Statistics

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1 Parametric Estimation

1.1 Review of IA Probability

1.1.1 Starting axioms

We observe some data $X_1, \ldots, X_n$ iid random variables taking values in a sample space $\mathcal{X}$. Let $X = (X_1, \ldots, X_n)$. We assume that X_1 belongs to a *statistical model* $\{p(x;\theta) : \theta \in \Theta\}$ with θ unknown. For example $p(x;\theta)$ could be a pdf.

Let's see some examples

(i) Suppose that $X_1 \sim \text{Poisson}(\lambda)$ where $\theta = \lambda \in \Theta = (0, \infty)$.

(ii) Suppose that $X_1 \sim \mathcal{N}(\mu, \sigma^2)$, where $\theta = (\mu, \sigma^2) \in \Theta = \mathbb{R} \times (0, \infty)$.

We have some common questions about these statistical models.

(i) We want to give an estimate $\hat{\theta} : \mathcal{X}^n \to \Theta$ of the true value of θ.

(ii) We also want to give an interval estimator $(\hat{\theta}_1(X), \hat{\theta}_2(X))$ of θ.

(iii) Further we want to test of hypothesis about θ. For example we might make the hypothesis that $H_0 : \theta = 0$.

Let's do a quick reivew of IA Probability. Let $X : \Omega \to \mathbb{R}$ be a random variable defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. So Ω is the sample space, $\mathcal{F}$ is the set of events, and $\mathbb{P} : \mathcal{F} \to [0, 1]$ is the probability measure.

The cumulative distribution function (cdf) of X is $F_X(s) = \mathbb{P}(X \leq x)$. A discrete random variable takes values in a countable set $\mathcal{X}$ and has probability mass function (pmf) given by $p_X(x) = \mathbb{P}(X = x)$. A continuous random variable has probability density function (pdf) f_X satisfying $P(X \in A) = \int_A f_X(x)\mathrm{d}x$ (for measurable sets A). We say that $X_1, \ldots, X_n$ are independent if $\mathbb{P}(X_1 \leq x_1, \ldots, X_n \leq x_n) = \prod_{i=1}^n \mathbb{P}(X_i \leq x_i)$ for all choices $x_1, \ldots, x_n$. If $X_1, \ldots, X_n$ have pdfs (or pmfs) $f_{X_1}, \ldots, f_{X_n}$, then this is equivalent to $f_X(x) = \prod_{i=1}^n f_{X_i}(x_i)$ for all x_i. The expectation of X is,

$$\mathbb{E}(x) = \begin{cases} \sum_{x \in \mathcal{X}} x p_X(x) & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{\infty} x f_X(x) & \text{if } X \text{ is continuous} \end{cases}.$$

The variance of X is $\text{Var}(X) = \mathbb{E}[(X - \mathbb{E}(X))^2]$. The moment generating function of X is $M(t) = \mathbb{E}[e^{tX}]$ and can be used to generate the momentum of a random varaible by taking derivatives. If two random variables have the same moment generating functions, then they have the same distribution.

The expectation operator is linear and

$$\text{Var}(a_1 X_1 + \cdots + a_n X_n) = \sum_{i,j=1}^{n} a_i a_j \,\text{Cov}(X_i, X_j),$$

where $\text{Cov}(X_i, X_j) = \mathbb{E}[(X_i - \mathbb{E}(X_i)(X_j - \mathbb{E}(X_j))]$. In vector notation writing X as the column vector of X_i and a as the column vector for a_i we get that

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

Similar for the variance we get that

$$\text{Var}\left(a^T X\right) = a^T \,\text{Var}(X)\, a$$

where $\mathrm{Var}(X)$ is the covariance matrix for X with entries $\mathrm{Cov}(X_i, X_j)$.

1.1.2 Joint random variables

If X is a discrete random variable with pmf $P_{X,Y}(x,y) = \mathbb{P}(X = x, Y = y)$ and marginal pmf $P_Y(y) = \sum_{x \in X} P_{X,Y}(x,y)$, then the conditional pmf is

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

If X, Y are continuous then the join pdf $f_{X,Y}$ satifies

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

and 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 of X given Y is

$$E(X \mid Y) = \begin{cases} \sum_{x \in X} x \mathbb{P}_{X|Y}(x \mid Y) & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{\infty} x f_{X|Y}(x \mid Y) \mathrm{d}y & \text{if } Y \text{ is continuous} \end{cases}.$$

Remark. $\mathbb{E}(X \mid Y)$ is a function of Y so $\mathbb{E}(X \mid Y)$ is a random variable.

We also have the law of total expectation,

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

This is a consequence of the law of total probability which is

$$p_X(x) = \sum_y p_{X|Y}(x \mid y) p_Y(y).$$

Now we have a new (but less useful) theorem similar to the tower property of expectation.

