta_0} d\mu = K \int p_{\theta_0} d\mu = 1 \Rightarrow K = 1$$

#### Correspondence theorem

Tests  $\longleftrightarrow$  Confidence regions C(x)

$$\Pr_{\theta}(\theta \in C(x)) \ge 1 - \alpha$$

If 
$$\Pr_{\theta}(\phi_{\theta}=1)=\alpha$$

**Theorem:** Let  $(P_{\theta}: \theta \in \Theta)$  be a statistical model,  $\alpha \in (0,1)$ .

(i) Let C = C(X) be a level- $\alpha$  confidence set, then

$$\phi_{\theta_0}(x) = 1 \left\{ \theta_0 \notin C(x) \right\}$$

is a level- $\alpha$  test of  $\theta = \theta_0$  vs.  $\theta \neq \theta_0$ .

(ii) Suppose  $\{\phi_{\theta_0}: \theta_0 \in \Theta\}$  is a family of level- $\alpha$  tests, then

$$C(X) = \{ \theta \in \Theta : \phi_{\theta}(X) = 0 \}$$

is a  $(1 - \alpha)$  confidence set.

#### **Proof:**

- (i)  $\operatorname{Pr}_{\theta_0}(\phi_{\theta_0} = 1) = \operatorname{Pr}_{\theta_0}(\theta_0 \notin C(X)) = \alpha$
- (ii)  $\operatorname{Pr}_{\theta}(\theta \notin C(X)) = \operatorname{Pr}_{\theta}(\theta \notin \{\tilde{\theta} \in \Theta : \phi_{\tilde{\theta}}(X) = 0\}) = \operatorname{Pr}_{\theta}(\phi_{\theta}(X) = 1) \le \alpha$

### UMPT Tests in Models with Monotone Likelihoods

**Proposition:** Let  $\Theta \subseteq \mathbb{R}$ . Consider testing  $H_0: \theta \leq \theta_0$  vs.  $H_1: \theta > \theta_0$ , for some  $\theta_0 \in \mathbb{R}$ . Assume there exists some test statistic  $T: X \to \mathbb{R}$  and a function  $h: \mathbb{R} \times \Theta \times \Theta$  such that

$$\frac{P_{\theta}(X)}{P_{\tilde{\theta}}(X)} = h(T(X), \theta, \tilde{\theta})$$

and for all  $\theta \geq \tilde{\theta}, t \mapsto h(t, \theta, \tilde{\theta})$  is monotone increasing.

The simplest model for the relationship between  $Y_i$  and  $X_i$  assumes a linear relationship:

$$Y_i = aX_i + b + \varepsilon_i$$

for i = 1, ..., n, where  $\varepsilon_i$  is centered, i.e.,  $E(\varepsilon) = 0$  and  $Var(\varepsilon) = \sigma^2$ . Suppose  $\varepsilon \sim N(0, \sigma^2)$  with  $\sigma$  known.

The statistical model is given by

$$(\mathbb{R}, B(\mathbb{R}), (\bigotimes_{i=1}^{n} N(ax_i + b, \sigma^2))_{(a,b) \in \mathbb{R}^2})$$

The likelihood within the statistical model is

$$L((a,b)|y) = \prod_{i=1}^{n} (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - ax_i - b)^2\right)$$

The MLE satisfies the optimization problem

$$(\hat{a}, \hat{b}) = \arg\min_{(a,b) \in \mathbb{R}^2} \sum_{i=1}^n (y_i - (ax_i + b))^2$$

Provided that  $x_i \neq x_j$  for  $i \neq j$ , the least squares problem has a solution with minimum given by (Gauss, 1801):

$$(\hat{a}, \hat{b}) = \left(\frac{\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2}, \ \bar{y} - \hat{a}\bar{x}\right)$$

**Definition 8** (Linear Model). A random vector  $Y = (Y_1, ..., Y_n)^T \in \mathbb{R}^n$  stems from a linear model if there exists a parameter vector  $\beta \in \mathbb{R}^p$ , a matrix  $X \in \mathbb{R}^{n \times p}$ , and a random vector  $\varepsilon \in \mathbb{R}^n$  such that

$$Y = X\beta + \varepsilon$$

- 1. A linear model is called regular if
  - (a)  $p \le n$  (parameter size is smaller than sample size),
  - (b) X has full rank.  $rank(X) = p \le n$  (design with full rank)
  - (c)  $E(\varepsilon) = 0$  (noise is controlled)
  - (d) The covariance matrix is positive definate,  $\Sigma = (Cov(\varepsilon_i, \varepsilon_i))_{i,i \in [n]}$
- 2. A linear model is called ordinary if  $\Sigma = \sigma^2 E_n$  (and is usually the noise is Gaussian)

#### Remark 3. 1. There are several synonyms

- (a) Y a dependent variable, response, regressand
- (b) X, a independent variable, predictor, design matrix, regressor
- (c)  $\varepsilon$  Error, perturbation, reression function
- 2. The matrix  $\Sigma$  is symmetric and diagonalizable, i.e.  $\Sigma = UDU^T$  for some diagonal matrix,  $D = diag(\lambda_1, \ldots, \lambda_n) \in \mathbb{R}^{n \times n}$
- 3. Positive semi-definate, i.e.  $\lambda_i \geq 0$

$$\langle \Sigma u, u \rangle = \langle E[(\varepsilon - E[\varepsilon])(\varepsilon - E[\varepsilon])^T]u, u \rangle$$
$$= E[(\varepsilon - E[\varepsilon])^2] \ge 0, u \in \mathbb{R}^n$$

item If  $\Sigma$  is positive definate  $(\lambda_i > 0)$  for i = 1, ..., n, then there exists the inverse  $\Sigma^{-1} = UD^{-1}U^T$  and  $\Sigma^{-1/2} = UD^{-1/2}U^T$ .

4. If X is not deterministic, we speak of random design.

In the regular linear model,  $\hat{\beta}$  is called weighted least squares estimate, (LSE). if

$$||\sigma^{-1/2}(Y - X\hat{\beta})||^2 = \inf_{\beta \in \mathbb{R}^n} ||\sigma^{-1/2}(Y - X\beta)||^2 = \inf_{\beta \in \mathbb{R}^n} ||\sigma^{-1/2}Y - X_{\Sigma}\beta||^2$$

where  $X_{\Sigma} = \Sigma^{-1/2} X$ .  $X_{\Sigma} \hat{\beta}$  is the point within the subspace,

$$U = \{X_{\Sigma}\beta \mid \beta \in \mathbb{R}^n\} \subseteq \mathbb{R}^n$$

with the smallest distance to the vector  $\Sigma^{-1/2}Y$ . Thus,  $X_{\Sigma}\hat{\beta} = \Pi_U(\Sigma^{-1/2}Y)$  where  $\Pi_U$  is the orthogonal projection onto U.  $\Pi_U u = u$  for all  $u \in U$   $\langle \Pi_U v - v, u \rangle = 0$  for all  $u \in U$  and  $r \in \mathbb{R}^n$ . Provided that  $(X_{\Sigma}^T X_{\Sigma})^{-1}$  exists, we can confirm by direct computation that the projection satisfies

$$\Pi_U = X_{\Sigma} (X_{\Sigma}^T X_{\Sigma})^{-1} X_{\Sigma}^T$$

For  $u = X_{\Sigma}\beta$  we have,

$$X_{\Sigma}(X_{\Sigma}^T X_{\Sigma})^{-1} X_{\Sigma}^T X_{\Sigma} \beta = X_{\Sigma} \beta = u$$

By symmetry,

$$\langle \Pi_U v - v, u \rangle = \langle v, \Pi_U u \rangle - \langle v, u \rangle = \langle v, u \rangle - \langle v, u \rangle = 0$$

for all  $u \in U$ .

**Lemma 1.** Representation for the LSE Consider a regular linear model, then the LSE exists uniquely, and is given by

$$\hat{\beta} = (X_{\Sigma}^T X_{\Sigma})^{-1} X_{\Sigma}^T \Sigma^{-1/2} Y = X_{\Sigma}^+ \Sigma^{-1/2} Y$$

*Proof.*  $\ker(X_{\Sigma}^T X_{\Sigma})$  is invertible. Suppose that  $X_{\Sigma}^T X_{\Sigma} v = 0$   $(v \in \ker(X_{\Sigma}^T X_{\Sigma}))$ 

$$0 = v^T X_{\Sigma}^T X_{\Sigma} v = (X_{\Sigma}^T v)^T X_{\Sigma} v = \langle X_{\Sigma} v, X_{\Sigma} v \rangle = ||X_{\Sigma} v||^2 = ||\Sigma^{-1/2} X v||^2 \implies ||X v||^2 = 0 \implies v = 0$$

So then

$$X_{\Sigma}\hat{\beta} = \Pi_{u}\Sigma^{-1/2}Y = X_{\Sigma}(X_{\Sigma}^{T}X_{\Sigma})^{-1}X_{\Sigma}^{T}\Sigma^{-1/2}Y$$
$$X_{\Sigma}^{T}X_{\Sigma}\hat{\beta} = X_{\Sigma}^{T}X_{\Sigma}(X_{\Sigma}^{T}X_{\Sigma})^{-1}X_{\Sigma}^{T}\Sigma^{-1/2}Y$$
$$\implies \hat{\beta} = (X_{\Sigma}^{T}X_{\Sigma})^{-1}X_{\Sigma}^{T}\Sigma^{-1/2}Y$$

