IB Statistics

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1 Introduction

Statistics is the science of making informed decisions. It can include:

- Design of experiments,
- Graphical exploration of data,
- Formal statistical inference (part of Decision theory),
- Communication of results.

Let $X_1, X_2, ..., X_n$ be independent observations from a distribution $f(x \mid \theta)$, with parameter θ . We wish to make inferences about the value of θ from $X_1, X_2, ..., X_n$. Such inference can include:

- Estimating θ ,
- Quantifying uncertainty in estimates,
- Testing a hypothesis about θ .

1.1 Probability Review

Let Ω be the *sample space* of outcomes in an experiment. A measurable subset of Ω is called an *event*. We denote the set of events as \mathcal{F} .

A function $\mathbb{P}: \mathcal{F} \to [0,1]$ is called a *probability measure* if:

- $\mathbb{P}(\emptyset) = 0$,
- $\mathbb{P}(\Omega) = 1$.
- $\mathbb{P}(\bigcup_i A_i) = \sum_i \mathbb{P}(A_i)$, if (A_i) are disjoint and countable.

A random variable is a (measurable) function $X: \Omega \to \mathbb{R}$.

The distribution function of X is

$$F_X(x) = \mathbb{P}(X \le x).$$

A discrete random variable takes values in a countable subset $E \subset \mathbb{R}$, and its probability mass function or pmf is $p_X(x) = \mathbb{P}(X = x)$.

We say X has continuous distribution if it has a probability density function or pdf, satisfying

$$\mathbb{P}(X \in A) = \int_A f_X(x) \, \mathrm{d}x,$$

for any measurable A. The expectation of X is defined

$$\mathbb{E}[X] = \begin{cases} \sum_{x \in X} x \cdot p_X(x) & X \text{ discrete,} \\ \int x \cdot f_X(x) \, \mathrm{d}x & X \text{ continuous.} \end{cases}$$

If $g: \mathbb{R} \to \mathbb{R}$, then

$$\mathbb{E}[g(x)] = \int g(x) f_X(x) \, \mathrm{d}x.$$

The variance of X is

$$Var(X) = \mathbb{E}[(X - \mathbb{E}[X])^2].$$

We say that X_1, X_2, \ldots, X_n are independent if for all x_1, x_2, \ldots, x_n ,

$$\mathbb{P}(X_1 \le x_1, \dots, X_n \le x_n) = \mathbb{P}(X_1 \le x_1) \cdots \mathbb{P}(X_n \le x_n).$$

If the variables have probability density functions, then

$$f_X(x) = \prod_{i=1}^n f_{X_i}(x_i),$$

where X is the vector of variables (X_1, \ldots, X_n) and x is the vector (x_1, \ldots, x_n) . Importantly, if $a_1, \ldots, a_n \in \mathbb{R}$,

$$\mathbb{E}[a_1X_1 + \dots + a_nX_n] = a_1\mathbb{E}[X_1] + \dots + a_n\mathbb{E}[X_n].$$

Moreover,

$$\operatorname{Var}(a_1 X_1 + \dots + a_n X_n) = \sum_{i,j} a_i a_j \operatorname{Cov}(X_i, X_j).$$

Here the *covariance* of X_i and X_j is

$$Cov(X_i, X_j) = \mathbb{E}[(X_i - \mathbb{E}[X_i])(X_j - \mathbb{E}[X_j])].$$

If $X = (X_1, \dots, X_n)^T$ and $\mathbb{E}[X] = (\mathbb{E}[X_1], \dots, \mathbb{E}[X_n])$, then the linearity of expectation can be rewritten as

$$\mathbb{E}[a^T X] = a^T \mathbb{E}[X],$$

and moreover

$$\operatorname{Var}(a^T X) = a^T \operatorname{Var}(X)a,$$

where Var(X) is the covariance matrix: $(Var(X))_{ij} = Cov(X_i, X_j)$.

1.2 Moment Generating Functions

The moment generating function of a variable X is

$$M_X(t) = \mathbb{E}[e^{tx}].$$

This may only exist for t in some neighbourhood of 0. The important properties of MGFs is that

$$\mathbb{E}[X^n] = \frac{\mathrm{d}^n}{\mathrm{d}t^n} M_X(0),$$

and from this we obtain $M_X = M_Y \iff F_x = F_y$.

MGFs also make it easy to find the distribution function of sums of iid variables.

Example 1.1.

Let X_1, \ldots, X_n be iid Poisson (μ) . Then

$$M_{X_1}(t) = \mathbb{E}[e^{tX_1}] = \sum_{x=0}^{\infty} e^{tx} \cdot \frac{e^{-\mu}\mu^x}{x!}$$
$$= e^{-\mu} \sum_{x=0}^{\infty} \frac{(e^t\mu)^x}{x!} = e^{-\mu} e^{\mu \exp(t)} = e^{-\mu(1-e^t)}.$$

If $S_n = X_1 + \cdots + X_n$, then

$$M_{S_n}(t) = \mathbb{E}[e^{t(X_1 + \dots + X_n)}] = \prod_{i=1}^n \mathbb{E}[e^{tX_i}]$$

= $e^{-\mu(1 - e^t)n}$

This is the same as a $Poisson(\mu n)$ MGF, so $S_n \sim Poisson(\mu \cdot n)$.

1.3 Limit Theorems

We list some important limit theorems, starting with the weak law of large numbers (WLLN). This says if X_1, \ldots, X_n are iid with $\mathbb{E}[X_1] = \mu$, then let $\overline{X_n} = \frac{1}{n} \sum_{i=1}^n X_i$ be the sample mean. WLLN says that for all $\varepsilon > 0$,

$$\mathbb{P}(|\overline{X_n} - \mu| > \varepsilon) \to 0,$$

as $n \to \infty$.