Theorem. (Law of total variance)

$$\mathrm{Var}(X) = \mathbb{E}[\mathrm{Var}(X \mid Y)] + \mathrm{Var}(\mathbb{E}[X \mid Y]).$$

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

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

We also have the change of variables formula. If we have a mapping $(x,y) \to (u,v)$, a bijection from $\mathbb{R}^2 \to \mathbb{R}^2$, then

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

where J is the Jacobian matrix.

1.1.3 Limit theorems

Suppose $X_1, \ldots, X_n$ are iid random variables with mean μ and variance σ^2. Define the sum $S = \sum_{i=1}^n X_i$ and the sample mean $\bar{X}_n = \frac{S_n}{n}$. We have the following theorems.

Theorem. (Weak Law of Large Numbers)

$$\bar{X}_n \to \mu$$

where $\to$ means that $\mathbb{P}\left(|\bar{X}_n - \mu| > \varepsilon\right) \to 0$ as $n \to \infty$ for all $\varepsilon > 0$.

Theorem. (Strong Law of Large Numbers)

$$\bar{X}_n \to \mu$$

almost surely. So $\mathbb{P}\left(\lim_{n\to\infty} \bar{X}_n = \mu\right) = 1$.

Theorem. (Central Limit Theorem) The random variables

$$Z_n = \frac{S_n - n\mu}{\sigma\sqrt{n}}$$

is approximately $\mathcal{N}(0,1)$ for large n. Or we can write this as

$$S_n \approx \mathcal{N}(n\mu, n\sigma^2).$$

Formally this means that $\mathbb{P}\left(Z_n \leq z\right) \to \Phi(z)$ for all $z \in \mathbb{R}$ where $\Phi(z)$ is the cdf of $\mathcal{N}(0,1)$.

1.2 Estimators

Suppose that $X_1, \ldots, X_n$ are iid with pdf $f_X(x \mid \theta)$ and parameter θ unknown.

Definition. (Estimator) A function of the data $T(X) \to \hat{\theta}$ which is used to approximate the true parameter θ is called an *estimator* (or sometimes a *statistic*). The distribution of $T(X)$ is the *sampling distribution*

For an example suppose that $X_1, \ldots, X_n \sim \mathcal{N}(\mu, 1)$ and let $\hat{\mu} = T(x) = \frac{1}{n}\sum_{i=1}^n X_i$. The sampling distribution of $\hat{\mu}$ is $T(X) \sim \mathcal{N}(\mu, \frac{1}{n})$.

Definition. (Bias) The *bias* of a random variable $\hat{\theta} = T(X)$ is

$$\text{bias}(\hat{\theta}) = \mathbb{E}_\theta(\hat{\theta}) - \theta,$$

where the expectation is taken over the model $X_1 \sim f_X(\cdot \mid \theta)$.

Remark. In general the bias might be a function of θ which is not explicit in the notation.

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

So for our estimator from before, $\hat{\mu}$, is unbiased since

$$\mathbb{E}_\mu(\hat{\mu}) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_\mu(X_i) = \mu.$$

1.2.1 Bias-variance decomposition

Definition. (Mean squared error) The *mean squared error* of an estimator $\hat{\theta}$ is

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

Remark. Note that the MSE is generally a function of θ like the bias. Again this is not clear from the notation.

Proposition. (Bias-variance decomposition) For an estimator $\hat{\theta}$ of a parameter θ, we have that

$$\text{mse}(\hat{\theta}) = \Big(\text{bias}(\hat{\theta})\Big)^2 + \text{Var}_\theta(\hat{\theta}).$$

Proof.

$$\begin{aligned}
\text{mse}(\hat{\theta}) &= \mathbb{E}_\theta[(\hat{\theta} - \theta)^2] \\
&= \mathbb{E}_\theta\left[\Big(\hat{\theta} - \mathbb{E}_\theta(\hat{\theta}) + \mathbb{E}_\theta(\hat{\theta}) - \theta\Big)^2\right] \\
&= \mathbb{E}_\theta[(\hat{\theta} - \mathbb{E}_\theta(\hat{\theta}))^2] + (\mathbb{E}_\theta(\hat{\theta}) - \theta)^2 + 2(\mathbb{E}_\theta(\hat{\theta}) - \theta)\cdot\mathbb{E}_\theta[\hat{\theta} - \mathbb{E}_\theta(\hat{\theta})] \\
&= \Big(\text{bias}(\hat{\theta})\Big)^2 + \text{Var}_\theta(\hat{\theta}). \quad \square
\end{aligned}$$

Let's see an example. Suppose that $X \sim \text{Binomial}(n, \theta)$ where is n is known and we want to estimate $\theta \in [0, 1]$. Let $T_u = \frac{X}{n}$ be an estimator, so $\mathbb{E}_\theta(T_u) = \frac{\mathbb{E}(X)}{n} = \frac{n\theta}{n} = \theta$, hence this estimator is unbiased. And $\text{mse}(T_u) = \text{Var}\,(T_u) + \text{bias}(T_u) = \frac{\theta(1-\theta)}{n}$.

