STAT 241 Course Notes

Statistics (Advanced Level)

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1 Review

1.1 Cumulative distribution function

DEFINITION 1.1. The **cumulative distribution function (CDF)** of a random variable X is defined by

$$F(x) = P(X \le x), \quad x \in \mathbb{R}.$$

Properties of the CDF. Let F be the CDF of a random variable X. Then:

(1) F is non-decreasing; that is, $F(x_1) \le F(x_2)$ for all $x_1 < x_2$.

(2) $\lim_{x\to-\infty} F(x) = 0$ and $\lim_{x\to\infty} F(x) = 1$.

(3) F is right-continuous; that is, $\lim_{x\to a^+} F(x) = F(a)$ for $a \in \mathbb{R}$.

(4) For $a < b \in \mathbb{R}$, we have $P(a < X \le b) = P(X \le b) - P(X \le a) = F(b) - F(a)$.

(5) Given $b \in \mathbb{R}$, we have $P(X = b) = P(X \le b) - P(X < b) = F(b) - \lim_{a\to b^-} F(a)$.

Note that the definition and the above properties hold for any random variable X regardless of whether X is discrete or continuous.

1.2 Discrete random variables and their probability functions

DEFINITION 1.2. If X takes finitely or countably many values, then X is said to be a **discrete random variable**. In this case, the CDF F of X is a right-continuous step function.

DEFINITION 1.3. If X is a discrete random variable, then the **probability function (PF)** of X is given by

$$f(x) = P(X = x), \quad x \in A.$$

The set $A = \{x \in \mathbb{R} : f(x) > 0\}$ is called the **support set** of X.

Properties of the PF. Let f be the PF of a discrete random variable X. Then:

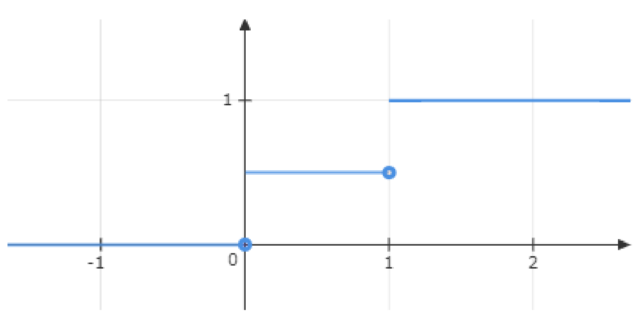
(1) For all $x \in \mathbb{R}$, we have $f(x) \ge 0$, and the inequality is strict if $x \in A$.

(2) $\sum_{x\in A} f(x) = 1$.

EXAMPLE 1.4. Suppose that X only takes the values 0 and 1, with $P(X = 0) = P(X = 1) = 1/2$. Then the CDF of X is given by

$$F(x) = P(X \le x) = \begin{cases} 0 & x < 0 \\ 1/2 & 0 \le x < 1 \\ 1 & x \ge 1. \end{cases}$$

As seen in the graph below, F is indeed a right-continuous step function.



1.3 More examples of discrete random variables

The discrete random variable X in Example 1.4 can naturally be extended to other discrete random variables that we are familiar with.

Bernoulli. Suppose that $X \sim \text{Bernoulli}(\theta)$ for some $0 < \theta < 1$. Then $P(X = 1) = \theta$ and $P(X = 0) = 1 - \theta$, where a 1 is a success, and a 0 is a failure.

Binomial. Let $0 < \theta < 1$. Suppose that $X_i \sim \text{Bernoulli}(\theta)$ for all $1 \leq i \leq n$, and that the X_i's are independent. Then, we may define the discrete random variable

$$X = \sum_{i=1}^{n} X_i.$$

Essentially, this is the number of successes in a sequence of independent and identically distributed (i.i.d.) Bernoulli(θ) random variables. This is the binomial distribution; that is, $X \sim \text{Bin}(n, \theta)$. The support set of X is $A = \{0, 1, \ldots, n\}$, and we have

$$P(X = x) = \binom{n}{x} \theta^x (1 - \theta)^{n-x}.$$

Multinomial. Suppose that $(X_1, X_2, \ldots, X_k) \sim \text{Multi}(n, \theta_1, \theta_2, \ldots, \theta_k)$. For each trial, there are $k + 1$ possible outcomes, with corresponding probabilities $(\theta_1, \theta_2, \ldots, \theta_k, 1 - \sum_{i=1}^{k} \theta_i)$. For convenience, it is useful to denote $\theta_{k+1} := 1 - \sum_{i=1}^{k} \theta_i$. Then, for each $1 \leq i \leq k$, we let X_i be the number of times outcome i occurs in n trials. Writing $x_{k+1} := n - \sum_{i=1}^{k} x_i$, the probability function of X is given by

$$P(X_1 = x_1, \ldots, X_k = x_k) = \frac{n!}{x_1! x_2! \cdots x_k! x_{k+1}!} \theta_1^{x_1} \theta_2^{x_2} \cdots \theta_k^{x_k} \theta_{k+1}^{x_{k+1}}$$

Poisson. Suppose that $X \sim \text{Poi}(\mu)$ for some $\mu > 0$. Often, X denotes the number of events during a time period, and μ is the occurrence rate (that is, $\mu = E(x)$). The probability function of X is given by

$$f(x) = P(X = x) = \frac{\mu^x e^{-\mu}}{x!}, \quad x \in \mathbb{Z}_{\geq 0}.$$

Notice that we have

$$\sum_{x=0}^{\infty} f(x) = \sum_{x=0}^{\infty} \frac{\mu^x e^{-\mu}}{x!} = e^{-\mu} \sum_{x=0}^{\infty} \frac{\mu^x}{x!} = e^{-\mu} e^{\mu} = 1.$$

1.4 Continuous random variables and their probability density functions

Definition 1.5. Suppose X is a random variable with CDF F. If F is continuous at each $x \in \mathbb{R}$ and F is differentiable except possibly at countably many points, then X is said to be a **continuous random variable**.

Definition 1.6. If X is a continuous random variable with CDF F, then the **probability density function (PDF)** of X is given by

$$f(x) = \begin{cases} F'(x) & \text{if } F \text{ is differentiable at } x \\ 0 & \text{otherwise.} \end{cases}$$

The set $A = \{x \in \mathbb{R} : f(x) > 0\}$ is called the **support set** of X.

Properties of the PDF. Suppose f is the PDF of a continuous random variable X. Then:

(1) For all $x \in \mathbb{R}$, we have $f(x) \geq 0$.

(2) $\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = \lim_{x\to\infty} F(x) - \lim_{x\to-\infty} F(x) = 1 - 0 = 1$.

(3) For all $x \in \mathbb{R}$, we have $F(x) = \int_{-\infty}^{x} f(t)\,\mathrm{d}t$.

(4) $P(a < X \leq b) = P(X \leq b) - P(X \leq a) = F(b) - F(a) = \int_a^b f(x)\,\mathrm{d}x$.

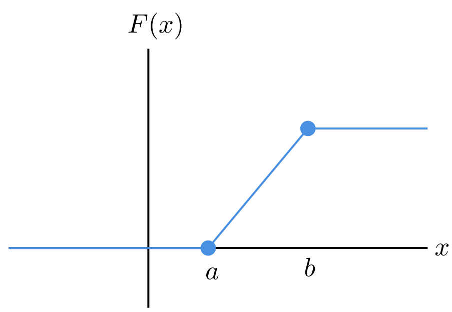
(5) $P(X = b) = F(b) - \lim_{a\to b^-} F(a) = F(b) - F(b) = 0$ (since F is continuous).

1.5 Examples of continuous random variables

Uniform. Suppose X is a random variable with CDF

$$F(x) = \begin{cases} 0 & x \leq a \\ \frac{x-a}{b-a} & a < x < b \\ 1 & x \geq b, \end{cases}$$

where $a < b$. The graph of the CDF is below.



Notice that F is continuous at every $x \in \mathbb{R}$ and differentiable except at the points $x = a$ and $x = b$, so X is a continuous random variable. In fact, we have that $X \sim \text{UNIF}(a, b)$. Now, the PDF of X is given by

$$f(x) = \begin{cases} \frac{1}{b-a} & a < x < b \\ 0 & \text{otherwise.} \end{cases}$$

Namely, the support set of X is $A = (a, b)$, and the PDF is constant there.

Exponential. Let $\theta > 0$ and suppose that $X \sim \text{EXP}(\theta)$. Then X is a continuous random variable, and the PDF of X is given by

$$f(x) = \frac{1}{\theta}\exp(-x/\theta), \quad x \geq 0.$$

EXAMPLE 1.7. An insurance agent has sold n policies. For each $1 \leq i \leq n$, let X_i be the amount of time passed before policy holder i makes the first claim. Assume that each $X_i \sim \text{EXP}(\lambda_i)$. Let T be the amount of time the insurance agent can stay "claim free". Find the distribution of T.

Solution. We have $T = \min\{X_1, \ldots, X_n\}$. Then, observe that

$$\begin{aligned} P(T \geq t) &= P(X_1 \geq t, \ldots, X_n \geq t) \\ &= \prod_{i=1}^{n} P(X_i \geq t) \\ &= \prod_{i=1}^{n} \int_t^\infty \frac{1}{\lambda_i} \exp(-x/\lambda_i)\,\mathrm{d}x \\ &= \prod_{i=1}^{n} \exp(-t/\lambda_i) = \exp(-(\textstyle\sum_{i=1}^n 1/\lambda_i)t). \end{aligned}$$

From this, we see that $T \sim \mathrm{EXP}(1/(\sum_{i=1}^n 1/\lambda_i))$.

Gaussian/Normal. Suppose $X \sim \mathrm{N}(\mu, \sigma^2)$ where $\mu \in \mathbb{R}$ and $\sigma > 0$. The PDF of X is

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\Big(-\frac{(x-\mu)^2}{2\sigma^2}\Big), \quad x \in \mathbb{R}.$$

Example 1.8. It is reasonable to model the IQ of University of Waterloo math students using a normal distribution. Suppose that Y is the IQ of a randomly selected math student; that is, $Y \sim \mathrm{N}(\mu, \sigma^2)$. Suppose we have a random sample of 16 IQs $\{127, 108, \ldots, 134\}$ such that $\sum_{i=1}^{16} y_i = 1916$ and $\sum_{i=1}^{16} y_i^2 = 231618$. Using some knowledge from later in the course, we can find that

$$\begin{aligned} \widehat{\mu}_{\mathrm{MLE}} &= \bar{y} = \frac{\sum_{i=1}^n y_i}{n} = \frac{1916}{16} = 119.75 \\ \widehat{\sigma}^2_{\mathrm{MLE}} &= \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2 = \frac{1}{15}\left(\sum_{i=1}^{16} y_i^2 - 16(\bar{y})^2\right) \approx 145.13, \end{aligned}$$

and so $\widehat{\sigma}_{\mathrm{MLE}} \approx \sqrt{145.13} \approx 12.05$. In summary, we obtain $Y \sim \mathrm{N}(145.13, (12.05)^2)$. Now, what is the probability of observing an IQ greater than 120?

Solution. We have

$$P(Y > 120) = P\left(\frac{Y - 119.75}{12.05} > \frac{120 - 119.75}{12.05}\right) = P(Z > 0.021) = 1 - \Phi(0.021) = 1 - 0.50798 = 0.49202,$$

where Φ is the CDF of $Z \sim \mathrm{N}(0,1)$.

Gamma. The **gamma function**, denoted by $\Gamma(\alpha)$ for all $\alpha > 0$, is given by

$$\Gamma(\alpha) = \int_0^\infty y^{\alpha-1} e^{-y}\,\mathrm{d}y.$$

Some properties of the gamma function include:

(1) $\Gamma(n) = (n-1)!$ for all $n \in \mathbb{Z}_{>0}$.

(2) $\Gamma(\alpha) = (\alpha - 1)\Gamma(\alpha - 1)$ for all $\alpha > 1$.

(3) $\Gamma(1) = 1$.

(4) $\Gamma(1/2) = \sqrt{\pi}$.

Now, suppose X is a random variable with PDF

$$f(x) = \frac{x^{\alpha-1}e^{-x/\beta}}{\Gamma(\alpha)\beta^\alpha}, \quad x > 0, \quad \alpha, \beta > 0.$$

We say that X has a **gamma distribution** with parameters α and β, and we write $X \sim \mathrm{GAM}(\alpha, \beta)$.

We verify that $\int_0^\infty f(x) = 1$. Indeed, we have

$$\begin{aligned}
\int_0^\infty f(x) &= \int_0^\infty \frac{1}{\Gamma(\alpha)\beta^\alpha} x^{\alpha-1} e^{-x/\beta}\,\mathrm{d}x \\
&= \int_0^\infty \frac{1}{\Gamma(\alpha)} y^{\alpha-1} e^{-y}\,\mathrm{d}y \text{ (using } y = x/\beta) \\
&= \frac{1}{\Gamma(\alpha)} \int_0^\infty y^{\alpha-1} e^{-y}\,\mathrm{d}y = \frac{\Gamma(\alpha)}{\Gamma(\alpha)} = 1.
\end{aligned}$$

Chi-square. Suppose $X \sim \chi^2(k)$, where $k \in \mathbb{Z}_{>0}$ (the number of degrees of freedom). The PDF of X is

$$f(x) = \frac{x^{k/2-1} e^{-x/2}}{\Gamma(k/2) 2^{k/2}}, \quad x > 0.$$

Notice that this is a special case of the gamma distribution; namely, we have $\chi^2(k) = \mathrm{GAM}(k/2, 2)$. On the other hand, we can also see that $\mathrm{EXP}(\theta) = \mathrm{GAM}(1, \theta)$.