The strong law of large numbers (SLLN) says a stronger result, namely

$$\mathbb{P}(\overline{X_n} \to \mu) = 1,$$

i.e. $\overline{X_n}$ converges to μ almost surely.

The central limit theorem is another important limit theorem. If we take

$$Z_n = \frac{\sqrt{n}(\overline{X_n} - \mu)}{\sigma},$$

where $\sigma^2 = \text{Var}(X_i)$, then Z_n is "approximately" N(0,1) as $n \to \infty$.

What this means is that $\mathbb{P}(Z_n \leq z) \to \Phi(z)$ as $n \to \infty$ for all $z \in \mathbb{R}$, where Φ is the distribution function of a N(0,1) variable.

1.4 Conditioning

Let X and Y be discrete random variables. Their *joint pmf* is

$$p_{X,Y}(x,y) = \mathbb{P}(X = x, Y = y).$$

The marginal pmf is

$$p_X(x) = \mathbb{P}(X = x) = \sum_{y \in Y} p_{X,Y}(x, y).$$

The conditional pmf of X given Y = y is

$$p_{X|Y}(x \mid y) = \mathbb{P}(X = x \mid Y = y) = \frac{\mathbb{P}(X = x, Y = y)}{\mathbb{P}(Y = y)} = \frac{p_{X,Y}(x, y)}{p_Y(y)}.$$

This is defined to be 0 if $p_Y(y) = 0$.

For continuous random variables X, Y, the joint pdf $f_{X,Y}$ has

$$\mathbb{P}(X \le x', y \le y') = \int_{-\infty}^{x'} \int_{-\infty}^{y'} f_{X,Y}(x, y) \, \mathrm{d}y \, \mathrm{d}x.$$

The marginal pdf of Y is

$$f_Y(y) = \int_{-\infty}^{\infty} f_{X,Y}(x,y) \, \mathrm{d}x.$$

The conditional pdf of X given Y is

$$f_{X|Y}(x \mid y) = \frac{f_{X,Y}(x,y)}{f_{Y}(y)}.$$

The *conditional expectation* is given by

$$\mathbb{E}[X \mid Y] = \begin{cases} \sum_{x} x \cdot p_{X|Y}(x \mid y) & X, Y \text{ discrete,} \\ \int_{-\infty}^{\infty} x \cdot f_{X|Y}(x \mid y) \, \mathrm{d}x & X, Y \text{ continuous.} \end{cases}$$

This is a random variable, which is a function of Y. The tower property says that

$$\mathbb{E}[\mathbb{E}[X \mid Y]] = \mathbb{E}[X].$$

Hence we can write the variance of X as follows:

$$\begin{aligned} \operatorname{Var}(X) &= \mathbb{E}[X^2] - (\mathbb{E}[X])^2 \\ &= \mathbb{E}[\mathbb{E}[X^2 \mid Y]] - (\mathbb{E}[\mathbb{E}[X \mid Y]])^2 \\ &= \mathbb{E}[\mathbb{E}[X^2 \mid Y] - (\mathbb{E}[X \mid Y])^2] + \mathbb{E}[\mathbb{E}[X \mid Y]^2] - \mathbb{E}[\mathbb{E}[X \mid Y]]^2 \\ &= \mathbb{E}[\operatorname{Var}(X \mid Y)] + \operatorname{Var}(\mathbb{E}[X \mid Y]). \end{aligned}$$

1.5 Change of Variables

The *change of variables* formula is as follows:

Let $(x,y) \mapsto (u,v)$ be a differentiable bijection. Then,

$$f_{U,V}(u,v) = f_{X,Y}(x(u,v),y(u,v)) \cdot |\det J|,$$

$$J = \frac{\partial(x,y)}{\partial(u,v)} = \begin{pmatrix} \partial x/\partial u & \partial x/\partial v \\ \partial y/\partial u & \partial y/\partial v \end{pmatrix}.$$

1.6 Important Distributions

 $X \sim \text{Negbin}(k, p)$ if X models the time in successive iid Ber(p) trials to achieve k successes. If k = 1, this is the same as a geometric distribution.

 $X \sim \text{Poisson}(\lambda)$ is the limit of $\text{Bin}(n, \lambda/n)$ random variables, as $n \to \infty$.

If $X_i \sim \Gamma(\alpha_i, \lambda)$ for i = 1, ..., n with $X_1, ..., X_n$ independent, then if $S_n = X_1 + \cdots + X_n$,

$$M_{S_n}(t) = \prod_{i=1}^n M_{X_i}(t) = \left(\frac{\lambda}{\lambda - 1}\right)^{\alpha_1 + \dots + \alpha_n}$$

which is the mgf of a $\Gamma(\sum \alpha_i, \lambda)$ random variable. Hence $S_n \sim \Gamma(\sum \alpha_i, \lambda)$.

Also, if $X \sim \Gamma(a, \lambda)$, then for any $b \in (0, \infty)$, $bX \sim \Gamma(a, \lambda/b)$.

Special cases of the Gamma distribution include $\Gamma(1,\lambda) = \text{Exp}(\lambda)$, and $\Gamma(\frac{k}{2},\frac{1}{2}) = \chi_k^2$, the Chi-squared distribution with k degrees of freedom. This can be thought of as the sum of k independent squared N(0,1) random variables.

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2 Estimation

Suppose we observe data X_1, X_2, \ldots, X_n , which are iid from some pdf (or pmf) $f_X(x \mid \theta)$, with θ unknown. We let $X = (X_1, \ldots, X_n)$.