Instead if we used the estimator $T_b = \frac{X+1}{n+2} = \omega\frac{X}{n} + (1-\omega)\frac{1}{2}$ where $\omega = \frac{n}{n+2}$. We get that

$$\begin{aligned}
\text{bias}(T_b) &= (1-\omega)(\frac{1}{2} - \theta) \\
\text{Var}\,(T_b) &= \omega^2\frac{\theta(1-\theta)}{n}.
\end{aligned}$$

Giving that

$$\text{mse}(T_b) = \omega^2\theta(1-\theta)n + (1-\omega)^2(\frac{1}{2} - \theta)^2$$

1.3 Sufficient statistics

Suppose $X_1, \dots, X_n$ are iid random variables taking values in χ with pdf $f_{X_1}(\cdot \mid \theta)$. Consider θ as fixed. Denote $X = (X_1, \dots, X_n)$.

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

Remark. The parameter θ may be a vector, and $T(X)$ may be a vector.

Suppose $X_1, \dots, X_n \sim \text{Binomial}(1, \theta)$ iid for some $\theta \in [0, 1]$. Then

$$\begin{aligned} f_X(x \mid \theta) &= \prod_{i=1}^{n} \theta^{x_i}(1-\theta)^{1-x_i} \\ &= \theta^{\sum x_i}(1-\theta)^{n-\sum x_i} \end{aligned}$$

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

$$\begin{aligned} f_{X|T=t}(x \mid T(x) = t) &= \frac{\mathbb{P}_\theta(X = x, T(X) = t)}{\mathbb{P}_\theta(T(X) = t)} \\ &= \frac{\mathbb{P}_\theta(X = x)}{\mathbb{P}_\theta(T(X) = t)} = \frac{\theta^{\sum x_i}(1-\theta)^{n-\sum x_i}}{\binom{n}{t}\theta^t(1-\theta)^{n-t}} = \frac{1}{\binom{n}{t}}. \end{aligned}$$

Theorem. (Factorisation criterion) The statistics T is sufficient for θ if and only if $f_X(x \mid \theta) = g(T(x), \theta)h(x)$ for some suitable g and h.

Proof. Suppose that $f_X(x \mid \theta) = g(T(x), \theta)h(x)$. We can compute

$$\begin{aligned} f_{X|T=t}(x \mid T = t) &= \frac{\mathbb{P}_\theta(X = x, T(x) = t)}{\mathbb{P}_\theta(T(x) = t)} \\ &= \frac{g(T(x), \theta)h(x)}{\sum_{x';T(x')=t} g(t, \theta)h(x')} \\ &= \frac{h(x)}{\sum_{x';T(x')=t} h(x')} \end{aligned}$$

which doesn't depend on θ, so $T(X)$ is sufficient.

Conversely, suppose $T(X)$ is sufficient. We can write

$$\begin{aligned} \mathbb{P}_\theta(X = x) &= \mathbb{P}_\theta(X = x, T(X) = T(x)) \\ &= \mathbb{P}_\theta(X = x \mid T(X) = T(x))\mathbb{P}\,()\,\theta(T(X) = T(x)) \\ &= h(x)g(T(X), \theta). \end{aligned}$$

So we're done. □

Remark. For our example before we can define $T(x) = \sum x_i$ and $g(t, \theta) = \theta^t(1-\theta)^{n-t}$ and $h(x) = 1$.

Let's see another example. Let $X_1, \dots, X_n$ be iid uniform on $[0, \theta]$ for some $\theta \in (0, \infty)$. So

$$\begin{aligned} f_X(x = \theta) &= \prod_{i=1}^{n} \frac{1}{\theta} \mathbf{1}\{x_i \in [0, \infty]\} \\ &= \frac{1}{\theta^n} \mathbf{1}\{\max x_i \leq \theta\} \mathbf{1}\{\min x_i \geq 0\} \\ &= g(T(x), \theta) h(x). \end{aligned}$$

1.4 Minimal sufficiency

Definition. (Minimal sufficient) A sufficient statistics $T(X)$ is *minimal sufficient* if it is a function of every other sufficient statistic. So if $T'(X)$ is also sufficient, then $T'(x) = T'(y) \implies T(x) = T(y)$ for all $x, y \in \chi$.

Remark. Minimal sufficient statistics are unique up to bijection.

Theorem. Suppose $T(X)$ is a statistics such that $\frac{f_X(x|\theta)}{f_X(y|\theta)}$ is constant a function of θ if and only if $T(x) = T(y)$. Then T is minimal sufficient.

Let's see an example before we prove this. Suppose that $X_1, \dots, X_n \sim \mathcal{N}(\mu, \sigma^2)$. Then

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

This is constant in (μ, σ^2) if and only if $\sum_i x_i = \sum_i y_i$ and $\sum_i x_i^2 = \sum_i y_i^2$ therefore $T(X) = \left(\sum_{i=1}^n X_i, \sum_{i=1}^n X_i^2\right)$ is minimal sufficient.

