STAT 566 Fall 2013 Statistical Inference Lecture Notes

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Contents

1 Lecture 1: Introduction

1.1 Incomplete Repertory of Tasks

- Estimation. E.g. estimating someone's weight.
- Testing. E.g. testing whether a treatment will work.
- Classification. E.g. email spam filter.
- Ranking...

1.2 Decision-theoretic Framework

- **Data** $x \in \mathcal{X}$, an outcome of random element X, a point in the sample space $\mathcal{X}$.
- **Action space** $\mathcal{A}$, the space of decisions
  - For classification, $\mathcal{A}$ is finite with at least two elements.
  - For testing, two possible elements: accept/reject.
- **Decision rule** δ, procedure, any (possibly randomized) function. $\delta : \mathcal{X} \mapsto \mathcal{A}$.
- **Model** P, from which X is drawn, an element of some collection of distributions $\mathcal{P}$.
  - **Parametric model** $\mathcal{P} = \{P_\theta\}$, with θ in some space Θ (say $\mathbb{R}^n$).
- **Loss function** $l(\delta(x), P)$, the loss incurred when action $a = \delta(x)$ is chosen, and X is from P. Usually $l \geqslant 0$.

2 Lecture 2: Evaluation of Statistical Procedures I

2.1 How to compare δ?

- If $a = \delta(x)$ is randomized, then first average the loss over all possible a:

$$\overline{l}(\delta(x), P) = E_a(l(\delta(x), P)).$$

- Compare based on **risk**:

$$r_\delta(P) = E_{x\sim P}[l(\delta(x), P)] = \int l(\delta(x), P) dP(x).$$

  - If δ is randomized, then replace l by $\overline{l}$ first.
  - It depends on P.

Estimation of the mean of normal.

$X \sim \mathcal{N}(\theta, 1)$, to estimate θ with quadratic loss $l(\widehat{\theta}, \theta) = (\widehat{\theta} - \theta)^2$. Given an observation X, consider two estimators:

$$\widehat{\delta}(X) = \widehat{\theta}(X) = X; \quad \tilde{\delta}(X) = \tilde{\theta}(X) = 0.$$

Their respective risks are given by

$$r_{\widehat{\theta}}(P) = E[(X - \theta)^2] = Var(X) = 1$$
$$r_{\tilde{\theta}}(P) = E[(0 - \theta)^2] = E^2(X) = \theta^2$$

Therefore, none of $\widehat{\theta}(x)$ and $\tilde{\theta}$ is dominant, because the risks depend on θ, that is, P, the distribution of X.

2.2 Comparing risk function I: Bayes risk

- Prior distribution Π of P over distribution space $\mathcal{P}$.
  - In parametric case, prior Π of θ over its space Θ.
  - Bayes inference, given X, we can update our belief on P

$$\Pr(P|X) = \frac{\Pr(X|P)\Pr(P)}{\Pr(X)} \propto \Pr(X|P)\Pi(P)$$

- **Bayes risk** is defined by

$$R_\delta^\Pi = E_{P\sim\Pi}[r_\delta(P)] = \int r_\delta(P) d\Pi(P).$$

- It only depends on the decision rule δ and the prior Π.

2.3 Bayes theorem

- Suppose that $f_{U,V}(u, v)$ is a joint density of random elements U and V. The (marginal) density of V is

$$f_V(v) = \int f_{U,V}(u, v) du.$$

The conditional density of U given V is

$$f_{U|V}(u|v) = \frac{f_{U,V}(u, v)}{f_V(v)} = \frac{f_{U,V}(u, v)}{\int f_{U,V}(u, v) du}.$$

The **Bayes theorem** states

$$f_{V|U}(v|u) = \frac{f_{U,V}(u, v)}{f_U(u)} = \frac{f_{U,V}(u, v)}{\int f_{U,V}(u, v) dv} = \frac{f_{U|V}(u|v) f_V(v)}{\int f_{U|V}(u|v) f_V(v) dv}.$$

2.4 Bayes risk revisited

- Let the **posterior risk** be

$$R^\Pi(\delta(X)|P) = E_{P\sim\Pi}[l(\delta(X), P)|X].$$

- Bayes risk can be computed via posterior distribution

$$\begin{aligned}
R_\delta^\Pi &= E_{P\sim\Pi}[r_{\delta(P)}] & R_\delta^\Pi &= \int r_\delta(P) d\Pi(P) = \int r_\delta(p) f_P(p) dp \\
&= E_{P\sim\Pi}[E_{X\sim P}[l(\delta(X), P)|P)]] & &= \int \left(\int l(\delta(x), P) f_{X|P}(x|p) dx \right) f_P(p) dp \\
&= E_{(X,P)\sim(P,\Pi)}[l(\delta(X), P)] & &= \int \int l(\delta(x), P) f_{X,P}(x, p) dx dp \\
&= E_{X\sim P}[E_{P\sim\Pi}[l(\delta(X), P)|X)]] & &= \int \left(\int l(\delta(x), P) f_{P|X}(p|x) dp \right) f_X(x) dx \\
&= E_{X\sim P}[R^\Pi(\delta(X)|P)] & &= \int R^\Pi(\delta(X)|P) f_X(x) dx.
\end{aligned}$$

This will be favourable when posterior distribution $f_{P|X}(p, x)$ is easily accessible.

3 Lecture 3: Location Estimation, Bayes Rules for Parametric Models

3.1 Prerequisites & Bayes risk revisited

- Assume that $X \sim Q$ and we are interested in estimating some characteristic quantity of the distribution Q, say $\theta(Q)$, where $\theta(\cdot)$ is a functional.
- Characteristic quantity of the distribution Q
  - **Mean**: $\theta(Q) = \int x dQ(x)$. Not always exists (e.g. Cauchy).
  - **Median**: $\theta(Q)$ satisfies
$$\Pr\left(X \leqslant \theta(Q)\right) \geqslant \frac{1}{2}, \Pr\left(X \geqslant \theta(Q)\right) \geqslant \frac{1}{2}.$$
  - **Quantile**: For $\tau \in (0,1)$, $\theta_\tau(Q)$ satisfies
$$\Pr\left(X \leqslant \theta_\tau(Q)\right) \geqslant \tau, \Pr\left(X \geqslant \theta_\tau(Q)\right) \geqslant 1-\tau.$$
    When $\tau = \frac{1}{2}$, it is median.
- Evaluation of estimation quality: losses in question
  - **Quadratic loss**: $l^{(2)}(a, Q) = (a - \theta(Q))^2$, then $r_\delta^{(2)}(Q) = E_{X\sim Q}^{(2)}[(\delta(X) - \theta(Q))^2]$.
  - **Absolute loss**: $l^{(1)}(a, Q) = |a - \theta(Q)|$, then $r_\delta^{(1)}(Q) = E_{X\sim Q}^{(1)}[|\delta(X) - \theta(Q)|]$.
  - **0-1 loss**: $l^{(0)}(a, Q) = I(a \neq \theta(Q))$, then
$$\begin{aligned} r_\delta^{(0)}(Q) &= E_{X\sim Q}^{(0)}[I(\delta(X) \neq \theta(Q))] \\ &= \Pr(\delta(X) \neq \theta(Q)) \cdot I(\delta(X) \neq \theta(Q)) + \Pr(\delta(X) = \theta(Q)) \cdot I(\delta(X) \neq \theta(Q)) \\ &= \Pr(\delta(X) \neq \theta(Q)) \cdot 1 + \Pr(\delta(X) = \theta(Q)) \cdot 0 \\ &= \Pr(\delta(X) \neq \theta(Q)). \end{aligned}$$
    The second equation is because X can choose two types of values, those $\delta(X) \neq \theta(Q)$ and those $\delta(X) = \theta(Q)$
- Bayes approach
  - Get the posterior distribution given X.
    - Know the posterior distribution of Q, then compute $\theta(Q)$.
    - Or know the posterior distribution of θ directly.
  - Observe the loss function in question and determine its corresponding characteristic value.
    - For $l^{(2)}$, the solution is the mean of posterior distribution.
    - For $l^{(1)}$, the solution is the median of posterior distribution.
    - For $l^{(0)}$, the solution is the mode of posterior distribution.

3.2 Estimation in parametric models

- Assume we have n independent variables $X_i, i = 1, \cdots, n$ jointly from distribution P, which is determined by Q, the identical distribution of X_i. Further assume that $\theta(Q)$ is one-to-one map.
- To estimate the quantity $\theta(P)$ given data, we need its posterior distribution. (No loss function for the moment)

Posterior of normal.