1.6 Moments of the gamma distribution

Discrete case. Recall that if X is a discrete random variable with support set A, we have that

$$E(x) = \sum_{x \in A} x \cdot f(x).$$

More generally, for a function $h(x)$, we have

$$E(h(x)) = \sum_{x \in A} h(x) \cdot f(x).$$

Continuous case. On the other hand, if X is a continuous random variable with support set A, then

$$E(x) = \int_A x \cdot f(x)\,\mathrm{d}x.$$

Similarly, for a function $h(x)$, we have

$$E(h(x)) = \int_A h(x) \cdot f(x)\,\mathrm{d}x.$$

Moments of the gamma distribution. Suppose that $Y \sim \mathrm{GAM}(\alpha, \beta)$ for some $\alpha, \beta > 0$. Then we have

$$\begin{aligned}
E(Y^p) &= \int_0^\infty y^p \cdot \frac{1}{\Gamma(\alpha)\beta^\alpha} y^{\alpha-1} e^{-y/\beta}\,\mathrm{d}y \\
&= \frac{1}{\Gamma(\alpha)\beta^\alpha} \int_0^\infty y^{p+\alpha-1} e^{-y/\beta}\,\mathrm{d}y \\
&= \frac{1}{\Gamma(\alpha)\beta^\alpha} \int_0^\infty x^{p+\alpha-1} \cdot \beta^{p+\alpha-1} \cdot e^{-x} \cdot \beta\,\mathrm{d}x \text{ (using } x = y/\beta) \\
&= \frac{\beta^p}{\Gamma(\alpha)} \int_0^\infty x^{p+\alpha-1} e^{-x}\,\mathrm{d}x \\
&= \frac{\Gamma(p+\alpha)}{\Gamma(\alpha)} \cdot \beta^p \text{ (as long as } p + \alpha > 0).
\end{aligned}$$

REMARK 1.9. An alternative way of solving this integral is as follows: recall that if $X \sim \text{GAM}(\alpha, \beta)$, then

$$f(x) = \frac{1}{\Gamma(\alpha)\beta^\alpha} x^{\alpha-1} e^{-x/\beta}$$

with $\int_0^\infty f(x) = 1$. Now, consider

$$E(Y^p) = \frac{1}{\Gamma(\alpha)\beta^\alpha} \int_0^\infty \underbrace{y^{p+\alpha-1} e^{-y/\beta}}_{(\star)} \, \mathrm{d}y,$$

and observe that $(\star)$ is part of the PDF of $\text{GAM}(p+\alpha, \beta)$. By our above observation, we see that

$$\int_0^\infty \frac{1}{\Gamma(p+\alpha)\beta^{p+\alpha}} y^{p+\alpha-1} e^{-y/\beta} \, \mathrm{d}y = 1,$$

and it follows that

$$\int_0^\infty y^{p+\alpha-1} e^{-y/\beta} \, \mathrm{d}y = \Gamma(p+\alpha)\beta^{p+\alpha}.$$

Putting everything together, we finally obtain

$$E(Y^p) = \frac{1}{\Gamma(\alpha)\beta^\alpha} \cdot \Gamma(p+\alpha)\beta^{p+\alpha} = \frac{\Gamma(p+\alpha)}{\Gamma(\alpha)} \cdot \beta^p.$$

1.7 Moment generating functions

Recall that the **moment generating function** of a random variable X is given by

$$M_X(t) = E[e^{tX}], \quad t \in \mathbb{R}.$$

Suppose X is a continuous random variable and let $f(x)$ be the PDF of X. Then

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} M_X(t) &= \frac{\mathrm{d}}{\mathrm{d}t} \int_A e^{tx} f(x) \, \mathrm{d}x \\ &= \int_A \frac{\mathrm{d}}{\mathrm{d}t} [e^{tx} f(x)] \, \mathrm{d}x \text{ (by Leibniz's rule)} \\ &= \int_A f(x) \cdot x \cdot e^{tx} \, \mathrm{d}x. \end{aligned}$$

Notice that

$$\frac{\mathrm{d}}{\mathrm{d}t} M_X(t)\Big|_{t=0} = \int_A f(x) \cdot x \cdot e^{0x} \, \mathrm{d}x = \int_A f(x) \cdot x \, \mathrm{d}x = E(x).$$

Similarly, we can find that

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} M_X(t) = \int_A \frac{\mathrm{d}^2}{\mathrm{d}t^2} [e^{tx} f(x)] \, \mathrm{d}x = \int_A f(x) \cdot x^2 \cdot e^{tx} \, \mathrm{d}x$$

and hence

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2} M_X(t)\Big|_{t=0} = E(x^2).$$

Moment generating function of the normal distribution. Suppose that $X \sim \text{N}(\mu, \sigma^2)$. Recall that the PDF of X is

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\Big(-\frac{(x-\mu)^2}{2\sigma^2}\Big), \quad x \in \mathbb{R}.$$

Then, the moment generating function is given by

$$\begin{aligned}
M_X(t) = E(e^{tX}) &= \int_{-\infty}^{\infty} \exp(tx) \cdot \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x-\mu)^2 - 2t\sigma^2 x}{2\sigma^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2 - 2x\mu - 2t\sigma^2 x + \mu^2}{2\sigma^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{x^2 - 2(\mu + t\sigma^2)x + \mu^2}{2\sigma^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x - (\mu + t\sigma^2))^2 - (\mu + t\sigma^2)^2 + \mu^2}{2\sigma^2}\right) \mathrm{d}x \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(\frac{(\mu + t\sigma^2)^2 - \mu^2}{2\sigma^2}\right) \int_{-\infty}^{\infty} \exp\left(-\frac{(x - (\mu + t\sigma^2))^2}{2\sigma^2}\right) \mathrm{d}x \qquad (\star) \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \cdot \exp\left(\frac{2\mu t\sigma^2 + t^2\sigma^4}{2\sigma^2}\right) \cdot \sqrt{2\pi\sigma^2} \\
&= \exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right)
\end{aligned}$$

for all $t \in \mathbb{R}$. At step $(\star)$, we use a similar trick to Remark 1.9. Namely, note that the term in the integral is part of the PDF of $\mathrm{N}(\mu + t\sigma^2, \sigma^2)$, and so the integral is equal to the reciprocal of the constant term of the PDF, which is $\sqrt{2\pi\sigma^2}$.

With this out of the way, we can now compute the expectation and variance of X. We have

$$\begin{aligned}
E(X) &= \frac{\mathrm{d}}{\mathrm{d}t} M_X(t)\bigg|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t} \exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right)\bigg|_{t=0} \\
&= \exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right) \cdot (\mu + t\sigma^2)\bigg|_{t=0} = \mu.
\end{aligned}$$

Then, to compute the variance, we first need to compute $E(X^2)$. We obtain

$$\begin{aligned}
E(X^2) &= \frac{\mathrm{d}^2}{\mathrm{d}t^2} M_X(t)\bigg|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{\mathrm{d}}{\mathrm{d}t} M_X(t)\right]\bigg|_{t=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\left[\exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right) \cdot (\mu + t\sigma^2)\right]\bigg|_{t=0} \\
&= \exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right) \cdot (\mu + t\sigma^2)^2 + \exp\left(\mu t + \frac{1}{2}t^2\sigma^2\right) \cdot \sigma^2\bigg|_{t=0} \\
&= \mu^2 + \sigma^2.
\end{aligned}$$

Finally, we see that

$$\mathrm{Var}(X) = E(X^2) - (E(X))^2 = \mu^2 + \sigma^2 - \mu^2 = \sigma^2.$$

2 Joint CDFs and independence

2.1 Definitions and properties

DEFINITION 2.1. The **joint CDF** of random variables X and Y is given by

$$F(x,y) = P[X \leq x, Y \leq y], \quad (x,y) \in \mathbb{R}^2.$$

Note that the comma means "and". In particular, we mean that

$$P(X \leq x, Y \leq y) = P((X \leq x) \cap (Y \leq y)).$$

Properties of the joint CDF. Let $F(x,y)$ be the joint CDF of random variables X and Y.

(1) For fixed y, we have that F is non-decreasing in x; that is, $F(x_1,y) \leq F(x_2,y)$ if $x_1 < x_2$.

(2) For fixed x, we have that F is non-decreasing in y; that is, $F(x,y_1) \leq F(x,y_2)$ if $y_1 < y_2$.

(3) $\lim_{x\to-\infty} F(x,y) = 0$ and $\lim_{y\to-\infty} F(x,y) = 0$.

(4) $\lim_{(x,y)\to(-\infty,-\infty)} F(x,y) = 0$.

(5) $\lim_{(x,y)\to(+\infty,+\infty)} F(x,y) = 1$.

DEFINITION 2.2. Suppose F is the joint CDF of random variables X and Y. The **marginal CDF of** X is given by

$$F_1(x) = \lim_{y\to+\infty} F(x,y) = P[X \leq x], \quad x \in \mathbb{R}.$$

Similarly, the **marginal CDF of** Y is given by

$$F_2(y) = \lim_{x\to+\infty} F(x,y) = P[Y \leq y], \quad y \in \mathbb{R}.$$

Note that the definition and properties of the joint CDF, as well as how to find the marginal CDFs, hold for both discrete and continuous random variables X and Y. In this course, we will assume that X and Y are either both discrete or both continuous.

DEFINITION 2.3. Suppose X and Y are discrete random variables. The **joint PF** of X and Y is given by

$$f(x,y) = P[X = x, Y = y], \quad (x,y) \in \mathbb{R}^2.$$

The set $A = \{(x,y) \in \mathbb{R}^2 : f(x,y) > 0\}$ is called the **support set** of (X,Y).

Properties of the joint PF. Let $f(x,y)$ be the joint PF of discrete random variables X and Y.

(1) $f(x,y) \geq 0$ for all $(x,y) \in \mathbb{R}^2$.

(2) $\sum_{(x,y)\in A} f(x,y) = 1$.

Note that (2) actually has a double summation; that is,

$$\sum_{(x,y)\in A} f(x,y) = \sum_{x\in\mathbb{R}} \sum_{y\in\mathbb{R}:(x,y)\in A} f(x,y).$$

DEFINITION 2.4. Let $f(x,y)$ be the joint PF of discrete random variables X and Y. The **marginal PF of** X is given by

$$f_1(x) = P[X = x] = \sum_{\text{all } y} f(x,y), \quad x \in \mathbb{R}.$$

The **marginal PF of** Y is given by

$$f_2(x) = P[Y = y] = \sum_{\text{all } x} f(x, y), \quad y \in \mathbb{R}.$$

The **conditional PF of** X **given** $Y = y$ is

$$P[X = x \mid Y = y] = f_1(x \mid y) = \frac{f(x, y)}{f_2(y)} = \frac{P[X = x, Y = y]}{P[Y = y]}$$

for all $(x, y) \in A$, provided that $f_2(y) \neq 0$. Similarly, the **conditional PF of** Y **given** $X = x$ is

$$P[Y = y \mid X = x] = f_2(y \mid x) = \frac{f(x, y)}{f_1(x)} = \frac{P[X = x, Y = y]}{P[X = x]}$$

for all $(x, y) \in A$, given that $f_1(x) \neq 0$.

Properties of the conditional PF.

(1) $f_1(x \mid y) = P[X = x \mid Y = y] \geq 0$.

(2) For fixed y, we have $\sum_{x:(x,y)\in A} f_1(x \mid y) = 1$. Similarly, for fixed x, we have $\sum_{y:(x,y)\in A} f_2(y \mid x) = 1$.

Definition 2.5. Let X and Y be continuous random variables with joint CDF F. The **joint PDF** of X and Y is given by

$$f(x, y) = \frac{\partial^2}{\partial x \partial y} F(x, y).$$

The set $A = \{(x, y) \in \mathbb{R}^2 : f(x, y) > 0\}$ is called the **support set** of (X, Y).

First, note that the order of partials does not matter. Secondly, for convenience, when $\frac{\partial^2}{\partial x \partial y} F(x, y)$ does not exist, we arbitrarily define $f(x, y) = 0$, and we only have countably many such cases.

Properties of the joint PDF.

(1) $f(x, y) \geq 0$ for all $(x, y) \in \mathbb{R}^2$.

(2) $\iint_A f(x, y) \, \mathrm{d}x \, \mathrm{d}y = 1$.

Note that given the joint PDF $f(x, y)$ of two continuous random variables X and Y, we can find the joint CDF $F(x, y)$ of X and Y by computing

$$F(x', y') = P[X \leq x', Y \leq y'] = \int_{-\infty}^{x'} \int_{-\infty}^{y'} f(x, y) \, \mathrm{d}x \, \mathrm{d}y.$$

Definition 2.6. Let $f(x, y)$ be the joint PDF of continuous random variables X and Y. The **marginal PDF of** X is given by

$$f_1(x) = \int_{-\infty}^{\infty} f(x, y) \, \mathrm{d}y, \quad x \in \mathbb{R}.$$

The **marginal PDF of** Y is given by

$$f_2(y) = \int_{-\infty}^{\infty} f(x, y) \, \mathrm{d}x, \quad y \in \mathbb{R}.$$

The **conditional PDF of** X **given** $Y = y$ is

$$f_1(x \mid y) = \frac{f(x, y)}{f_2(y)}$$

for all $(x, y) \in A$ with $f_2(y) \neq 0$. The **conditional PDF of** Y **given** $X = x$ is

$$f_2(y \mid x) = \frac{f(x, y)}{f_1(x)}$$

for all $(x, y) \in A$ where $f_1(x) \neq 0$.

Properties of the conditional PDF.

(1) $f_1(x \mid y) \geq 0$.

(2) For fixed y, we have $\int_{-\infty}^{\infty} f_1(x \mid y)\, \mathrm{d}x = 1$.

2.2 Examples

Example 2.7. The Hardy-Weinberg law of genetics states that under certain conditions, the relative frequencies of which three genotypes AA, Aa, and aa occur in the population will be θ^2, $2\theta(1-\theta)$, and $(1-\theta)^2$ respectively, where $0 < \theta < 1$.

Suppose n members of the population are selected at random. Let X be the number of AA types selected, and let Y be the number of Aa types selected.

(1) Find the joint PF of X and Y.

Solution: Let us denote $p_1 = \theta^2$, $p_2 = 2\theta(1-\theta)$, and $p_3 = (1-\theta)^2$. Notice that we have $p_1+p_2+p_3 = 1$, and so $(X, Y) \sim \text{Multi}(n, p_1, p_2)$. Hence, the joint PF of X and Y is

$$P[X = x, Y = y] = \frac{n!}{x!y!(n-x-y)!} p_1^x p_2^y p_3^{n-x-y}.$$

(2) Find the marginal PF of X.

Solution: First, note that $0 \leq y \leq n$ and $0 \leq x + y \leq n$, which implies that $y \leq n - x$. Then we have

$$\begin{aligned} f_1(x) = P[X = x] &= \sum_{\text{all } y} f(x, y) \\ &= \sum_{y=0}^{n-x} \frac{n!}{x!y!(n-x-y)!} p_1^x p_2^y p_3^{n-x-y} \\ &= \frac{n! p_1^x}{x!(n-x)!} \sum_{y=0}^{n-x} \frac{(n-x)!}{y!((n-x)-y)!} p_2^y p_3^{(n-x)-y} \\ &= \frac{n!}{x!(n-x)!} p_1^x (p_2 + p_3)^{n-x} \\ &= \frac{n!}{x!(n-x)!} p_1^x (1 - p_1)^{n-x}, \end{aligned}$$

where the second last equality follows from $(a+b)^k = \sum_{y=0}^{k} \binom{k}{y} a^y b^{k-y}$ where we have $k = n-x$, $a = p_2$, and $b = p_3$. In particular, we have $X \sim \text{Bin}(n, p_1)$. (Similarly, one can show that $Y \sim \text{Bin}(n, p_2)$.)