Definition 2.1. An *estimator* is a statistic or a function of the data $T(X) = \hat{\theta}$, which we use to approximate the true parameter θ . The distribution of T(X) is called the *sampling distribution*.

Example 2.1.

If X_1, \ldots, X_n are iid $N(\mu, 1)$, we can define an estimator for the mean as

$$\hat{\mu} = T(X) = \frac{1}{n} \sum_{i=1}^{n} X_i.$$

The sampling distribution of $\hat{\mu}$ is $N(\mu, \frac{1}{n})$.

Definition 2.2. The bias of $\hat{\theta} = T(X)$ is

$$bias(\hat{\theta}) = \mathbb{E}_{\theta}[\hat{\theta}] - \theta.$$

Remark. In general, the bias is a function of θ , even if the notation bias($\hat{\theta}$) does not make that explicit.

Definition 2.3. We say that $\hat{\theta}$ is *unbiased* if $bias(\hat{\theta}) = 0$ for all $\theta \in \Theta$.

Example 2.2.

Out previous estimator

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

is unbiased because $\mathbb{E}_{\mu}[\hat{\mu}] = \mu$ for all $\mu \in \mathbb{R}$.

Definition 2.4. The mean squared error (mse) of $\hat{\theta}$ is

$$mse(\hat{\theta}) = \mathbb{E}_{\theta}[(\hat{\theta} - \theta)^2].$$

Like the bias, the mean squared error of $\hat{\theta}$ is a function of θ .

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2.1 Bias-Variance Decomposition

We can write the mean squared error as

$$\begin{split} \operatorname{mse}(\hat{\theta}) &= \mathbb{E}_{\theta}[(\hat{\theta} - \theta)^2] = \mathbb{E}_{\theta}[(\hat{\theta} - \mathbb{E}_{\theta}[\hat{\theta}] + \mathbb{E}_{\theta}[\hat{\theta}] - \theta)^2] \\ &= \operatorname{Var}_{\theta}(\hat{\theta}) + \operatorname{bias}^2(\hat{\theta}) + 2\underbrace{\left[\mathbb{E}_{\theta}[(\hat{\theta} - \mathbb{E}_{\theta}[\hat{\theta}])]\right]}_{0}(\mathbb{E}_{\theta}[\hat{\theta}] - \theta). \end{split}$$

The two terms on the right hand side are non-negative, so there is a trade off between bias and variance.

$\overline{\text{Example 2.3}}$.

Let $X \sim \text{Bin}(n, \theta)$, where n is known, and we wish to estimate θ . The standard estimator is

$$T_u = \frac{X}{n}, \quad \mathbb{E}_{\theta}[T_u] = \frac{\mathbb{E}_{\theta}[X]}{n} = \theta.$$

Hence T_u is unbiased. We can also calculate the mean squared error as

$$\operatorname{mse}(T_u) = \operatorname{Var}_{\theta}(T_u) = \frac{\operatorname{Var}_{\theta}(X)}{n^2} = \frac{n\theta(1-\theta)}{n^2} = \frac{\theta(1-\theta)}{n}.$$

Consider a second estimator

$$T_B = \frac{X+1}{n+2} = w\frac{X}{n} + (1-w)\frac{1}{2},$$

for $w = \frac{n}{n+2}$. In this case T_B is interpolating between our unbiased estimator, and the constant estimator. The bias of T_B is

bias
$$(T_B) = \mathbb{E}_{\theta}[T_B] - \theta = \mathbb{E}[\frac{X+1}{n+2}] - \theta = \frac{1}{n+2} - \frac{2}{n+2}\theta.$$

This is not equal to zero for all but one value of θ . Hence, T_B is biased. We can also calculate the variance

$$\operatorname{Var}_{\theta}(T_B) = \frac{1}{(n+2)^2} n\theta (1-\theta) - w^2 \frac{\theta (1-\theta)}{n},$$

$$\operatorname{mse}(T_B) = \operatorname{Var}_{\theta}(T_B) + \operatorname{bias}^2(T_B)$$

$$= w^2 \frac{\theta (1-\theta)}{n} + (1-w)^2 \left(\frac{1}{2} - \theta\right)^2.$$

Hence the mse of the biased estimator is a weighted average of the mse of the unbiased estimator, and a parabola. For θ around 1/2, the biased estimator has a lower mse than the unbiased estimator.

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The message here is that our prior judgements about θ affect our choice of estimator, and unbiasedness is not always desirable.

Example 2.4.

Suppose $X \sim \text{Poisson}(\lambda)$. We wish the estimate $\theta = \mathbb{P}(X = 0)^2 = e^{-2\lambda}$. For an estimator T(X) to be unbiased, we must have for all λ ,

$$\mathbb{E}_{\lambda}[\hat{\theta}] = \sum_{x=0}^{\infty} T(x) \frac{e^{-\lambda} \lambda^{x}}{x!} = e^{-2\lambda} = \theta$$

$$\iff \sum_{x=0}^{\infty} T(x) \frac{\lambda^{x}}{x!} = e^{-\lambda} = \sum_{x=0}^{\infty} (-1)^{x} \frac{\lambda^{x}}{x!}.$$

For this to hold for all $\lambda \geq 0$, we should take $T(X) = (-1)^X$. But this estimator makes no sense.

2.2 Sufficiency

Suppose X_1, \ldots, X_n are iid random variables from a distribution with pdf (or pmf) $f_X(\cdot \mid \theta)$. Let $X = (X_1, \ldots, X_n)$.

The question is: is there a statistic T(X) which contains all the information in X needed to estimate θ ?

Definition 2.5. A statistic T is *sufficient* for θ if the conditional distribution of X given T(X) does not depend on θ .