**Remark 4.** 1. If p > n, then  $(X_{\Sigma}^T X_{\Sigma})^{-1}$  does not exist and the LSE is not unique.

$$\left\{\beta \cdot ||\Sigma^{-1/2}Y - X_{\Sigma}\beta||^2 = 0\right\}$$

is a p-n dim subspace and each solution interpolates the data

**Theorem 1.** Optimality of the LSE, Gauss-Markov Theorem Consider an ordinary linear model for  $\sigma > 0$ , then

- 1. The least squares estimator  $\hat{\beta} = (X^T X)^{-1} X^T Y$  is linear and the unbiased parameter for the parameter  $\beta$ .
- 2. For the desired parameter  $\alpha = \langle \beta, v \rangle$  for  $v \in \mathbb{R}$ , the estimator  $\hat{\alpha} = \langle \hat{\beta}, v \rangle$  is the best linear unbiased estimator (BLUE), meaning that  $\hat{\alpha}$  has the optimal value within the class of linear unbiased estimators for  $\alpha$
- 3.  $\hat{\sigma}^2 = \frac{||Y X\hat{\beta}||^2}{n-p}$  is an unbiased estimator of  $\sigma^2$

Proof.

$$\hat{\beta}(y+\tilde{y}) = \hat{\beta}(y) + \hat{\beta}(\tilde{y})$$
 for  $y, \tilde{y} \in \mathbb{R}^n$ 

$$E[\hat{\beta}] = (X^T X)^{-1} X^T E[Y] \tag{1}$$

$$= (X^T X)^{-1} X^T E[X\beta + \varepsilon] \tag{2}$$

$$= (X^T X)^{-1} (X^T X)\beta \tag{3}$$

$$=\beta$$
 (4)

Suppose that  $\tilde{\alpha}$  is some other linear unbiased estimator of  $\alpha$ . Since the estimator is linear, there exists some element w such that  $\tilde{\alpha} = \langle y, w \rangle$ 

$$\langle \beta, v \rangle = \alpha = E[\tilde{\alpha}] = E[\langle y, w \rangle] = \langle X\beta, w \rangle = \langle \beta, X^T w \rangle$$

This implies that  $v = X^T w$ , therefore we have,

$$Var = Var(\langle x\beta, w \rangle + \langle \varepsilon, w \rangle) \tag{5}$$

$$= \operatorname{Var}(\langle \varepsilon, w \rangle) + E\left[\left(\sum_{i=1}^{n} \varepsilon w\right)^{2}\right]$$
 (6)

$$= \sigma^2 \sum_{i=1}^p w_i^2 = \sigma^2 ||w||^2 \tag{7}$$

$$Var(\hat{\alpha}) = E[\langle \hat{\beta} - \beta, v \rangle^2]$$
(8)

$$= E[\langle (X^T X)^{-1} X^T \beta + (X^T X)^{-1} X^T \varepsilon - \beta, v \rangle^2]$$
(9)

$$= E[\langle (X^T X)^{-1} X^T \varepsilon, v \rangle^2] \tag{10}$$

$$= \sigma^{2} ||X(X^{T}X)^{-1}v||^{2} = \sigma^{2} ||X(X^{T}X)^{-1}X^{T}w||^{2}$$
(11)

$$= \sigma^2 ||\Pi_u w||^2 \tag{12}$$

Thus,  $Var(\hat{\alpha}) \leq Var\tilde{\alpha}$ 

#### 7 Lecture 8

Recall linear model

$$Y = X\beta + \varepsilon$$

where  $cov(\varepsilon) = \Sigma$ .

OLD: 
$$\beta = (X_{\Sigma}^T X_{\Sigma})^{-1} X_{\varepsilon}^T \Sigma^{-1/2} Y$$
.

OLD:  $\hat{\beta} = (X_{\Sigma}^T X_{\Sigma})^{-1} X_{\varepsilon}^T \Sigma^{-1/2} Y$ .  $X\hat{\beta} = \text{Projection of } \Sigma^{-1/2} Y \text{ onto span } \{X_{\varepsilon,1}, \dots, X_{\varepsilon,p}\}$ 

1.  $\hat{\beta}_{OLS}$  is the best linear unbiased est (BLUE) Theorem 2 (Gauss-Markov).

- 2.  $\alpha_i = \langle \beta, v \rangle$  is BLUE.
- 3.  $\hat{\sigma}^2 = \frac{||Y X\hat{\beta}||^2}{n-p}$  is unbiased est for  $\sigma^2 > 0$

$$\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{pmatrix}^T + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix} \text{ Where our data is } (Y_i, X_i)_{i=1}^n \in (\mathbb{R} \times \mathbb{R}^p)^{\otimes p}$$

Remark 5. Is this an iid model? Depends!

- 1. Typically  $\varepsilon_i$  are iid.
- 2. If  $X_i$  are random then "random design".
- 3. If  $X_i$  are iid, then linear model is iid model.
- 4. If  $X_i$  are deterministic, then not iid model.

$$\beta \mapsto ||Y - X\hat{\beta}||.$$

*Proof.* This is a continuation of point 3 in our theorem above.

We already introduced  $\Pi_U = X(X^TX)^{-1}X^T$  projection onto col space U of X. Thus  $I_n - \Pi_U$  is another projection operator, onto  $U^{\perp}$  (othrogonal complement),

$$U^{\perp} = \{ z \in \mathbb{R}^n \mid \langle z, X_k \rangle \forall k = 1, \dots, p \}.$$

Choose a basis  $e_1, \ldots e_{n-p}$ , orthonormal, of  $U^{\perp}$ , then

$$(I_n - \Pi_U)z = \Pi_{U^{\perp}}z = \sum_{n=1}^{n-p} \langle z, e_k \rangle e_k.$$

$$||Y - X\hat{\beta}|| = ||Y - \underbrace{X(X^T X)^{-1} X^T}_{\Pi_U} Y||^2$$
(13)

$$= ||(I_n - \Pi_n)Y||^2 \tag{14}$$

$$= ||(I_n - \Pi_n)(X\beta + \varepsilon)||^2 \tag{15}$$

$$=||(I_n - \Pi_n)\varepsilon||^2\tag{16}$$

$$=\sum_{i=1}^{n-p}\langle \varepsilon, e_i \rangle^2 \tag{17}$$

(18)

Hence,

$$E[||Y - X\hat{\beta}||^2] = \sum_{i=1}^{n-p} E[\langle \varepsilon, e_i \rangle^2] = n - p \implies E[\hat{\sigma}] = n - p$$

**Remark 6.** Recall the  $N(\mu, \sigma^2)$  model, where the MLE is

 $\hat{\mu} = \frac{1}{n} \sum_{i=1}^{n} X_i, \quad \hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \hat{\mu})^2.$ 

The unbiased estimator for  $\sigma^2$  was  $\frac{1}{n-1}\sum_{i=1}^n (X-i-\hat{\mu})^2$ . This is related to the n-p factor in point 3.

**Remark 7.** 1. If linearity is dropped, there exists better estimators than  $\hat{\beta}_{OLS}$ . For example a connstant estimator,  $\hat{\beta} = \beta^*$ 

2. The MSE of  $\hat{\beta}_{OLS}$  is

$$E[||\hat{\beta}_{OLS} - \beta||^2] = E\left[\sum_{i=1}^p \langle \hat{\beta}_{OLS} - \beta, \underbrace{e_i}_{ONBof\mathbb{R}^n} \rangle^2\right] = \sum_{i=1}^n Var_{\beta}(\langle \hat{\beta}_{OLS}, e_i \rangle) = \sum_{i=1}^n \sigma^2 ||X(X^TX)^{-1}e_k||^2$$

We say X satisfies orthogonal design if

$$X^T X = nI_n$$

"The different covariants are uncorrelated.="  $(X^TX)_{ij} = \langle X_i, X_j \rangle = n\delta_{ij}$  For orthogonal design,

$$E_{\beta}[||\hat{\beta}_{OLS} - \beta||^2] = \frac{1}{n^2} \sigma^2 \sum_{i=1}^n \underbrace{||xe_i||^2}_n = \frac{\sigma^2 P}{n}.$$

and this is equal to noise level times the number of parameters, divided by the number of data points.

**Theorem 3** (Bayes in Linear Models). Consider a linear model  $Y = X\beta + \varepsilon$ , and  $\varepsilon \sim N(0, \sigma^2 I_n)$  with  $\sigma > 0$  known and  $\beta \sim N(m, M)$  where  $m \in \mathbb{R}^p, M \in \mathbb{R}^{p \times p}$  positive semi definate. Then, the posterior  $\Pi(\beta|Y_iX)$  is given by

$$\begin{split} \Pi(\beta|Y,X) &= N(\mu_{past}, \Sigma_{past}) \ for \\ \mu_{past} &= \sigma_{past}(\sigma^{-2}X^Ty + M^{-1}m) \quad \Sigma_{past} = (\sigma^{-2}X^TX + M^{-2})^{-1} \end{split}$$

Remark 8.  $\Sigma_{past}$  independent of Y. For " $M^{-2} \to 0$ ", then " $\mu_{past} \to \hat{beta}_{OLS}$ "

Proof.

$$L(X,Y,\beta)\pi(\beta) \propto \exp\left(-\frac{1}{2\sigma^2}||Y-X\beta|| - \frac{1}{2}(\beta-m)^T M^{-1}(\beta-m)\right)$$

We want this to be proportional to  $\exp\left(-\frac{1}{2}(\beta - \mu_{\text{past}})^T \sigma_{\text{past}}^{-1}(\beta - \mu_{\text{past}})\right)$ . Now.

$$\exp\left(-\frac{1}{2}(\beta-\mu_{\text{past}})^T\sigma_{\text{past}}^{-1}(\beta-\mu_{\text{past}})\right) \propto \exp\left(-\frac{1}{\sigma^2}\beta^TX^TX\beta-\frac{1}{2}\beta^TM^{-1}\beta+\frac{1}{\sigma^2}\beta^TX^TY+\beta^TM^{-1}m\right)$$

and this is equal to

$$\exp\left(-\frac{1}{2}\beta^T\left(\frac{1}{\sigma^2}X^TX + M^{-1}\right)\beta + \beta^T(\frac{1}{\sigma^2}X^TY + M^{-1}m\right)$$

and this is

$$\propto \exp\left(-\frac{1}{2}(\beta - \mu_{\mathrm{past}})^T \sigma_{\mathrm{past}}^{-1}(\beta - \mu_{\mathrm{past}})\right)$$

Corollary 1. For  $\ell = ||\cdot||^2$ , the Bayes estimator is  $\hat{\beta}_{\Pi} = \mu_{past}$ 

**Proposition 1.** Consider the previous setting (from the theorem), with m=0, and  $M=\tau^2 I_p$  (centered, isotropic, normal prior). The,  $\mu_{past}=\hat{\beta}_{\Pi}$  minimizes

$$\beta \mapsto ||Y - X\beta||_{\mathbb{R}^n}^2 + \underbrace{\frac{\sigma^2}{\tau^2} ||\beta||_{\mathbb{R}^p}^2}_{"penalty" \ or "regularization"}$$

Proof.