$X_i \sim \mathcal{N}(\mu, \sigma)$, to estimate μ given $X_i = x_i$. Assume normal prior for μ: $\mu \sim \mathcal{N}(\mu_0, \sigma_0)$. That is,

$$\pi(\mu) = \frac{1}{\sigma_0\sqrt{2\pi}} \exp\left(-\frac{(\mu-\mu_0)^2}{2\sigma_0^2}\right)$$
$$q(x|\mu) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

The posterior of μ given data $x_1, \cdots, x_n$ is

$$\begin{aligned} f(\mu) &\propto \prod_{i=1}^{n} q(x|\mu)\pi(\mu) \\ &= \exp\left(-\frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\sigma^2} - \frac{(\mu-\mu_0)^2}{2\sigma_0^2}\right) \\ &= \exp\left(-\frac{1}{2}\left(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}\right)\mu^2 + \left(\frac{n\bar{x}}{\sigma^2}+\frac{\mu_0}{\sigma_0^2}\right)\mu\right). \end{aligned}$$

That is,

$$\mathcal{N}\left(\frac{\frac{\bar{x}}{\sigma^2}+\frac{\mu_0}{n\sigma_0^2}}{\frac{1}{\sigma^2}+\frac{1}{n\sigma_0^2}}, \frac{1}{\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}}\right).$$

In general, if a random variable X has a density of the form $K\exp(ax^2+bx+c)$, then

- $a < 0$, otherwise the integral will not converge to 1;
- The density can be expressed as

$$K\exp(ax^2+bx+c) = K\exp\left(\frac{c}{a}-\frac{b^2}{4a^2}\right)\exp a\left(x-\left(-\frac{b}{2a}\right)\right)^2,$$

  which is the density of a normal distribution with $\mu = -\frac{b}{2a}$ and $\sigma^2 = -\frac{1}{2a}$;
- c is free and $K = K(a,b,c)$ is a normalizing positive constant.

4 Lecture 4: Evaluation of Statistical Procedures II

4.1 Comparing risk function II: minimax

- The **minimax risk** ("worst case")

$$\bar{R}_\delta = \sup_{P\in\mathcal{P}} r_\delta(P).$$

- **Minimax rule** is the rule that minimize minimax risk.

4.2 Connection between minimax and Bayes

- Suppose δ^Π is the Bayes rule for some prior Π, i.e., $R^\Pi_{\delta^\Pi} = \inf_\delta R^\Pi_\delta$ and suppose that for all P, $r_{\delta^\Pi}(P) \leqslant R^\Pi_{\delta^\Pi}$, then δ^Π is minimax (and Π is called a least favourable prior).
  - Proof: If δ^Π were not minimax, then there would exist δ such that

$$\sup_P r_\delta(P) < \sup_P r_{\delta^\Pi}(P) \leqslant R^\Pi_{\delta^\Pi}.$$

    As the average never exceeds sup, and the average of a constant is that constant, we would have a contradiction with the assumptions:

$$R^\Pi_\delta = E_{P\sim\mathcal{P}}[r_\delta(P)] \leqslant \sup_P r_\delta(P) < \sup_P r_{\delta^\Pi}(P) \leqslant R^\Pi_{\delta^\Pi}.$$

- If δ is the Bayes rule with respect to some prior Π, and if it has constant risk, $r_\delta(P) = c$ for all P, then δ is minimax.
  - In fact, $r_{\delta^\Pi}(P) = R^\Pi_{\delta^\Pi} = c$ in such cases.

4.3 Admissibility

- δ is **admissible** if there is no $\tilde{\delta}$ such that $r_{\tilde{\delta}}(P) \leqslant r_\delta(P)$ with strict inequality $<$ at least for one P.
- Connection to Bayes rule: if δ^Π is the unique Bayes rule with respect to a prior Π, then δ^Π is admissible.
  - Proof: If not, there exists δ such that $r_\delta(P) \leqslant r_{\delta^\Pi}(P)$ with strict inequality for some P, which implies

    $$R_\delta^\Pi = E_{P\sim\Pi}[r_\delta(P)] \leqslant E_{P\sim\Pi}[r_{\delta^\Pi}(P)] = R_{\delta^\Pi}^\Pi.$$

    Not necessarily the middle inequality is $<$, despite the strict inequality for at least one P (because difference at single point may not influence their integral; but if $\mathcal{P}$ is discrete or continuous, then strict inequality will hold); however, the result is a contradiction with uniqueness.
- Connection to minimax rule: if δ has constant risk and is admissible, then it is minimax.
  - Proof: Let δ_c be an admissible rule with constant risk c, i.e., $r_{\delta_c}(P) = c, \forall P \in \mathcal{P}$. Because δ_c is admissible, for any other rule δ, there exists $P_0 \in \mathcal{P}$, such that

    $$r_{\delta_c}(P_0) \leqslant r_\delta(P_0).$$

    Now we prove the claim by contradiction. Assume that δ_c is not minimax, then there exists δ, such that

    $$\sup_{P\in\mathcal{P}} r_\delta(P) < \sup_{P\in\mathcal{P}} r_{\delta_c}(P).$$

    Since the supremum should be larger than or equal to the risk at any specific P, we have

    $$r_\delta(P_0) \leqslant \sup_{P\in\mathcal{P}} r_\delta(P)$$

    To combine, we have

    $$c = r_{\delta_c}(P_0) \leqslant r_\delta(P_0) \leqslant \sup_{P\in\mathcal{P}} r_\delta(P) < \sup_{P\in\mathcal{P}} r_{\delta_c}(P) = c.$$

    A contradiction. Therefore, the assumption is false. δ_c is minimax.

James-Stein estimator.

$X_i \sim \mathcal{N}(\theta_i, 1), i = 1, \cdots, p$, to estimate θ_i with quadratic loss $l(\widehat{\theta}, \theta) = (\widehat{\theta} - \theta)^2$. The natural estimator is $\theta_i = X_i$. It is admissible for $p = 1, 2$, but not for $p > 3$; in that case, the James-Stein estimator

$$\widehat{\theta}_i^{JS} = \left(1 - \frac{p-2}{\sum_{i=1^p} X_i^2}\right)^+ X_i$$

has smaller risk. However, James-Stein estimator is not admissible either.

4.4 Unbiasedness

- δ is unbiased with respect to a loss l if for every P

  $$r_\delta(P) = E_{X\sim P}[l(\delta(X), P)] \leqslant E_{X\sim P}[l(\delta(X), Q)], \text{for all } Q.$$

  That is, $E_{X\sim P}[l(\delta(X), Q)]$ is minimized at $Q^* = P$.
- When P is parametrized, δ is unbiased with respect to a loss l if for every θ

  $$E_{X\sim P_\theta}[l(\delta(X), \theta)] \leqslant E_{X\sim P_\theta}[l(\delta(X), \tilde{\theta})], \text{for all } \tilde{\theta}.$$

Unbiasedness for quadratic loss.
If l is quadratic loss, then unbiasedness means

$$\begin{aligned}\theta &= \text{argmin}_{\tilde{\theta}} E_{X\sim P_\theta}[(\delta(X)-\tilde{\theta})^2] \\ &= \text{argmin}_{\tilde{\theta}} \tilde{\theta}^2 + 2\tilde{\theta}E_{X\sim P_\theta}[\delta(X)] \\ &= E_{X\sim P_\theta}[\delta(X)].\end{aligned}$$

Bias-variance decomposition.
If l is quadratic loss, then the risk is

$$\begin{aligned}r_\delta(P) &= E_X[(\delta(X)-\theta(P))^2] \\ &= E[(\delta(X)-E(\delta(X))+E(\delta(X))-\theta(P))^2] \\ &= E[((\delta(X)-E(\delta(X)))^2]+[E(\delta(X))-\theta(P)]^2 \\ &= Var(\delta(X))+Bias^2(\delta(X))\end{aligned}$$

5 Lecture 5: Building Statistical Procedure I

5.1 Sufficient statistics

- A **statistic** is a function $T:\mathcal{X}\mapsto\mathbb{R}$.
- A statistic T is called **sufficient** for the model $\mathcal{P}$, if the conditional distribution of the data X given the value of $T(X)=T(x)$ does not depend on $\mathcal{P}$.

Sufficient statistic for binomial distribution.
Suppose $X\in\{0,1\}^n$ with independent and entries, where $P(X_i=1)=p,\forall i$. Then $T(X)=X^T\mathbf{1}$ is sufficient:

$$\begin{aligned}P(X|X^T\mathbf{1}=s) &= \frac{P(X,X^T\mathbf{1}=s)}{X^T\mathbf{1}=s} \\ &= \begin{cases}\frac{p^s(1-p)^{n-s}}{\binom{n}{s}p^s(1-s)^{n-s}}=\binom{n}{s}^{-1} & \text{if } X^T\mathbf{1}=s \\ 0 & \text{if } X^T\mathbf{1}\neq s\end{cases}\end{aligned}$$

which does not depend on p.

- If $T(\cdot)$ is a sufficient statistic for $\mathcal{P}$ and S is a one-to-one function, then $S(T(\cdot))$ is also a sufficient statistic for $\mathcal{P}$.
- A sufficient statistic which is a function of every other sufficient statistic is called **minimal sufficient**.
  - May not exist.
  - In the binomial example, $T(X)=X$ is not, but $T(X)=X^T\mathbf{1}$ is.
- Let Π be a prior distribution on $\mathcal{P}$. A statistic $T(\cdot)$ is called **Bayes sufficient** for Π, if the posterior distribution of P given $X=x$ is the same as the posterior distribution of P given $T(X)=T(x)$, for all x.
- (Kolmogorov) If $T(X)$ is sufficient for $\mathcal{P}$, it is Bayes sufficient for every Π.
  - The converse is also true, but not in general.
- (Rao-Blackwell) **Construct decision rule from sufficient statistics**. Suppose that the loss function is convex for fixed P:

$$l(\alpha_1 a_1+\alpha_2 a_2,P)\leqslant\alpha_1 l(a_1,P)+\alpha_2 l(a_2,P)$$

where $\alpha_1,\alpha_2\geqslant 0$ and $\alpha_1+\alpha_2=1$. If $T(X)$ is sufficient for $\mathcal{P}$ and δ is a decision rule, then the decision rule $\delta^*(X)=E_{\delta(X)}(\delta(X)|T(X))$ has uniformly smaller risk:

$$r_{\delta*}(P)\leqslant r_\delta(P),\forall P.$$

Also, if δ is unbiased, so is δ^*.