Note θ and T(X) may be vector-valued.

Example 2.5.

Let X_1, \ldots, X_n be iid $Ber(\theta)$ for $\theta \in [0, 1]$. Then,

$$f_X(\cdot \mid \theta) = \prod_{i=1}^n \theta^{x_i} (1 - \theta)^{1 - x_i} = \theta^{x_1 + \dots + x_n} (1 - \theta)^{n - x_1 - \dots - x_n}.$$

This only depends on X through

$$T(X) = \sum_{i=1}^{n} x_i.$$

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Indeed, for x with $x_1 + \cdots + x_n = t$,

$$f_{X|T=t}(x \mid T(x) = t) = \frac{\mathbb{P}_{\theta}(X = x, T(X) = t)}{\mathbb{P}_{\theta}(T(X) = t)} = \frac{\mathbb{P}_{\theta}(X = x)}{\mathbb{P}_{\theta}(T(x) = t)}$$
$$= \frac{\theta^{x_1 + \dots + x_n} (1 - \theta)^{n - x_1 - \dots - x_n}}{\binom{n}{t} \theta^t (1 - \theta)^{n - t}} = \binom{n}{t}^{-1},$$

and otherwise this probability is 0. As this doesn't depend on θ , T(X) is sufficient for θ .

Theorem 2.1 (Factorization criterion). T is sufficient for θ if and only if

$$f_X(x \mid \theta) = g(T(x), \theta) \cdot h(x),$$

for suitable functions g, h.

Proof: We only do the discrete case.

Suppose that $f_X(x \mid \theta) = g(T(x), \theta)h(x)$. If T(x) = t, then

$$f_{X|T=t}(x \mid T=t) = \frac{\mathbb{P}_{\theta}(X=x, T(X)=t)}{\mathbb{P}_{\theta}(T(X)=t)}$$

$$= \frac{g(T(x), \theta)h(x)}{\sum_{T(x')=t} g(T(x'), \theta)h(x')}$$

$$= \frac{g(t, \theta)}{g(t, \theta)} \cdot \frac{h(x)}{\sum_{T(x')=t} h(x')}.$$

This doesn't depend on θ , so T(X) is sufficient. Conversely, if T(X) is sufficient, then

$$\mathbb{P}_{\theta}(X = x) = \mathbb{P}_{\theta}(X = x, T(X) = t)$$

$$= \underbrace{\mathbb{P}_{\theta}(T(X) = t)}_{g(t,\theta)} \cdot \underbrace{\mathbb{P}_{\theta}(X = x \mid T(X) = t)}_{h(x)}.$$

Therefore the pmf of X factorizes.

Example 2.6.

Return to our example from before, where X_1, \ldots, X_n are iid Ber(θ). Then

$$f_X(x \mid \theta) = \theta^{x_1 + \dots + x_n} (1 - \theta)^{n - x_1 - \dots - x_n}.$$

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Hence if we take $g(t,\theta) = \theta^t(1-\theta)^{n-t}$, and h(x) = 1, we immediately get that $T(X) = \sum x_i$ is sufficient.

Example 2.7.

Let X_1, \ldots, X_n be iid $U([0, \theta])$, for $\theta > 0$. Then,

$$f_X(x \mid \theta) = \prod_{i=1}^n \frac{1}{\theta} \mathbb{1}(X_i \in [0, \theta])$$
$$= \underbrace{\frac{1}{\theta^n} \mathbb{1}(\max_i x_i \le \theta)}_{q(T(x), \theta)} \underbrace{\mathbb{1}(\min_i x_i \ge 0)}_{h(x)}.$$

Hence $T(x) = \max_i x_i$ is a sufficient statistic for θ .

2.3 Minimal Sufficiency

Sufficient statistics are not unique. Indeed, any one-to-one function of a sufficient statistic is also sufficient. Also T(X) = X is always sufficient, but not very useful.

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Definition 2.6. A sufficient statistic T is minimal sufficient if it is a function of any other sufficient statistic, so if T' is also sufficient, then

$$T'(x) = T'(y) \implies T(x) = T(y),$$

for all x, y in our space.

By this definition, any two minimal sufficient statistics T, T' are in bijection with each other, so

$$T(x) = T(y) \iff T'(x) = T'(y).$$

Theorem 2.2. Suppose that T(X) is a statistic such that

$$\frac{f_X(x\mid\theta)}{f_X(y\mid\theta)}$$

is constant as a function of θ , if and only if T(x) = T(y). Then T is minimal sufficient.

Let $x \stackrel{1}{\sim} y$ if

$$\frac{f_X(x \mid \theta)}{f_X(y \mid \theta)}$$

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is constant in θ . It is easy to check that $\stackrel{1}{\sim}$ is an equivalence relation.

Similarly, for a given statistic T, $x \stackrel{2}{\sim} y$ if T(x) = T(y) defines another equivalence relation.

The condition of the theorem says that $\stackrel{1}{\sim}$ and $\stackrel{2}{\sim}$ are the same for minimal sufficient statistics.

Remark. We can always construct a statistic T which is constant on the equivalence classes of $\stackrel{1}{\sim}$, which by the theorem is minimal sufficient.

Proof: For any value of T, let z_t be a representative from the equivalence class

$$\{x \mid T(x) = t\}.$$

Then,

$$f_X(x \mid \theta) = f_X(z_{T(x)} \mid \theta) \frac{f_X(x, \theta)}{f_X(z_{T(x)} \mid \theta)}.$$

This is exactly in the form g(T(x),t)h(x), so by the factorization criterion T is sufficient.

To prove that T is minimal, take any other sufficient statistic S. We want to show that if S(x) = S(y), then T(x) = T(y).