(3) Find the conditional PF of X given $Y = 1$.

Solution: We find this for general $Y = y$. We obtain

$$\begin{aligned} f_1(x \mid y) = \frac{f(x, y)}{f_2(y)} &= \frac{\frac{n!}{x!y!(n-x-y)!} p_1^x p_2^y p_3^{n-x-y}}{\frac{n!}{y!(n-y)!} p_2^y (1 - p_2)^{n-y}} \\ &= \frac{(n-y)!}{x!((n-y)-x)!} \cdot \frac{p_1^x p_3^{(n-y)-x}}{(1-p_2)^{x+(n-y)-x}} \\ &= \binom{n-y}{x} \left(\frac{p_1}{1-p_2}\right)^x \left(\frac{p_3}{1-p_2}\right)^{n-y}. \end{aligned}$$

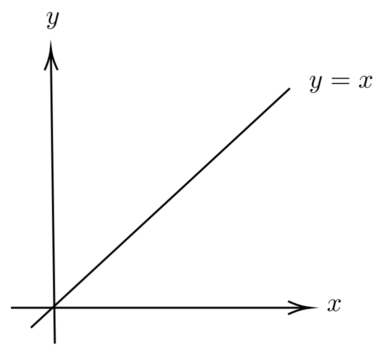
In particular, we have $(X \mid Y = y) \sim \text{Bin}(n-y, \frac{p_1}{1-p_2})$, and so $(X \mid Y = 1) \sim \text{Bin}(n-1, \frac{p_1}{1-p_2})$.

Example 2.8. Suppose X and Y are two continuous random variables with joint PDF

$$f(x,y) = \begin{cases} ke^{-x-y} & \text{if } 0 < x < y, \\ 0 & \text{otherwise.} \end{cases}$$

(1) Find k.

Solution: We first note that the support set of (X, Y) is the area above the $y = x$ line in the first quadrant in the following diagram.



Thus, we require

$$1 = k\int_0^\infty \left(\int_x^\infty e^{-x}e^{-y}\,\mathrm{d}y\right)\mathrm{d}x = k\int_0^\infty e^{-x}(e^{x} - 0)\,\mathrm{d}x = k\int_0^\infty e^{-2x}\,\mathrm{d}x = \frac{k}{2}(1-0) = \frac{k}{2},$$

and we obtain $k = 2$.

(2) Find the marginal PDF of X.

Solution: For $x \le 0$, we clearly have $f_1(x) = 0$. On the other hand, if $x > 0$, then

$$\begin{aligned} f_1(x) &= \int_{-\infty}^\infty f(x,y)\,\mathrm{d}y \\ &= \int_x^\infty f(x,y)\,\mathrm{d}y + \underbrace{\int_{-\infty}^x f(x,y)\,\mathrm{d}y}_{0 \text{ since } (x,y)\notin A \text{ here}} \\ &= \int_x^\infty 2e^{-x-y}\,\mathrm{d}y \\ &= 2e^{-x}\int_x^\infty e^{-y}\,\mathrm{d}y \\ &= 2e^{-x}(e^{-x} - 0) = 2e^{-2x}. \end{aligned}$$

(3) Find the conditional PDF of $(Y \mid X = x)$.

Solution: Given our result in (2), we obtain

$$f_2(y \mid x) = \frac{f(x,y)}{f_1(x)} = \frac{2e^{-x-y}}{2e^{-2x}} = \frac{e^{-y}}{e^{-x}} = e^{x-y},$$

if $(x, y) \in A$ and $f_1(x) \ne 0$. In particular, $(x, y) \in A$ if and only if $0 < x < y$, and in such a case we do not have $f_1(x) = 0$. Thus, we see that

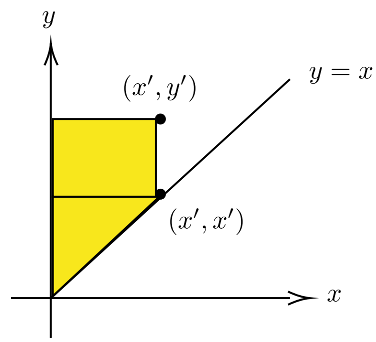
$$f_2(y \mid x) = e^{x-y}, \quad 0 < x < y.$$

(4) Find the joint CDF of X and Y.

Solution: We wish to compute $F(x', y') = P[X \le x', Y \le y']$. We consider three cases.

Case 1. If $x' \le 0$ or $y' \le 0$, then it is clear that $F(x', y') = 0$.

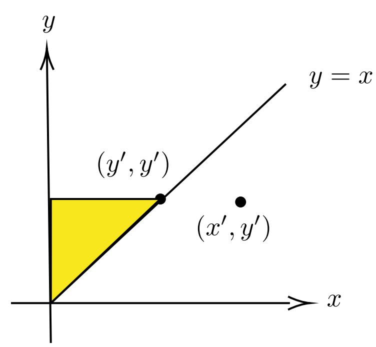
Case 2. Suppose that $0 < x' \le y'$. In this case, we would like to integrate the area indicated in the diagram below.



In particular, we see that

$$F(x', y') = \int_0^{x'} \left(\int_x^{y'} f(x, y)\, \mathrm{d}y \right) \mathrm{d}x = \int_0^{x'} \left(\int_x^{y'} 2e^{-x-y}\, \mathrm{d}y \right) \mathrm{d}x = (1 - e^{-2x'}) - 2e^{-y'}(1 - e^{-x'}).$$

Case 3. Suppose that $0 < y' < x'$. We now want to integrate the area below.



Notice that this case simply reduces to Case 2, as we have

$$F(x', y') = F(y', y') = (1 - e^{-2y'}) - 2e^{-y'}(1 - e^{-y'}) = 1 + e^{-2y'} - 2e^{-y'}.$$

Putting all these together, we have

$$F(x, y) = \begin{cases} 0 & x \le 0 \text{ or } y \le 0 \\ (1 - e^{-2x}) - 2e^{-y}(1 - e^{-x}) & 0 < x \le y \\ 1 + e^{-2y} - 2e^{-y} & 0 < y < x. \end{cases}$$

(5) Find the marginal CDF of X.

Solution: Note that taking $y \to +\infty$, the case $0 < y < x$ is not possible, while the cases $x \le 0$ and $0 < x \le y$ are. Namely, we have

$$F_1(x) = \lim_{y \to +\infty} F(x, y) = \begin{cases} 0 & x \le 0 \\ 1 - e^{-2x} & x > 0. \end{cases}$$

2.3 Product rule and independence

The **product rule** states that if $f(x, y)$ is the joint PF (respectively joint PDF) of two discrete (respectively continuous) random variables, then

$$f(x, y) = f_1(x \mid y) f_2(y) = f_2(y \mid x) f_1(x).$$

This is immediate from the definition.

We give an example of applying the product rule. Suppose we are given $f_2(y \mid x)$ and $f_1(x)$, and wish to find $f_2(y)$. We can do this with the following steps.

(i) Use the product rule to compute $f(x, y) = f_2(y \mid x) f_1(x)$.

(ii) Compute $f_2(y) = \int_{-\infty}^{\infty} f(x, y)\,\mathrm{d}x$ in the continuous case, or $f_2(y) = \sum_x f(x, y)$ in the discrete case.

Two random variables X and Y are **independent** if and only if one of the following holds:

(1) $F(x, y) = F_1(x) F_2(y)$ for all $(x, y) \in \mathbb{R}^2$;

(2) $f(x, y) = f_1(x) f_2(y)$ for all $(x, y) \in A_1 \times A_2$, where $A_1 = \{x \in \mathbb{R} : f_1(x) > 0\}$ and $A_2 = \{y \in \mathbb{R} : f_2(x) > 0\}$ (the joint support set is rectangular);

(3) $f_1(x \mid y) = f_1(x)$ for all $x \in A_1$;

(4) $f_2(y \mid x) = f_2(y)$ for all $y \in A_2$;

(5) $M_{(X,Y)}(t_1, t_2) = M_X(t_1) M_Y(t_2)$.

Example 2.9. Recall Example 2.7, where we had $(X, Y) \sim \text{Multi}(n, p_1, p_2)$ with joint PF

$$f(x, y) = \frac{n!}{x!y!(n - x - y)!} p_1^x p_2^y p_3^{n-x-y}.$$

In particular, we require that $0 \le x \le n$, $0 \le y \le n$, and $0 \le x + y \le n$. The condition $0 \le x + y \le n$ means that the support set is not rectangular (condition (2) fails), and hence X and Y are not independent.

Example 2.10. From Example 2.8, we had joint PF

$$f(x, y) = 2e^{-x-y}, \quad 0 < x < y.$$

Again, this support set is not rectangular, and so X and Y are not independent. We can also show this in another way; recall that we had

$$f_2(y \mid x) = e^{x-y},$$

and since this depends on x, it cannot be the case that $f_2(y \mid x) = f_2(y)$, as $f_2(y)$ does not depend on x. Thus, condition (4) above fails.

Example 2.11. Suppose that X and Y are discrete random variables with joint PF

$$f(x, y) = \frac{\theta^{x+y} e^{-2\theta}}{x!y!}, \quad x = 0, 1, 2, \ldots, \quad y = 0, 1, 2, \ldots, \quad \theta > 0.$$

Notice that the support set $A = \mathbb{Z}_{\ge 0} \times \mathbb{Z}_{\ge 0}$ is rectangular. We claim that X and Y are independent. Indeed, we have

$$f_1(x) = \sum_{y=0}^{\infty} f(x, y) = \frac{\theta^x e^{-2\theta}}{x!} \sum_{y=0}^{\infty} \frac{\theta^y}{y!} = \frac{\theta^x e^{-2\theta}}{x!} \cdot e^{\theta} = \frac{\theta^x}{x!} \cdot e^{-\theta}.$$

In particular, we have $X \sim \text{Poi}(\theta)$. Similarly, one can find that

$$f_2(y) = \frac{\theta^y}{y!} \cdot e^{-\theta},$$

and so $Y \sim \text{Poi}(\theta)$. Since $f(x, y) = f_1(x) f_2(y)$ for all $(x, y) \in A$, it follows that X and Y are independent, as claimed.

2.4 Largest and smallest order statistics

Let $X_1, \ldots, X_n$ be a sequence of i.i.d. random variables; that is, a random sample from some distribution. We denote the **smallest order statistic** as

$$X_{(1)} := \min(X_1, \ldots, X_n)$$

and the **largest order statistic** as

$$X_{(n)} := \max(X_1, \ldots, X_n).$$

Note that we have

$$\begin{aligned} P[X_{(1)} \geq t] &= \prod_{i=1}^{n} P[X_i \geq t], \\ P[X_{(n)} \leq t] &= \prod_{i=1}^{n} P[X_i \leq t], \end{aligned}$$

as $X_1, \ldots, X_n$ are i.i.d. random variables.

Let $X_1, \ldots, X_n$ be a random sample of *continuous* random variables with CDF $F(x)$, pdf $f(x)$, and support set A. The PDFs of $X_{(1)}$ and $X_{(n)}$ respectively are

$$\begin{aligned} f_{(1)}(t) &= nf(t)[1 - F(t)]^{n-1}, \quad t \in A, \\ f_{(n)}(t) &= nf(t)[F(t)]^{n-1}, \quad t \in A. \end{aligned}$$

We prove this for $X_{(1)}$. First, notice that

$$\begin{aligned} P[X_{(1)} \geq t] &= P[X_1 \geq t, X_2 \geq t, \ldots, X_n \geq t] \\ &= \prod_{i=1}^{n} P[X_i \geq t] \\ &= \prod_{i=1}^{n} 1 - P[X_i \leq t] \\ &= \prod_{i=1}^{n} 1 - F(t) = (1 - F(t))^n. \end{aligned}$$

Next, the CDF of $X_{(1)}$ is given by

$$F_{(1)}(t) = P(X_{(1)} \leq t) = 1 - P[X_{(1)} > t] = 1 - P[X_{(1)} \geq t] = 1 - (1 - F(t))^n.$$

Finally, we see that

$$f_{(1)}(t) = \frac{\mathrm{d}}{\mathrm{d}t} F_{(1)}(t) = -n(1 - F(t))^{n-1} \cdot \underbrace{(-f(t))}_{(1-F(t))'} = nf(t)[1 - F(t)]^{n-1}.$$

Example 2.12. Suppose that we have a random sample of size n from $\text{UNIF}(0, \theta)$. Find the PDFs of $X_{(1)}$ and $X_{(n)}$.

Solution: Let $X_1, \ldots, X_n \sim \text{UNIF}(0, \theta)$ be i.i.d. random variables where $\theta > 0$. Note that the support set is given by $A = (0, \theta)$. We have CDF

$$F(t) = \begin{cases} 0 & t \leq 0 \\ t/\theta & 0 < t < \theta \\ 1 & t \geq \theta. \end{cases}$$

and PDF $f(t) = 1/\theta$, where $t \in (0, \theta)$. Thus, we obtain

$$f_{(1)}(t) = n(1 - t/\theta)^{n-1} \cdot 1/\theta, \quad t \in (0, \theta);$$
$$f_{(n)}(t) = n(t/\theta)^{n-1} \cdot 1/\theta, \quad t \in (0, \theta).$$

2.5 Sum of independent random variables

Recall the following facts:

(1) The moment generating function of a random variable X is given by $M_X(t) = E(\exp(tX))$; note that this may not always exist, so we must specify the values of t where it does exist.

(2) If X and Y are independent, then $M_{(X,Y)}(t_1, t_2) = M_X(t_1)M_X(t_2)$ for all $t_1 \in (-h_1, h_1)$ and $t_2 \in (-h_2, h_2)$, where $h_1, h_2 > 0$.

(3) **Uniqueness Theorem.** Let X and Y be random variables. Then X and Y are identically distributed if and only if $M_X(t) = M_Y(t)$.

Example 2.13. Suppose that $X \sim \mathrm{N}(\mu_1, \sigma_1^2)$ and $Y \sim \mathrm{N}(\mu_2, \sigma_2^2)$ are independent. Find the distribution of $X + Y$.