Proof. Need to show that such a statistics is sufficient and minimal. First we'll show sufficiency. For each t pick a x_t such that $T(x_t) = t$. Now let $x \in \chi_N$ and let $T(x) = t$. So $T(x) = T(x_t)$, so by the hypothesis $\frac{f_X(x,\theta)}{f_X(x_t,\theta)}$ does not depend on θ. Let this be $h(x)$ and let $g(t, \theta) = f_X(x, \theta)$ then we have that $f_X(x, \theta) = g(t, \theta)h(x)$ so sufficient.

Now let S be any other sufficient statistic. By the factorisation criterion, there exists g_S, h_S such that $f_X(x \mid \theta) = G_S(S(x), \theta) h_S(x)$. Suppose $S(x) = S(y)$. Then

$$\frac{f_X(x \mid \theta)}{f_X(y \mid \theta)} = \frac{g_S(S(x), \theta) h_S(x)}{g_S(S(y), \theta) h_S(y)} = \frac{h_S(x)}{h_S(y)}$$

which does not depend on θ so $T(x) = T(y)$ so T is minimal sufficient. □

We know that bijections of minimal sufficient statistics are still minial sufficient statistics, so we can write our minimal sufficient statistic for $X_1, \dots, X_n \sim \mathcal{N}(\mu, \sigma^2)$ as

$$S(X) = (\overline{X}, S_{XX})$$

where $\overline{X} = \frac{1}{n} \sum_i X_i$ and $S_{XX} = \sum_i (X_i - \overline{X})^2$, since there is a bijection between them.

Until now we used $\mathbb{E}_\theta$ and $\mathbb{P}_\theta$ to denote expectation and probability when $X_1, \dots, X_n$ are iid from a distribution with pdf $f_X(x \mid \theta)$. From now on we drop the subscript θ to simplify notation.

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

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

This inequality is strict unless $\tilde{\theta}$ is a function of T.

Remark. We have that $\hat{\theta}(T) = \int \tilde{\theta}(x) f_{X|T}(x \mid T)\mathrm{d}x$. By sufficiency of T, the conditional pdf does *not* depend on θ so $\hat{\theta}$ does not depend on θ, and is valid estimator.

Proof. By the tower property of expectation,

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

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

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

So

$$\mathrm{mse}(\tilde{\theta}) \geq \mathrm{mse}(\hat{\theta}).$$

Equality is achieved only when $\mathrm{Var}\left(\tilde{\theta} \mid T\right) = 0$ with probability 1 which requiers $\tilde{\theta}$ to be a function of T. □

Let's see an example of this. Suppose that $X_1, \ldots, X_n \sim \mathrm{Poisson}(\lambda)$ iid. Let $\theta = \mathbb{P}(X_1 = 0) = e^{-\lambda}$. Then

$$f_X(x \mid \theta) = \frac{e^{-n\lambda}\lambda^{\sum x_i}}{\prod_i x_i!} = \frac{\theta^n(-\log\theta)^{\sum x_i}}{\prod_i x_i!}.$$

By the factorisation criterion, $T(X) = \sum_i x_i$ is sufficient. Recall that $\sum x_i \sim \mathrm{Poisson}(n\lambda)$. Let $\tilde{\theta} = \mathbf{1}\{X_1 = 0\}$. Then

$$\begin{aligned}
\hat{\theta} = \mathbb{E}[\tilde{\theta} \mid T = t] &= \mathbb{P}\left(X_1 = 0 \mid \sum_{i=1}^n X_i = t\right) \\
&= \frac{\mathbb{P}\left(X_1 = 0, \sum_{i=2}^n X_i = t\right)}{\mathbb{P}\left(\sum_{i=1}^n X_i = t\right)} \\
&= \frac{\mathbb{P}\left(X_1 = 0\right)\mathbb{P}\left(\sum_{i=2}^n X_i = t\right)}{\mathbb{P}\left(\sum_{i=1}^n X_i = t\right)} \\
&= \frac{e^{-\lambda}e^{-(n-1)\lambda}\frac{((n-1)\lambda)^t}{t!}}{e^{-n\lambda}\frac{(n\lambda)^t}{t!}} = \left(\frac{n-1}{n}\right)^t
\end{aligned}$$

Hence $\hat{\theta} = \left(1 - \frac{1}{n}\right)^{\sum x_i}$ has $\mathrm{mse}(\hat{\theta}) < \mathrm{mse}(\tilde{\theta})$ for all θ. We can see that as $n \to \infty$, $\hat{\theta} \to e^{-\overline{X}} = e^{-\lambda} = \theta$.

Let $X_1, \dots, X_n \sim \text{Uniform}([0, \theta])$ and suppose we want to estimate $\theta \geq 0$. Last time we saw that $T = \max X_i$ is sufficient for θ. Let $\tilde{\theta} = 2X_1$ be an estimator (unbias). Then

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

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

1.5 Likelihood

Definition. (Likelihood) Let $X = (X_1, \dots X_n)$ have a joint pdf $f_X(x \mid \theta)$. The *likelihood* of θ is the function

$$L : \theta \to f_X(x \mid \theta).$$

The max likelihood estimator (MLE) is the value of θ maximizing L.