By the factorization criterion, there are functions g_s, h_s such that

$$f_X(x,\theta) = g_s(S(x),\theta)h_s(x).$$

Suppose S(x) = S(y). Then the ratio

$$\frac{f_X(x \mid \theta)}{f_X(y \mid \theta)} = \frac{g_s(S(x), \theta)h_s(x)}{g_s(S(y), \theta)h_s(y)} = \frac{h_s(x)}{h_s(y)},$$

is independent of θ . Hence $x \stackrel{1}{\sim} y$. By the hypothesis, we get that T(x) = T(y).

Remark. Sometimes the range of X depends on θ . In this case we can interpret

$$\frac{f_X(x \mid \theta)}{f_Y(y \mid \theta)}$$
 constant in θ ,

to mean that

$$f_X(x \mid \theta) = c(x, y) f_X(y \mid \theta),$$

for some function c which does not depend on θ .

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Example 2.8.

Suppose that X_1, \ldots, X_n are iid $N(\mu, \sigma^2)$, with parameters (μ, σ^2) unknown. Then,

$$\frac{f_X(x \mid t)}{f_X(y \mid t)} = \frac{(2\pi\sigma^2)^{-n/2} \exp(-\frac{1}{2\sigma^2} \sum (x_i - \mu)^2)}{(2\pi\sigma^2)^{-n/2} \exp(-\frac{1}{2\sigma^2} \sum (y_i - \mu)^2)}$$
$$= \exp\left[-\frac{1}{2\sigma^2} \left(\sum x_i^2 - \sum y_i^2\right) + \frac{\mu}{\sigma^2} \left(\sum x_i - \sum y_i\right)\right].$$

Hence if $\sum x_i^2 = \sum y_i^2$ and $\sum x_i = \sum y_i$, this ratio does not depend on (μ, σ^2) . The converse is also true: if the ratio does not depend on (μ, σ^2) , then we must have $\sum x_i^2 = \sum y_i^2$ and $\sum x_i = \sum y_i$. By the theorem, $T(x) = (\sum x_i^2, \sum x_i)$ is minimal sufficient.

Recall that bijections of T are also minimal sufficient. A more common way of expressing a minimal sufficient statistic in this model is $S(X) = (\bar{X}, S_{xx})$, where

$$\bar{X} = \frac{1}{n} \sum_{i} X_{i}, \qquad S_{xx} = \sum_{i} (X_{i} - \bar{X})^{2}.$$

In this example, (μ, σ^2) and T(X) are both 2-dimensional. In general, the parameter and sufficient statistic can have different dimensions.

For example, if X_1, \ldots, X_n are iid $N(\mu, \mu^2)$, where $\mu \geq 0$, then the minimal sufficient statistic is $S(X) = (\bar{X}, S_{xx})$.

2.4 Rao-Blackwell Theorem

So far we have written \mathbb{E}_{θ} and \mathbb{P}_{θ} to denote the expectations and probabilities in the model where X_1, \ldots, X_n are iid drawn from $f_X(\cdot \mid \theta)$. From now on, we drop the subscript θ .

Theorem 2.3 (Rao-Blackwell Theorem). Let T be a sufficient statistic for θ . Let $\tilde{\theta}$ be some estimator for θ , with $\mathbb{E}[\tilde{\theta}^2] < \infty$ for all θ . Define a new estimator $\hat{\theta} = \mathbb{E}[\tilde{\theta} \mid T(X)]$. Then, for all θ ,

$$\mathbb{E}[(\hat{\theta} - \theta)^2] \le \mathbb{E}[(\tilde{\theta} - \theta)^2],$$

with equality if and only if $\tilde{\theta}$ is a function of T(X).

Remark. $\hat{\theta}$ is a valid estimator, as it does not depend on θ , only on X, as T is sufficient:

$$\hat{\theta}(T(x)) = \int \tilde{\theta}(x) f_{X|T}(x|T) dx,$$

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where neither $\tilde{\theta}$ nor the conditional distribution depend on θ .

The message is that we can improve the mean squared error of any estimator $\tilde{\theta}$ by taking a conditional expectation given T(X).

Proof: By the tower property,

$$\mathbb{E}[\hat{\theta}] = \mathbb{E}[\mathbb{E}[\tilde{\theta} \mid T]] = \mathbb{E}[\tilde{\theta}].$$

So $bias(\hat{\theta}) = bias(\tilde{\theta})$ for all θ . By the conditional variance formula,

$$Var(\tilde{\theta}) = \mathbb{E}[Var(\tilde{\theta} \mid T)] + Var(\mathbb{E}[\tilde{\theta} \mid T])$$
$$= \mathbb{E}[Var(\tilde{\theta} \mid T)] + Var(\hat{\theta}).$$

Hence $Var(\tilde{\theta}) \geq Var(\hat{\theta})$ for all θ . Hence $mse(\tilde{\theta}) \geq mse(\hat{\theta})$.

Note that $\operatorname{Var}(\hat{\theta} \mid T) > 0$ with some positive probability unless $\hat{\theta}$ is a function of T(X). So $\operatorname{mse}(\hat{\theta}) > \operatorname{mse}(\hat{\theta})$ unless $\tilde{\theta}$ is a function of T(X).

Example 2.9.