Solution: We recall that the moment generating functions of X and Y are given by

$$M_X(t_1) = \exp(t_1\mu_1 + \tfrac{1}{2}t_1^2\sigma_1^2), \quad t_1 \in \mathbb{R};$$
$$M_Y(t_2) = \exp(t_2\mu_2 + \tfrac{1}{2}t_2^2\sigma_2^2), \quad t_2 \in \mathbb{R}.$$

Let us denote $Z = X + Y$. Then

$$\begin{aligned}
M_Z(t) &= E[\exp(tZ)] = E[\exp(t(X + Y))] \\
&= E[\exp(tX + tY)] = E[\exp(tX)\exp(tY)] \\
&= E[\exp(tX)] \cdot E[\exp(tY)] \qquad (\star) \\
&= M_X(t)M_Y(t) \\
&= \exp(t\mu_1 + \tfrac{1}{2}t^2\sigma_1^2)\exp(t\mu_2 + \tfrac{1}{2}t^2\sigma_2^2) \\
&= \exp(t(\mu_1 + \mu_2) + \tfrac{1}{2}t^2(\sigma_1^2 + \sigma_2^2)).
\end{aligned}$$

We justify the equality at $(\star)$. Recall that if X and Y are independent, then $f(x, y) = f_1(x)f_2(y)$ for all $(x, y) \in A = A_1 \times A_2$. In particular, we see that

$$\begin{aligned}
E[h(X) \cdot g(Y)] &= \int_{A_1}\int_{A_2} h(x)g(y)f(x, y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \int_{A_1}\int_{A_2} h(x)g(y)f_1(x)f_2(y)\,\mathrm{d}x\,\mathrm{d}y \\
&= \left(\int_{A_1} h(x)f_1(x)\,\mathrm{d}x\right)\left(\int_{A_2} g(y)f_2(y)\,\mathrm{d}y\right) \\
&= E[h(X)] \cdot E[g(Y)].
\end{aligned}$$

Thus, we may conclude that $Z \sim N(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$.

Exercise 2.14. Suppose that $X \sim \mathrm{GAM}(\alpha_1, \beta)$ and $Y \sim \mathrm{GAM}(\alpha_2, \beta)$ are independent random variables. Find the distribution of $X + Y$.

3 Maximum likelihood estimates

Suppose that $Y \sim f(y;\theta)$. We obtain a random sample $Y_1,\dots,Y_n$ (i.i.d.) of size n, and denote the observed data by $y_1,\dots,y_n$.

(1) We know what f is; for example, it could be the PDF of a normal distribution, or the PF of a Poisson distribution.

(2) On the other hand, we do not know what θ is.

For now, we will focus on **point estimation** of θ (only one possible value of the unknown quantity) as opposed to **set estimation** (such as an interval). We wish to find θ based on the observed data $\mathbf{y} = (y_1,\dots,y_n)$. We use $\hat{\theta}$ to denote an estimate of the parameter θ; that is, $\hat{\theta} = \hat{\theta}(y_1,\dots,y_n) = \hat{\theta}(\mathbf{y})$.

Definition 3.1. The **likelihood function** (both discrete and continuous cases) for θ is defined as

$$L(\theta) = L(\theta;\mathbf{y}) = \prod_{i=1}^{n} f(y_i;\theta), \quad \theta \in \Omega,$$

where Ω is the **parameter space** which contains all possible values of θ.

Remark 3.2.

(1) When Y is *discrete*, the likelihood function is the probability that we observe the data $\mathbf{y}$, considered as a function of the parameter θ. In particular, $Y_1,\dots,Y_n$ are i.i.d., with $f(y_i;\theta) = P[Y_i = y_i;\theta]$ and

$$L(\theta) = \prod_{i=1}^{n} P[Y_i = y_i;\theta] = P[Y_1 = y_1,\dots,Y_n = y_n;\theta].$$

(2) The values of θ that make the observed data $\mathbf{y}$ more probable would be more credible or likely than those that make the data less probable.

(3) Hence, taking the largest of such θ seems like a sensible approach to find the point estimate of θ, and it turns out that it has some very nice properties.

Definition 3.3. The value of θ which maximizes $L(\theta)$ with the observed data $\mathbf{y}$ is called the **maximum likelihood estimate (MLE)** of θ. This value is denoted by $\hat{\theta}_{\text{MLE}}$ or just $\hat{\theta}$; that is,

$$\hat{\theta}_{\text{MLE}} = \hat{\theta} = \operatorname{argmax}_{\theta\in\Omega} L(\theta).$$

Remark 3.4.

(1) It is typically easier to work with the log (base e) of the likelihood function $L(\theta)$. We denote

$$\ell(\theta) := \log L(\theta).$$

(2) Since functions are often (but not always) maximized by setting their derivatives equal to zero, we can usually obtain θ by solving the **score equation**

$$\frac{\partial \ell(\theta)}{\partial \theta} = 0.$$

(3) The first derivative test can be used to verify that a solution to $\partial\ell(\theta)/\partial\theta = 0$ corresponds to a maximizer (and not a minimizer). In particular, if $\hat{\theta}$ is a solution, we need to check that

- $\partial\ell(\theta)/\partial\theta > 0$ when $\theta < \hat{\theta}$, and
- $\partial\ell(\theta)/\partial\theta < 0$ when $\theta > \hat{\theta}$.

EXAMPLE 3.5. During 2016, Nanos Research conducted a survey on Canadian adults to determine support for the legalization of marijuana. The 1000 participants were recruited across Canada, and were asked "Do you support, somewhat support, somewhat oppose, or oppose legalizing the recreational use of marijuana?" 39% of participants indicated that they supported the recreational use of marijuana, while 29% of participants indicated that they somewhat supported it.

Let θ denote the proportion of Canadian adults who support or somewhat support the recreational use of marijuana. Find the MLE of θ.

Solution: We have $X_1, \ldots, X_{1000}$ (i.i.d.) with each $X_i \sim \text{Bernoulli}(\theta)$. We have $X_i = 1$ when the recreational use of marijuana is supported or somewhat supported, and $X_i = 0$ otherwise. In particular, notice that

$$\sum_{i=1}^{1000} X_i \sim \text{Bin}(1000, \theta).$$

Observe that a total of $390 + 290 = 680$ participants from the sample support or somewhat support the use of recreational marijuana. This gives

$$\sum_{i=1}^{1000} x_i = 680.$$

Let $Y = \sum_{i=1}^{1000} X_i \sim \text{Bin}(1000, \theta)$, and we have a single observation $y = 680$. Then the likelihood function is given by

$$L(\theta) = L(\theta; y) = \binom{1000}{y} \theta^y (1-\theta)^{1000-y}.$$

The log of the likelihood function is then

$$\ell(\theta) = \log L(\theta) = \log \binom{1000}{y} + y \log \theta + (1000 - y) \log(1-\theta),$$

and taking the derivative, we get

$$\frac{\partial \ell(\theta)}{\partial \theta} = 0 + \frac{y}{\theta} - \frac{1000 - y}{1 - \theta} = \frac{y(1-\theta) - (100 - y)\theta}{\theta(1-\theta)} = \frac{y - 1000\theta}{\theta(1-\theta)}.$$

Solving $\partial \ell(\theta)/\partial \theta = 0$, we have

$$\hat{\theta} = \frac{y}{1000} = \frac{680}{1000} = 0.68.$$

Finally, we use the first derivative test to verify that this is a maximizer.

- If $\theta < \hat{\theta} = y/1000$, then $1000\theta < y$, which implies that $\partial \ell(\theta)/\partial \theta > 0$.
- If $\theta > \hat{\theta} = y/1000$, then $1000\theta > y$, so $\partial \ell(\theta)/\partial \theta < 0$.

In summary, we obtain $\hat{\theta}_{\text{MLE}} = \hat{\theta} = 0.68$.

Recall that to solve $f(x) = 0$ numerically, we can use Newton's method which iteratively computes

$$x^{(i+1)} = x^{(i)} - \frac{f(x^{(i)})}{f'(x^{(i)})},$$

and this converges to the solution.

Newton Raphson method. To find $\hat{\theta}$, we usually solve $\partial \ell(\theta)/\partial \theta = 0$. When this is not possible (there is no explicit solution), we must use numerical methods. We can do this using the Newton Raphson method, which is given by

$$\theta^{(i+1)} = \theta^{(i)} - \frac{S(\theta^{(i)}; \mathbf{y})}{I(\theta^{(i)}; \mathbf{y})},$$

where $S(\theta; \mathbf{y}) = \partial \ell(\theta)/\partial \theta$ is the **score function** and $I(\theta; \mathbf{y}) = -\partial^2 \ell(\theta)/\partial \theta^2$ is the **information function**.

Note that in STAT 241, we are not required to carry out the Newton Raphson method (using code or other methods). We only need to be able to give the iterative formula above within some provided model.

Likelihood functions for continuous random variables. Recall that for a continuous random variable X, we have $P[X = x; \theta] = 0$ for all $x \in \mathbb{R}$. Hence, we need to be more careful than in the discrete case.

Suppose that Y is a continuous random variable with PDF $f(y; \theta)$. We usually observe only the value of Y rounded to some degree of precision; for instance, we would round data on waiting time to the nearest second, and data on height to the nearest centimeter.

Suppose we observe $Y = y$ to one decimal place. Then we have

$$P[Y = 1.1; \theta] = \int_{1.05}^{1.15} f(y; \theta)\,\mathrm{d}y \approx 0.5 \cdot f(1.1; \theta),$$

provided that $f(y; \theta)$ is reasonably smooth between 1.05 and 1.15.

More generally, suppose that $y_1, \ldots, y_n$ are the observations from a random sample from $f(y; \theta)$ which have been rounded to the nearest Δ which is assumed to be small. Then

$$P[\mathbf{Y} = \mathbf{y}; \theta] \approx \prod_{i=1}^{n} \Delta \cdot f(y_i; \theta) = \Delta^n \prod_{i=1}^{n} f(y_i; \theta).$$

It is a reasonable assumption that the precision Δ does not depend on the unknown parameter θ, so the term Δ^n can be ignored when finding $\hat{\theta}$. In particular, similarly to the discrete case, we can find θ by maximizing

$$L(\theta) = L(\theta; \mathbf{y}) = \prod_{i=1}^{n} f(y_i; \theta).$$

Multiple unknown parameters. When there are multiple unknown parameters, we need to find the MLE by solving multiple equations simultaneously. More explicitly, if $\underline{\theta} = (\theta_1, \ldots, \theta_k)$ are unknowns for some $k \geq 1$, then we need to solve

$$\begin{cases} \partial \ell(\underline{\theta}) / \partial \theta_1 = 0, \\ \qquad \vdots \\ \partial \ell(\underline{\theta}) / \partial \theta_k = 0. \end{cases}$$

Invariance property of the MLE. If $\hat{\theta}$ is the MLE of θ, then $g(\hat{\theta})$ is the MLE of $g(\theta)$.

Example 3.6. Suppose we want to estimate attributes associated with BMI for some population of individuals. If the distribution of BMI values in the population is well described by a Gaussian model $Y \sim \mathrm{N}(\mu, \sigma^2)$, then by estimating μ and σ, we can estimate any attribute associated with the BMI distribution.

Suppose a random sample of 150 males gave observations $y_1, \ldots, y_{150}$ and that the MLEs based on the data are $\hat{\mu} = 27.1$ and $\hat{\sigma} = 3.56$.

(1) Find the median BMI in the population.

Solution: The median is clearly $\hat{\mu} = 27.1$.

(2) Find the 10% quantile of the BMI distribution.

Solution: Let τ be the 10% quantile of $\mathrm{N}(\mu, \sigma^2)$. Then

$$0.1 = P[Y \leq \tau] = P\left[\frac{Y - \mu}{\sigma} \leq \frac{\tau - \mu}{\sigma}\right] = \Phi\left(\frac{\tau - \mu}{\sigma}\right),$$

where Φ is the CDF of $\mathrm{N}(0, 1)$. Then we have $(\tau - \mu)/\sigma = -1.28$, which implies that $\tau = \mu - 1.28\sigma$. By the invariance property of the MLE, we then obtain

$$\hat{\tau} = \hat{\mu} - 1.28\hat{\sigma} = 22.54.$$

(3) Find the fraction of the population with BMI over 35.0.

Solution: Similar to (2), and is left as an exercise (the answer is 0.013).

4 Expectation-maximization algorithm

The **expectation-maximization (E-M) algorithm** was popularized by Dempster, Laird, and Rubin in 1977 and is a useful method for finding the MLE when (some of) the data are incomplete, and can also be applied to other contexts such as mixture models.

Suppose that

- the complete data $\mathbf{X}$ has log-likelihood function $\ell(\theta; \mathbf{x})$, and
- the incomplete data $\mathbf{Y} = \mathbf{Y}(\mathbf{X})$ has log-likelihood function $\ell^*(\theta; \mathbf{y})$.

Usually, maximizing $\ell(\theta; \mathbf{x})$ is easier than maximizing $\ell^*(\theta; \mathbf{y})$. However, suppose that we can only observe $\mathbf{Y} = \mathbf{y}$, while $\mathbf{X} = \mathbf{x}$ (and hence $\ell(\theta; \mathbf{x})$) is unavailable.

The E-M algorithm uses an iterative two-step method. We denote by $\theta^{(k)}$ the estimate of θ at the k-th iteration of the algorithm.

Step 0. Choose an initial value $\theta^{(0)}$ based on the complete part of the incomplete data. Usually, if $\mathbf{Y} = (Y_1, \ldots, Y_n)$ is the incomplete data and $(Y_1, \ldots, Y_j)$ is the complete part of the incomplete data, then it is reasonable to set

$$\theta^{(0)} = \frac{1}{j} \sum_{i=1}^{j} y_i.$$

Step 1. This is the first step of the two-step method, the **E-step**. We find

$$Q(\theta, \theta^{(k)}) := E[\ell(\theta; \mathbf{X}) \mid \mathbf{Y} = \mathbf{y}; \theta^{(k)}].$$

Step 2. This is the second step of the two-step method, the **M-step**. We let

$$\theta^{(k+1)} = \max_{\theta} Q(\theta, \theta^{(k)}).$$

Note that the max is with respect to θ, and not $\theta^{(k)}$. We can do this similarly to the usual method; solve $\partial Q(\theta, \theta^{(k)})/\partial\theta = 0$ and apply the first derivative test.

Step 3. We check for convergence. In particular, we verify that

$$|\theta^{(k+1)} - \theta^{(k)}| < \varepsilon$$

for some chosen tolerance level $\varepsilon > 0$. If not, go back to Step 1.

In Step 1, it is useful to note that if $\mathbf{X} = (X_1, \ldots, X_n)$ are independent, then $\mathbf{Y}(\mathbf{X}) = (Y_1, \ldots, Y_n)$ is also independent. Moreover, we have that

$$E[x_i \mid \mathbf{Y} = \mathbf{y}; \theta^{(k)}] = E[x_i \mid Y_i = y_i; \theta^{(k)}].$$

Indeed, we can verify this for the special case $n = 2$ which can then be generalized. Suppose that X_1 is independent of X_2. Then Y_1 and Y_2 are also independent. Also, we have

$$f(x_1 \mid y_1, y_2) = \frac{f(x_1, y_1, y_2)}{f(y_1, y_2)} = \frac{f(x_1, y_1 \mid y_2) f(y_2)}{f(y_1 \mid y_2) f(y_2)} = \frac{f(x_1, y_1)}{f(y_1)} = f(x_1 \mid y_1),$$

where the second equality is by the product rule, and the third equality follows from independence.