### 8 Lecture 9

#### **Proof:**

Take gradient of  $\mathcal{J}(\boldsymbol{\beta})$  w.r.t.  $\boldsymbol{\beta}$ :

$$\nabla_{\boldsymbol{\beta}} \mathcal{J}(\boldsymbol{\beta}) = 2\boldsymbol{X}^{\top} (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) + \frac{2\sigma^2}{\tau^2} \boldsymbol{\beta}$$

Set = 0:

$$\Rightarrow \nabla_{\boldsymbol{\beta}} \mathcal{J}(\boldsymbol{\beta}) = 2(\boldsymbol{X}^{\top} \boldsymbol{X} + \frac{\sigma^{2}}{\tau^{2}} \boldsymbol{I}) \boldsymbol{\beta} - 2\boldsymbol{X}^{\top} \boldsymbol{Y} = 0$$
$$\Rightarrow \boldsymbol{\beta} = (\boldsymbol{X}^{\top} \boldsymbol{X} + \frac{\sigma^{2}}{\tau^{2}} \boldsymbol{I})^{-1} \boldsymbol{X}^{\top} \boldsymbol{Y}$$

Posterior mean:

$$egin{aligned} &\mu_{ ext{post}} = oldsymbol{\Sigma}_{ ext{post}}^{-1}(oldsymbol{X}^{ op}oldsymbol{Y} + oldsymbol{M}_0^{-1}oldsymbol{\mu}_0) \ &= (\sigma^{-2}oldsymbol{X}^{ op}oldsymbol{X} + au^{-2}oldsymbol{I}_p)^{-1}\sigma^{-2}oldsymbol{X}^{ op}oldsymbol{Y} \ &= (oldsymbol{X}^{ op}oldsymbol{X} + rac{\sigma^2}{ au^2}oldsymbol{I})^{-1}oldsymbol{X}^{ op}oldsymbol{Y} \end{aligned}$$

### Remark:

 $\boldsymbol{\beta}$  is defined even if rank( $\boldsymbol{X}$ ) < p, in particular even for n < p.

#### **Definition:**

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = \operatorname*{argmin}_{\boldsymbol{\beta} \in \mathbb{R}^p} \| \boldsymbol{Y} - \boldsymbol{X} \boldsymbol{\beta} \|^2 + \lambda \| \boldsymbol{\beta} \|^2,$$

is called a **Ridge Regression** estimator. Here,  $\lambda > 0$  is called a regularization parameter.  $\hat{\beta}_{\text{ridge}}$  is always uniquely defined.

For 
$$Y = X\beta + \varepsilon$$
, UM:

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = (\boldsymbol{X}^{\top} \boldsymbol{X} + \lambda \boldsymbol{I}_p)^{-1} \boldsymbol{X}^{\top} \boldsymbol{Y}.$$

Estimator independent of  $\sigma^2$ .

### Proposition:

MSE of  $\hat{\boldsymbol{\beta}}_{\text{ridge}}$ .

Consider a linear model with  $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 \boldsymbol{I}_n)$ ,  $\sigma^2 > 0$  known, and  $\boldsymbol{X}^\top \boldsymbol{X} = n \boldsymbol{I}_p$  (orthonormal design). Let  $\mathcal{J} := \langle \boldsymbol{\beta}, \boldsymbol{v} \rangle$  for  $\boldsymbol{v} \in \mathbb{R}^p$ , and:

$$\delta_{\text{ridge}} = \langle \hat{\boldsymbol{\beta}}_{\text{ridge}}, \boldsymbol{v} \rangle.$$

Then:

1.

$$\mathbb{E}_{\boldsymbol{\beta}}[(\delta_{\mathrm{ridge}} - \mathcal{J})^2] = (1 + \lambda)^{-2} \langle \boldsymbol{\beta}_v, \boldsymbol{v} \rangle^2 + \frac{\sigma^2}{n} \|\boldsymbol{v}\|^2 (1 + \lambda)^{-2}.$$

2.

$$\mathbb{E}_{\boldsymbol{\beta}}[\|\hat{\boldsymbol{\beta}}_{\text{ridge}} - \boldsymbol{\beta}\|^2] = (1+\lambda)^{-2}\|\boldsymbol{\beta}\|^2 + \frac{p\sigma^2}{n} \frac{1}{(1+\lambda)^2}.$$

We have:

$$egin{aligned} \hat{oldsymbol{eta}}_{ ext{ridge}} &= (oldsymbol{X}^ op oldsymbol{X} + \lambda oldsymbol{I}_p)^{-1} oldsymbol{X}^ op oldsymbol{Y}. \ &= rac{1}{(1+rac{\lambda}{p})} (oldsymbol{X}^ op oldsymbol{X} oldsymbol{Y} oldsymbol{X} oldsymbol{A} + oldsymbol{X}^ op oldsymbol{arepsilon}, \end{aligned}$$

where  $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 \boldsymbol{I}_n)$ .

$$= \frac{1}{1 + \frac{\lambda}{n}} (\boldsymbol{X}^{\top} \boldsymbol{X} \boldsymbol{\beta} + \boldsymbol{X}^{\top} \boldsymbol{\varepsilon}),$$
  
$$= \frac{1}{1 + \frac{\lambda}{n}} \boldsymbol{\beta} + \frac{1}{1 + \frac{\lambda}{n}} \boldsymbol{X}^{\top} \boldsymbol{\varepsilon}.$$

### **Bias-Variance Decomposition:**

$$\mathbb{E}\left[(\hat{\boldsymbol{\beta}}_{\mathrm{ridge}} - \mathcal{J})^{2}\right] = (\mathbb{E}[\hat{\boldsymbol{\beta}}_{\mathrm{ridge}}] - \mathcal{J})^{2} + \mathrm{Var}(\hat{\boldsymbol{\beta}}_{\mathrm{ridge}}).$$

$$= ((1 + \frac{\lambda}{n})^{-1} \langle \boldsymbol{\beta}, \boldsymbol{v} \rangle)^{2} + \frac{\lambda^{2}}{(1 + \lambda)^{2}} \mathrm{Var}(\boldsymbol{X}^{\top} \boldsymbol{\varepsilon}, \nu).$$

Observe:

$$(1+\frac{\lambda}{n})^{-1} = \frac{1}{(1+\frac{\lambda}{n})}.$$

Also:

$$\operatorname{Var}(\boldsymbol{X}^{\top}\boldsymbol{\varepsilon}, \boldsymbol{\nu}) = \boldsymbol{\nu}^{\top}\boldsymbol{X}\operatorname{Cov}(\boldsymbol{\varepsilon})\boldsymbol{X}^{\top}\boldsymbol{\nu} = \sigma^{2}\|\boldsymbol{\nu}\|^{2}.$$

### Corollary:

Under the same assumptions:

$$\mathbb{E}[\|\hat{\boldsymbol{\beta}}_{\text{ridge}} - \boldsymbol{\beta}\|^2] = \mathbb{E}\left[\sum_{k=1}^p (\langle \boldsymbol{\beta}, \boldsymbol{e}_k \rangle - \beta_k)^2\right].$$
$$= \frac{1}{(1 + \frac{\lambda}{n})^2} \|\boldsymbol{\beta}\|^2 + \frac{p\sigma^2}{n(1 + \frac{\lambda}{n})^2}.$$

### Remark:

For small  $\|\beta\|$ , Ridge  $\to$  OLS. The optimal choice of  $\lambda$  depends on  $\|\beta\|$ .

### 1.7 Confidence Sets & Tests in Linear Model:

The estimators we studied are independent of  $\sigma^2$ , but uncertainty quantification will depend on  $\sigma^2$ ! Assume  $\varepsilon \sim N(0, \sigma^2 \mathbf{I}_n)$  throughout.

#### Easy Case:

For  $\sigma^2 > 0$  known:

$$\hat{\boldsymbol{\beta}}_{\text{OLS}} \sim N(\boldsymbol{\beta}, (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}).$$

Indeed:

$$\operatorname{Cov}((\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{\varepsilon}) = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}.$$

And for  $\mathcal{J} = \langle \boldsymbol{\beta}, \boldsymbol{\nu} \rangle$ ,

$$\hat{\mathcal{J}} = \langle \hat{\boldsymbol{\beta}}_{\mathrm{OLS}}, \boldsymbol{\nu} \rangle \sim N(\mathcal{J}, \sigma^2 \boldsymbol{\nu}^\top (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{\nu}).$$

Then a 95% confidence set for  $\mathcal{J}$  is:

$$I_{95\%}(\mathcal{J}) = \left[ \hat{\mathcal{J}} \pm 1.96 \sqrt{\boldsymbol{\nu}^{\top} (\boldsymbol{X}^{\top} \boldsymbol{X})^{-1} \boldsymbol{\nu}} \right].$$

### Notes on t- and F-distributions:

**BUT:** Normally,  $\sigma^2$  is unknown. Replace  $\sigma$  by its estimator  $\hat{\sigma}$ . We need the t- and F-distributions.