Say X_1, \ldots, X_n are iid Poisson(λ). We wish to estimate $\theta = \mathbb{P}(X_1 = 0) = e^{-\lambda}$. Then

$$f_X(x \mid \lambda) = \frac{e^{-n\lambda} \lambda^{x_1 + \dots + x_n}}{x_1! \cdots x_n!}$$
$$= \frac{\theta^n (-\log \theta)^{x_1 + \dots + x_n}}{x_1! \cdots x_n!}$$

Letting $h(x) = 1/(x_1! \cdots x_n!)$, $g(T(x), \theta) = \theta^n(-\log \theta)^{T(x)}$, by the factorization criterion, $T(x) = \sum x_i$ is a sufficient statistic. Let $\tilde{\theta} = \mathbb{1}(X_i = 0)$. This is unbiased, but only uses one observation X_1 . Using Rao-Blackwell, we can find

$$\hat{\theta} = \mathbb{E}[\tilde{\theta} \mid T = t] = \mathbb{P}\left(X_1 = 0 \mid \sum_{i=1}^n X_i = t\right)$$

$$= \frac{\mathbb{P}(X_1 = 0, X_1 + \dots + X_n = t)}{\mathbb{P}(X_1 + \dots + X_n = t)} = \frac{\mathbb{P}(X_1 = 0, X_2 + \dots + X_n = t)}{\mathbb{P}(X_1 + \dots + X_n = t)}$$

$$= \frac{\mathbb{P}(X_1 = 0)\mathbb{P}(X_2 + \dots + X_n = t)}{\mathbb{P}(X_1 + \dots + X_n = t)} = \frac{e^{-\lambda}\mathbb{P}(\text{Poisson}((n-1)\lambda) = t)}{\mathbb{P}(\text{Poisson}(n\lambda) = t)}$$

$$= \frac{e^{-n\lambda}((n-1)\lambda)^t/t!}{e^{-n\lambda}(n\lambda)^t/t!} = \left(1 - \frac{1}{n}\right)^t.$$

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So $\hat{\theta} = (1 - \frac{1}{n})^{x_1 + \dots + x_n}$ is an estimator which by the Rao-Blackwell theorem has $\operatorname{mse}(\hat{\theta}) < \operatorname{mse}(\tilde{\theta})$.

As $n \to \infty$,

$$\hat{\theta} = \left(1 - \frac{1}{n}\right)^{n\bar{x}} \stackrel{n \to \infty}{\to} e^{-\bar{x}},$$

and by the strong law of large numbers

$$\bar{x} \to \mathbb{E}[X_1] = \lambda.$$

so
$$\hat{\theta} \to e^{-\lambda}$$
.

Example 2.10.

Let X_1, \ldots, X_n be iid $U([0, \theta])$ where θ is unknown and $\theta \ge 0$. Then recall $T(X) = \max_i X_i$ is sufficient for θ .

Let $\tilde{\theta} = 2X_1$, which is unbiased. Then,

$$\begin{split} \hat{\theta} &= \mathbb{E}[\tilde{\theta} \mid T = t] = 2\mathbb{E}[X_1 \mid \max_i X_i = t] \\ &= 2\mathbb{E}[X_1 \mid \max_i X_i = t, \max_i X_i = X_1] \mathbb{P}(\max_i X_i = X_1 \mid \max_i X_i = t) \\ &+ 2\mathbb{E}[X_1 \mid \max_i X_i = t, \max_i X_i \neq X_1] \mathbb{P}(\max_i X_i \neq X_1 \mid \max_i X_i = t) \\ &= \frac{2t}{n} + \frac{2(n-1)}{n} \mathbb{E}[X_1 \mid X_1 \leq t, \max_{i>1} X_i = t] = \frac{2t}{n} + \frac{2(n-1)}{n} \frac{t}{2} = \frac{n+1}{n} t. \end{split}$$

So $\hat{\theta} = \frac{n+1}{n} \max_i X_i$ is a valid estimator with $\operatorname{mse}(\hat{\theta}) < \operatorname{mse}(\tilde{\theta})$.

2.5 Maximum Likelihood Estimation

Let $X = (X_1, ..., X_n)$ have joint pdf (or pmf) $f_X(X \mid \theta)$.

Definition 2.7. The likelihood function is

$$L: \theta \mapsto f_X(X \mid \theta).$$

The maximum likelihood estimator is any value of θ maximizing $L(\theta)$.

If X_1, \ldots, X_n are iid each with pdf (or pmf) $f_X(\cdot \mid \theta)$, then

$$L(\theta) = \prod_{i=1}^{n} f_X(x_i \mid \theta).$$

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We will denote the logarithm

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} \log f_X(x_i \mid \theta).$$

Example 2.11.

If X_1, \ldots, X_n are iid $Ber(\theta)$, then

$$\ell(\theta) = \left(\sum x_i\right) \log \theta = \left(n - \sum_{x_i}\right) \log(1 - \theta),$$

and the derivative

$$\frac{\partial \ell}{\partial \theta} = \frac{\sum x_i}{\theta} - \frac{n - \sum x_i}{1 - \theta}.$$

This is zero if and only if $\theta = \frac{1}{n} \sum x_i = \bar{X}$.

Hence \bar{X} is the maximum likelihood estimator for θ , and is unbiased as $\mathbb{E}[\bar{X}] = 0$.

Example 2.12.

If X_1, \ldots, X_n are iid $N(\mu, \sigma^2)$, then

$$\log(\mu, \sigma^2) = -\frac{n}{2}\log(2\pi) - \frac{n}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^n (x_i - \mu)^2.$$

This is maximized when $\partial \ell/\partial \mu = \partial \ell/\partial \sigma^2 = 0$. First, we get

$$\frac{\partial \ell}{\partial \mu} = -\frac{1}{\sigma^2} \sum_{i=1}^{n} (x_i - \mu),$$

which is equal to zero when $\mu = \bar{X}$. Then

$$\frac{\partial \ell}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (x_i - \mu)^2.$$

This is zero when

$$\sigma^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2 = \frac{1}{n} S_{xx}.$$

Hence $(\hat{\mu}, \hat{\sigma}^2) = (\bar{X}, S_{xx}/n)$ give the maximum likelihood estimator in this model.