Rao-Blackwell for binomial distribution.

Suppose $X \in \{0,1\}^n$ with independent and entries, where $P(X_i = 1) = p, \forall i$. Then $T(X) = X^T\mathbf{1}$ is sufficient for p. Consider $\delta(X) = X_1$ (estimating p, unbiased). Then

$$\begin{aligned}
\delta^*(X) &= E_{\delta(X)}[\delta(X)|T(X) = T(x)] \\
&= E_{X_1}(X_1|X^T\mathbf{1} = s) \\
&= 0 \cdot P(X_1 = 0|X^T\mathbf{1} = s) + 1 \cdot P(X_1|X^T\mathbf{1} = s) \\
&= P(X_1|X^T\mathbf{1} = s) \\
&= \frac{P(X_1 = 1, X^T\mathbf{1} = s)}{P(X^T\mathbf{1} = s)} \\
&= \frac{p \cdot \binom{n-1}{s-1} p^{s-1}(1-p)^{(n-1)-(s-1)}}{\binom{n}{s} p^s (1-p)^{n-s}} \\
&= \frac{s}{n} = \frac{X^T\mathbf{1}}{n}.
\end{aligned}$$

It is unbiased with respect to quadratic loss:

$$E_{X\sim P}\left(\frac{X^T\mathbf{1}}{n}\right) = \frac{1}{n}\sum_{i=1}^{n} E(X_i) = p.$$

Thus, its risk is the variance (see bias-variance decomposition):

$$r_{\delta*}(P) = Var\left(\frac{X^T\mathbf{1}}{n}\right) = \frac{1}{n^2}\sum_{i=1}^{n} Var(X_i) = \frac{1}{n^2} \cdot n \cdot p(1-p) = \frac{p(1-p)}{n}.$$

It has uniformly smaller risk than $\delta(X)$ for any p:

$$\begin{aligned}
r_{\delta*}(P) &= E_{X\sim P}\left[l\left(\frac{X^T\mathbf{1}}{n}, p\right)\right] \\
&\leqslant E_{X\sim P}[l(X_1, p)] \\
&= p \cdot (1-p)^2 + (1-p) \cdot (0-p)^2 \\
&= p(1-p).
\end{aligned}$$

- (Neyman-Savage) **Factorization criterion** for sufficient statistics. Suppose that X has a density (or mass). T is sufficient for θ iff there are g and h such that

$$f(x|\theta) = g(T(x), \theta)h(x).$$

  - T is sufficient for θ if and only if the following is true:

$$T(x) = T(y) \Rightarrow f(x|\theta) = c(x,y)f(y|\theta).$$

  - T is minimal sufficient for θ if and only if the following is true:

$$T(x) = T(y) \Leftrightarrow f(x|\theta) = c(x,y)f(y|\theta).$$

Neyman-Savage factorization criterion for binomial distribution.

Suppose $X \in \{0,1\}^n$ with independent and entries, where $P(X_i = 1) = p, \forall i$. Then $T(X) = X^T\mathbf{1}$ is sufficient for p, since if $T(X) = T(x) = s$,

$$f(x|p) = p^s(1-p)^{n-s} = g(s,p)h(x),$$

where

$$g(s,p) = p^s(1-p)^{n-s}; h(x) = 1.$$

T is minimal. Let

$$f(x|p) = p^{\sum_i x_i}(1-p)^{n-\sum_i x_i}; f(y|p) = p^{\sum_i y_i}(1-p)^{n-\sum_i y_i}.$$

T is minimal because

$$T(x) = T(y) = s \Leftrightarrow f(x|p) = c(x,y)f(y|p),$$

where $c(x,y) = 1$.

Neyman-Savage factorization criterion for normal distribution.

Suppose $X_i \sim \mathcal{N}(\mu, \sigma^2), i = 1, \cdots, n$, σ^2 is known, to estimate μ. Then $T(X) = X^T\mathbf{1}$ is sufficient for μ, since if $T(X) = T(x) = s$,

$$\begin{aligned} f(x|p) &= \frac{1}{\sigma^n(2\pi)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^n (x_i-\mu)^2\right) \\ &= \frac{1}{\sigma^n(2\pi)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^n x_i^2\right) \cdot \exp\left(\frac{1}{2\sigma^2}(2\mu\sum_{i=1}^n x_i - n\mu^2)\right) \\ &= h(x)g(s,p). \end{aligned}$$

where

$$\begin{aligned} g(s,p) &= \exp\left(\frac{1}{2\sigma^2}(2\mu s - n\mu^2)\right) \\ h(x) &= \frac{1}{\sigma^n(2\pi)^{n/2}} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^n x_i^2\right). \end{aligned}$$

T is minimal. To see this, set $c(x,y) = \exp\left(-\frac{1}{2\sigma^2}\sum_i (x_i^2 - y_i^2)\right)$.

5.2 Complete statistics

- Assume a parametric model $\{P_\theta\}$ and the quadratic loss function.
- A statistic S is **complete** if for every function g, independent of θ,

$$E_{X\sim P_\theta}[g(S(X))] = 0, \forall\theta \Rightarrow \Pr_{X\sim P_\theta}[g(S(X)) = 0] = 1, \forall\theta.$$

Roughly speaking, if the expectation with respect to all θ is 0, then g is identically zero.

Complete statistic for binomial distribution.

Suppose $X \in \{0,1\}^n$ with independent and entries, where $P(X_i = 1) = p, \forall i$. Then $T(X) = X^T\mathbf{1}$ is complete for p: if

$$E[g(T(X))] = \sum_{k=0}^n g(k)\Pr(T(X) = k) = \sum_{k=0}^n g(k)\binom{n}{k}p^k(1-p)^{n-k},$$

equals to zero for all $p \in [0,1]$, then $g(k) = 0$ for all k, because $E[g(T(X))]$ is a polynomial of p.

- (Lehmann-Scheffé) Any unbiased estimator based (only) on a complete, sufficient statistic is **minimum-variance unbiased estimator**. That is, it has the smallest variance (= MSE for unbiased), for all θ, among all unbiased estimators of θ.

5.3 Cramér-Rao bound

- In this part we only consider **regular** models, whose support ($\{x|f(x;\theta)>0\}$) does not depend on θ. Also assumed is that we may interchange integration and differentiation.
- The **score function** is

$$s(x;\theta)=\frac{\partial}{\partial\theta}\log f(x;\theta)=\frac{\frac{\partial}{\partial\theta}f(x;\theta)}{f(x;\theta)}.$$

  - Note that

$$\begin{aligned}E_{X\sim P_\theta}[s(X;\theta)]&=\int\frac{\frac{\partial}{\partial\theta}f(x;\theta)}{f(x;\theta)}f(x;\theta)dx\\&=\int\frac{\partial}{\partial\theta}f(x;\theta)dx\\&=\frac{\partial}{\partial\theta}\int f(x;\theta)dx\\&=\frac{\partial}{\partial\theta}1=0.\end{aligned}\tag{5.1}$$

  - When X consists of independent r.v.s then

$$s(x;\theta)=\frac{\partial}{\partial\theta}\log f(x;\theta)=\frac{\partial}{\partial\theta}\sum_{i=1}^n\log g(x_i;\theta)=\sum_{i=1}^n\frac{\partial}{\partial\theta}\log g(x_i;\theta)$$

- The **Fisher information** is defined by

$$\begin{aligned}I(\theta)&=Var_{X\sim P_\theta}[s(X;\theta)]\\&=E_{X\sim P_\theta}[s^2(X;\theta)]\\&=\int\left(\frac{\frac{\partial}{\partial\theta}f(x;\theta)}{f(x;\theta)}\right)^2f(x;\theta)dx\\&=\int\frac{(\frac{\partial}{\partial\theta}f(x;\theta))^2}{f(x;\theta)}dx\end{aligned}$$

  - Another way to compute $I(\theta)$ via second derivative. First note that

$$\frac{\partial^2}{\partial^2\theta}\log f=\frac{\partial}{\partial\theta}\frac{f'}{f}=\frac{f''f-f'f'}{f^2}.$$

    Also,

$$E_{X\sim P_\theta}\left(\frac{f''}{f}\right)=\int\frac{f''}{f}fdx=\int f''dx=0\text{ as }\int fdx=1.$$

    To combine, we have

$$\begin{aligned}E\left(-\frac{\partial^2}{\partial^2\theta}\log f\right)&=E\left(\frac{f'f'-f''f}{f^2}\right)\\&=E\left(\left(\frac{f'}{f}\right)^2\right)-E\left(\frac{f''}{f}\right)\\&=E(s^2)-0=I(\theta)\end{aligned}$$