#### **Definitions:**

**Definition** (t-distribution): The t-distribution with  $n \ge 1$  degrees of freedom on  $\mathbb{R}$  has density:

$$f_n(x) = C_n \left( 1 + \frac{x^2}{n} \right)^{-\frac{n+1}{2}},$$

where  $C_n$  is the normalizing constant.

**Note:** For n = 1:

$$f_1(x) = C_1 \frac{1}{1+x^2},$$

which corresponds to the Cauchy distribution.

**Definition (F-distribution):** The F-distribution with  $(m,n) \in \mathbb{N}^2$  degrees of freedom has density:

$$f_{m,n}(x) = C_{m,n} \frac{x^{\frac{m}{2}-1}}{(mx+n)^{\frac{m+n}{2}}}, \quad x \in (0,\infty),$$

where  $C_{m,n}$  is the normalizing constant.

#### Why is this useful?

**Lemma:** Let  $X_1, \ldots, X_n, Y_1, \ldots, Y_n$  be i.i.d.  $N(0, \Delta)$  random variables. Then:

1.

$$T_n := \frac{X_n}{\sqrt{\frac{1}{n} \sum_{i=1}^n Y_i^2}} \sim t_n.$$

2.

$$F_{m,n} := \frac{\frac{1}{m} \sum_{i=1}^{m} X_i^2}{\frac{1}{n} \sum_{j=1}^{n} Y_j^2} \sim F_{m,n}.$$

### Remarks:

- 1. The t-distribution arises when considering the "empirical mean" and "empirical variance."
- 2. For  $n \to \infty$ ,  $T_n \stackrel{d}{\to} N(0,1)$ .

### **Proof:**

(b) Observe:

$$T_n^2 = F_{1.n}$$
.

By a change of measure  $(y \mapsto y^2 \text{ in } (0, \infty))$ :

$$f_{F_{m,n}}(x) = f_{F_{m,n}}(x^2)2x, \quad x > 0.$$

Since t is symmetric around 0, we obtain for all  $x \in \mathbb{R}$ :

$$f_{T_n}(x) = f_{F_{m,n}}(x^2)|x| = C_n \left(1 + \frac{x^2}{n}\right)^{-\frac{n+1}{2}}.$$

It remains to show the claim for  $F_{m,n}$ .

 $\operatorname{Let}$ :

$$X = \sum_{i=1}^{m} X_i^2, \quad Y = \sum_{j=1}^{n} Y_j^2.$$

Then:

$$X \sim \chi_m^2, \quad Y \sim \chi_n^2,$$

where the density of  $\chi_m^2$  is:

$$f(x) \propto x^{m/2-1}e^{-x/2}, \quad x > 0.$$

#### **Derivation:**

Writing  $W = \frac{X}{Y}$ , we have:

$$\mathbb{P}\left(\frac{X}{Y} < z\right) = \int_0^\infty \int_0^{zy} 1 f_X(x) f_Y(y) dx dy.$$

Substituting x = wy, we get:

$$= \int_0^\infty \int_0^z 1 f_X(wy) f_Y(y) y \, dw \, dy$$
$$= \int_0^\infty f_X(zy) f_Y(y) y \, dy$$
$$\propto \int_0^\infty (zy)^{\frac{m}{2} - 1} y^{\frac{n}{2} - 1} e^{-(z+y)/2} \, dy.$$

#### Change of Variable:

Let  $a = \frac{z}{z+1}y$ , then:

$$\propto \int_0^\infty \left(\frac{z}{z+1}\right)^{\frac{m}{2}} a^{\frac{m}{2}-1} e^{-\frac{z}{z+1}a} \frac{1}{z+1} da$$
$$\propto z^{\frac{m}{2}-1} (z+1)^{-\frac{m+n}{2}} \int_0^\infty a^{\frac{m}{2}-1} e^{-a} da.$$

It follows:

$$\frac{\partial}{\partial z} \mathbb{P}\left(\frac{X}{Y} < z\right) = f_{X,Y}(z) = \int_0^\infty f_X(zy) f_Y(y) \frac{1}{y} dy$$
$$\propto z^{\frac{m}{2} - 1} (z+1)^{-\frac{m+n}{2}}.$$

#### Change of Variable:

Let  $F = \frac{X}{Y}$ , given  $f_F(z) = \frac{m}{n} f_{X,Y}\left(\frac{m}{n}z\right) = f_{m,n}(z)$ .

#### 9 Lecture 10

$$\begin{split} t\text{-distribution} & \cdot t_n(x) \propto \left(\frac{n^2}{n}+1\right)^{-(n+1)/2} \\ & F \cdot \cdot f_{m,n}(x) \propto \frac{x^{m/2-1}}{(n+mx)^{(m+n)/2}} \\ & \text{In the linear model } Y = X\beta + \varepsilon, \, \varepsilon \sim N(0,\sigma^2 I_n), \end{split}$$

$$F - f_{m,n}(x) \propto \frac{x^{m/2-1}}{(n+mx)^{(m+n)/2}}$$

$$\hat{\beta} = (X^T X)^{-1} X^T Y \sim N(0, \sigma^2 A)$$

where

$$\sigma^2 = \hat{\sigma}^2 = \left| \left| \frac{||Y - X\beta|}{n - p} \sim \sigma^2 \frac{\chi^2(n - p)}{n - p} \right| \right|$$

We now have

$$t_n = \frac{N(0,1)}{\chi^2(n)n}$$
  $f_{m,n} = \frac{n\chi^2(m)}{m\chi^2(n)}$ 

**Lemma 2.** Let  $\xi \sim N(0, I_n)$ , a ramdom variable in  $\mathbb{R}^n$ , and let  $R \in \mathbb{R}^{n \times n}$  be an orthogonal projection  $(R = R^2, R = R^T)$ , with  $rank(R) = r \le n$ .

- 1.  $\xi^T R \xi = ||R\xi||^2 \sim \chi^2(r)$ .
- 2. If  $B \in \mathbb{R}^{p \times n}$  is such that BR = 0, then  $B\xi$  is independent from  $R\xi$
- 3. If  $S \in \mathbb{R}^{n \times n}$  is another orthogonal projection,  $rank(S) = s \leq n$  and RS = 0, then

$$\frac{s}{r} \frac{\xi^T R \xi}{\xi^T S \xi} \sim F(r, s)$$

1. Since R is an othrogonal projection, there exists an orthogonal matrix  $T^T = T^{-1}$  such that Proof.

$$R = T \begin{pmatrix} I_r & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} T^T = T D_r T^T.$$

Then we have  $T^T \sim N(0, T^T T) = N(0, I_n)$ .

$$\xi^T R \xi = \xi^T (T D_r T^T) \xi = (T^T \xi)^T D_r T^T \xi = \sum_{i=1}^n (T^T \xi)_i^2 \sim \chi^2(r).$$

2. Let  $A_1 = B\xi$ ,  $A_2 = R\xi$ , then

$$Cov(A_1, A_2) = Cov(B\xi, R\xi) = BCov(\xi, \xi)R^T = BR^T = BR = 0$$

3. By (2), we know  $S\xi$  and  $R\xi$  are independent. By (1),  $\xi^T S\xi \sim \chi^2(s)$ ,  $\xi R\xi \sim \chi^2(r)$ . The claim follows from the definition of F(r, s). 

**Theorem 4.** Linear Model Confidence Sets -unknown  $\sigma^2$  Assume regular linear model,  $Y = X\beta + \varepsilon$ ,  $rank(X) = p \le n, \ \varepsilon \sim N(0, \sigma^2 I_n). \ Let \ \alpha \in (0, 1)$ 

- $1. \ \ Let \ q_{F_{p,n-p},1-\alpha} \ be \ the \ 1-\alpha \ quantile \ of \ F_{p,n-p} \ distribution. \ \ Then \ C(Y,X) = \left\{\beta \in \mathbb{R}^p \ | \ \frac{||X(\beta \hat{\beta}_{OLS})||^2}{p\hat{\sigma}^2} \leq q_{F_{p,n-p},1-\alpha} \right\}$ is a level  $1 - \alpha$  confidence set.
- 2. Let  $\alpha = \langle \beta, v \rangle$ , for some  $v \in \mathbb{R}^p$ . Then a  $1 \alpha$  confidence set is

$$C = C(Y, X) = \left\{ \alpha \in \mathbb{R} \mid \left| \frac{\alpha - \hat{\alpha}}{\hat{\sigma} \sqrt{v^T (X^T X)^{-1} v}} \right| < q \right\}$$

where  $\hat{\alpha} = \langle \hat{\beta}_{OLS}, v \rangle$  and q is the  $1 - \alpha/2$  quantile of  $t_n$ .

