IB Statistics

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Based on Lectures by Dr. Sergio Bacallado

February 2, 2023

Contents

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

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

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

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

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

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

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 $a_1, \ldots, a_n \in \mathbb{R}$,

$$\mathbb{E}[a_1 X_1 + \cdots + a_n X_n] = a_1 \mathbb{E}[X_1] + \cdots + a_n \mathbb{E}[X_n].$$

Moreover,

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

Here the *covariance* of X_i and X_j is

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

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

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

and moreover

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

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

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

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

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

$$\begin{aligned} M_{S_n}(t) = \mathbb{E}[e^{t(X_1+\cdots+X_n)}] &= \prod_{i=1}^{n} \mathbb{E}[e^{tX_i}] \\ &= e^{-\mu(1-e^t)n} \end{aligned}$$

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

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 $\sigma^2 = \mathrm{Var}(X_i)$, 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

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

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:

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

1.5 Change of Variables

The *change of variables* formula is as follows:

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

$$\begin{aligned} f_{U,V}(u, v) &= f_{X,Y}(x(u, v), y(u, v)) \cdot |\det J|, \\ J &= \frac{\partial(x, y)}{\partial(u, v)} = \begin{pmatrix} \partial x/\partial u & \partial x/\partial v \\ \partial y/\partial u & \partial y/\partial v \end{pmatrix}. \end{aligned}$$

1.6 Important Distributions

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

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

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

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

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 $\Gamma(1, \lambda) = \mathrm{Exp}(\lambda)$, and $\Gamma(\frac{k}{2}, \frac{1}{2}) = \chi^2_k$, 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.

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

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

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

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

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

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

2.1 Bias-Variance Decomposition

We can write the mean squared error as

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

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

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

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

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

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

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

$$\begin{aligned}\text{Var}_\theta(T_B) &= \frac{1}{(n+2)^2}n\theta(1-\theta) - w^2\frac{\theta(1-\theta)}{n}, \\ \text{mse}(T_B) &= \text{Var}_\theta(T_B) + \text{bias}^2(T_B) \\ &= w^2\frac{\theta(1-\theta)}{n} + (1-w)^2\left(\frac{1}{2}-\theta\right)^2.\end{aligned}$$

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.

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 $\text{Ber}(\theta)$ for $\theta \in [0, 1]$. Then,

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

This only depends on X through

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

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

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

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

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

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,

$$\begin{aligned} f_X(x \mid \theta) &= \prod_{i=1}^{n} \frac{1}{\theta} \mathbb{1}(X_i \in [0,\theta]) \\ &= \underbrace{\frac{1}{\theta^n} \mathbb{1}(\max_i x_i \leq \theta)}_{g(T(x),\theta)} \underbrace{\mathbb{1}(\min_i x_i \geq 0)}_{h(x)}. \end{aligned}$$

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.

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 $x \overset{1}{\sim} y$ if

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

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

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

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

Remark. We can always construct a statistic T which is constant on the equivalence classes of $\overset{1}{\sim}$, 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 $x \overset{1}{\sim} y$. 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

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

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.

Example 2.8.

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

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

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 $X_1, \dots, X_n$ 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 $\mathbb{E}_\theta$ and $\mathbb{P}_\theta$ to denote the expectations and probabilities in the model where $X_1, \dots, X_n$ 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,*

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

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:

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

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

$$\begin{aligned}\text{Var}(\tilde{\theta}) &= \mathbb{E}[\text{Var}(\tilde{\theta} \mid T)] + \text{Var}(\mathbb{E}[\tilde{\theta} \mid T]) \\ &= \mathbb{E}[\text{Var}(\tilde{\theta} \mid T)] + \text{Var}(\hat{\theta}).\end{aligned}$$

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

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

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

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

$$\begin{aligned}\hat{\theta} &= \mathbb{E}[\tilde{\theta} \mid T = t] = \mathbb{P}\left(X_1 = 0 \;\middle|\; \sum_{i=1}^n X_i = t\right) \\ &= \frac{\mathbb{P}(X_1 = 0, X_1 + \cdots + X_n = t)}{\mathbb{P}(X_1 + \cdots + X_n = t)} = \frac{\mathbb{P}(X_1 = 0, X_2 + \cdots + X_n = t)}{\mathbb{P}(X_1 + \cdots + X_n = t)} \\ &= \frac{\mathbb{P}(X_1 = 0)\mathbb{P}(X_2 + \cdots + X_n = t)}{\mathbb{P}(X_1 + \cdots + X_n = t)} = \frac{e^{-\lambda}\mathbb{P}(\text{Poisson}((n-1)\lambda) = t)}{\mathbb{P}(\text{Poisson}(n\lambda) = t)} \\ &= \frac{e^{-n\lambda}((n-1)\lambda)^t/t!}{e^{-n\lambda}(n\lambda)^t/t!} = \left(1 - \frac{1}{n}\right)^t.\end{aligned}$$

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

As $n \to \infty$,

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

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 $\theta \geq 0$. Then recall $T(X) = \max_i X_i$ is sufficient for θ.

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

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

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

2.5 Maximum Likelihood Estimation

Let $X = (X_1, \ldots, X_n)$ 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

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

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 $\text{Ber}(\theta)$, 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.

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

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

hence

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

which is biased, but asymptotically unbiased.

Example 2.13.

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

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

We can see from the plot that $\hat{\theta}_{\text{mle}} = \max_i X_i$ 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,

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

   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

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,

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

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

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

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

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

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

Rearranging,

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

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 $z_1 = \Phi^{-1}(0.025), z_2 = \Phi^{-1}(0.975)$.

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