  - When X consists of independent r.v.s then

$$\begin{aligned}I(\theta)&=Var_{X\sim P_\theta}[s(X;\theta)]\\&=Var_{X\sim P_\theta}[\sum_{i=1}^n\frac{\partial}{\partial\theta}\log g(x_i;\theta)]\\&=\sum_{i=1}^nVar_{X\sim P_\theta}[\frac{\partial}{\partial\theta}\log g(x_i;\theta)]\\&=\sum_{i=1}^n\int\frac{(\frac{\partial}{\partial\theta}g(x_i;\theta))^2}{g(x_i;\theta)}dx_i\end{aligned}$$

If all g_i are identical, then

$$I(\theta) = n \int \frac{(\frac{\partial}{\partial\theta} g(y;\theta))^2}{g(y;\theta)} dy$$

- **Cramér-Rao inequality** provides a lower bound on the variance of *any* statistic $U(X)$. Consider the covariance of $s(X;\theta)$ and $U(X)$. By Cauchy-Schwartz inequality

$$\begin{aligned}[Cov_{X\sim P_\theta}(s(X;\theta), U(X))]^2 &\leqslant Var_{X\sim P_\theta}(s(X;\theta)) \cdot Var_{X\sim P_\theta}(U(X)) \\ &= I(\theta) \cdot Var_{X\sim P_\theta}(U(X))\end{aligned}$$

To compute $Cov_{X\sim P_\theta}(s(X;\theta), U(X))$ (note Eq.(5.1)):

$$\begin{aligned}Cov_{X\sim P_\theta}(s(X;\theta), U(X)) &= E_{X\sim P_\theta}[s(X;\theta)U(X)] - E_{X\sim P_\theta}(s(X;\theta))E_{X\sim P_\theta}[U(X)] \\ &= E_{X\sim P_\theta}[s(X;\theta)U(X)] \\ &= \int \frac{\frac{\partial}{\partial\theta} f(x;\theta)}{f(x;\theta)} U(x) f(x;\theta) dx \\ &= \int \frac{\partial}{\partial\theta} f(x;\theta) U(x) dx \\ &= \frac{\partial}{\partial\theta} \int U(x) f(x;\theta) dx = \frac{\partial}{\partial\theta} E_{X\sim P_\theta}[U(X)].\end{aligned}$$

Therefore, **Cramér-Rao lower bound** gives

$$Var_{X\sim P_\theta}(U(X)) \geqslant \frac{\{\frac{\partial}{\partial\theta} E_{X\sim P_\theta}[U(X)]\}^2}{I(\theta)}$$

  - When $U(X)$ is unbiased w.r.t. quadratic loss:

$$E_{X\sim P_\theta}(U(X)) = \theta.$$

Because $\frac{\partial}{\partial\theta} E_{X\sim P_\theta}[U(X)] = \frac{\partial}{\partial\theta}\theta = 1$, we have

$$Var_{X\sim P_\theta}(U(X)) \geqslant \frac{1}{I(\theta)}.$$

Cramér-Rao lower bound for binomial distribution.

Suppose $X \in \{0,1\}^n$ with independent and entries, where $P(X_i = 1) = p, \forall i$. $g(x_i;p) = p^{x_i}(1-p)^{1-x_1}$. To compute the Fisher information

$$\begin{aligned}I(p) &= n \times E_{X_i}\left[\left[\frac{\partial}{\partial\theta} \log g(x_i;p)\right]^2\right] \\ &= n \cdot E_{X_i}\left[\left(\frac{x_i}{p} - \frac{1-x_i}{1-p}\right)^2\right] \\ &= \frac{n}{p^2(1-p)^2} E_{X_i}[(x_i - p)^2] \\ &= \frac{n}{p^2(1-p)^2} Var_{X_i}(x_i) = \frac{n}{p(1-p)}.\end{aligned}$$

Therefore, any unbiased estimator of p must have a variance (which equals its mean square error) greater than $\frac{1}{I(p)} = \frac{p(1-p)}{n}$.
Now let's compute the variance (also MSE) of an unbiased estimator $T(X) = \frac{X^T\mathbf{1}}{n}$:

$$Var_X(T(X)) = \frac{1}{n^2}\sum_{i=1}^n Var_{X_i}(X_i) = \frac{p(1-p)}{n}.$$

Therefore, this estimator makes the Cramér-Rao lower bound tight.

- When Cramér-Rao an equality? The inequality is the result of Cauchy-Schwartz. Therefore, if the score function has the form

$$s(x;\theta) = \frac{\partial}{\partial\theta} \log f(x;\theta) = c(\theta) + d(\theta)U(x),$$

equality will hold. Then

$$f(x;\theta) = \exp(\eta(\theta)U(X) - a(\theta) + g(x)).$$

That is, exponential families preserve equality in Cramér-Rao. For the exponential family, if we define $\eta = \eta(\theta)$ as a new parameter, then $a(\theta) = b(\eta)$. For the density, we have

$$\int f(x;\eta)dx = \int \exp(\eta U(X) - b(\eta) + g(x))dx = 1.$$

Differentiating in η on both sides (assuming we can interchange integration and differentiation), we have

$$\begin{aligned} 0 &= \int \exp(\eta U(X) - b(\eta) + g(x))(U(x) - b'(\eta))dx \\ &= \int U(x)\exp(\eta U(X) - b(\eta) + g(x))dx - b'(\eta)\exp(\eta U(X) - b(\eta) + g(x))dx \\ &= E_X(U(x)) - b'(\eta). \end{aligned}$$

Therefore, we have $E_X(U(x)) = b'(\eta)$. Similarly, we can show that $Var_X(T(X)) = b''(\eta)$.

Cramér-Rao for exponential distribution.

Exponential distribution is specified by

$$f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x} & \text{when } x \geqslant 0 \\ 0 & \text{otherwise} \end{cases}$$

where $\lambda > 0$ is the parameter. Note that it can be also expressed as

$$f(x;\theta) = \begin{cases} \frac{1}{\theta} e^{-\frac{1}{\theta}x} & \text{when } x \geqslant 0 \\ 0 & \text{otherwise} \end{cases}$$

for $\theta > 0$. With this new parametrization, we can see that $U(X) = X$ is unbiased for θ, with least variance (MSE) one can have because of Cramér-Rao inequality.
Note that if we use old parametrization with λ, then $U(X) = -X$ and

$$\lambda e^{-\lambda x} = e^{-\lambda x - (-\ln \lambda)}.$$

Thus $b'(\lambda) = \frac{-1}{\lambda}$, so is $E_X(U(X)) = E_X(-X) = -E_X(X) = \frac{-1}{\lambda}$.
(Side note: having an estimator, $\widehat{\theta}$ of θ, with some properties does not mean that $g(\widehat{\theta})$ is the estimator of $g(\theta)$ with the same properties (unless g is very simple - say, a linear function). For instance, an unbiased estimator for σ^2 may not be unbiased for σ)

Cramér-Rao for binomial distribution: revisited.

Suppose $X \in \{0,1\}^n$ with independent and entries, where $P(X_i = 1) = p, \forall i$. $g(x_i;p) = p^{x_i}(1-p)^{1-x_1}$. The joint distribution is

$$\begin{aligned} f(x;p) &= p^{\sum_i x_i}(1-p)^{n-\sum_i x_i} \\ &= \left(\frac{p}{1-p}\right)^{\sum_i x_i}(1-p)^n \\ &= \exp\left(\ln\frac{p}{1-p}\sum_i x_i + n\ln(1-p)\right). \end{aligned}$$

Let $\eta = \ln\frac{p}{1-p}$, we have

$$f(x;p) = \exp\left(\eta\sum_i x_i - n\ln(1+e^\eta)\right)$$

Therefore, it is also a member of exponential family. As a result, Cramér-Rao bound is sharp (as we already shown).

6 Lecture 6: Building Statistical Procedure II

6.1 Substitution principle

- Let $x = (x_1, x_2, \cdots, x_n)$, which is a realization of $X = (X_1, X_2, \cdots, X_n))$, where X_i is a r.v. with distribution P. We want to estimate $\theta(P)$, some characteristic quantity of P. Typically, X_i are independent, but it is not absolutely necessary; some permutational invariance (exchangeability) is enough.
- An **empirical distribution** by x is the discrete distribution that assigns probability $\frac{1}{n}$ to every point x_i, denoted $\mathbb{P}_x$:

$$\mathbb{P}_x(E) = \frac{1}{n}\text{card}\{i | x_i \in E\}.$$

- The **substitution principle** states that to estimate $\theta(P)$, replace P by $\mathbb{P}_x$.

Moment estimation.

Suppose we want to estimate the kth moment

$$\theta(P) = \int z^k dP(z), k = 1, 2, \cdots .$$

The resultant estimators with substitution principle is

$$\theta(\mathbb{P}_x) = \int z^k d\mathbb{P}_x(z) = \frac{1}{n}\sum_{i=1}^{n} x_i^k.$$

Variance estimation.

Suppose we want to estimate the variance

$$\theta(P) = \int \left(z - \int u dP(u)\right)^2 dP(z).$$

The resultant estimator with substitution principle is

$$\theta(\mathbb{P}_x) = \frac{1}{n}\sum_{i=1}^{n}\left(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i\right)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2.$$

Linear regression.