*Proof.* 1. We know  $X\hat{\beta}_{OLS} = \Pi_U Y = \Pi_U X\beta + \Pi_U \varepsilon = X\beta + \Pi_U \varepsilon$  Moreover,

$$\hat{\sigma}^2 = \frac{||X(\beta - \hat{\beta}_{OLS})||^2}{n - p} = \frac{(||I_n - \Pi_U)Y||^2}{n - p} = \frac{||\Pi_{U^{\perp}}Y||^2}{n - p} = frac||\Pi_{U^{\perp}}\varepsilon||^2 n - p$$

This implies

$$\frac{||X\beta - X\hat{\beta}_{OLS}|}{p\hat{\sigma}^2} = \frac{|n-p|||\Pi_U\varepsilon||^2}{p||\Pi_{U^\perp}\varepsilon||^2} \sim \frac{(n-p)\sigma^2\chi^2(p)}{p\sigma^2\chi^2(n-p)} \sim F(p,n-p).$$

2. We know

$$\hat{\sigma} = \langle \hat{\beta}_{OLS}, v \rangle = v^T \hat{\beta}_{OLS} \sim v^T N(\beta, (X^T X)^{-1} \sigma^2) = N(\alpha, v^T (X^T X)^{-1} v \sigma^2)$$

And this implies

$$\frac{\alpha - \hat{\alpha}}{\sigma \sqrt{v^T (X^T X)^{-1} v}} \sim N(0, 1).$$

Finally, also, as in (1),  $\hat{\sigma}^2 \sim \sigma^2 \chi^2(n-p)$ . This implies

$$\frac{\alpha - \hat{\alpha}}{\hat{\sigma}\sqrt{v^T(X^TX)^{-1}v}} \sim t_{n-p}.$$

9.1 The t- and F-test

**Remark 9** (Method (t-test)). In a regular linear model with  $\varepsilon \sim N(0, \sigma I_n)$ , consider  $H_0: \gamma = \gamma_0$  vs  $H_1 \gamma \neq \gamma_0$  ( $\gamma = \langle \beta, v \rangle$ ). The two sided t-test is

$$\varphi_{\alpha_0}(Y, X) = \mathbf{1}(\{|T_{\alpha_0, n-p}(Y, X)| > q\}),$$

where

$$T_{\alpha_0, n-p} = \frac{\alpha_0 - \hat{\alpha}}{\hat{\sigma} \sqrt{v^T (X^T X)^{-1} v}}$$

and q is the  $1 - \alpha/2$ -quantile of  $t_{n-p}$ .

**Remark 10** (Method (F-test)). Same setting as before for t-test,  $H_0: \beta = \beta_0$  vs  $H_1\beta \neq \beta_0$  since  $\beta_0 \in \mathbb{R}^p$ . Then the F-test is

$$\varphi_{\beta_0}(Y,X) = \mathbb{1}(|F_{\beta_0,n-p}(Y,X)| > q)$$

where

$$F_{\beta_0, n-p}(Y, X) = \frac{||X(\beta - \hat{\beta}_{OLS})||^2}{p\hat{\sigma}^2}$$

and  $q = (1 - \alpha)$ -quantile of  $F_{p,n-p}$ .

### 9.2 General linear hypothesis testing problems

**Definition 9.** A linear hypothesis testomng pb. is of the form  $H_0: K\beta = d$  vs  $H_1: K\beta \neq d$ , where  $K \in \mathbb{R}^{r \times p}$  with  $rank(K) = r \leq p$ ,  $d \in \mathbb{R}^p$ . In other words "r linear constrations on  $\beta$ " K os called the "contrast matrix"

**Theorem 5.** Assume regular linear model, with  $\varepsilon \sim N(0, \sigma^2 I_n)$ , and consider  $H_0: K\beta = d$  vs.  $K\beta \neq d$ . Defin residual sum of squares as  $RSS = ||Y - X\beta_{OLS}||^2$  and  $RSS_{H_0} = ||Y - X\beta_{H_0}||^2$  and  $\hat{\beta}_{H_0}$  over  $\{\beta: K\beta = d\}$ .

Proof. 1.

$$\hat{\beta}_{H_0} = \hat{\beta}_{OLS} - (X^T X)^{-1} K^T (K(X^T X)^{-1} K^T)^{-1} (K \hat{\beta}_{OLS} - d)$$

2. 
$$RSS_{H_0} - RSS = (K\hat{\beta}_{OLS} - d)(K(X^TX)^{-1}K^T)^{-1}(K\hat{\beta}_{OLS} - d), \quad \frac{RSS_{H_0} - RSS}{\sigma^2} \sim \chi^2(r)$$

3. Define

$$F = \frac{n-p}{r} = \frac{RSS_{H_0} - RSS}{RSS} = \frac{RSS_{H_0} - RSS}{r\hat{\sigma}^2} \sim F_{r,n-p}$$

under  $H_0$ .

# 10 Lecture 11

#### Theorem:

Assume regular LM,  $\varepsilon \sim N(0, \sigma^2 I_n)$ , and consider:

$$H_0: K\beta = d$$
 vs.  $H_1: K\beta \neq d$ 

Define:

$$RSS = ||Y - X\beta||^2$$
,  $RSS_{H_0} = ||Y - X\beta_{H_0}||^2$ 

where  $\beta_{H_0}$  is the OLS estimator over  $K\beta = d$ :

$$\beta_{H_0} = \hat{\beta} - (X^{\top}X)^{-1}K^{\top} (K(X^{\top}X)^{-1}K^{\top})^{-1} (K\hat{\beta} - d)$$

1.

$$RSS_{H_0} - RSS = ||X(\beta_{H_0} - \hat{\beta})||^2 = (K\hat{\beta} - d)^{\top} (K(X^{\top}X)^{-1}K^{\top})^{-1} (K\hat{\beta} - d)$$

2. Under  $H_0$ :

$$RSS_{H_0} \sim \chi^2(n)$$

3. Define:

$$F = \frac{1}{p} \frac{RSS_{H_0} - RSS}{RSS/n} = \frac{RSS_{H_0} - RSS}{c \cdot RSS}$$

Under  $H_0$ :

$$F \sim F_{n-p}$$

#### **Proof:**

1. To show  $K\hat{\beta}_{H_0} = d$ , note that  $\beta_{H_0}$  is the minimizer. Observe:

$$K\beta_{H_0} - K\beta = K(X^{\top}X)^{-1}K^{\top} (K(X^{\top}X)^{-1}K^{\top})^{-1} (K\beta - d) - K\beta - (K\beta - d) = d$$

Second part: Let  $Y \in \mathbb{R}^n$ ,  $K\beta = d$ . By Pythagoras:

$$||Y - X\hat{\beta}||^2 = ||Y - X\beta_{H_0}||^2 + ||X(\beta - \beta_{H_0})||^2$$

where:

$$A = \left( X(\hat{\beta} - \beta_{H_0}) \right)^{\top} X \beta_{H_0} - Y = (K\hat{\beta} - d)^{\top} \left( K(X^{\top}X)^{-1} K^{\top} \right)^{-1} K(X^{\top}X)^{-1} (X^{\top}Y)$$

This implies:

$$(K\hat{\beta} - d)^{\top} \left( K(X^{\top}X)^{-1}K^{\top} \right)^{-1} (K\hat{\beta} - d) = 0$$

Overall:

$$||Y - X\beta_{H_0}||^2 = ||Y - X\hat{\beta}||^2 + ||X(\hat{\beta} - \beta_{H_0})||^2 \ge 0$$

### Continuation:

2) Under  $H_0$ :

$$RSS_{H_0} - RSS = ||Y - X\beta_{H_0}||^2 - ||Y - X\hat{\beta}||^2$$
$$= ||X(\hat{\beta} - \beta_{H_0})||^2 = (K\hat{\beta} - d)^{\top} (K(X^{\top}X)^{-1}K^{\top})^{-1} (K\hat{\beta} - d)$$

Let  $Z = K\hat{\beta} - d$ . Then:

$$\mathbb{E}[Z] = \mathbb{E}[K\hat{\beta} - d] = K\mathbb{E}[\hat{\beta}] - d = K(X^{\top}X)^{-1}X^{\top}Y - d$$

(Substitute  $K\beta = d$  into the expectation)

$$\operatorname{Var}(Z) = K \operatorname{Var}(\hat{\beta}) K^{\top} = \sigma^2 K (X^{\top} X)^{-1} K^{\top}$$

Thus:

$$Z \sim \mathcal{N}(0, \sigma^2 K(X^\top X)^{-1} K^\top)$$

Finally:

$$RSS_{H_0} - RSS = ||X(\hat{\beta} - \beta_{H_0})||^2 = Z^{\top} (\sigma^2 K(X^{\top} X)^{-1} K^{\top})^{-1} Z$$

$$\sim \chi^2(p)$$

$$RSS \sim \sigma^2 \chi^2(n-p), \quad RSS_{H_0} \sim \sigma^2 \chi^2(n).$$

3) We know:

$$\frac{RSS_{H_0} - RSS}{\sigma^2} \sim \chi^2(p), \quad \frac{RSS}{\sigma^2} \sim \chi^2(n-p)$$

To show independence: We have:

$$RSS_{H_0} \perp Y$$
 while  $RSS_{H_0} - RSS$  only depends on  $\hat{\beta}$ .

(Since  $\hat{\beta} \propto X^{\top}Y$  and  $T_n = 0$  by the lemma from last time, independence follows.)

# ANOVA (Analysis of Variance)

**Motivation:** We have data from k different groups. Are the means equal?

**Definition:** ANOVA We are given data:

$$Y_{ij} = \mu_i + \varepsilon_{ij}, \quad i = 1, \dots, k, \quad j = 1, \dots, n_i$$

Assume:

$$\varepsilon_{ij} \sim \mathcal{N}(0, \sigma^2)$$

# ANOVA (Analysis of Variance)

**Index:** i = 1, ..., k is called the factor.

The model is a  $factor\ model$  with 1 categorical variable.

 $n = \sum_{i=1}^{k} n_i$  is the total sample size.

The model is balanced (design) if  $n_1 = n_2 = \ldots = n_k$ .

Remark: ANOVA is a linear model:

$$\begin{pmatrix} Y_{1,1} \\ Y_{1,2} \\ \vdots \\ Y_{k,n_k} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{n_1} & 0 \\ 0 & \mathbf{1}_{n_k} \end{pmatrix} \begin{pmatrix} \mu_1 \\ \mu_k \end{pmatrix} + \varepsilon$$

### Hypothesis Testing:

$$H_0: \mu_1 = \ldots = \mu_k$$
 vs.  $H_a: \exists i, j \text{ with } \mu_i \neq \mu_j$ 

Basic Idea: Compare variation within groups vs. variation across groups.