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Note that $\hat{\mu} = \bar{X}$ is unbiased. Now we want to see if $\hat{\sigma}^2$ is biased. We could compute it directly, but later in the course we will show that

$$\frac{S_{xx}}{\sigma^2} = \frac{n\hat{\sigma}^2}{\sigma^2} \sim \chi_{n-1}^2,$$

hence

$$\mathbb{E}[\hat{\sigma}^2] = \mathbb{E}[\chi_{n-1}^2] \frac{\sigma^2}{n} = \frac{n-1}{n} \sigma^2 \neq \sigma^2,$$

which is biased, but asymptotically unbiased.

$\overline{\text{Example 2.13}}$.

Let X_1, \ldots, X_n be iid $U([0, \theta])$. Then

$$L(\theta) = \frac{1}{\theta^n} \mathbb{1}(\max_i X_i \le \theta).$$

We can see from the plot that $\hat{\theta}_{mle} = \max_i X_i$ is the maximum likelihood estimator for θ . We also started from an unbiased estimator, and using Rao-Blackwellization we found an estimator

$$\hat{\theta} = \frac{n+1}{n} \max_{i} X_{i}.$$

This is also unbiased. So in this model the mle is biased as

$$\mathbb{E}[[\hat{\theta}_{\text{mle}}] = \mathbb{E}\left[\frac{n+1}{n}\hat{\theta}\right] = \frac{n}{n+1}\theta,$$

however it is asymptotically unbiased.

The maximum likelihood estimator has the following properties:

1. If T is a sufficient statistic, then the maximum likelihood estimator is a function of T(X). By the factorization criterion,

$$L(\theta) = q(T(X), \theta)h(X).$$

If T(x) = T(y), then the likelihood function with data x and y is the same up to a multiplicative constant. Hence the maximum likelihood estimator in each case is the same.

2. If $\phi = h(\theta)$ where h is a bijection, then the maximum likelihood estimator of

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 ϕ is

$$\hat{\phi} = h(\hat{\theta}),$$

where $\hat{\theta}$ is the maximum likelihood estimator of θ .

3. Asymptotically, we have normality. This says $\sqrt{n}(\hat{\theta} - \theta)$ is approximately normal with mean 0 when n is large. Under some regularity conditions, for a measurable set A,

$$\mathbb{P}(\sqrt{n}(\hat{\theta} - \theta) \in A) \stackrel{n \to \infty}{\to} \mathbb{P}(Z \in A),$$

where $Z \sim N(0, \Sigma)$. This holds for all regular values of θ .

Here Σ is some function of ℓ , and there is a theorem (Cramer-Rao) which says this is the smallest variance attainable.

4. Sometimes, if the maximum likelihood estimator is not available analytically, we can find it numerically.

2.6 Confidence Intervals

Definition 2.8. A $(100 \cdot \gamma)\%$ confidence interval for a parameter θ is a random interval (A(X), B(X)) such that

$$\mathbb{P}(A(X) \le \theta \le B(X)) = \gamma,$$

for all values of θ .

The frequentist interpretation of the confidence interval is:

There exists some fixed true parameter θ . We repeat the experiment many times. On average, $100 \cdot \gamma\%$ of the time the interval (A(X), B(X)) contains θ .

The incorrect interpretation is:

Having observed X = x, there is a probability γ that θ is in (A(x), B(x)).

Example 2.14.

Let X_1, \ldots, X_n be iid $N(\theta, 1)$. To find a 95% confidence interval for θ , we know that

$$\bar{X} = \frac{1}{n} \sum_{x_i} \sim N\left(\theta, \frac{1}{n}\right).$$

Hence

$$Z = \sqrt{n}(\bar{X} - \theta) \sim N(0, 1).$$

Z has this distribution for all θ . Then let z_1, z_2 be any two numbers such

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that $\Phi(z_2) - \Phi(z_1) = 0.95$. Then,

$$\mathbb{P}(z_1 \le \sqrt{n}(\bar{X} - \theta) \le z_2) = 0.95.$$

Rearranging,

$$\mathbb{P}\left(\bar{X} - \frac{z_2}{\sqrt{n}} \le \theta \le \bar{X} - \frac{z_1}{\sqrt{n}}\right) = 0.95.$$

Therefore $(\bar{X} - \frac{z_2}{\sqrt{n}}, \bar{X} - \frac{z_1}{\sqrt{n}})$ is a 95% confidence interval.

There are multiple ways to choose z_1, z_2 . Usually we minimise the width of the interval, which is achieved by $z_1 = \Phi^{-1}(0.025), z_2 = \Phi^{-1}(0.975)$.

To find a confidence interval, we can do the following:

1. Find some quantity $R(X, \theta)$ such that the \mathbb{P}_{θ} distribution of $R(X, \theta)$ does not depend on θ . This is called a *pivot*.

For example, we chose $Z = \sqrt{n}(\bar{X} - \mu) \sin N(0, 1)$.

2. Write down a probabilistic statement about the pivot of the form

$$\mathbb{P}(c_1 \le R(x, \theta) \le c_2) = \gamma,$$

by using quantiles c_1, c_2 of the distribution of $R(X, \theta)$ (typically N(0, 1) or χ_p^2).

3. Rearrange the inequalities to leave θ in the middle.

Proposition 2.1. If T is a monotone increasing function $T: \mathbb{R} \to \mathbb{R}$, and (A(X), B(X)) is a $100 \cdot \gamma\%$ confidence interval for θ , then (T(A(X)), T(B(X))) is a confidence interval for $T(\theta)$.