5 Sampling distributions

To investigate properties of estimates, we note that our estimate $\hat{\theta} = \hat{\theta}(\mathbf{y})$ depends on the observed sample $\mathbf{Y} = \mathbf{y}$. In particular, if we take different samples $\mathbf{y}^1, \dots, \mathbf{y}^M$ where

$$\mathbf{y}^j = (y_1^j, \dots, y_{n_j}^j)$$

and n_j is the sample size of $\mathbf{y}^j$, then we obtain different estimates $\hat{\theta}_1 = \hat{\theta}(\mathbf{y}^1)$, ..., $\hat{\theta}_M = \hat{\theta}(\mathbf{y}^M)$.

Moreover, we can think of each estimate $\hat{\theta}(\mathbf{y})$ as a realization of a random variable $\hat{\theta}(\mathbf{Y})$, which has its own distribution, mean, and variance, among other properties.

How close to θ could we expect $\hat{\theta}(\mathbf{Y})$ to be? How do we quantify the uncertainty in $\hat{\theta}(\mathbf{Y})$? To answer these questions, we introduce estimators and sampling distributions.

Definition 5.1. A **point estimator** is a random variable which is a function $\hat{\theta}(\mathbf{Y})$ of a random sample $\mathbf{Y} = (Y_1, \dots, Y_n)$.

Note that a **point estimate** $\hat{\theta}(\mathbf{y})$ is the value of this function $\hat{\theta}(\cdot)$ based on a particular observed sample $\mathbf{y} = (y_1, \dots, y_n)$.

Definition 5.2. The distribution of an estimator $\hat{\theta}(\mathbf{Y})$ is called the **sampling distribution** of the estimator.

Remark 5.3. Observe that $\hat{\theta}(\mathbf{Y})$ is random as the sample $\mathbf{Y}$ is random. Consequently, $\hat{\theta}(\mathbf{y})$ is a realization of $\hat{\theta}(\mathbf{Y})$ since $\mathbf{y}$ is a realization of $\mathbf{Y}$.

Example 5.4. Suppose that $(Y_1, \dots, Y_n)$ is a random sample from $\mathrm{N}(\mu, \sigma^2)$. Find the sampling distribtuion of $\hat{\mu}(\mathbf{Y}) = \overline{Y} = \frac{1}{n}\sum_{i=1}^n Y_i$.

Solution: Recall that in Week 1, we derived the moment generating function of $Y \sim \mathrm{N}(\mu, \sigma^2)$, which is given by

$$M_Y(t) = \exp\left(t\mu + \frac{1}{2}t^2\sigma^2\right), \quad t \in \mathbb{R}.$$

Moreover, recall that X and Y are independent if and only if $M_X(t_1) \cdot M_Y(t_2) = M_{(X,Y)}(t_1, t_2)$ for all $t_1 \in (-h_1, h_1)$ and $t_2 \in (-h_2, h_2)$ for some $h_1, h_2 > 0$.

Therefore, since $(Y_1, \dots, Y_n)$ are independent, we have

$$\begin{aligned}
M_{(Y_1,\dots,Y_n)}(t_1, \dots, t_n) &= E[\exp(t_1Y_1 + t_2Y_2 + \cdots + t_nY_n)] \\
&= E[\exp(t_1Y_1)]E[\exp(t_2Y_2)] \cdots E[\exp(t_nY_n)] \\
&= M_{Y_1}(t_1)M_{Y_2}(t_2) \cdots M_{Y_n}(t_n) \\
&= \prod_{i=1}^n M_{Y_i}(t_i) \\
&= \prod_{i=1}^n M_Y(t_i) \\
&= \prod_{i=1}^n \exp\left(t_i\mu + \frac{1}{2}t_i^2\sigma^2\right) \\
&= \exp\left(\mu\sum_{i=1}^n t_i + \frac{1}{2}\sigma^2\sum_{i=1}^n t_i^2\right).
\end{aligned}$$

Now, note that we are trying to find the moment generating function of $\hat{\mu}(\mathbf{Y}) = \frac{1}{n}\sum_{i=1}^{n} Y_i$, which we will denote by $M(t)$. We have

$$\begin{aligned}
M(t) &= E[\exp(t \cdot \hat{\theta}(\mathbf{Y}))] \\
&= E\left[\exp\left(t \cdot \frac{1}{n}\sum_{i=1}^{n} Y_i\right)\right] \\
&= E\left[\exp\left(\frac{t}{n} \cdot Y_1 + \frac{t}{n} \cdot Y_2 + \cdots + \frac{t}{n} Y_n\right)\right] \\
&= M_{(Y_1,\ldots,Y_n)}\left(\frac{t}{n}, \frac{t}{n}, \ldots, \frac{t}{n}\right) \\
&= \exp\left(\mu \sum_{i=1}^{n} \frac{t}{n} + \frac{1}{2}\sigma^2 \sum_{i=1}^{n}\left(\frac{t}{n}\right)^2\right) \\
&= \exp\left(\mu t + \frac{1}{2}\sigma^2 \frac{t^2}{n}\right).
\end{aligned}$$

Observe that this is the moment generating function of $\mathrm{N}(\mu, \sigma^2/n)$. Due to the Uniqueness Theorem of moment generating functions, it follows that

$$\hat{\mu}(\mathbf{Y}) = \overline{Y} \sim \mathrm{N}(\mu, \sigma^2/n).$$

Example 5.5. Suppose that $(Y_1, \ldots, Y_n)$ is a random sample from $\mathrm{EXP}(\theta)$. Find the sampling distribution of $\hat{\theta}(\mathbf{Y}) = \overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$.

Solution: Recall that the PDF of $Y \sim \mathrm{EXP}(\theta)$ is given by

$$f(y;\theta) = \frac{1}{\theta}\exp\left(-\frac{y}{\theta}\right), \quad y > 0, \quad \theta > 0.$$

Then, we see that

$$\begin{aligned}
M_Y(t) = E[\exp(t \cdot Y)] &= \int_0^\infty \exp(t \cdot y) \cdot \frac{1}{\theta}\exp\left(-\frac{y}{\theta}\right)\,\mathrm{d}y \\
&= \frac{1}{\theta}\int_0^\infty \exp\left(\left(t - \frac{1}{\theta}\right)y\right)\,\mathrm{d}y \qquad (\star) \\
&= \frac{1}{\theta} \cdot \frac{1}{t - 1/\theta}\left[\exp\left(\left(t - \frac{1}{\theta}\right)y\right)\right]_{y=0}^{y\to\infty} \\
&= \frac{1}{\theta} \cdot \frac{1}{t - 1/\theta}[0 - 1] \\
&= \frac{1}{1 - \theta t}, \quad t < \frac{1}{\theta}.
\end{aligned}$$

Note that $M_Y(t)$ only exists for $t < 1/\theta$ as the integral at $(\star)$ is finite only when $t - 1/\theta < 0$.

Now, the moment generating function of $\overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$ is

$$\begin{aligned} M(t) &= E\left[\exp\left(t \cdot \frac{1}{n}\sum_{i=1}^{n} Y_i\right)\right] \\ &= E\left[\exp\left(\frac{t}{n}\cdot Y_1 + \cdots + \frac{t}{n}\cdot Y_n\right)\right] \\ &= \prod_{i=1}^{n} M_y\left(\frac{t}{n}\right) \\ &= \prod_{i=1}^{n} \frac{1}{1-\theta\cdot t/n} \\ &= \left(\frac{1}{1-\theta\cdot t/n}\right)^n, \quad \frac{t}{n} < \frac{1}{\theta}. \end{aligned}$$

As an exercise, verify that if $X \sim \mathrm{GAM}(\alpha, \beta)$, then the moment generating function of X is

$$M_X(t) = \frac{1}{(1-\beta t)^\alpha}, \quad t < \frac{1}{\beta}.$$

In particular, we see that $M(t)$ is the moment generating function of $\mathrm{GAM}(n, \theta/n)$. By the Uniqueness Theorem of moment generating functions, we have

$$\hat{\theta}(\mathbf{Y}) = \overline{Y} \sim \mathrm{GAM}(n, \theta/n).$$

Now, suppose we have a random sample $(Y_1, \ldots, Y_n)$ from $\mathrm{Poi}(\theta)$, and we wish to find the sampling distribution of $\hat{\theta}(\mathbf{Y}) = \overline{Y} = \frac{1}{n}\sum_{i=1}^{n} Y_i$.

As usual, we start by finding the moment generating function of $Y \sim \mathrm{Poi}(\theta)$; as an exercise, we can find that

$$M_y(t) = e^{\theta(e^t - 1)}, \quad t \in \mathbb{R}.$$

Then, for $\hat{\theta}(\mathbf{Y}) = \overline{Y}$, the moment generating function is given by

$$M(t) = \prod_{i=1}^{n} M_Y\left(\frac{t}{n}\right) = \prod_{i=1}^{n} e^{\theta(e^{t/n}-1)} = e^{n\theta(e^{t/n}-1)}, \quad t \in \mathbb{R}.$$

What random variable has this moment generating function? This is certainly not a Poisson distribution due to the t/n term. In fact, this is not any of the commonly seen random variables. Hence, we cannot apply the same techniques which we used in Example 5.4 and Example 5.5.

This shows us that the sampling distribution often has to be determined approximately, using results such as the Central Limit Theorem.

Theorem 5.6 (Central Limit Theorem). Suppose that $(Y_1, \ldots, Y_n)$ is a random sample with $E(Y_i) = \mu$ and $\mathrm{Var}(Y_i) = \sigma^2 < \infty$. Then, we have

$$\frac{\sqrt{n}(\overline{Y} - \mu)}{\sigma} \sim \mathrm{N}(0, 1)$$

approximately/for large n.

Note that larger n or smaller σ results in a smaller approximation $\mathrm{Var}(\overline{Y})$, which means that our estimate is more likely to be close to the true value μ (estimated by $\overline{Y}$).

Let us consider how we can apply the Central Limit Theorem to our situation. Suppose that $Z = \sqrt{n}(\overline{Y} - \mu)/\sigma \sim \mathrm{N}(0,1)$ approximately/for large n. Then, by the Central Limit Theorem, we have

$$M_Z(t) \approx \exp\left(t\cdot 0 + \frac{1}{2}t^2 \cdot 1\right) = \exp\left(\frac{1}{2}t^2\right).$$

Consequently, we obtain

$$\begin{aligned}
M_{\overline{Y}}(t) &= E[\exp(t \cdot \overline{Y})] \\
&= E\left[\exp\left(t \cdot \left(\frac{\sigma Z}{\sqrt{n}} + \mu\right)\right)\right] \\
&= \exp(t\mu) \cdot E\left[\exp\left(\frac{t\sigma}{\sqrt{n}} \cdot Z\right)\right] \\
&\approx \exp(t\mu) \cdot \exp\left(\frac{1}{2}\left(\frac{t\sigma}{\sqrt{n}}\right)^2\right) \\
&= \exp\left(t\mu + \frac{1}{2}t^2\frac{\sigma^2}{n}\right),
\end{aligned}$$

where we have the approximation since $E[\exp(t\sigma/\sqrt{n} \cdot Z)]$ is the moment generating function of Z applied at $t\sigma/\sqrt{n}$. In particular, this is the moment generating function of $\mathrm{N}(\mu, \sigma^2/n)$, so we have $\overline{Y} \sim \mathrm{N}(\mu, \sigma^2/n)$ approximately/for large n.

Remark 5.7. The variation σ^2/n of $\overline{Y}$ is small (which is desirable) when σ is small or n is large.

It is important to note that we only have an approximate sampling distribution when doing this. We now take a look at Markov's Inequality and Chebyshev's Inequality to help us quantify how good these approximations are.

Theorem 5.8 (Markov's Inequality). For any random variable X such that $E(|X|^k)$ is finite, we have

$$P(|X| \geq c) \leq \frac{E(|X|^k|)}{c^k}$$

for all $c > 0$ and $k > 0$. We often call $P(|X| \geq c)$ the **tail probability**.

Proof. We prove Markov's Inequality in the case where X is a continuous random variable; the proof is similar in the discrete case by replacing the integral with the summation. Indeed, for all $c > 0$ and $k > 0$, we have

$$\begin{aligned}
\frac{E(|X|^k|)}{c^k} &= E\left[\left(\frac{|x|}{c}\right)^k\right] \\
&= E\left[\left|\frac{x}{c}\right|^k\right] \\
&= \int_{-\infty}^{\infty} \left|\frac{x}{c}\right|^k f(x)\,\mathrm{d}x \\
&= \int_{\{x:|x/c|\geq 1\}} \left|\frac{x}{c}\right|^k f(x)\,\mathrm{d}x + \int_{\{x:|x/c|<1\}} \left|\frac{x}{c}\right|^k f(x)\,\mathrm{d}x \\
&\geq \int_{\{x:|x/c|\geq 1\}} \left|\frac{x}{c}\right|^k f(x)\,\mathrm{d}x \\
&\geq \int_{\{x:|x/c|\geq 1\}} f(x)\,\mathrm{d}x \\
&= \int_{\{x:|x|\geq c\}} f(x)\,\mathrm{d}x = P(|X| \geq c). \qquad \square
\end{aligned}$$

Theorem 5.9 (Chebyshev's Inequality). For any random variable X such that $E(X) = \mu$ and $\mathrm{Var}(X) = \sigma^2$ are finite, we have

$$P(|X - \mu| \geq \beta\sigma) \leq \frac{1}{\beta^2}$$

for all $\beta > 0$.

Proof. Let $Y = X - \mu$. Then $E(Y) = 0$ and $\mathrm{Var}(Y) = \mathrm{Var}(X) = \sigma^2$. Let $\beta > 0$. By Markov's Inequality, for all $k > 0$, we have

$$P(|Y| \geq \beta\sigma) \leq \frac{E(|Y|^k)}{(\beta\sigma)^k}.$$

In particular, for $k = 2$, it follows that

$$P(|Y| \geq \beta\sigma) \leq \frac{E(Y^2)}{(\beta\sigma)^2} = \frac{E[(X-\mu)^2]}{\beta^2\sigma^2} = \frac{\mathrm{Var}(X)}{\beta^2\sigma^2} = \frac{\sigma^2}{\beta^2\sigma^2} = \frac{1}{\beta^2}. \qquad \square$$

We can now return to the example where we could not find an exact sampling distribution.

Example 5.10. Suppose that $(Y_1, \ldots, Y_n)$ is a random sample from $\mathrm{Poi}(\theta)$. Find the approximate sampling distribution of $\hat{\theta}(\mathbf{Y}) = \overline{Y} = \frac{1}{n}\sum_{i=1}^n Y_i$.