If $X_1, \dots, X_n \sim f_X(\cdot \mid \theta)$ iid, then $L(\theta) = \prod_{i=1}^n f_X(x_i \mid \theta)$.

It's usually easier to work with the log-likelihood, since this reduces to a sum. So in the iid case,

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

For example let $X_1, \dots, X_n \sim \text{Bernoulli}(p)$ iid. Then we get that

$$\ell(p) = \left(\sum_{i=1}^n X_i\right) \log p + \left(n - \sum_{i=1}^n X_i\right) \log(1-p).$$

Taking the derivative with respect to p,

$$\frac{\partial \ell}{\partial p} = \frac{\sum_i X_i}{p} - \frac{n - \sum_i X_i}{1-p}.$$

So setting the derivative to zero we get that

$$p = \frac{\sum X_i}{n}.$$

Hence the MLE is

$$\hat{p} = \frac{\sum_i X_i}{n},$$

and since $\mathbb{E}[\hat{p}] = p$, this is unbiased.

Now suppose $X_1, \dots, X_n \sim \mathcal{N}(\mu, \sigma^2)$.

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

So

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

which is zero when $\mu = \frac{\sum_i X_i}{n}$ regardless of σ. Also

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

If we set $\mu = \frac{\sum_i X_i}{n}$ then we get $\frac{\partial \ell}{\partial \sigma^2} = 0$ if $\sigma^2 = \frac{1}{n}\sum(X_i - \bar{X})^2 = \frac{S_{xx}}{n}$. Hence the MLE is

$$(\hat{\mu}, \hat{\sigma}^2 = (\bar{X}, \frac{S_{xx}}{n}).$$

Notte that μ is unbiased, but we will see later that

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

So $\mathbb{E}[\hat{\sigma}^2] = \mathbb{E}\left(\frac{S_{xx}}{n}\right) = \frac{n-1}{n}\sigma^2$. So $\hat{\sigma}^2$ is not unbiased, but is asymptotically unbiased as $n \to \infty$.

Suppose now that $X_1, \ldots, X_n \sim \text{Uniform}([0, \theta])$ iid. Then

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

Hence the MLE is $\hat{\theta}_{\text{MLE}} = \max_i X_i$. Recall that last time, we had an aunbiased estimator $\tilde{\theta}$ and by the Rao-Blackwell Theorem we found the estimator $\hat{\theta} = \mathbb{E}[\tilde{\theta} \mid T] = \frac{n+1}{n}\max_i X_i$. Note that $\hat{\theta}_{\text{MLE}} = \frac{n}{n+1}\hat{\theta}$, so $\mathbb{E}[\hat{\theta}_{\text{MLE}}] = \frac{n}{n+1}\mathbb{E}[\hat{\theta}] = \frac{n}{n+1}\theta$. Again this not unbiased, but is asymptotically unbiased.

Let's see some properties of the MLE.

(i) If T is a sufficient statistic, the MLE is a function of T. We can factorise $L(\theta) = g(T(x), \theta)h(x)$.

(ii) If $\phi = h(\theta)$ where h is a bijection, the MLE of ϕ is $\hat{\phi} = h(\hat{\theta})$ where $\hat{\theta}$ is the MLE of θ.

(iii) Asymptotic normality: $\sqrt{n}(\hat{\theta}_{\text{MLE}} - \theta)$ is approximately normal with mean 0 for large n. The covariance matrix is the "smallest attainable" (see II Principles of Statistics).

1.6 Confidence intervals

Definition. (Confidence intervals) A $(100\gamma)\%$ confidience interval for a paramter θ is a random interval $(A(X), B(X))$ such that $\mathbb{P}(A(X) \leq \theta \leq B(X)) = \gamma$ for some $\gamma \in (0, 1)$ and all values of the true parameter θ.

Remark. The incorrect interperatation: Having observed $X = x$, there is a $1 - \gamma$ probability that θ is in $(A(X), B(X))$. This is wrong.

Suppose that $X_1, \ldots, X_n \sim \mathcal{N}(\theta, 1)$ iid. We want to find a 95% confidence interval for θ. We know that $\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i \sim \mathcal{N}(\theta, \frac{1}{n})$. If we define $Z = \sqrt{n}(\overline{X} - \theta)$ Then $Z \sim \mathcal{N}(0, 1)$ no matter

the value of θ. Let z_1, z_2 be numbers with $\Phi(z_1) - \Phi(z_2) = 0.95$ where Φ is the cdf of the standard normal. $\mathbb{P}\left(z_1 \leq \sqrt{n}(\overline{X} - \theta) \leq z_2\right) = 0.95$ rearranging we get that

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

hence

$$\left(\overline{X} - \frac{z_2}{\sqrt{n}}, \overline{X} - \frac{z_1}{\sqrt{n}}\right)$$

is a 95% confidence interval.