Theorem (Decomposition of RSS): Define the group means:

$$\bar{Y}_{i.} = \frac{1}{n_i} \sum_{j=1}^{n_i} Y_{ij}, \quad i = 1, \dots, k$$

and the overall mean:

$$\bar{Y}_{\cdot \cdot} = \frac{1}{n} \sum_{i,j} Y_{ij}.$$

Furthermore, let:

$$SSB = \sum_{i=1}^{k} n_i (\bar{Y}_{i.} - \bar{Y}_{..})^2 \quad \text{(Sum of squares between groups)},$$

$$SSW = \sum_{i=1}^{k} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i.})^2 \quad \text{(Sum of squares within groups)}.$$

Then:

$$SST = \sum_{i=1}^{k} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{..})^2 = SSB + SSW,$$

where SST is the total sum of squares.

**Proof:** 

$$SST = \sum_{i=1}^{k} \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i.} + \bar{Y}_{i.} - \bar{Y}_{..})^2$$

$$= \sum_{i,j} (Y_{ij} - \bar{Y}_{i.})^2 + (\bar{Y}_{i.} - \bar{Y}_{..})^2 + 2(Y_{ij} - \bar{Y}_{i.})(\bar{Y}_{i.} - \bar{Y}_{..})$$

$$= SSB + SSW + C,$$

where:

$$C = \sum_{i=1}^{k} (\bar{Y}_{i.} - \bar{Y}_{..}) \sum_{j=1}^{n_i} (Y_{ij} - \bar{Y}_{i.}).$$

By construction:

$$\sum_{i=1}^{n_i} (Y_{ij} - \bar{Y}_{i.}) = 0 \quad \text{for each } i,$$

so:

$$C = 0.$$

### Theorem:

1. The least square estimator for  $\mu = (\mu_1, \dots, \mu_k) \in \mathbb{R}^k$  is:

$$\hat{\mu} = (\bar{Y}_{1.}, \dots, \bar{Y}_{k.})^{\top}.$$

2. Under  $H_0$ :

$$\frac{SSW}{\sigma^2} \sim \chi^2(n-k).$$

3. Under  $H_0$ :

$$\frac{SSB}{\sigma^2} \sim \chi^2(k-1).$$

4. SSW and SSB are independent under  $H_0$ , and:

$$F = \frac{\frac{n-k}{k-1}SSB}{SSW} \stackrel{H_0}{\sim} F(k-1, n-k).$$

### 11 Lecture 12

ANOVA

linear model, factor/category, F-test for equality of means,  $Y_{i,j} = \mu_i + \varepsilon_{ij}$  for i = 1, ..., k and j = 1, ..., k.

First a note,  $X^TX = ||X||_{\mathbb{R}^n}^2$ 

**Theorem 6.** In the ANOVA model with  $\varepsilon_{ij} \sim N(0, \sigma^2)$ :

1. The OLS estimate is

$$\hat{\mu} = (\bar{y}_{1,.}, \dots \bar{y}_{k,.}) \quad Recall \ \bar{y}_{i,.} = \frac{1}{n_i} \sum_{j=1}^{n_i} y_{ij}$$

2.

$$\frac{SSW}{\sigma^2} = \frac{1}{\sigma^2} \sum_{i} \sum_{j} (y_{ij} - \bar{y}_{i,\cdot})^2 \sim \chi^2(n-k)$$

- 3. Under  $H_0$ :  $\mu_0 = \mu_1 = \dots = \mu_k$ ,  $\frac{SSB}{\sigma^2} = \frac{1}{\sigma^2} \sum_i n_i(\bar{y}_{i,\cdot} \bar{y}) \sim \chi^2(k-1)$
- 4. SSW and SSB are independent and under  $H_0$ ,

$$\frac{n-k}{k-1} \frac{SSB}{SSW} \sim F(k-1, n-k)$$

*Proof.* (a) We have  $\hat{\mu} = (X^T X)^{-1} X^T Y$ , with

$$(X^T X)^{-1} = \begin{pmatrix} \frac{1}{n_1} & \dots & 0\\ 0 & \dots & 0\\ 0 & \dots & \frac{1}{n_k} \end{pmatrix}$$

and this implies that

$$\hat{\mu} = \begin{pmatrix} \frac{1}{n_1} & \dots & 0 \\ 0 & \dots & 0 \\ 0 & \dots & \frac{1}{n_k} \end{pmatrix} \begin{pmatrix} \begin{bmatrix} 1 & \dots & 0 \\ 0 & \dots & 0 \\ 0 & \dots & \end{bmatrix} Y = \begin{pmatrix} \frac{1}{n_1} & \dots & 0 \\ 0 & \dots & 0 \\ 0 & \dots & \frac{1}{n_k} \end{pmatrix} \begin{pmatrix} \sum_j Y_{1,j} \\ \vdots \\ \sum_j Y_{k,j} \end{pmatrix} = \begin{pmatrix} \bar{Y_{1,j}} \\ \vdots \\ \bar{Y_{k,j}} \end{pmatrix}$$

- (b)  $SSW = ||Y X\hat{\mu}||_{\mathbb{R}^n}^2 = \sum_i \sum_j (y_j y_{i,\cdot})^2 = RSS \implies \frac{SSW}{\sigma^2} \sim \chi^2(n k).$
- (c) We know that SSW = RSS and we know that  $SSW + SSB = SST = \sum_{ij} (y_{ij} \bar{y}_{i,\cdot})^2$ . We also know  $\frac{RSS_{H_0} RSS}{\sigma^2} \sim \chi^2(k-1)$  from before, it suffices to show  $SST = RSS_{H_0}$ ,

$$RSS_{H_0} = \min_{\mu \in \mathbb{R}} ||Y - \mu||_{\mathbb{R}^2}^2 = ||Y - \bar{Y}_{\cdot \cdot \cdot \mathbb{R}^n}|^2 = SST.$$

(d) Follows from general lin hypotheses testing theorem, Theorem 2.2.30 in Methoden der Statistik book.

11.1 Exponential Families

General  $Model(P_{\theta} : \theta \in \Theta) \supseteq Exp.$  families  $\supseteq Linear Model$ 

Regularity Assumptions:

Let  $(P_{\theta}: \theta \in \Theta)$  be a statistical model

- 1. Dominated, there exists  $\mu$  such that  $P_{\theta} \ll \mu$  for all  $\theta \in \Theta$
- 2.  $\Theta \in \mathbb{R}^p$  is an open set  $p \geq 1$ .
- 3. Likelihood  $p_{\theta}(x) > 0$  for all  $\theta \in \Theta, x \in X$ , in particular  $\log p_{\theta}(x)$  is well defined.

**Definition 10.** Score The score vector is  $U_{\theta}(x) = \nabla_{\theta} \log p_{\theta}(x) = \begin{pmatrix} \frac{\partial}{\partial \theta_1} \log p_{\theta}(x) \\ \vdots \\ \frac{\partial}{\partial \theta_p} \log p_{\theta}(x) \end{pmatrix}$  whenever it exists

**Definition 11.** Fisher Information For  $\theta \in \Theta$ , the FI, whenever it exists, is  $I(\theta) = E(U_{\theta}(x)U_{\theta}(x)^T) \in \mathbb{R}^{p \times p}$ 

More Regularity Assumptions

- 1.  $p_{\theta}(x)$  is twice differentiable, in particular,  $U_{\theta}(x)$  is well defined.
- 2.  $E_{\theta}[||U_{\theta}(x)||_{\mathbb{R}^p}^2] < \infty$  for all  $\theta \in \Theta$ , so  $I(\theta)$  is well defined.

3.

$$\int h(x)\nabla_{\theta}p_{\theta}(x)\mu(dx) = \nabla_{\theta} \int h(x)$$

for relevant h(x).

**Lemma 3.**  $(P_{\theta} \in \Theta)$  regular model (as above),

1. 
$$E_{\theta}(U_{\theta}(x)) = 0$$

2. 
$$I(\theta) = Cov(U_{\theta})$$

Proof.

$$E_{\theta}[U_{\theta}(x)] = \int_{X} \frac{\nabla_{\theta} p_{\theta}(x)}{p_{\theta}(x)} p_{\theta}(x) d\mu(x) = \int_{X} \nabla_{\theta} p_{\theta}(x) d\mu(x) = \nabla_{\theta}[\theta \mapsto 1] = 0$$

**Definition 12.** Uniform minimum variance unbiased estimators (UMVUE) Let  $p(\theta) \in \mathbb{R}$  be some quantity of interest,  $T: X \to \mathbb{R}$  is a UMVUE if  $E_{\theta}[T(x)] = g(\theta)$  and for all other unbiased estimators,  $S: X \to \mathbb{R}$ ,  $Var_{\theta}(T) \leq Var_{\theta}(S)$  for all  $\theta \in \Theta$ .