Solution: Note that we have $E(Y_i) = \mathrm{Var}(Y_i) = \theta < \infty$. Then by the Central Limit Theorem, we have

$$Z = \frac{\sqrt{n}(\overline{Y} - E(Y_i))}{\sqrt{\mathrm{Var}(Y_i)}} = \frac{\sqrt{n}(\overline{Y} - \theta)}{\sqrt{\theta}} \sim \mathrm{N}(0,1)$$

approximately/for large n. Then $M_Z(t) \approx \exp(\frac{1}{2}t^2)$, and hence

$$\begin{aligned}
M_{\overline{Y}}(t) &= E\left[\exp\left(t \cdot \frac{\sqrt{\theta}\cdot Z}{\sqrt{n}} + \theta\right)\right] \\
&= \exp(t\theta) \cdot E\left[\exp\left(\frac{t\sqrt{\theta}}{\sqrt{n}} \cdot Z\right)\right] \\
&\approx \exp(t\theta) \cdot \exp\left(\frac{1}{2} \cdot \frac{t^2\theta}{n}\right) \\
&= \exp\left(t\theta + \frac{1}{2}t^2 \cdot \frac{\theta}{n}\right).
\end{aligned}$$

This is the moment generating function of $\mathrm{N}(\theta, \theta/n)$, so we have $\overline{Y} \sim \mathrm{N}(\theta, \theta/n)$, approximately.

We now use Chebyshev's Inequality to discuss how close $\overline{Y}$ is to the true value of θ. Indeed, for all $\beta > 0$, we have (approximately)

$$P\left(|\overline{Y} - \theta| \geq \beta \cdot \sqrt{\theta/n}\right) \leq \frac{1}{\beta^2}.$$

Let the sample size be $n = 81$, that is, $\overline{Y}_{81} = \frac{1}{81}\sum_{i=1}^{81} Y_i$. Choose $\beta = 3$. Then

$$P\left(|\overline{Y}_{81} - \theta| \geq 3 \cdot \sqrt{\theta/81}\right) = P\left(|\overline{Y}_{81} - \theta| \geq \frac{1}{3}\sqrt{\theta}\right) \leq \frac{1}{9},$$

which implies that

$$P\left(|\overline{Y}_{81} - \theta| \leq \frac{1}{3}\sqrt{\theta}\right) \geq 1 - \frac{1}{9} = \frac{8}{9}.$$

Similarly, taking $n = 49$, we obtain

$$P\left(|\overline{Y}_{49} - \theta| \leq \frac{3}{7}\sqrt{\theta}\right) \geq \frac{8}{9}.$$

Clearly we have $\frac{1}{3}\sqrt{\theta} < \frac{3}{7}\sqrt{\theta}$, so $\overline{Y}_{81}$ is more likely to be close to the true value of θ.

6 Unbiased estimators and the Cramer-Rao lower bound

DEFINITION 6.1 (Bias). The **bias** of an estimator $\hat{\theta}(\mathbf{Y})$ is given by

$$\text{Bias}(\hat{\theta}) = E(\hat{\theta}) - \theta.$$

If the bias equals 0, then the estimator is said to be **unbiased**.

Intuitively, an unbiased estimator will be correct "on average". Moreover, if we have multiple unbiased estimators, we ideally want to choose the one with the smallest variance, as smaller variance leads to estimates that are closer to the true value of θ.

What happens if we do not have unbiased estimators? Also, if we have an unbiased estimator with high variance and a biased estimator with low variance, which one do we choose?

DEFINITION 6.2 (Mean squared error). The **mean squared error (MSE)** of an estimator is given by

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

THEOREM 6.3. We have $\text{MSE}(\hat{\theta}) = E[(\hat{\theta} - \theta)^2] = \text{Var}(\hat{\theta}) + (\text{Bias}(\hat{\theta}))^2$.

PROOF. Observe that

$$\begin{aligned}
\text{MSE}(\hat{\theta}) &= E[(\hat{\theta} - \theta)^2] \\
&= E[(\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta)^2] \\
&= E[(\hat{\theta} - E(\hat{\theta}))^2 + (E(\hat{\theta}) - \theta)^2 + 2(\hat{\theta} - E(\hat{\theta}))(E(\hat{\theta}) - \theta)] \\
&= E[(\hat{\theta} - E(\hat{\theta}))^2] + E[(E(\hat{\theta}) - \theta)^2] + 2E[(\hat{\theta} - E(\hat{\theta})(E(\hat{\theta}) - \theta)] \\
&= \text{Var}(\hat{\theta}) + E[(\text{Bias}(\hat{\theta}))^2] + 2(E(\hat{\theta}) - \theta)(E(\hat{\theta}) - E(E(\hat{\theta}))) \\
&= \text{Var}(\hat{\theta}) + (\text{Bias}(\hat{\theta}))^2.
\end{aligned}$$

□

REMARK 6.4.

(i) Large variance and bias are both undesirable. We compute the MSE to strike a balance between these two quantities.

(ii) If an estimator is unbiased, then the MSE is simply the variance of the estimator.

EXAMPLE 6.5. Suppose that $X_1, \dots, X_n$ is a random sample from $\text{UNIF}(0, \theta)$. Compare the MSEs of the three estimators $2\bar{X}$, $X_{(n)}$, and $(n+1)X_{(1)}$ for θ.

Solution: Let $T_1 = 2\bar{X}$, $T_2 = X_{(n)}$, and $T_3 = (n+1)X_{(1)}$. For each $1 \le i \le 3$, we need to find $\text{Var}(T_i)$ and $E(T_i)$ in order to comptute $\text{MSE}(T_i)$.

(1) For $T_1 = 2\bar{X}$, we have

$$E(T_1) = 2E[\bar{X}] = 2E\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{2nE[X_1]}{n} = 2 \cdot \frac{\theta}{2} = \theta.$$

It follows that $\text{Bias}(T_1) = E(T_1) - \theta = 0$, so T_1 is unbiased. Moreover, we obtain

$$\text{Var}(T_1) = \text{Var}(2\bar{X}) = 4\,\text{Var}\left(\frac{1}{n}\sum_{i=1}^{n} X_i\right) = \frac{4}{n^2}\sum_{i=1}^{n} \text{Var}(X_i) = \frac{4}{n}\,\text{Var}(X_1) = \frac{4}{n} \cdot \frac{\theta^2}{12} = \frac{\theta^2}{3n}.$$

Finally, we get

$$\text{MSE}(T_1) = \frac{\theta^2}{3n} + 0^2 = \frac{\theta^2}{3n}.$$

(2) Recall that $X \sim \text{UNIF}(0,\theta)$ has PDF $f(x) = 1/\theta$ for $0 \le x \le \theta$ and CDF given by

$$F(x) = \begin{cases} 0 & x < 0, \\ x/\theta & 0 \le x \le \theta, \\ 1 & x \ge \theta. \end{cases}$$

Hence, the PDF of $T_2 = X_{(n)}$ is

$$f_{T_2}(t) = nf(t)(F(t))^{n-1} = n \cdot \frac{1}{\theta} \cdot \left(\frac{t}{\theta}\right)^{n-1} = \frac{nt^{n-1}}{\theta^n}, \quad 0 \le t \le \theta.$$

Now, we obtain

$$E(T_2) = \int_0^\theta t \cdot \frac{nt^{n-1}}{\theta^n}\,\mathrm{d}t = \frac{n}{n+1}\theta,$$

and we see that T_2 is biased. Similarly, we have

$$E(T_2^2) = \int_0^\theta t^2 \cdot \frac{nt^{n-1}}{\theta^n}\,\mathrm{d}t = \frac{n}{\theta^n} \cdot \frac{\theta^{n+2}}{n+2} = \frac{n}{n+2}\theta^2,$$

so it follows that

$$\text{Var}(T_2) = E(T_2^2) - (E(T_2))^2 = \frac{n\theta^2}{(n+2)(n+1)^2}.$$

Finally, we get

$$\text{MSE}(T_2) = \frac{n\theta^2}{(n+2)(n+1)^2} = \left(\frac{n}{n+1}\theta - \theta\right)^2 = \frac{2\theta^2}{(n+1)(n+2)}.$$

(3) Recall that the PDF of $X_{(1)}$ is given by

$$f_{X_{(1)}}(t) = nf(t)[1-F(t)]^{n-1}, \quad 0 \le x \le \theta.$$

We leave it as an exercise to show that

$$\text{MSE}(T_3) = \frac{n}{n+2}\theta^2.$$

Putting these together, we have

$$\text{MSE}(T_1) = \frac{\theta^2}{3n}, \qquad \text{MSE}(T_2) = \frac{\theta^2}{(n+1)(n+2)/2}, \qquad \text{MSE}(T_3) = \frac{\theta^2}{(n+2)/n}.$$

To compare the MSEs, it suffices to look at the denominators. Indeed, note that $3n \ge (n+2)/n$ for all $n \ge 1$, and $3n \le (n+1)(n+2)/2$ for all $n \ge 1$, so we can conclude that

$$\text{MSE}(T_2) \le \text{MSE}(T_1) \le \text{MSE}(T_3).$$

Theorem 6.6 (Cramer-Rao lower bound). Suppose that $\mathbf{X} = (X_1, \ldots, X_n)$ is a random sample from $f(x;\theta)$. Denote $J(\theta) = E[I(\theta;\mathbf{X})]$, where

$$I(\theta;\mathbf{x}) = -\frac{\partial}{\partial\theta}S(\theta;\mathbf{x}) = -\frac{\partial^2}{\partial\theta^2}\ell(\theta;\mathbf{x}).$$

We call $J(\theta)$ the **Fisher information**. For any *unbiased* estimator $T(\mathbf{X})$ of $\tau(\theta)$ (which is a function of θ we wish to examine), its variance has the lower bound

$$\text{Var}[T(\mathbf{X})] \ge \frac{[\tau'(\theta)]^2}{J(\theta)},$$

where $\tau'(\theta) = d\tau(\theta)/d\theta$.

Proof. We will make use of the Cauchy-Schwarz inequality which is given by

$$\mathrm{Cov}^2(X, Y) \leq \mathrm{Var}(X) \cdot \mathrm{Var}(Y),$$

as well as the following claims.

Claim 1. We have $E[S(\theta; \mathbf{X})] = 0$.

Proof of Claim 1. We prove this in the continuous case; the discrete case is analogous. We have

$$\begin{aligned} E\left[\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})\right] &= \int \frac{\partial}{\partial\theta}\ell(\theta; \mathbf{x}) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int \frac{\partial}{\partial\theta} \log L(\theta; \mathbf{x}) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int \frac{\frac{\partial}{\partial\theta} L(\theta; \mathbf{x})}{L(\theta; \mathbf{x})} \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int \frac{\partial}{\partial\theta} L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \frac{\partial}{\partial\theta} \int L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \frac{\partial}{\partial\theta} 1 = 0. \end{aligned}$$

■

Claim 2. We have $J(\theta) = \mathrm{Var}(\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X}))$.

Proof of Claim 2. Note that

$$J(\theta) = E[I(\theta; \mathbf{X})] = E\left[-\frac{\partial^2}{\partial\theta^2}\ell(\theta; \mathbf{X})\right].$$

By Claim 1, we have $E[\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})] = 0$, so it follows that

$$\mathrm{Var}\left[\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})\right] = E\left[\left(\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})\right)^2\right].$$

Therefore, to prove the claim, it suffices to show that

$$E\left[-\frac{\partial^2}{\partial\theta^2}\ell(\theta; \mathbf{X})\right] = E\left[\left(\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})\right)^2\right].$$

Indeed, we have

$$\begin{aligned} E\left[-\frac{\partial^2}{\partial\theta^2}\ell(\theta; \mathbf{X})\right] &= \int \left(-\frac{\partial^2}{\partial\theta^2}\ell(\theta; \mathbf{x})\right) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int -\frac{\partial}{\partial\theta}\left(\frac{\partial}{\partial\theta} \log L(\theta; \mathbf{x})\right) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int -\frac{\partial}{\partial\theta} \frac{L'(\theta; \mathbf{x})}{L(\theta; \mathbf{x})} \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int -\frac{L''(\theta; \mathbf{x}) \cdot L(\theta; \mathbf{x}) - (L'(\theta; \mathbf{x}))^2}{(L(\theta; \mathbf{x}))^2} \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int -\left(L''(\theta; \mathbf{x}) - \frac{(L'(\theta; \mathbf{x}))^2}{L(\theta; \mathbf{x})}\right) \, \mathrm{d}\mathbf{x} \\ &= \int \frac{(L'(\theta; \mathbf{x}))^2}{L(\theta; \mathbf{x})} \, \mathrm{d}\mathbf{x} - \int \frac{\partial^2}{\partial\theta^2} L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\ &= \int \left(\frac{L'(\theta; \mathbf{x})}{L(\theta; \mathbf{x})}\right)^2 \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} = \int \left(\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{x})\right)^2 \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} = E\left[\left(\frac{\partial}{\partial\theta}\ell(\theta; \mathbf{X})\right)^2\right]. \end{aligned}$$

■

Now, we show that $\tau'(\theta) = \operatorname{Cov}(T(\mathbf{X}), S(\theta; \mathbf{X}))$. Indeed, recall that

$$\tau(\theta) = E[T(\mathbf{X})] = \int T(\mathbf{x}) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x}.$$

Then we have

$$\begin{aligned}
\tau'(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta}\tau(\theta) = \frac{\mathrm{d}}{\mathrm{d}\theta} \int T(\mathbf{x}) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\
&= \int \frac{\partial}{\partial\theta}(T(\mathbf{x}) \cdot L(\theta; \mathbf{x})) \, \mathrm{d}\mathbf{x} \\
&= \int T(\mathbf{x}) \cdot \frac{\partial}{\partial\theta} L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\
&= \int T(\mathbf{x}) \cdot \frac{\frac{\partial}{\partial\theta} L(\theta; \mathbf{x})}{L(\theta; \mathbf{x})} \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\
&= \int T(\mathbf{x}) \cdot \frac{\partial}{\partial\theta} \ell(\theta; \mathbf{x}) \cdot L(\theta; \mathbf{x}) \, \mathrm{d}\mathbf{x} \\
&= E[T(\mathbf{X}) \cdot S(\theta; \mathbf{X})] \\
&= E[T(\mathbf{X}) \cdot S(\theta; \mathbf{X})] - E[T(\mathbf{X})]E[S(\theta; \mathbf{X})] \\
&= \operatorname{Cov}(T(\mathbf{X}), S(\theta; \mathbf{X})).
\end{aligned}$$

We note that in the second last step, we use the fact that $E[S(\theta; \mathbf{X})] = 0$ from Claim 1. Finally, by the Cauchy-Schwarz inequality, we obtain

$$\operatorname{Var}[T(\mathbf{X})] \cdot J(\theta) = \operatorname{Var}[T(\mathbf{X})] \cdot \operatorname{Var}[S(\theta; \mathbf{X})] \geq \operatorname{Cov}^2(T(\mathbf{X}), S(\theta; \mathbf{X})) = (\tau'(\theta))^2,$$

which is exactly what we needed to prove. $\square$

Definition 6.7 (Efficiency). The ratio of the Cramer-Rao lower bound to the variance of an unbiased estimator $T(\mathbf{X})$ is called the **efficiency** of the estimator; that is,

$$\operatorname{Eff}(T(\mathbf{X})) = \frac{(\tau'(\theta))^2 / J(\theta)}{\operatorname{Var}(T(\mathbf{X}))}.$$

Note that $0 \leq \operatorname{Eff}(T(\mathbf{X})) \leq 1$. If $\operatorname{Eff}(T(\mathbf{X})) = 1$, then $T(\mathbf{X})$ attains the Cramer-Rao lower bound, and we call $T(\mathbf{X})$ an **efficient estimator**.