This is the recipe for confidence intervals.

(i) Find a quantity $R(X, \theta)$ such that this $\mathbb{P}_\theta$ distribution of $R(X, \theta)$ does not depend on θ. This is called a *pivot* for example $R(X, \theta) = \sqrt{n}(\overline{X} - \theta)$.

(ii) Write down the statement

$$\mathbb{P}\left(c_1 \leq R(X, \theta) \leq c_2\right) = \gamma$$

where (c_1, c_2) are quantiles of the distribution of $R(X, \theta)$.

(iii) Rearranging the above to leave θ in the middle of the inequality, so we get something in the form

$$\mathbb{P}\left(A(X) \leq \theta \leq B(X)\right).$$

Remark. When θ is a vector, we talk about *confidence sets* rather than intervals.

Suppose that $X_1, \ldots, X_n \sim \mathcal{N}(0, \sigma^2)$ iid. We want a 95% confidence interval for σ^2. Note that

$$\frac{X_i}{\sigma} \sim \mathcal{N}(0, 1),$$

so $\sum_{i=1}^n \frac{X_i^2}{\sigma^2} \sim \chi_n^2$. Hence

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

is a *pivot*. Let $F^{-1}_{\chi_n^2}(0.025)$ and $F^{-1}_{\chi_n^2}(0.975)$. Then

$$\mathbb{P}\left(c_1 \leq \sum_{i=1}^n \frac{X_i^2}{\sigma^2} \leq c_2\right) = 0.95,$$

so rearranging we get that

$$\mathbb{P}\left(\frac{\sum X_i^2}{c_2} \leq \sigma^2 \leq \frac{\sum X_i^2}{c_1}\right) = 0.95$$

gives our confidence interval.

Now suppose that $X_1, \ldots, X_n \sim$ Bernoulli(p) for large n. We will find an approximate 95% confidence interval for p. The maximium likelihood estimator of p is $\hat{p} = \frac{1}{n}\sum_{i=1}^n X_i$. By the central limit theorem $\hat{p} \sim \mathcal{N}\left(p, \frac{p(1-p)}{n}\right)$ approximately. Thus

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

for large n. So we have our pivot, which gives

$$\mathbb{P}\left(-z_{0.025} \leq \frac{\sqrt{n}(\hat{p}-p)}{\sqrt{p(1-p)}} \leq z_{0.025}\right) \approx 0.95$$

Instead of inverting directly, if n is large $\hat{p} \approx p$, so switching p with $\hat{p}$ on the denominator we get that

$$\mathbb{P}\left(\hat{p} - z_{0.025}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}} \leq p \leq \hat{p} + z_{0.025}\sqrt{\frac{\hat{p}(1-\hat{p})}{n}}\right) \approx 0.95$$

which gives our confidence interval. Since for all $\hat{p} \in [0,1]$ we have $\hat{p}(1-\hat{p}) \leq \frac{1}{4}$ we would also report a conservative confidence interval of $\hat{p} \pm z_{0.025}\sqrt{\frac{1}{4n}}$.

1.7 Bayesian estimation

So far we've been using frequentist methods treating $\theta \in \Theta$ as fixeed. For Bayesian methods, we treat θ as random with a prior distribution $\pi(\theta)$. Conditional on θ the data X has pdf $f_X(\cdot \mid \theta)$. Having observed that $X = x$, we combine with the prior to form a posterior distribution $\pi(\theta \mid X)$. By Bayes' rule,

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

where $f_X(x)$ is the marginal distribution of X, so

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

More simply,

$$\pi(\theta \mid x) \propto \pi(\theta) f_X(x \mid \theta).$$

Often is it easier to reconginise the RHS as propotional to a known distribution.

Remark. By the factorisation criterion, the posterior only depends on X through a sufficient statistic.

$$\begin{aligned} \pi(\theta \mid x) &\propto \pi(\theta) \cdot f_X(x \mid \theta) = \pi(\theta) \cdot g(T(x), \theta)h(x) \\ &\propto \pi(\theta) g(T(x), \theta). \end{aligned}$$

Suppose $\theta \in [0,1]$ is the mortality rate for some procedure at Addenbrooks. In the first 10 operations there are no deaths. In other hospitals across the country the mortality rate is between $3 - 20\%$, with average of 10%. Consider the prior distribution $\pi(\theta) \sim \text{Beta}(a,b)$ we can choose $(a,b) = (3,27)$ so $\pi(\theta)$ as mean 0.1 and $\pi(0.03 < \theta < 0.2) = 0.9$.