Consider the linear regression model:

$$Y = \alpha X + \beta + U, \tag{6.1}$$

where X is input variable and Y is output variable (jointly with U from some distribution), α, β are the parameters of the model, and U is an error term independent of X (so they are also uncorrelated, $E(XU) = 0$) with $E(U) = 0$. Taking expectation on both sides, we have

$$E(Y) = \alpha E(X) + \beta. \tag{6.2}$$

Moreover, we can multiply Eq.(6.1) by X, then take expectation:

$$E(XY) = \alpha E(X^2) + \beta E(X). \tag{6.3}$$

With Eq.(6.2) and Eq.(6.3), we can solve α, β as

$$\alpha = \frac{E(XY) - E(X)E(Y)}{E(X^2) - (E(X))^2} = \frac{Cov(X, Y)}{Var(X)}$$
$$\beta = E(Y) - \alpha E(X).$$

By substitution principle, all expectations (variance/covariance) can be computed from sample $\{(x_1, y_1), (x_2, y_2), \cdots, (x_n, y_n)\}$:

$$\widehat{\alpha} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$
$$\widehat{\beta} = \bar{y} - \widehat{\alpha}\bar{x}.$$

break.

Quantile estimation.

For $\tau \in (0,1)$, suppose we are going to estimate the quantile q_τ such that

$$P((-\infty, q_\tau]) \geqslant \tau; P([q_\tau, +\infty)) \geqslant 1-\tau.$$

We can see quantile in a different way. Define check function as

$$\rho_\tau(z) = |z| + (2\tau - 1)z = \begin{cases} 2\tau z & \text{for } z > 0 \\ 2(1-\tau)z & \text{for } z \leqslant 0 \end{cases}$$

Then

$$q_\tau = \text{argmin}_c \, E[\rho_\tau(Z-c)] = \int \rho_\tau(z-c) dP(z).$$

Therefore, given $\tau \in (0,1)$, to estimate q_τ, find the minimizer c^* of

$$\int \rho_\tau(z-c) d\mathbb{P}_x(z) = \frac{1}{n}\sum_{i=1}^{n} \rho_\tau(x_i - c).$$

For instance, if $\tau = 0.5$, we are trying to estimate the median, then

$$\text{card}\{i | x_i \leqslant c^*\} \geqslant \frac{n}{2}; \text{card}\{i | x_i \geqslant c^*\} \geqslant \frac{n}{2}.$$

That is, c^* is just sample median.

- Can be used to estimate non-parametric model. If we want to estimate the accumulative distribution $F(z) = P((-\infty, z])$, by substitution principle, we have

$$\mathbb{F}_n(z) = \mathbb{P}_x(z) = \frac{1}{n}\text{card}\{i | x_i \leqslant z\},$$

which is essentially a step function.

  - $E(\mathbb{F}_n(z)) = F(z)$.
  - $Var(\mathbb{F}_n(z)) = \frac{F(z)(1-F(z))}{n}$.
  - $\mathbb{F}(z) \to F(z)$ as $n \to \infty$ (in probability, almost surely).
  - $\sup_z |\mathbb{F}(z) - F(z)| \to 0$ as $n \to \infty$ (in probability, almost surely).

6.2 Consistency

- If the estimator $\widehat{\theta}_n$ converges to the target/estimated quantity θ as $n \to \infty$, where convergence is determined by

  - Convergence in probability

$$\Pr(|\widehat{\theta} - \theta| \geqslant \epsilon) \to 0 \text{ for every } \epsilon > 0.$$

  - Almost surely (with probability 1) convergence

$$\Pr(|\widehat{\theta} - \theta| \to 0) = 1.$$

  - Convergence in some mean sense

$$E(|\widehat{\theta} - \theta|^p) \to 0.$$

then we say $\widehat{\theta}_n$ is **consistent**.

Consistent estimator for mean and variance.

Assume that X_i are iid r.v.s and the mean $\mu = E(X_i)$ exists. Then $\bar{X}_n$ is a consistent estimator for μ. By a **law of large numbers** (have different versions),

$$\bar{X}_n \xrightarrow{p} \mu$$

as $n \to \infty$.
Now further assume that the variance $\sigma^2 = Var(X_i)$ exists. Consider the quantity

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} (X_i - \mu) = \sqrt{n}(\bar{X}_n - \mu).$$

A **central limit theorem** (again, many versions) states that

$$\frac{\bar{X}_n - E(\bar{X}_n)}{\sqrt{Var(X_n)}} = \frac{\bar{X}_n - \mu}{\sqrt{\frac{\sigma^2}{n}}} = \sqrt{n}\frac{\bar{X}_n - \mu}{\sigma}$$

converges in distribution to the standard normal distribution $\mathcal{N}(0,1)$. It follows that $\sqrt{n}(\bar{X}_n - \mu)$ converges *in distribution* to $\mathcal{N}(0, \sigma^2)$.

6.3 Asymptotic normality

- If the estimator, $\widehat{\theta}_n$, of θ, has the property that $\sqrt{n}(\widehat{\theta}_n - \theta)$ converges in distribution to $\mathcal{N}(0, \sigma^2)$, then we call that estimator **asymptotically normal** with asymptotic variance σ^2.
  - The smaller σ^2 is, the better (more accurate).
- To compare two asymptotically normal estimator $\widehat{\theta}$ and $\widetilde{\theta}$, with

$$\sqrt{n}(\widehat{\theta} - \theta) \xrightarrow{d} Z \sim \mathcal{N}(0, \sigma^2); \quad \sqrt{n}(\widetilde{\theta} - \theta) \xrightarrow{d} Z \sim \mathcal{N}(0, \widetilde{\sigma}^2).$$

The **asymptotic relative efficiency** (ARE) of $\widetilde{\theta}$ to $\widehat{\theta}$ is defined as

$$\text{ARE}(\widetilde{\theta}, \widehat{\theta}) = \frac{\sigma^2}{\widetilde{\sigma}^2}.$$

ARE of sample mean versus sample median.

Assume that X_i are iid r.v.s whose mean and median are both μ.

- Suppose that the variance of X_i is σ^2; from the central limit theorem, we know that σ^2 is the asymptotic variance of the sample mean.
- Suppose that the common density, f, of X_i exists and is positive at μ. For the sample median, Kolmogorov proved that under these assumptions, it is asymptotically normal with the asymptotic variance $\frac{1}{4(f(\mu))^2}$.

For instance, if the distribution of X_i is normal, then the asymptotic variance of sample mean is σ^2, while the asymptotic variance of sample median is

$$\frac{1}{4(f(\mu))^2} = \frac{\pi}{2}\sigma^2.$$

Therefore,

$$ARE(\mu_{\text{median}}, \mu_{\text{mean}}) = \frac{\sigma^2}{\frac{\pi}{2}\sigma^2} = \frac{2}{\pi} \approx 0.6366,$$

which means sample mean μ_{mean} is more efficient.
For any unimodal f (only has one mode), the ratio is $\geqslant 1/3$ and there are f with > 1, i.e., the sample median is more efficient (t distribution with 3 or 4 degrees of freedom, for instances).

6.4 Maximum likelihood estimate

- Likelihood
$$L(\theta) = f(x;\theta).$$
If we have independent r.v.s, then
$$L(\theta) = f(x;\theta) = \prod_{i=1}^{n} g(x_i;\theta).$$

- **Maximum likelihood estimate** is given by
$$\widehat{\theta} = \text{argmax}_\theta \, L(\theta).$$
Usually take the logarithm when we have independent r.v.s.

- Suppose that $\widehat{\theta}_n$ are maximum likelihood estimators of θ, from iid sample where the distribution of X_i is specified by θ. Then typically,
  - Maximum likelihood estimators are consistent (in probability): $\widehat{\theta}_n \xrightarrow{p} \theta$.
  - They are asymptotically normal, and asymptotically efficient:
$$\sqrt{n}(\widehat{\theta}_n - \theta) \xrightarrow{d} Z \sim \mathcal{N}\left(0, \frac{1}{I(\theta)}\right),$$
where $I(\theta)$ is the Fisher information for one observation from the family parametrized by θ. (Note that the Fisher information for the whole sample $X_1, X_2, \cdots, X_n$ is $nI(\theta)$.)

7 Lecture 7: Estimating the precision of estimates

7.1 Bootstrap

- We care about how accurate our prediction is.

Standard error: a canonical example.

Consider an example where $X_1, \cdots, X_n$ are i.i.d. r.v.s with the same distribution P with mean μ and variance σ^2. We are estimating the mean μ by $\bar{X}$. It is known that $Var(\bar{X}) = \frac{\sigma^2}{n}$. So the standard error of sample mean is given by
$$se_{X\sim P}(\bar{X}) = \frac{\sigma}{\sqrt{n}}.$$
However, we don't know σ, so we can estimate this by substitution principle, we have
$$se_{X\sim \mathbb{P}_x}(\bar{X}) = \frac{1}{\sqrt{n}}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2}.$$
(Sometimes, $n-1$ is preferable.)

Unlike the example above, standard error (standard deviation) of estimator $\widehat{\theta}$ may not be calculated in closed form. So we can estimate its standard error via bootstrap.