7 Confidence intervals

The estimates and estimators we have discussed so far (namely, maximum likelihood estimates) are often referred to as point estimates and point estimators. This is because of a consist of a single value or "point".

However, an issue with point estimates is that while they are precise (as they consist of a single value), we do not have the confidence that they are correct since

$$P[\hat{\theta}_{\text{MLE}} = \theta] = 0$$

when $\hat{\theta}_{\text{MLE}}$ is continuous. Instead, we turn to set estimation. In STAT 241, we focus on interval estimates.

DEFINITION 7.1. An **interval estimate** takes the form $[L(\mathbf{y}), U(\mathbf{y})]$ where the endpoints $L(\mathbf{y})$ and $U(\mathbf{y})$ are both functions of the observed data $\mathbf{y}$. Then $[L(\mathbf{Y}), U(\mathbf{Y})]$ is called a **random interval** since the endpoints (based on a random sample $\mathbf{Y}$) are random variables.

The probability that the parameter θ falls in the random interval $[L(\mathbf{Y}), U(\mathbf{Y})]$ tells us how good the rule is by which the interval estimate was obtained. For instance, we might have

$$P[L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y})] = 0.95.$$

Note that the probability depends only on $\mathbf{Y}$, whereas θ is a fixed but unknown parameter. Therefore, for a given observed sample $\mathbf{y}$, we either have $P[L(\mathbf{y}) \leq \theta \leq U(\mathbf{y})] = 1$ or $P[L(\mathbf{y}) \leq \theta \leq U(\mathbf{y})] = 0$.

REMARK 7.2. We can think of the above probability as an expectation; namely, we have

$$P[L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y})] = E[I(L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y}))].$$

DEFINITION 7.3. A $100p\%$ **confidence interval** for a parameter θ is an interval $[L(\mathbf{y}), U(\mathbf{y})]$ such that

$$P[L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y})] = p,$$

where p is called the **confidence level** (or **confidence coefficient**).

REMARK 7.4.

(i) Common choices for p are 0.90, 0.95, and 0.99.

(ii) Suppose that $P[L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y})] = 0.95$. If we draw a large number of random samples, then each time we construct the interval $[L(\mathbf{y}), U(\mathbf{y})]$ from the observed data $\mathbf{y}$, we would expect the true value of the parameter θ to lie in $[L(\mathbf{y}), U(\mathbf{y})]$ approximately 95% of the time. In other words, we are 95% confident that the interval $[L(\mathbf{y}), U(\mathbf{y})]$ contains the true value of the parameter θ.

EXAMPLE 7.5. Suppose that $Y_1, \ldots, Y_n$ are i.i.d. random variables from $\mathrm{N}(\theta, 1)$. Consider the interval

$$\left[\underbrace{\overline{Y} - \frac{1.96}{\sqrt{n}}}_{L(\mathbf{Y})}, \underbrace{\overline{Y} + \frac{1.96}{\sqrt{n}}}_{U(\mathbf{Y})}\right]$$

where $\overline{Y}$ is the sample mean. What is the confidence level of this confidence interval for θ?

Solution: We need to find $P[L(\mathbf{Y}) \leq \theta \leq U(\mathbf{Y})]$. First, recall that $\overline{Y} \sim \mathrm{N}(\theta, 1/n)$. It follows that

$$\frac{\overline{Y} - \theta}{\sqrt{1/n}} \sim \mathrm{N}(0, 1).$$

Note that 1.96 is the 97.5% quantile of $\mathrm{N}(0,1)$ and -1.96 is the 2.5% quantile of $\mathrm{N}(0,1)$ since the PDF of $\mathrm{N}(0,1)$ is symmetric, so

$$P\left[-1.96 \leq \frac{\overline{Y} - \theta}{\sqrt{1/n}} \leq 1.96\right] = 0.95.$$

We can rewrite the above in the form

$$P\left[-1.96 \le \frac{\overline{Y}-\theta}{\sqrt{1/n}} \le 1.96\right] = P\left[-\frac{1.96}{\sqrt{n}} - \overline{Y} \le -\theta \le \frac{1.96}{\sqrt{n}} - \overline{Y}\right] = P\left[\overline{Y} - \frac{1.96}{\sqrt{n}} \le \theta \le \overline{Y} + \frac{1.96}{\sqrt{n}}\right],$$

so 0.95 is the confidence level of the confidence interval $[L(\mathbf{Y}), U(\mathbf{Y})]$ for θ.

Notice that in Example 7.5, neither of $L(\mathbf{Y})$ or $U(\mathbf{Y})$ depended on the unknown parameter θ. In addition, the confidence level (or coverage probability) did not depend on θ either. This is a highly desirable property to have, since we would like to know the coverage probability without having to know the value of the unknown parameter.

This nice property occurred in Example 7.5 due to the fact that

$$\frac{\overline{Y}-\theta}{1/\sqrt{n}} \sim \mathrm{N}(0,1),$$

and this distribution is free of any unknown parameters. This motivates the following definition.

DEFINITION 7.6. A **pivotal quantity** $Q = Q(\mathbf{Y};\theta)$ is a function of the random sample $\mathbf{Y}$ and the unknown parameter θ such that the distribution of Q is fully known.

As we saw in Example 7.5, a pivotal quantity can be used to construct a confidence interval by setting

$$P[a \le Q(\mathbf{Y};\theta) \le b] = p$$

and re-expressing it in the form

$$P[L(\mathbf{Y}) \le \theta \le U(\mathbf{Y})] = p.$$

EXAMPLE 7.7. Suppose that $Y_1, \ldots, Y_n$ are i.i.d. random variables from $N(\mu, \sigma^2)$.

(a) Construct a 95% confidence interval for σ^2.

Solution: We need to find a pivotal quantity $Q(\mathbf{Y};\sigma^2)$. Recall that

$$Q(\mathbf{Y};\sigma^2) = \frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\sigma^2} \sim \chi^2(n-1)$$

which is free of any unknown parameters. Then letting $\chi^2_{0.025}(n-1)$ and $\chi^2_{0.975}(n-1)$ be the 2.5% and 97.5% quantiles of $\chi^2(n-1)$ respectively, we have

$$P\left[\chi^2_{0.025}(n-1) \le \frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\sigma^2} \le \chi^2_{0.975}(n-1)\right] = 0.95,$$

and hence

$$P\left[\frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\chi^2_{0.975}(n-1)} \le \sigma^2 \le \frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\chi^2_{0.025}(n-1)}\right] = 0.95.$$

Thus, a 95% confidence interval for σ^2 is

$$\left[\frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\chi^2_{0.975}(n-1)}, \frac{\sum_{i=1}^n (Y_i - \overline{Y})^2}{\chi^2_{0.025}(n-1)}\right].$$

(b) Construct a 95% confidence interval for μ.

Solution: We have $\sum_{i=1}^n (Y_i - \overline{Y})^2/\sigma^2 \sim \chi^2(n-1)$ and

$$\frac{\overline{Y}-\mu}{\sqrt{\sigma^2/n}} \sim \mathrm{N}(0,1).$$

It can be shown (using STAT 330 materials) that

$$\frac{\mathrm{N}(0,1)}{\sqrt{\chi^2(k)/k}} \sim t(k)$$

where k is the number of degrees of freedom. In particular, observe that

$$\frac{\sum_{i=1}^n (Y_i - \overline{Y})^2/\sigma^2}{n-1} \sim \frac{\chi^2(n-1)}{n-1},$$

so it follows that

$$\frac{\frac{\overline{Y}-\mu}{\sqrt{\sigma^2/n}}}{\sqrt{\frac{\sum_{i=1}^n (Y_i-\overline{Y})^2/\sigma^2}{n-1}}} = \frac{\sqrt{n}(\overline{Y}-\mu)}{\sqrt{\sum_{i=1}^n (Y_i-\overline{Y})^2/(n-1)}} = \frac{\sqrt{n}(\overline{Y}-\mu)}{s} \sim t(n-1),$$

where $s^2 = \sum_{i=1}^n (Y_i - \overline{Y})^2/(n-1)$ is the sample variance. Now, we have

$$P\left[t_{0.025}(n-1) \leq \frac{\sqrt{n}(\overline{Y}-\mu)}{s} \leq t_{0.975}(n-1)\right] = 0.95.$$

Since the t-distribution is symmetric, it follows that $t_{0.025} = -t_{0.975}$. Using this fact and rearranging the above inequalities gives

$$P\left[\overline{Y} - \frac{s}{\sqrt{n}} t_{0.975}(n-1) \leq \mu \leq \overline{Y} + \frac{s}{\sqrt{n}} t_{0.975}(n-1)\right] = 0.95,$$

so we see that

$$\left[\overline{Y} - \frac{s}{\sqrt{n}} t_{0.975}(n-1), \overline{Y} + \frac{s}{\sqrt{n}} t_{0.975}(n-1)\right]$$

is an equal-tail 95% confidence interval for μ.

For most models, it is not possible to find exact pivotal quantities. Moreover, not all pivotal quantities are useful for finding confidence intervals. However, we can generally find quantities $Q_n = Q_n(\mathbf{Y};\theta)$ such that as $n \to \infty$, the asymptotic distribution of Q_n does not depend on the unknown parameter θ.

Definition 7.8. An **approximate pivotal quantity** $Q_n = Q_n(\mathbf{Y};\theta)$ is a function of the random sample $\mathbf{Y}$ and the unknown parameter θ such that the asymptotic distribution of Q_n is fully known.

Example 7.9. Suppose that $Y \sim \mathrm{Bin}(n,\theta)$. By the Central Limit Theorem, we have approximately

$$Q_{1n} = \frac{Y - n\theta}{\sqrt{n\theta(1-\theta)}} \sim \mathrm{N}(0,1).$$

It can also be shown that approximately

$$Q_n = \frac{Y - n\theta}{\sqrt{n(Y/n)(1-Y/n)}} \sim \mathrm{N}(0,1)$$

by replacing θ by Y/n and applying the Continuous Mapping Theorem and Slutsky's Theorem, which are beyond the scope of the course. Now, we have

$$P\left[-1.96 \leq \frac{Y - n\theta}{\sqrt{n(Y/n)(1-Y/n)}} \leq 1.96\right] \approx 0.95,$$

and hence we obtain

$$P\Bigg[\underbrace{\frac{Y}{n} - \frac{1.96}{n}\sqrt{n\left(\frac{Y}{n}\right)\left(1-\frac{Y}{n}\right)}}_{L(\mathbf{Y})} \leq \theta \leq \underbrace{\frac{Y}{n} + \frac{1.96}{n}\sqrt{n\left(\frac{Y}{n}\right)\left(1-\frac{Y}{n}\right)}}_{U(\mathbf{Y})}\Bigg] \approx 0.95.$$

Suppose we want n large enough so that the width of a 95% confidence interval for θ is no wider than 0.06. We see that the width of the above interval is

$$2 \cdot \frac{1.96}{n}\sqrt{n\left(\frac{Y}{n}\right)\left(1-\frac{Y}{n}\right)},$$

so we need to find n such that

$$\frac{1.96}{n}\sqrt{n\left(\frac{Y}{n}\right)\left(1-\frac{Y}{n}\right)} \leq 0.03.$$

This is equivalent to saying that

$$n \geq \left(\frac{1.96}{0.03}\sqrt{\frac{Y}{n}\left(1-\frac{Y}{n}\right)}\right)^2.$$

Note that $a(1-a) \leq 1/4$ for all $a \in \mathbb{R}$, so it follows that

$$n \geq \left(\frac{1.96}{0.03}\sqrt{\frac{1}{4}}\right)^2 \geq 1068.$$

In practice, many polls are based on 1050 to 1100 people, giving "accuracy to within 3 percent" with probability 0.95. This is explained by the above computation.

Moreover, rewriting the width of the confidence interval as

$$2 \cdot \frac{1.96}{\sqrt{n}}\sqrt{\frac{Y}{n}\left(1-\frac{Y}{n}\right)}$$

and noting that Y/n converges to θ, we see that the width is decreasing as n is increasing.

EXAMPLE 7.10. Suppose that $X \sim f(x;\theta)$ where

$$f(x;\theta) = \frac{2(\theta - x)}{\theta^2},\ x \in (0,\theta),\ \theta > 0.$$

(a) Show that X/θ is a pivotal quantity.

Solution: To show that X/θ is a pivotal quantity, it suffices to show that the CDF, PDF, or moment generating function of X/θ is free of unknown parameters. In this case, we shall look at the CDF of X/θ. Note that

$$P[X/\theta \leq y] = P[X \leq \theta y],$$

which is the CDF of X evaluated at θy. In particular, the CDF of X is given by

$$P[X \leq x^*] = \begin{cases} 0 & x^* \leq 0 \\ \Delta & 0 < x^* < \theta \\ 1 & x^* \geq \theta, \end{cases}$$

where we have

$$\Delta = \int_0^{x^*} f(x)\,\mathrm{d}x = \int_0^{x^*} \frac{2(\theta - x)}{\theta^2}\,\mathrm{d}x = \frac{1}{\theta^2}(2\theta x^* - (x^*)^2).$$

Therefore, it follows that

$$P[X/\theta \leq y] = P[X \leq \theta y] = \begin{cases} 0 & \theta y \leq 0 \\ \frac{1}{\theta^2}(2\theta \cdot \theta y - (\theta y)^2) & 0 < \theta y < \theta \\ 1 & \theta y \geq \theta \end{cases} = \begin{cases} 0 & y \leq 0 \\ 2y - y^2 & 0 < y < 1 \\ 1 & y \geq 1. \end{cases}$$

Thus, the CDF of X/θ is free of unknown parameters, so X/θ is a pivotal quantity.