**Remark 11.** 1. UMUVE are the best possible among unbiased estimators.

2. Compare to Gauss Markov,  $\hat{\beta}_{OLS}$  is UMVUE

3.

$$E_{\theta}[||T(x) - \rho(\theta)||^2] = Bias^2 + Var(T) = Var(T) \le E_{\theta}[|S(x) - \rho(\theta)|^2]$$

**Theorem 7.** Let  $(P_{\theta} \mid \theta \in \theta)$  be regular. Let  $\rho \colon \Theta \to \mathbb{R}$  continuous differentiable, then for any unbiased estimator T of S,  $E_{\theta}[T] = S(\theta)$ ,

$$Var_{\theta} \ge \nabla_{\theta} \rho(\theta)^T I(\theta)^{-1} \nabla_{\theta} \rho(\theta)$$

Remark 12. If  $\Theta = \mathbb{R}$ ,  $\rho(\theta) = \theta$ ,  $Var_{\theta}(T) \geq I(\theta)^{-1}$ 

*Proof.* Let us assume  $\Theta \subseteq \mathbb{R}$ ,

$$Cov_{\theta}(U_{\theta}, T) = E_{\theta}[U_{\theta}T] - E_{\theta}[U_{\theta}]E_{\theta}[T] = E_{\theta}[U_{\theta}T]$$

More over, by Cauchy Swartz,

$$\operatorname{Cov}_{\theta}(U_{\theta}T) \leq \operatorname{Var}_{\theta}(U_{\theta})^{1/2} \operatorname{Var}_{\theta}(T)^{1/2} I(\theta)^{1/2} \operatorname{Var}_{\theta}(T)^{1/2}$$

But then

$$E_{\theta}[U_{\theta}T] = \int_{X} \nabla_{\theta} \log p_{\theta}(x) T(x) p_{\theta}(x) d\mu(x)$$

$$= \int_{X} T(x) \nabla_{\theta} p_{\theta}(x) d\mu(x)$$

$$= \nabla_{\theta} \int \int_{X} T(x) p_{\theta}(x) d\mu(x)$$

$$= E_{\theta}[T] \qquad = \rho'(\theta)$$

Thus,  $\operatorname{Var}_{\theta}(T) \geq I(\theta)^{-1} \rho'(\theta)^2$ 

Another regularity condition,  $I(\theta)$  is invertible.

#### Lecture 13

### Regular Stat Model

- $\Theta \subset \mathbb{R}^p$  open
- $p_{\vartheta}(x) > 0$  for all  $\vartheta \in \Theta$ ,  $x \in \mathcal{X}$  and  $p_{\vartheta}$  is continuously differentiable.

$$I(\vartheta) = \mathbb{E}_{\vartheta} \left[ \nabla_{\vartheta} \log p_{\vartheta}(x) \ \nabla_{\vartheta} \log p_{\vartheta}(x)^T \right]$$

exists  $\forall \vartheta \in \Theta$ , and  $I(\vartheta)$  is positive definite ( $\Rightarrow I(\vartheta)^{-1}$  exists). Interchange  $\nabla_{\vartheta}$  and  $\int$ . 

#### Theorem

 $(p_{\vartheta}, \vartheta \in \Theta \text{ regular.})$  Let  $g: \Theta \to \mathbb{R}$  be continuously differentiable. Let  $T: \mathcal{X} \to \mathbb{R}$  be an unbiased estimator,  $\mathbb{E}_{\vartheta}[T] = g(\vartheta) \ \forall \vartheta \in \Theta$ . Then

$$\operatorname{Var}_{\vartheta}(T) \ge (g'(\vartheta))^T I(\vartheta)^{-1} g'(\vartheta) \quad \forall \vartheta \in \Theta.$$

#### Cramér-Rao / Information Inequality

#### Score Vector

$$U_{\vartheta}(x) = \nabla_{\vartheta} \log p_{\vartheta}(x)$$

#### **Fisher Information Matrix**

#### Remarks

- If  $I(\vartheta)$  is large, better estimation seems possible: "more information contained in the data."
- Another interpretation.

#### Derivation

Let  $\Theta \subseteq \mathbb{R}$ . Suppose  $p_{\vartheta}$  is twice differentiable in  $\vartheta$ :

$$(\log p_{\vartheta}(x))' = \frac{p_{\vartheta}'(x)}{p_{\vartheta}(x)}$$

$$(\log p_{\vartheta}(x))'' = \frac{p_{\vartheta}''(x)p_{\vartheta}(x) - (p_{\vartheta}'(x))^{2}}{p_{\vartheta}(x)^{2}}$$

$$\mathbb{E}_{\vartheta} \left[ (\log p_{\vartheta}(x))' \right] = \int_{x} \frac{p_{\vartheta}'(x)}{p_{\vartheta}(x)} p_{\vartheta}(x) dx = \int_{x} p_{\vartheta}'(x) dx = \frac{d}{d\vartheta} \int_{x} p_{\vartheta}(x) dx = 0.$$

Thus.

$$\mathbb{E}_{\vartheta}\left[\left(\log p_{\vartheta}(x)\right)^{2}\right] = -\mathbb{E}_{\vartheta}\left[\left(\log p_{\vartheta}(x)\right)^{"}\right] = -\mathbb{E}_{\vartheta}\left[U_{\vartheta}(x)^{2}\right] = -I(\vartheta).$$

**Theorem 8.** Let  $(P_{\theta}, \theta \in \Theta)$  be a regular model,  $\Theta \subseteq \mathbb{R}$  and let  $\rho : \Theta \to \mathbb{R}$ , be a continuous differentiable function, an unbiased estimator T,  $E_{\theta}[T] = \rho(\theta)$  attains equality in the CR-bound iff and only if

$$T(x) = \rho(\theta) + \rho'(\theta)I(\theta)^{-1}U_{\theta}(x)$$

almost surely for all  $\theta \in \Theta$ 

*Proof.* Define  $v(\theta) = \rho'(\theta)I(\theta)^{-1}$ , then let T as above,

$$0 \le \operatorname{var}(T - v(\theta)U_{\theta}) = \operatorname{var}(T) + v(\theta)^{2} E_{\theta}[U_{\theta}^{2}] - 2v(\theta) \underbrace{\operatorname{Cov}_{\theta}(T, U_{\theta})}_{\rho'(\theta)}$$

$$= \operatorname{Var} - \rho'(\theta)^2 I(\theta)^{-1} = 0$$

This implies

$$T - v(\theta)U_{\theta} = Constant$$

Since T is unbiased we have  $E_{\theta}[T] = \rho(\theta)$  so,  $T = \rho(\theta) + v(\theta)U_{\theta}$  almost surely. This shows  $\Longrightarrow$ ,  $\Longleftrightarrow$  is a straightforward computation.

**Remark 13.** 1. T(x) is not always a measureable feature of x in the equation above.

2. If T attains the CR-bound, we say that T is the Cramer-Rao coefficent

**Corollary 2.** Assume previous scaling and assume  $\rho(\theta) \neq 0$  for all  $\theta \in \Theta$  then the likelihood can be written in the form

$$p_{\theta}(x) = c(x) \exp(n(\theta)T(x) - \Psi(\theta))$$

where  $n:\theta\to\mathbb{R}$ , such that  $n'(\theta)=\frac{I(\theta)}{\rho'(\theta)}$  and c(x) and  $\Psi(\theta)$  are invertible.

*Proof.* By the above equation, from the last theorem, we have

$$T(x) = \rho(\theta) + \rho(\theta)I^{-1}(\theta)(\log p_{\theta}(x))'$$

and this implies

$$(T(x) - \rho(\theta))\frac{I(\theta)}{\rho(\theta)} = (\log p_{\theta}(x))'$$

and then we get

$$T(x) \int_{\theta_0}^{\theta} \frac{I(\theta)}{\rho(\theta)} dt + \Psi(\theta) = \log(p_{\theta}(\theta)) + constant$$

which implies

$$p_{\theta}(x) = \exp(constant(x)) = \exp(n(\theta)T(x) - \Psi(\theta))$$

**Definition 13.** Exponential Families A regular model  $(P_{\theta} : \theta \in \Theta)$  is called the k-parameter Exponential family  $(k \ge 1)$  if there exists measurable functions

- 1.  $n:\Theta\to\mathbb{R}^k$
- 2.  $T: C \to \mathbb{R}^k$
- 3.  $c: X \to [0, \infty)$

such that

$$p_{\theta}(x) = \frac{dP_{\theta}}{d\mu}(x) = c(x) \exp(\langle n(\theta)T(x)\rangle_{\mathbb{R}^k} - \Psi(\theta))$$

for all  $\theta$ , x where

$$\Psi(\theta) = \log \left( \int_X c(x) \exp\left( \langle n(\theta) T(x) \rangle_{\mathbb{R}^k} \right) d\mu(x) \right)$$

**Remark 14.** 1. Key features is the factorization of  $\langle n(\theta)T(x)\rangle_{\mathbb{R}^k}$ .

2. Exponential forms are motivated by finding general models in which CR-efficent procedures exists.

Example 2. Binomial  $p_{\theta} = Bin(n, \theta)$ 

$$p_{\theta}(k) = \binom{n}{k} \theta^{k} (1 - \theta)^{n-k}$$

$$= \binom{n}{k} \exp(k \log \theta + (n+k) \log(1 - \theta))$$

$$= \underbrace{\binom{n}{k}}_{\ell} c(k) \exp(\underbrace{k}_{T(k)} \underbrace{\log \frac{\theta}{n - \theta}}_{n(\theta)} + \underbrace{n \log(n - k)}_{\Psi(\theta)})$$

Example 3. Normal  $\theta = (\mu, \sigma^2) \in \mathbb{R} \times (0, \infty), p_{\theta} = N(\mu, \sigma^2)$ 

$$p_{\mu,\sigma^2} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2 - 2x\mu - \mu^2}{2\sigma^2}\right)$$

Take  $T(x) = {x^2 \choose x}$ ,  $n(\theta) = {-\frac{1}{2\sigma^2} \choose \frac{\mu}{\sigma^2}}$  for k = 2, then

$$p_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\langle n(\theta), T(x) \rangle - \frac{\mu^2}{2\sigma^2}\right)$$

Example 4. Poisson  $X = \{0, 1, ...\}, p_{\theta} = Poisson(\theta), \theta > 0,$ 

$$p_{\theta}(k) = e^{-\theta} \frac{\theta^k}{k!} = \exp(-\theta + k \log \theta) \frac{1}{k!}$$

Take  $n(v) = \log \theta$ , T(k) = k,  $c(k) = \frac{1}{k!}$ ,  $\Psi(\theta) = \theta$ .