Let $X_i \sim \text{Bernoulli}(\theta)$ be indicator for whether ith patient at Addenbrookes dies.

$$f_X(x \mid \theta) = \theta^{\sim x_i}(1-\theta)^{n - \sum x_i}.$$

The posterior is

$$\begin{aligned} \pi(\theta \mid X) &\propto \pi(\theta) f_X(x \mid \theta) \\ &\propto \theta^{a-1}(1-\theta)^{b-1}\theta^{\sum x_i}(1-\theta)^{n-\sum x_i} \\ &= \theta^{\sum x_i + a - 1}(1-\theta)^{b+n-\sum x_i - 1}. \end{aligned}$$

Hence

$$\pi(\theta \mid X) \sim \text{Beta}(a + \sum x_i, b + n - \sum x_i)$$

so pluggin in $a = 3, b = 27, n = 10, \sum X_i = 0$, so the posterior is $\text{Beta}(3, 37)$.

Remark. In the example the prior and posterior were from the same family of distributions known as conjugacy.

Supposewe put a $\text{Beta}(a, b)$ prior on the parameter θ of kidney cancer death rates in each county. We can estimate $(a, b) = (27, 58000)$ with $\frac{a}{a+b} \approx 4.65 \times 10^{-9}$ being the kidney cancer death rate in the United States. The previous example shows that if we observe $\sum_{i=1}^{n} X_i$ deaths in a county, the posterior mean estimate is $\frac{a+\sum X_i}{a+b-n}$. This is equal to

$$\frac{n}{a+b+n} \cdot \frac{\sum X_i}{n} + \frac{a+b}{a+b+n} \cdot \frac{a}{a+b}.$$

For large n, we use $\approx \frac{\sum X_i}{n}$ as our estimate, for small n we use $\frac{a}{a+b}$ and in between we shrink our estimate between them.

What is the use of the posterior distribution? This opens us to decision theory.

(i) We must pick a decision $\delta \in D$;

(ii) We have a loss function $L(\theta, \delta)$ which gives loss incurred in making decision δ when the true paramter value is θ.

(iii) Von-Neumann-Morgenstern Theorem: Under axioms of rational behaviour, pick δ that minimises expected loss under posterior.

Definition. (Bayes estimator) The *Bayes estimator* $\hat{\theta}^{(b)}$ is defined by

$$h(\delta) = \int_{\Theta} L(\theta, \delta)\pi(\theta \mid X)\mathrm{d}\theta$$

and

$$\hat{\theta}^{(b)} = \arg\min h(\delta)$$

Consider the case where we have quadartic loss, so $L(\theta, \delta) = (\theta - \delta)^2$. Then we have that

$$h(\delta) = \int_{\Theta} (\theta - \delta)^2 \pi(\theta \mid X)\mathrm{d}\theta.$$

Differentiating with resepct to δ we get that $h'(\delta) = 0$ if

$$\int_{\Theta} (\theta - \delta)\pi(\theta \mid X)\mathrm{d}\theta = 0$$

so

$$\delta = \int_{\Theta} \theta\pi(\theta \mid x)\mathrm{d}\theta$$

is the posterior mean. Now suppose we have absolute loss, so $L(\theta, \delta) = |\theta - \delta|$. So

$$\begin{aligned} h(\delta) &= \int_\Theta |\theta - \delta| \pi(\theta \mid X) \mathrm{d}\theta \\ &= \int_{-\infty}^{\delta} -(\theta - \delta)\pi(\theta \mid X \mathrm{d}\theta + \int_{\delta}^{\infty} (\theta - \delta)\pi(\theta \mid X)\mathrm{d}\theta \\ &= -\int_{\infty}^{\delta} \theta\pi(\theta \mid X)\mathrm{d}\theta + \int_{\delta}^{\infty} \theta\pi(\theta \mid X)\mathrm{d}\theta + \delta\int_{-\infty}^{\delta} \pi(\theta \mid X)\mathrm{d}\theta - \delta\int_{\delta}^{\infty} \pi(\theta \mid X)\mathrm{d}\theta \end{aligned}$$

Taking derivatives and applying FTC we get that

$$h'(\delta) = \int_{-\infty}^{\delta} \pi(\theta \mid X)\mathrm{d}\theta - \int_{\delta}^{\infty} \pi(\theta \mid X)\mathrm{d}\theta.$$

Hence $h'(\delta) = 0$ if and only if

$$\int_{-\infty}^{\delta} \pi(\theta \mid X)\mathrm{d}\theta = \int_{\delta}^{\infty} \pi(\theta \mid X)\mathrm{d}\theta$$

so $\hat{\theta}^{(b)}$ is the posterior median.

Supose we have $X_1, \ldots, X_n \overset{\text{idd}}{\sim} \mathcal{N}(\mu, 1)$ and prior $\pi(\mu)$ that is $\mathcal{N}(0, \frac{1}{\tau^2})$ for some known $\tau > 0$. Then

$$\begin{aligned} \pi(\mu \mid X) &\propto f_X(x \mid \mu)\pi(\mu) \\ &\propto \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(X_i - \mu)^2\right)\exp\left(-\frac{-\mu^2\tau^2}{2}\right) \\ &\propto \exp\left(-\frac{1}{2}(n+\tau^2)\left(\mu - \frac{\sum X_i}{n+\tau^2}\right)^2\right) \end{aligned}$$

This is the pdf of a $\mathcal{N}\left(\frac{\sum X_I}{n+\tau^2}, \frac{1}{n+\tau^2}\right)$ distribution. The posterior mean and median are both $\frac{\sum X_i}{n+\tau^2}$.