- Generate B bootstrap samples of size n (sampling from $\mathbb{P}_x$ with replacement.)
- We estimate $se_{\mathbb{P}_x}(\widehat{\theta})$ by the standard derivative of $\widehat{\theta}^*$, the estimation from bootstrap sample:
$$se_{\mathbb{P}_x}(\widehat{\theta}) \approx \sqrt{\frac{1}{B}\sum_{i=1}^{B}(\widehat{\theta}_b^* - \frac{1}{B}\sum_{i=1}^{B}\widehat{\theta}_b^*)^2}. \tag{7.1}$$
- In theory, there are $\binom{2n-1}{n}$ distinct bootstrap samples of size n (place $n-1$ boards in between n balls). However, their probabilities are different. The probability of a bootstrap sample in which x_i appears k_i times, with $k_i > 0$ and $k_1 + k_2 + \cdots + k_n = n$ is
$$\frac{n!}{n^n k_1! k_2! \cdots k_n!}.$$
The most probable sample is the one with $k_i = 1$ - the original one.

- Bias correction via bootstrap.
  - The bias of $\widehat{\theta}$ is
$$b_{X\sim P}(\widehat{\theta}) = E_{X\sim P}(\widehat{\theta}) - \theta.$$
If it is known, then we can use
$$\widetilde{\theta} = \widehat{\theta} - b_{X\sim P}(\widehat{\theta})$$
as a "corrected" estimate: $E_{X\sim P}(\widetilde{\theta}) = E_{X\sim P}(\widehat{\theta}) - E_{X\sim P}(b_{X\sim P}(\widehat{\theta})) = [\theta + b_{X\sim P}(\widehat{\theta})] - b_{X\sim P}(\widehat{\theta}) = \theta$.
  - When $b_{X\sim P}(\widehat{\theta})$ is unknown, we estimate it by
$$b_{X\sim \mathbb{P}_x}(\widehat{\theta}) = E_{X\sim \mathbb{P}_x}(\widehat{\theta}) - \widehat{\theta},$$
where $E_{X\sim \mathbb{P}_x}(\widehat{\theta})$ can be estimated by bootstrap $\frac{1}{B}\sum_{i=1}^{B}\theta_b^*$. That is, we can correct bias by
$$\widetilde{\theta} = 2\widehat{\theta} - E_{X\sim \mathbb{P}_x}(\widehat{\theta}).$$

- **Parametric bootstrap**
  - Non-parametric bootstrap is to substitute P by $\mathbb{P}_x$.
  - Parametric bootstrap assumes that the distribution P comes from a model $\{P_\theta\}_{\theta\in\Theta}$, and substitutes $P_{\widehat{\theta}}$ for P. In Monte Carlo approximation, it means that we do not draw random samples from $\mathbb{P}_x$, but from P_θ instead.

7.2 Delta method

- Suppose we have an asymptotic normality theorem for $\widehat{\theta} = \widehat{\theta}_n$ (for example, CLT with $\widehat{\theta} = \bar{X}$):
$$\sqrt{n}(\widehat{\theta}_n - \theta) \xrightarrow{\mathcal{L}} N(0, \sigma^2),$$
then we have
$$\widehat{\theta}_n \dot{\sim} N(\theta, \frac{\sigma^2}{n}).$$
where $\dot{\sim}$ is "approximately distributed as". σ can be known or estimated, then we can use $\sigma/\sqrt{n}$ as standard error of $\widehat{\theta}_n$.

- Sometimes we care about $g(\theta)$ instead of θ itself. Then we may estimate $g(\theta)$ by $g(\widehat{\theta})$ (MLE works for instance). If g is differentiable (which implies continuous) at θ and $g'(\theta) \neq 0$, then
$$\sqrt{n}\frac{g(\widehat{\theta}_n) - g(\theta)}{\sigma|g'(\theta)|} \xrightarrow{\mathcal{L}} N(0,1),$$
and then
$$g(\widehat{\theta}_n) \dot{\sim} N\left(g(\theta), \frac{\sigma^2(g'(\theta))^2}{n}\right),$$
which implies the standard error of $g(\widehat{\theta}_n)$ is $\frac{\sigma g'(\theta)}{\sqrt{n}}$.

- θ is unknown, so $g'(\theta)$ is also unknown. If $\widehat{\theta}_n$ is consistent ($\xrightarrow{p}\theta$), and g' is continuous (at θ), then we have (by Slutsky's Theorem)
$$\sqrt{n}\frac{g(\widehat{\theta}_n) - g(\theta)}{\sigma|g'(\widehat{\theta})|} \xrightarrow{\mathcal{L}} N(0,1),$$
and then
$$g(\widehat{\theta}_n) \dot{\sim} N\left(g(\theta), \frac{\sigma^2(g'(\widehat{\theta}))^2}{n}\right).$$

8 Lecture 8: Confidence interval

8.1 Bayesian confidence/probability intervals

- Bayesian approach: everything is in posterior distribution.
- Percentile method.
  - Take two quantiles, q_β and $q_{1-\gamma}$, set β, γ such that
$$Pr(q_\beta \leqslant \theta \leqslant q_{1-\gamma}) = 1 - \alpha.$$
Usually, $\beta = \gamma = \alpha/2$.
  - **HPD** (**highest posterior density**). With posterior density $f_{\theta|x}(u)$, find c such that the region is $E = \{u | f_{\theta|x}(u) \geqslant c\}$, where
$$Pr_{\theta|x}(E) = \int_E f_{\theta|x}(u)du = 1 - \alpha \quad (\text{or} \geqslant 1 - \alpha \text{ if discrete}).$$
It is the shortest interval if $f_{\theta|x}(u)$ is unimodal.

8.2 General confidence intervals

- Main idea: find the distribution of the estimates.

Normal observations: unknown μ, known σ.
Consider an example where $X_1, \cdots, X_n$ are i.i.d. r.v.s with $N(\mu, \sigma^2)$. We are estimating the mean μ by $\bar{X}$. We know that $\bar{X} \sim N\left(\mu, \frac{\sigma^2}{n}\right)$, so $\frac{\bar{X}-\mu}{\sigma/\sqrt{n}} \sim N(0,1)$. Then
$$1 - \alpha = Pr\left[\left|\frac{\bar{X} - \mu}{\sigma/\sqrt{n}}\right| \leqslant z_{\alpha/2}\right] = Pr\left[\bar{X} - \frac{\sigma}{\sqrt{n}} z_{\alpha/2} \leqslant \mu \leqslant \bar{X} + \frac{\sigma}{\sqrt{n}} z_{\alpha/2}\right],$$
where $z_{\alpha/2}$ is the $\alpha/2$-quantile of standard normal $N(0,1)$.

Generally, if $\widehat{\theta}$ is (approximately) $N(\theta, (se(\widehat{\theta}))^2)$, then
$$Pr\left[\widehat{\theta} - se(\widehat{\theta}) z_{\alpha/2} \leqslant \theta \leqslant \widehat{\theta} + se(\widehat{\theta}) z_{\alpha/2}\right] = 1 - \alpha.$$

  - **Bootstrap confidence intervals** (normal case). If $se(\widehat{\theta})$ is unknown (σ is unknown), then we can estimate it via bootstrap (7.1). This works if $\widehat{\theta}$ is (approximately) normal.
  - **Bootstrap "percentile" confidence intervals** (normal case). We can estimate the end points $\widehat{\theta} \pm se(\widehat{\theta}) z_{\alpha/2}$ directly by bootstrap estimates $\widehat{\theta}^*_{\alpha/2}, \widehat{\theta}^*_{1-\alpha/2}$. Recall that we have B bootstrap sample estimates $\widehat{\theta}^*$. $\widehat{\theta}^*_{\alpha/2}$ corresponds to the $\alpha/2$ sample quantile of these B estimates.
  - **Bootstrap pivotal confidence intervals**. We can estimate the $\alpha/2$ and $1-\alpha/2$ quantiles ($q_{\alpha/2}$ and $q_{1-\alpha/2}$) of $\widehat{\theta} - \theta$, by $\widehat{\theta}^*_{\alpha/2} - \widehat{\theta}, \widehat{\theta}^*_{1-\alpha/2} - \widehat{\theta}$. Then
$$\begin{aligned} 1 - \alpha &= \Pr[q_{\alpha/2} \leqslant \widehat{\theta} - \theta \leqslant q_{1-\alpha/2}] \\ &= \Pr[\widehat{\theta} - q_{1-\alpha/2} \leqslant \theta \leqslant \widehat{\theta} - q_{\alpha/2}] \\ &\approx \Pr[\widehat{\theta} - (\widehat{\theta}^*_{1-\alpha/2} - \widehat{\theta}) \leqslant \theta \leqslant \widehat{\theta} - (\widehat{\theta}^*_{\alpha/2} - \widehat{\theta})] \\ &= \Pr[2\widehat{\theta} - \widehat{\theta}^*_{1-\alpha/2} \leqslant \theta \leqslant 2\widehat{\theta} - \widehat{\theta}^*_{\alpha/2}] \end{aligned}$$

Normal observations: unknown μ, unknown σ.