**Definition 14.** Natural Exponential Family Define

$$\Xi = \left\{ n \in \mathbb{R}^k \mid \int_X c(x) \exp\left(\langle n(\theta) T(x) \rangle_{\mathbb{R}^k}\right) d\mu(x) < \infty \right\}$$

A model  $(P_n \mid n \in \theta)$  is called an natural Exponential family if  $\Theta = \Xi$ ,

$$\frac{dP_n}{du} = c(x) \exp(\langle n, T(x) \rangle_{\mathbb{R}^k} - \Psi(n))$$

for all  $x \in X, n \in \Xi$ .

**Remark 15.** A natural Exponential family is specificed by c(x), T(x), and  $\Xi$ .

**Lemma 4.** Let  $(P_n \mid n \in \Xi)$  be a 1-parameter natural Exponential form. For all  $n \in int(\Xi)$ 

1. 
$$\Psi'(n) = E_n[T]$$

2. 
$$\Psi''(n) = var_n[T]$$

*Proof.* Let  $n \in \text{int}(\Xi)$ , and define

$$\gamma(n) = e^{\Psi(n)} = \int_X c(x) \exp(nT(x)) d\mu(x).$$

We show that  $\gamma$  is infinitely differentiable at n. Observe that

$$\frac{d}{dn}(c(x)\exp(nT(x))) = c(x)T(x)\exp(nT(x))$$

To use dominated convergence theorem, we want

$$\sup_{t} |c(x)T(x)\exp(n+t)T(x)|$$

is integrable for some  $\varepsilon > 0$ . But for some  $\varepsilon$  small enough,  $n \neq t \in textint(\Xi)$  and

$$T(x) \exp(nT(x)) \le C \exp((n+\varepsilon)T(x))$$

for some constant C > 0, using that  $x \leq Ce^{\varepsilon x}$  for all  $\varepsilon$ .

Thus, by using DCT

$$\frac{d}{d\mu}\gamma(n) - \int_X c(x)T(x)\exp(nT(x))d\mu(x),$$

$$\frac{d}{dn}\Psi(n) = \frac{d}{dn}\log\gamma(n) = \frac{\gamma'(n)}{\gamma(n)} = E_n[T].$$

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Exponential Families: Assume  $\Theta \subseteq \mathbb{R}$  open,

1. 
$$p_{\theta}(x) = c(x) \exp\{n(\theta)T(x) - \Psi(\theta)\}\$$

2. Natural EF:  $p_n(x) = c(x) \exp\{nT(x) - \Psi(n)\}$ 

3. Natural Parameter Space:  $\Xi=\{t\mid\underbrace{\int_X c(x)\exp(tT(x))d\mu(x)}_{e^{\Psi(n)}}<\infty\}$  we need to check that  $\Xi$  is an open interval.

4.  $p_{\theta}(x)$  satisfies the regularity assumptions.

**Lemma 5.**  $(P_n)_{n\in\Xi}$  a natural and regular EF, then for every  $n\in\Xi=\Xi_0$ ,

1. 
$$\varphi'(n) = E_n[T]$$

2. 
$$\varphi''(n) = Var_n(T)$$

*Proof.* 1. Done in last Lecture

2. Recall that  $\alpha(n) = \int_X c(x) \exp(nT(x)) d\mu(x) = e^{\Psi(n)}$  we had shown that  $\alpha$  is  $C^{\infty}$  on this natural parameter space  $\Xi$ . as well as  $\Psi'(n) = \frac{\alpha'(n)}{\alpha(n)} = E_n[T]$ . Similarly,

$$\Psi''(n) = \frac{\alpha''(n)}{\alpha(n)} - \frac{\alpha'(n)^2}{\alpha(n)^2} = \int_X c(x)T(x)^2 \exp(nT(x))d\mu(x) - E_n[T]^2 = E_n[T^2] - E_n[T]^2 = \operatorname{Var}_n(T)$$

**Example 5.** Often T(x) = x, like with the Poisson, Normal, etc.

1.  $P_{\theta} = Bin(n, \theta), T(k) = k, n = \log \frac{\theta}{1-\theta}$ 

Recall 
$$p_{\theta}(k) = \binom{n}{k} \theta^{k} (1 - \theta)^{n-k} = \binom{n}{k} \exp\left(k \log \frac{\theta}{1-\theta} + n \log(1-\theta)\right)$$

$$\Psi(n) = -n\log(1-\theta) = -n\log\left(1 - \frac{e^n}{1+e^n}\right)$$

$$\theta = \frac{e^n}{1+e^n}$$

$$= -n\log\left(\frac{1}{1+e^n}\right) = n\log(1+e^n)$$

Hence,

$$\Psi'(n) = n \frac{e^n}{1 + e^n} = n\theta = E_n[T] = Mean \ of \ Bin(n, \theta)$$

$$\Psi(n) = Var_n[T] = n\theta(1-\theta)$$

2.  $P_{\lambda} = Poisson(\lambda)$ ,

$$P_{\lambda}(k) = e^{-\lambda} \frac{\lambda^{k}}{k!} = \frac{1}{k!} \exp(\underbrace{k}_{T(k)} \underbrace{\log \lambda}_{n} - \underbrace{\lambda}_{\Psi(n)})$$

with  $\Psi(n) = e^n$ , then  $\Psi' = \Psi'' = e^n$ . Hence,

$$E_n[T] = e^n = \lambda, Var_n(T) = e^n = \lambda$$

**Theorem 9.** MLEs in Internal EF and UMVUE Estimators Let  $(P_{\theta})_{n \in \Xi}$  be a natural 1-parameter regular EF, then

- 1. If a unique MLE  $\hat{n}_{MLE}$  exists then  $(\Psi')^{-1}(T) = \hat{n}_{MLE}$
- 2. Define  $\rho(n) = E_n[T]$  where T is the UMVUE for  $\rho(n)$

Proof. 1.

$$\hat{n}_{MLE} = \hat{n} = \arg \max_{n \in \Xi} p_n(x)$$

$$= \arg \max_{n} \log p_n(x)$$

$$= \arg \max_{n} nT(x) - \Psi(n)$$

Therefore,

$$\frac{d}{d\mu} \left( nT(x) - \Psi(n) \right) \bigg|_{n=\hat{n}} = 0 \implies T(x) = \Psi'(\hat{n})$$

Moreover,  $\Psi''(n) = \operatorname{Var}_n(T) > 0$  results from inverting  $\Psi'$ .

2. Recall CR lower bound  $\operatorname{Var}_n(S) \geq \rho'(n)^2 I'(n)$  for any unbiased estimator S. It holds that

$$\rho'(n) = \frac{d}{dn}(E_n[T]) = \Psi''[n]$$

where  $I(n) = E_n[\log p_n(x)'^2] = -E_n[\log p_n(x)'']$  Then

$$(\log p_n(x))' = (nT(x) - \Psi(n))' = T(x) - \Psi'(n) = T(x) - E_n[T(x)]$$

$$E_n[(\log p_n(x))'^2] = \text{Var}_n(T) = \Psi''(n).$$

Therefore the CR-bound  $\operatorname{Var}_n(S) \ge \Psi(n) = \operatorname{Var}_n(T)$ 

# 13 Generalized Linear Models (GLMs)

establish relations,  $x_i \to y_i, X\beta + \varepsilon = Y$  flexible classescontinuous (normal)discrete (Poisson)Binomial (Bernoulli) Note, General (X, F) are allowed, but  $\Theta$  will still be an open set in  $\mathbb{R}^p$ 

**Example 6.** Suppose we have binary data,  $Y_i \in \{0,1\}, i = 1,...,n$ 

- 1. Covariates  $X_i \in \mathbb{R}^p$
- 2. Logistic Regression for  $\beta \in \mathbb{R}^p$ ,

$$p_{\beta}(Y_i = 1|X_i) = \frac{\exp(X_i^T \beta)}{1 + \exp(X_i^T \beta)}$$

Equivalently,

$$X_i^T \beta = \log \left( \frac{P_{\beta}(Y_i = 1 | X_i)}{1 - P_{\beta}(Y_i = 1 | X_i)} \right) = \log it(P_{\beta}(Y_i = 1 | X)).$$

Example 7. Poisson Regression

- 1.  $Y_i \sim Poission(\lambda_i), \lambda_i > 0.$
- 2.  $\log \lambda_i = X_i^T \beta$
- 3.  $X_i \in \mathbb{R}^p$ ,  $\beta \in \mathbb{R}^p$
- 4. Used for count data

**Definition 15.** Generalized Linear Models We have the data  $(X_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$  In a GLM,

$$dP_{n_i}^{Y_i}(y_i) = c(y_i) \exp(n_i y_i - \Psi(n_i))$$

where  $n_i$  and  $x_i$  are linked through some link function

$$g \colon \mathbb{R} \to \mathbb{R},$$

$$g(E_{n_i}[Y_i]) = X_i^T \beta.$$

Intuition,  $n_i \iff E_{n_i}[Y_i] = \mu_i \iff X_i^T \beta \text{ with } g' > 0.$ 

When  $g(E_{n_i}[Y_i]) = n_i$ , then g is called the canonical link, or the natural link function.

Remark 16. 1. Under the canonical link,

$$p_{\beta}^{Y_i}(Y_i) = c(y_i) \exp(Y_i X_i^T \beta - \Psi(X_i^T \beta)).$$

2. Link function links the linear predictors  $X_i$  to the mean of the outcome.

$$E[Y_i|X_i,\beta] = g^{-1}(X_i^T\beta)$$