Definition. (Credible interval) A $100\gamma\%$ *credible interval* satifies that

$$\pi(A(X) \leq \theta \leq B(X) \mid X = x) = \gamma.$$

2 Hypothesis Testing

Definition. (Hypothesis) A *hypothesis* is an assumption about a distribution of data X taking values in χ.

Definition. (Null/Alternative hypothesis) The *null hypothesis* H_0 is the base case. The *alternative hypothesis* is the positive or negative effect the interesting case, denoted by H_1.

For example let $X_1, \ldots, X_n \overset{\text{idd}}{\sim} \text{Bernoulli}(\theta)$. We may have the null hypothesis $H_0 : \theta = \frac{1}{2}$ and then make alternative hypothesis $H_1 : \theta = \frac{3}{4}$ or $H_1 : \theta \neq \frac{1}{2}$ for example.

Suppose that $X_1, \ldots, X_n$ are iid. Then we have the hypotheses:

$$H_0 : X_i \text{ has pdf } f_0$$
$$H_1 : X_i \text{ has pdf } f_1$$

This is called a goodness of fit test.

Now suppose that X has pdf $f(\cdot \mid \theta)$ for some $\theta \in \Theta$.

$$H_0 : \theta \in \Theta_0 \subsetneq \Theta$$
$$H_1 : \theta \notin \Theta_0$$

Definition. (Simple/composite hypothesis) A *simple hypothesis* fully specifies the distribution of X. Otherwise we say the hypothesis is *composite*.

Definition. (Test and critical regions) A *test* of H_0 is defined by a *critical region*, C. When $X \in C$, we reject H_0, otherwise we do not reject H_1.

Definition. (Type I Error) A *Type I Error* occurs when we reject H_0 when H_0 is true.

Definition. (Type II Error) A *Type II Error* occurs when we fail to reject H_0 when H_1 is true.

When H_0 and H_1 are simple hypotheses we have the following.

Definition. (Size) We define α as the *size* of the test, defined as

$$\alpha = \mathbb{P}_{H_0}(H_0 \text{ rejected}) = \mathbb{P}_{H_0}(X \in C).$$

Definition. (Power) We define the *power* of the test as $1 - \beta$ where

$$\beta = \mathbb{P}_{H_1}(H_0 \text{ not rejected}) = \mathbb{P}_{H_1}(X \notin C).$$

Remark. Note that α is the probability of a Type I error and β is the probability of a Type II error.

Remark. Type I and Type II errors correspond to a false positive and a false negative respectively.

Usually we set α at an acceptable level for example 1%, and choose a test that minimises β subject to $\alpha \leq 1\%$.

Definition. (Likelihood ratio statistic) Let H_0 and H_1 be simple hypotheses with X

having pdf f_i under H_i. The *likelihood ratio statistic* is

$$\Lambda_X(H_0, H_1) = \frac{f_1(X)}{f_0(X)}.$$

Definition. (Likelihood ratio test) A *Likelihood ratio test* (LRT) rejects H_0 when $X \in C = \{x \in \Lambda_X(H_0, H_1) > k\}$ for some $k > 0$.

Theorem. (Neyman-Pearson Lemma) Suppose that f_0 and f_1 are nonzero on the same sets and $\exists k$ such that the LRT with critical region $C = \{x : \frac{f_1(x)}{f_0(x)} > k\}$ has size α. Out of all tests with size $\leq \alpha$ the LRT is the test with smallest β.

Proof. Let $\overline{C}$ be the complement of C. Then

$$\alpha = \mathbb{P}_{H_0}(X \in C) = \int_C f_0(x)\mathrm{d}x$$
$$\beta = \mathbb{P}_{H_1}(X \in C) = \int_{\overline{C}} f_1(x)\mathrm{d}x$$

Let C^* be the critical region of another test of size $\alpha^* \leq \alpha$. We want to show that $\beta \leq \beta^*$.

$$\begin{aligned}
\beta - \beta^* &= \int_{\overline{C}} f_1(x)\mathrm{d}x - \int_{\overline{C^*}} f_1(x)\mathrm{d}x \\
&= \int_{\overline{C} \cap \overline{C}^*} f_1(x)\mathrm{d}x - \int_{\overline{C}^* \cap C} f_1(x)\mathrm{d}x \\
&= \int_{\overline{C} \cap C^*} \frac{f_1(x)}{f_0(x)} f_0(x)\mathrm{d}x - \int_{\overline{C}^* \cap C} \frac{f_1(x)}{f_0(x)} f_0(x)\mathrm{d}x
\end{aligned}$$