Consider an example where $X_1, \cdots, X_n$ are i.i.d. r.v.s with $N(\mu, \sigma^2)$. We are estimating the mean μ by $\bar{X}$. Let

$$s^2 = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2}.$$

We know that

$$Z = \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \sim N(0,1)$$

$$\chi^2 = \frac{(n-1)s^2}{\sigma^2} \sim \chi^2(n-1)$$

$$t = \frac{Z}{\sqrt{\chi^2/(n-1)}} = \frac{\frac{\bar{X}-\mu}{\sigma/\sqrt{n}}}{\sqrt{\frac{(n-1)s^2}{\sigma^2(n-1)}}} = \sqrt{n}\frac{\bar{X}-\mu}{s} \sim \frac{N(0,1)}{\sqrt{\frac{\chi^2(n-1)}{n-1}}} = t(n-1),$$

since Z and χ^2 are independent. Then

$$\begin{aligned} 1-\alpha &= Pr\left[|t| \leqslant t_{\alpha/2}(n-1)\right] \\ &= Pr\left[\bar{X} - \frac{s}{\sqrt{n}}t_{\alpha/2}(n-1) \leqslant \mu \leqslant \bar{X} + \frac{s}{\sqrt{n}}t_{\alpha/2}(n-1)\right], \end{aligned}$$

where $t_{\alpha/2}(n-1)$ is the $\alpha/2$-quantile of $t(n-1)$, t distribution with $(n-1)$ degree of freedom.

9 Lecture 9: Hypothesis testing

9.1 Setup

- Null hypothesis set $\mathcal{P}_0$; alternative hypothesis set $\mathcal{P}_A$. (Θ_0 and Θ_A if parametric).
- $\mathcal{P}_0 \bigcap \mathcal{P}_0 = \varnothing$; $\mathcal{P}_0 \bigcup \mathcal{P}_0 = \mathcal{P}$.
- Rejection region $\mathcal{R} \subseteq \mathcal{X}$: if data X falls into $\mathcal{R}$, then **reject** null hypothesis; accept null hypothesis if $X \in \mathcal{X}\backslash\mathcal{R}$.
- Errors

Table 1: Testing errors

		Decision	
		Accept H_0	Reject H_0
Truth	H_0	Correct	Type I Error
	H_A	Type II Error	Correct

9.2 Testing evaluation

- Power function, level, size
  - The **power function** is defined as

$$\beta(P) = Pr(X \in \mathcal{R}),$$

where $X \sim P$ and $\mathcal{R}$ is calculated based on the testing method. Note that

$$\beta(P) = \begin{cases} Pr(\text{Type I error}) & \text{if } P \in \mathcal{P}_0 \\ 1 - Pr(\text{Type II error}) & \text{if } P \in \mathcal{P}_A \end{cases}$$

We say that a test is **powerful** if $\beta(P)$ is "large" for $P \in \mathcal{P}_A$.

  - Given $0 \leqslant \alpha \leqslant 1$, a test is of (significance) **level** α if $\sup_{P\in\mathcal{P}_0}\beta(P) \leqslant \alpha$.

– Given $0 \leqslant \alpha \leqslant 1$, a test is of **size** α if $\sup_{P\in\mathcal{P}_0} \beta(P) = \alpha$.

- **Most powerful test**. A test at level α that has higher or equal power than all other tests at level α for all $P \in \mathcal{P}_A$ is called **uniformly most powerful** at level α.

- **Neyman-Pearson lemma**. To test *one* simple hypothesis P_0 against *one* simple alternative hypothesis P_A. Assuming they can be represented by density $f_0(x), f_A(x)$, respectively. On the basis of observed x, the (uniformly) most powerful test exists and is

$$\text{reject } H_0 \text{ if } \frac{f_A(x)}{f_0(x)} \geqslant c,$$

where c is set so that

$$P_0\left[x \in \mathcal{R}\right] = P_0\left[\frac{f_A(x)}{f_0(x)} \geqslant c\right] = \alpha.$$

– Randomized version:

$$\begin{aligned}\text{reject } H_0 \text{ if } \frac{f_A(x)}{f_0(x)} &> c,\\ \text{reject } H_0 \text{ with probability } d \text{ if } \frac{f_A(x)}{f_0(x)} &= c,\\ \text{accept } H_0 \text{ if } \frac{f_A(x)}{f_0(x)} &< c,\end{aligned}$$

where c and $d \in [0,1]$ are set so that

$$P_0\left[x \in \mathcal{R}\right] = P_0\left[\frac{f_A(x)}{f_0(x)} > c\right] + P_0\left[\frac{f_A(x)}{f_0(x)} = c\right] \cdot d = \alpha.$$

Normal observations: most powerful test.

Consider an example where $X_1, \cdots, X_n$ are i.i.d. r.v.s with $N(\mu, \sigma^2)$, where σ is known. We are testing $H_0 : \mu = \mu_0$ against $H_A : \mu = \mu_A$. The most powerful test has rejection region

$$\frac{\frac{1}{\sigma^n(2\pi)^{n/2}} e^{-\frac{1}{2\sigma^2}\sum(X_i-\mu_A)^2}}{\frac{1}{\sigma^n(2\pi)^{n/2}} e^{-\frac{1}{2\sigma^2}\sum(X_i-\mu_0)^2}} = \exp\left(\sum(X_i-\mu_0)^2 - \sum(X_i-\mu_A)^2\right) \geqslant c,$$

which is equivalent to

$$\bar{X} = \frac{1}{n}\sum X_i \geqslant k \text{ if } \mu_A > \mu_0; \bar{X} = \frac{1}{n}\sum X_i \leqslant k \text{ if } \mu_A < \mu_0.$$

The constant k is chosen so that $P_0(\bar{X} \geqslant k) = \alpha$. We know that under H_0 (so that we compute P_0 based on μ_0), $\bar{X} \sim N(\mu_0, \sigma^2/n)$. That is, $\sqrt{n}\frac{\bar{X}-\mu_0}{\sigma} \sim N(0,1)$. Therefore, $k = \mu_0 + \frac{\sigma}{\sqrt{n}} z_\alpha$.
The result here can be extended to composite testing where $H_0 : \mu \leqslant \mu_0$ and $H_A : \mu > \mu_A$.

- **Unbiased test**. A test with power function $\beta(P)$ is unbiased if $\beta(P_A) \geqslant \beta(P_0)$ for every $P_A \in \mathcal{P}_A, P_0 \in \mathcal{P}_0$.

9.3 p-value

- Suppose we have nested rejection regions $\mathcal{R}_{\alpha_1} \subseteq \mathcal{R}_{\alpha_2}$ whenever $\alpha_1 \leqslant \alpha_2$. Given the observed data x, **the observed significance level** (or **p-value**) is defined as

$$p(x) = \inf\{\alpha | x \in \mathcal{R}_\alpha\}.$$

10 Lecture 10: Multiple testing

Suppose we have K tests, $k = 1, 2, \cdots, K$: testing $H_{0k} : \mathcal{P}_{0k}$ against $H_{Ak} : \mathcal{P}_{Ak}$ with rejection region $\mathcal{R}_k$.

10.1 Union-intersection test

- Testing $H_0 : \mathcal{P}_0 = \bigcap_k \mathcal{P}_{0k}^c$ against $H_A : \mathcal{P}_A = (\bigcap_k \mathcal{P}_{0k})^c = \bigcup_k \mathcal{P}_{0k}$.
- Rejection region is $\mathcal{R} = \bigcup_k \mathcal{R}_k$.
- Union bound: $P_0(X \in \mathcal{R}) = P_0(X \in \bigcup_k \mathcal{R}_k) \leqslant \sum_k P_0(X \in \mathcal{R}_k)$.

10.2 Intersection-union test

- Testing $H_0 : \mathcal{P}_0 = \bigcup_k \mathcal{P}_{0k}$ against $H_A : \mathcal{P}_A = (\bigcup_k \mathcal{P}_{0k})^c = \bigcap_k \mathcal{P}_{0k}$.
- Rejection region is $\mathcal{R} = \bigcap_k \mathcal{R}_k$.

10.3 Controlling family-wise error rate

Family-wise error rate (**FWER**): the probability of committing *at least* one error of the first kind. We want to bound it as

$$\text{FWER} = P_0\left(X \in \bigcup_{k=1}^{K} \mathcal{R}_k\right) \leqslant \alpha.$$

- **Bonferroni method**: reject all null hypotheses whose p-value p_k is smaller than α/K. By union bound,

$$\text{FWER} = P_0(X \in \mathcal{R}) = P_0\left(X \in \bigcup_{k=1}^{K} \mathcal{R}_k\right) \leqslant \sum_{k=1}^{K} P_0(X \in \mathcal{R}_{k=1}^K) \leqslant \sum_{k=1}^{K} \frac{\alpha}{K} = \alpha.$$

- **Holm method**.
  - Order p-values as $p_{(1)} \leqslant p_{(2)} \leqslant \cdots \leqslant p_{(K)}$.
  - If $\frac{\alpha}{K} \leqslant p_{(1)}$, then accept all null hypotheses and stop; otherwise reject $H_{0(1)}$ and continue.
  - If $\frac{\alpha}{K-1} \leqslant p_{(2)}$, then accept all remaining null hypotheses and stop; otherwise reject $H_{0(2)}$ and continue.
  - $\cdots$
  - If $\frac{\alpha}{1} \leqslant p_{(K)}$, then accept $H_{0(K)}$ and stop; otherwise reject $H_{0(K)}$ and stop.