Remark. When θ is a vector, we talk about confidence sets.

Example 2.15.

Let X_1, \ldots, X_n be iid $N(0, \sigma^2)$. We want to find a 95% confidence interval for σ^2 .

Note that $\frac{X_i}{\sigma} \sim N(0,1)$, so using all the data points,

$$R(X, \sigma^2) = \sum_{i=1}^n \frac{X_i^2}{\sigma^2} \sim \chi_n^2$$

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is a pivot. Let $c_1 = F_{\chi_n^2}^{-1}(0.025)$, $c_2 = F_{\chi_n^2}^{-1}(0.975)$. Then,

$$\mathbb{P}(c_1 \le R(X, \sigma^2) \le c_2) = 0.95.$$

Rearranging,

$$\mathbb{P}\left(\frac{\sum x_i^2}{c_2} \le \sigma^2 \le \frac{\sum x_i^2}{c_1}\right) = 0.95.$$

Hence $\left[\sum x_i^2/c_2, \sum x_i^2/c_1\right]$ is a 95% confidence interval σ^2 .

Applying the proposition, $[\sqrt{\sum x_i^2/c_2}, \sqrt{\sum x_i^2/c_1}]$ is a 95% confidence interval for σ .

Example 2.16.

Let X_1, \ldots, X_n be Ber(p), for n. To find an approximate 95% for confidence interval p.

Recall that the maximum likelihood estimator for p is

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

By the central limit theorem, when n is large, \hat{p} is approximately $N(p, \frac{p(1-p)}{n})$. Hence,

$$\sqrt{n} \frac{(\hat{p}-p)}{\sqrt{p(1-p)}} \sim N(0,1),$$

approximately. If $z = \Phi^{-1}(0.975)$, then

$$\mathbb{P}\left(-z \le \frac{\sqrt{n}(\hat{p} - p)}{\sqrt{p(1 - p)}} \le z\right) \approx 0.95.$$

Rearranging this is tricky. Instead, we argue that $n \to \infty$, $\hat{p}(1-\hat{p}) \to p(1-p)$. So replacing this in the denominator,

$$\mathbb{P}\left(-z \le \frac{\sqrt{n}(\hat{p} - p)}{\sqrt{\hat{p}(1 - \hat{p})}} \le z\right) \approx 0.95.$$

Rearranging this, we get

$$\mathbb{P}\bigg(\hat{p} - z \frac{\sqrt{\hat{p}(1-\hat{p})}}{\sqrt{n}} \le p\hat{p} + z \frac{\sqrt{\hat{p}(1-\hat{p})}}{\sqrt{n}}\bigg) \approx 0.95.$$

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Hence this is an approximate 95% confidence interval for p.

Note that $z\approx 1.96$ and $\sqrt{\hat{p}(1-\hat{p})}\leq \frac{1}{2}$ for all $\hat{p}\in (0,1)$. So a conservative confidence interval is $[\hat{p}\pm 1.96\cdot \frac{1}{2}\cdot \frac{1}{\sqrt{n}}]$.

2.7 Interpreting Confidence Intervals

Suppose X_1, X_2 are iid $U[\theta - \frac{1}{2}, \theta + \frac{1}{2}]$. We find a sensible 50% confidence interval for θ . Consider

$$\mathbb{P}(\theta \text{ between } X_1, X_2) = \mathbb{P}(\min(X_1, X_2) \le \theta \le \max(X_1, X_2))$$
$$= \mathbb{P}(X_1 \le \theta \le X_2) + \mathbb{P}(X_2 \le \theta \le X_1)$$
$$= \frac{1}{4} + \frac{1}{4} = \frac{1}{2}.$$

Hence we can immediately conclude that $(\min(X_1, X_2), \max(X_1, X_2))$ is a 50% confidence interval for θ .

This does not mean for specific $X_1 = x_1$, $X_2 = x_2$ the value θ lies in $(\min(x_1, x_2), \max(x_1, x_2))$ with probability $\frac{1}{2}$: consider when $|x_1 - x_2| > \frac{1}{2}$.

In this case, we can be sure that θ is in $(\min(x_1, x_2), \max(x_1, x_2))$, as the value θ can be at most distance $\frac{1}{2}$ from x_1 and x_2 .

However the frequentist interpretation makes sense: if we repeat the experiment many times, we see $\theta \in (\min(X_1, X_2), \max(X_1, X_2))$ exactly 50% of the time. We cannot say, given a specific observation that we are 50% certain that θ is in the confidence interval.

3 Bayesian Inference

So far, we have assumed there is some true parameter θ . That data X has pdf (or pmf) $f_X(\cdot \mid \theta)$.

Bayesian analysis is a different framework, where we treat θ as a random variable, taking values in Θ .

We begin by assigning to θ a prior distribution $\pi(\theta)$, which represents the opinions or information about θ before seeing on any data.

Conditional on θ , the data X has pdf (or pmf) $f_X(x \mid \theta)$. Having observed a specific value of X = x, this information is combined with the prior to form the *posterior distribution* $\pi(\theta \mid x)$, which is the conditional distribution of θ given X = x. By Bayes' rule,

$$\pi(\theta \mid x) = \frac{\pi(\theta) \cdot f_X(x \mid \theta)}{f_X(x)},$$

where $f_X(x)$ is the marginal probability of X, and

$$f_X(x) = \begin{cases} \int_{\Theta} f_X(x \mid \theta) \pi(\theta) d\theta & \theta \text{ continuous,} \\ \sum_{\Theta} f_X(x \mid \theta) \pi(\theta) & \theta \text{ discrete.} \end{cases}$$

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