10.4 Controlling false discovery rate

Rejecting null hypothesis when it is true means "false discovery" (Type I error).

- **False discovery proportion** (**FDP**) is defined as

$$\text{FDP} = \frac{\#\text{ of false discoveries}}{\#\text{ of all discoveries}},$$

  where the # is counted from K tests.

- **False discovery rate** (**FDR**) is defined as the expectation of FDP, i.e.,

$$\text{FDR} = E(\text{FDP}).$$

  We want to control FDR as FDR$\leqslant \alpha$.

- **Benjamini and Hochberg method**.
  - Order p-values as $p_{(1)} \leqslant p_{(2)} \leqslant \cdots \leqslant p_{(K)}$.
  - Let $l_i = \frac{i\alpha}{KC_K}$, where

$$C_K = \begin{cases} 1 & \text{if tests are independent} \\ \sum_{i=1}^{K} \frac{1}{i} & \text{otherwise} \end{cases}$$

    Let $r = \max\{i | p_{(i)} < l_i\}$.
  - Set $t = p_{(r)}$ as the Benjamini-Hochberg rejection threshold. Reject all null hypotheses whose $p_k \leqslant t$.

11 Lecture 11: Hypothesis testing, practical procedures

11.1 Wald test

- $\widehat{\theta}$ is an estimator of θ. To test $H_0 : \theta = \theta_0$, against the alternative $H_A : \theta \neq \theta_0$. $\frac{\widehat{\theta}-\theta}{se(\widehat{\theta}|\theta)}$ is a good indicator of discrepancy.
- Suppose $\widehat{\theta}$ is (approximately) normal:

$$\sqrt{n}(\widehat{\theta}-\theta) \xrightarrow{\mathcal{L}} N(0,\sigma^2) \Longrightarrow \widehat{\theta} \dot{\sim} N(\theta,(se(\widehat{\theta}|\theta))^2) \Longrightarrow \frac{\widehat{\theta}-\theta}{se(\widehat{\theta}|\theta)} \dot{\sim} N(0,1).$$

- If $se(\widehat{\theta}|\theta)$ is unknown (because θ is unknown), then we can estimate it by

$$se(\widehat{\theta}|\theta) \approx se(\widehat{\theta}|\widehat{\theta}) = \sqrt{Var(\widehat{\theta})}, \text{ or } \sigma^2 \approx \widehat{\sigma}^2.$$

  We reject H_0 if $\frac{\widehat{\theta}-\theta_0}{\sqrt{Var(\widehat{\theta})}}$ is too large or too small. Equivalently, reject H_0 if

$$\frac{(\widehat{\theta}-\theta_0)^2}{Var(\widehat{\theta})} \dot{\sim} \chi^2(1)$$

  is too large.

- In multidimensional case, with (approximately) normality,

$$\sqrt{n}(\widehat{\theta}-\theta) \xrightarrow{\mathcal{L}} N(0,V),$$

  where $V_{p\times p}$ is variance matrix. Then the Wald test becomes reject H_0 if

$$n(\widehat{\theta}-\theta_0)^T V^{-1}(\widehat{\theta}-\theta_0) \dot{\sim} \chi^2(p).$$

  If V unknown, estimate it as $\widehat{V} = V(\widehat{\theta})$ or $\widehat{V} = V(\theta_0)$.

- If $\widehat{\theta}$ is an **MLE** of θ, then

$$V(\theta) = I^{-1}(\theta),$$

  where $I(\theta)$ is the Fisher information matrix for *ONE observation.*
  - In one dimensional case, $Var(\widehat{\theta}) = \frac{1}{nI(\theta)}$.

11.2 Likelihood ratio test

Consider parametric model and its hypotheses $H_0 : \theta \in \Theta_0$ and $H_A : \theta \in \Theta_A$.

- From Neyman-Pearson lemma, the optimal test is based on

$$\frac{f_A(x)}{f_0(x)} = \frac{L(\theta_A)}{L(\theta_0)} \geqslant c.$$

  Or equivalently

$$\log L(\theta_A) - \log L(\theta_0) = l(\theta_A) - l(\theta_0) \geqslant c.$$

- To extend this to multiple hypotheses case, the **likelihood ratio test statistic** is defined as: reject H_0 if

$$\frac{\sup_{\theta\in\Theta_A} L(\theta)}{\sup_{\theta\in\Theta_0} L(\theta)} \geqslant c.$$

  Or alternatively, reject H_0 if

$$\frac{\sup_{\theta\in\Theta} L(\theta)}{\sup_{\theta\in\Theta_0} L(\theta)} \geqslant c.$$

- Let $\widehat{\theta}$ and $\widehat{\theta}_0$ be unconstrained and constrained MLE, respectively. Then the test in logarithm form: reject H_0 if

$$2(l(\widehat{\theta}) - l(\widehat{\theta}_0)) \geqslant c,$$

  where the 2 is to ensure that the statistic has the approximate distribution $\chi^2(p)$, where p is the number of restrictions imposed by the null hypothesis. $l(\theta)$

11.3 Rao score test via Lagrange multipliers

If the null hypothesis is interpreted as a restriction on parameters: $H_0 : g(\theta) = 0$, and the alternative is again $H_A : g(\theta) \neq 0$, then following the idea of Neyman-Pearson, we can check the magnitude of Lagrange multiplier as an indicator of how much the constraint is violated.

- Consider maximizing $l(\theta) - \lambda g(\theta)$. Setting the derivative (in θ) to zero, we have

$$\lambda(\theta) = \frac{l'(\theta)}{g'(\theta)} = \frac{f'(x;\theta)}{f(x;\theta)} \frac{1}{g'(\theta)}.$$

  We reject null if $\left|\frac{\lambda(\theta)}{se(\lambda(\theta))}\right|$ or $\frac{\lambda^2(\theta)}{Var(\lambda(\theta))}$ is too large.

- When $g(\theta) = \theta - \theta_0$, $g'(\theta) = 1$, $Var(\lambda(\theta_0)) = nI(\theta_0)$. Then

$$\frac{\lambda(\theta_0)}{\sqrt{nI(\theta_0)}} \dot{\sim} N(0,1), \frac{\lambda^2(\theta_0)}{nI(\theta_0)} \dot{\sim} \chi^2(1).$$

  Quantiles can be applied to find rejection region.

Score test for Binomial.

$X \sim Bin(n,p)$. To compute the score function and Fisher information:

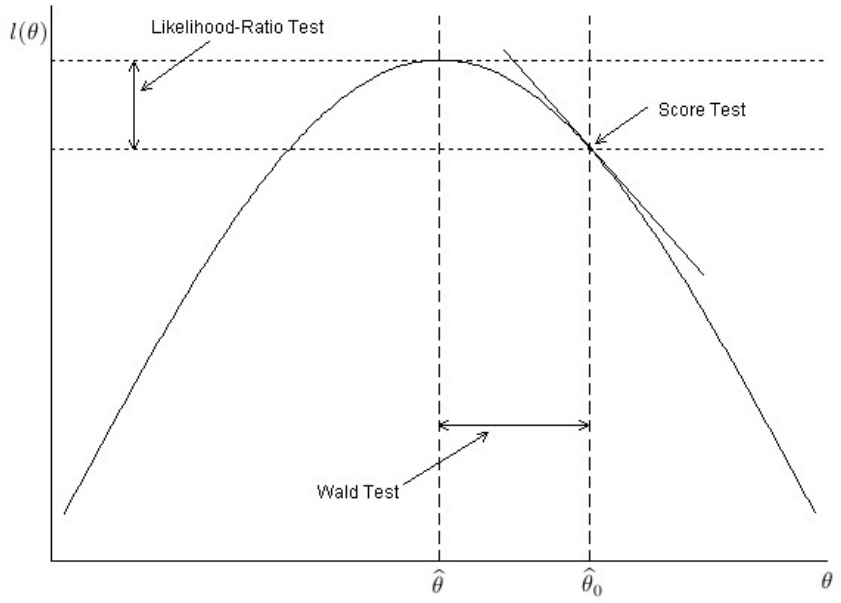
$$\lambda(p) = s(p) = \frac{n(\widehat{p} - p)}{p(1-p)}, nI(p) = \frac{n}{p(1-p)}.$$

Therefore,

$$Z = \frac{\widehat{p} - p_0}{\sqrt{\frac{p_0(1-p_0)}{n}}} \dot{\sim} N(0,1),$$

which is equivalent to Wald test with $se(\widehat{p}|p)$ estimated as $se(\widehat{p}|p_0)$ instead of $se(\widehat{p}|\widehat{p})$.

Figure 1: Illustration of Wald, LRT and Rao tests.



11.4 Bayes factor

To interpret Neyman-Pearson in Bayesian formula, consider averaging instead of maximization: reject H_0 if

$$\frac{\int_{\Theta_A} L(\theta)\pi_A(\theta)d\theta}{\int_{\Theta_0} L(\theta)\pi_0(\theta)d\theta} \geqslant c,$$

where π_A and π_0 are priors over Θ_A and Θ_0.