(b) Find an equal-tail $100p\%$ confidence interval for θ using X/θ.

Solution: We have $P[a \leq X/\theta \leq b] = p$ where

$$P[X/\theta \geq b] = P[X/\theta \leq a] = \frac{1-p}{2}$$

since we want an equal-tail confidence interval. Now, to find b, we have

$$P[X/\theta \leq b] = 1 - P[X/\theta > b] = 1 - \frac{1-p}{2}.$$

This quantity is in the interval $[0, 1]$ since $0 \leq p \leq 1$, so we solve

$$2b - b^2 = 1 - \frac{1-p}{2}$$

to get $b = (2 - \sqrt{2-2p})/2$. Similarly, we can find that $a = (2 - \sqrt{2+2p})/2$. Thus, we have

$$P\left[\frac{2-\sqrt{2+2p}}{2} \leq \frac{X}{\theta} \leq \frac{2-\sqrt{2-2p}}{2}\right] = p$$

so that

$$P\left[\frac{2X}{2-\sqrt{2-2p}} \leq \theta \leq \frac{2X}{2-\sqrt{2+2p}}\right] = p.$$

Therefore, it follows that

$$\left[\frac{2X}{2-\sqrt{2-2p}}, \frac{2X}{2-\sqrt{2+2p}}\right]$$

is an equal-tail $100p\%$ confidence interval for θ.

8 Hypothesis testing

Suppose a statement has been formulated such as "This drug that a pharmaceutical company developed reduces pain better than those currently available." Then an experiment (in this case, a clinical trial) is conducted to determine how credible the statement is in light of the observed data.

How do we measure credibility? With hypothesis testing!

To understand a test of hypothesis, it may be helpful to draw an analogy from the criminal court system used in many places in the world.

There are two hypotheses: "the defendant is innocent" and "the defendant is guilty". These two hypotheses are not treated symmetrically. In these courts, the court assumes that the first hypothesis is true, and then the prosecution attempts to find sufficient evidence to show that this hypothesis of innocence is not plausible. At the end of the trial, the judge or jury may conclude that there is insufficient evidence that the defendant is guilty and the defendant is then acquitted.

Of course, there are two types of errors that this court system can make: convicting an innocent defendant or failing to convict a guilty defendant. These two types of errors have very different consequences (the former is worse than the latter). We will need to deal with these cases differently.

A test of hypothesis is analogous to this example. We often begin by specifying a default hypothesis (in the legal context, this is the statement "the defendant is innocent") and then checking whether the data collected does not agree with this hypothesis (or whether the data collected is unlikely under this hypothesis).

The default hypothesis is often referred to as the **null hypothesis** and is denoted by H_0. Correspondingly, there is an **alternative hypothesis** which is denoted by H_1; it is often simply the statement that H_0 is not true, but this is not always the case.

If the data agrees with the null hypothesis, then we **fail to reject the null hypothesis**. On the other hand, if there is strong evidence against the null hypothesis or inconsistency with the null hypothesis, then we **reject the null hypothesis**. Notice that we do not claim that the null hypothesis is true.

EXAMPLE 8.1. Suppose we toss a coin 100 times and record the outcome of every toss. In an effort to prove or disprove the claim that this is a fair coin, we count the number of heads Y, which has a binomial distribution with $n = 100$. The probability of getting heads on a given toss is an unknown parameter θ.

If this is a fair coin, we would expect to have $\theta = 0.5$, whereas if the coin is unfair, then $\theta \neq 0.5$. What is the null hypothesis H_0, and what observed values of Y are highly inconsistent with H_0?

Solution: The null hypothesis H_0 is that $\theta = 0.5$, and when H_0 is true, we would expect Y to be close to $100 \times 0.5 = 50$. Then, in order to be inconsistent, we either have $Y \gg 50$ or $Y \ll 50$.

In general, how do we measure inconsistency? We require test statistics, p-values, and significance levels.

DEFINITION 8.2 (Test statistic). A **test statistic** D is a non-negative function of the data Y that is constructed to measure the degree of "disagreement" between Y and the null hypothesis H_0.

- Often, D is defined so that $D = 0$ represents the best possible agreement between the data Y and the null hypothesis H_0.
- Values of D not close to 0 (that is, $D \gg 0$) indicate poor agreement.

In Example 8.1, a good choice of a test statistic is $D(Y) = |Y - 50|$. Let $D(y) = |y - 50|$ be the value of D of a given sample y. Consider the tail probability $P[D(Y) \geq D(y) \mid H_0]$. Note that when H_0 is true (so that $\theta = 0.5$), then $Y \sim \text{Bin}(100, 0.5)$.

If $D(y)$ is large, then the tail probability $P[D(Y) \geq D(y) \mid H_0]$ will be small. On the other hand, in the case that $y = 52$, when $D(y) = 2$, we have

$$P[|Y - 50| \geq d \mid H_0] = P[Y \geq 52 \mid H_0] + P[Y \leq 48 \mid H_0] = 0.76.$$

In particular, if we toss this coin 100 times repeatedly, then if the coin is fair, roughly 76% of the time, it will result in some $D(y)$ at least as large as the observed value of 2. This does not prove that the coin is fair, but it indicates that we have failed to find evidence in the data to support rejecting H_0.

Definition 8.3. Suppose we use the test statistic $D(\mathbf{Y})$ to test the null hypothesis H_0. Suppose that $d = D(\mathbf{y})$ is the observed value of D. The ***p*-value** (or **observed significance level**) of the test of the null hypothesis using test statistic D is

$$p\text{-value} = P[D(\mathbf{Y}) \geq D(\mathbf{y}) \mid H_0] = P[D \geq d \mid H_0].$$

Remark 8.4.

- The p-value is the probability (when assuming H_0) of the test statistic being greater or equal to the observed value (based on the observed data).
- If d is large and consequently the p-value is small, then we have evidence in the data to support rejecting H_0. We compare the p-value with a given significance level (in other words, a cutoff for the p-value).

The following table gives a rough guideline for interpreting p-values.

p-value	Interpretation
$p\text{-value} > 0.10$	No evidence against H_0 based on the observed data
$0.05 < p\text{-value} \leq 0.10$	Weak evidence against H_0 based on the observed data
$0.01 < p\text{-value} \leq 0.05$	Evidence against H_0 based on the observed data
$0.001 < p\text{-value} \leq 0.01$	Strong evidence against H_0 based on the observed data
$p\text{-value} \leq 0.001$	Very strong evidence against H_0 based on the observed data

In STAT 241, we reject the null hypothesis if the p-value is less than or equal to the given significance level.

Example 8.5. Suppose we test the null hypothesis $H_0 : \theta = 0.5$ versus the alternative hypothesis $H_1 : \theta \neq 0.5$ for $n = 200$, $y = 90$, and $D(Y) = |Y - 100|$ where $Y \sim \text{Bin}(n, \theta)$. Do we reject H_0 at the significance level 0.05?

Solution: We have

$$\begin{aligned}
p\text{-value} &= P[D(Y) \geq D(y) \mid H_0] \\
&= P[|Y - 100| \geq |90 - 100| \mid H_0] \\
&= P[|Y - 100| \geq 10 \mid H_0] \\
&= P[Y \geq 110 \mid H_0] + P[Y \leq 90 \mid H_0] \\
&= F(90) + (1 - F(109)) \\
&= 0.0894 + 0.0894 = 0.1788 > 0.05,
\end{aligned}$$

where F above is the CDF of $Y \sim \text{Bin}(200, 0.5)$. Thus, we fail to reject the null hypothesis $H_0 : \theta = 0.5$.

Example 8.6. Suppose we test the null hypothesis $H_0 : \theta = 0.5$ versus the alternative hypothesis $H_1 : \theta > 0.5$ (called a one-sided alternative) for $n = 200$, $y = 130$, and $D(Y) = \max\{Y - 100, 0\}$ where $Y \sim \text{Bin}(n, \theta)$. Do we reject H_0 at the significance level 0.05?

Solution: We have

$$\begin{aligned}
p\text{-value} &= P[D(Y) \geq D(y) \mid H_0] \\
&= P[\max(Y - 100, 0) \geq \max(130 - 100, 0) \mid H_0] \\
&= P[Y - 100 \geq 30 \mid H_0] \\
&= P[Y \geq 130 \mid H_0] \\
&= 1 - F(129) \\
&= 1.33 \times 10^{-5} \leq 0.01,
\end{aligned}$$

where F above is the CDF of $Y \sim \text{Bin}(200, 0.5)$. Thus, we reject the null hypothesis and claim the alternative.

EXAMPLE 8.7. Suppose that $X_1, \ldots, X_n$ is a random sample from $\mathrm{N}(\mu, \sigma^2)$.

(1) $H_0 : \mu = \mu_0$ versus $H_1 : \mu \neq \mu_0$ (two-sided alternative), where μ_0 is fixed and known.

(2) $H_0 : \mu = \mu_0$ versus $H_1 : \mu > \mu_0$ (one-sided alternative), where μ_0 is fixed and known.

(3) $H_0 : \sigma^2 = \sigma_0^2$ versus $H_1 : \sigma^2 \neq \sigma_0^2$ (two-sided alternative), where σ_0^2 is fixed and known.

(4) $H_0 : \sigma^2 = \sigma_0^2$ versus $H_1 : \sigma^2 > \sigma_0^2$ (one-sided alternative), where σ_0^2 is fixed and known.

Solution: First, recall that $\overline{X} \sim \mathrm{N}(\mu, \sigma^2/n)$.

(1) Consider the test statistic

$$D(\mathbf{X}) = \frac{|\overline{X} - \mu_0|}{S/\sqrt{n}}$$

where $S^2 = \frac{1}{n-1}\sum_{i=1}^n (X_i - \overline{X})^2$ is the sample variance. Note that $\overline{X} \sim N(\mu_0, \sigma^2/n)$ under the null hypothesis H_0 and recall that

$$\frac{\overline{X} - \mu_0}{S/\sqrt{n}} \sim t(n-1).$$

Then, we have

$$\begin{aligned}
p\text{-value} &= P[D(\mathbf{X}) \geq D(\mathbf{x}) \mid H_0] \\
&= P\left[\frac{|\overline{X} - \mu_0|}{S/\sqrt{n}} \geq \frac{|\overline{x} - \mu_0|}{s/\sqrt{n}} \;\middle|\; H_0\right] \\
&= P\left[|t(n-1)| \geq \frac{|\overline{x} - \mu_0|}{s/\sqrt{n}}\right] \\
&= 2 \cdot P\left[t(n-1) \geq \frac{|\overline{x} - \mu_0|}{s/\sqrt{n}}\right],
\end{aligned}$$

where the last equality follows from the symmetry of the t-distribution.

(2) This time, consider the test statistic

$$D(\mathbf{X}) = \max\left(\frac{\overline{X} - \mu_0}{S/\sqrt{n}}, 0\right).$$

We see that

$$\begin{aligned}
p\text{-value} &= P\left[\max\left(\frac{\overline{X} - \mu_0}{S/\sqrt{n}}, 0\right) \geq \max\left(\frac{\overline{x} - \mu_0}{s/\sqrt{n}}, 0\right) \;\middle|\; H_0\right] \\
&= \begin{cases} P\left[\frac{\overline{X} - \mu_0}{S/\sqrt{n}} \geq \frac{\overline{x} - \mu_0}{s/\sqrt{n}} \;\middle|\; H_0\right] = P\left[t(n-1) \geq \frac{\overline{x} - \mu_0}{s/\sqrt{n}}\right] & \text{if } \overline{x} - \mu_0 > 0, \\ P\left[\max\left(\frac{\overline{X} - \mu_0}{S/\sqrt{n}}, 0\right) \geq 0 \;\middle|\; H_0\right] = 1 & \text{if } \overline{x} - \mu_0 \leq 0. \end{cases}
\end{aligned}$$

(3) Consider the test statistic

$$D(\mathbf{X}) = \left|\frac{S^2}{\sigma_0^2} - 1\right|$$

where $S^2 = \frac{1}{n-1}\sum_{i=1}^n (X_i - \overline{X})^2$ is the sample variance. Note that

$$\frac{(n-1)S^2}{\sigma^2} = \frac{\sum_{i=1}^n (X_i - \overline{X})^2}{\sigma^2} \sim \chi^2(n-1)$$

since the X_i are a random sample from $\mathrm{N}(\mu, \sigma^2)$. In particular, under the null hypothesis H_0, we have

$$\frac{(n-1)S^2}{\sigma_0^2} \sim \chi^2(n-1).$$

Hence, we obtain

$$\begin{aligned}
p\text{-value} &= P[D(\mathbf{X}) \geq D(\mathbf{x}) \mid H_0] \\
&= P\left[\left|\frac{S^2}{\sigma_0^2} - 1\right| \geq \left|\frac{s^2}{\sigma_0^2} - 1\right| \,\middle|\, H_0\right] \\
&= P\left[\left|\frac{(n-1)S^2}{\sigma_0^2} - (n-1)\right| \geq \underbrace{(n-1)\left|\frac{s^2}{\sigma_0^2} - 1\right|}_{(\star)} \,\middle|\, H_0\right] \\
&= P\left[\frac{(n-1)S^2}{\sigma_0^2} - (n-1) \geq (\star) \,\middle|\, H_0\right] + P\left[\frac{(n-1)S^2}{\sigma_0^2} - (n-1) \leq -(\star) \,\middle|\, H_0\right] \\
&= P\left[\frac{(n-1)S^2}{\sigma_0^2} \geq (\star) + (n-1) \,\middle|\, H_0\right] + P\left[\frac{(n-1)S^2}{\sigma_0^2} \leq (n-1) - (\star) \,\middle|\, H_0\right] \\
&= P\left[\chi^2(n-1) \geq (\star) + (n-1)\right] + P\left[\chi^2(n-1) \leq (n-1) - (\star)\right].
\end{aligned}$$

(4) Consider the test statistic

$$D(\mathbf{X}) = \max\left(\frac{S^2}{\sigma_0^2} - 1, 0\right).$$

Hence, we have

$$\begin{aligned}
p\text{-value} &= P[D(\mathbf{X}) \geq D(\mathbf{x}) \mid H_0] \\
&= P\left[\max\left(\frac{S^2}{\sigma_0^2} - 1, 0\right) \geq \max\left(\frac{s^2}{\sigma_0^2} - 1, 0\right) \,\middle|\, H_0\right] \\
&= \begin{cases} (\star\star) & \text{if } \dfrac{s^2}{\sigma_0^2} > 1, \\[2ex] P\left[\max\left(\dfrac{S^2}{\sigma_0^2} - 1, 0\right) \geq 0\right] = 1 & \text{if } \dfrac{s^2}{\sigma_0^2} \leq 1, \end{cases}
\end{aligned}$$

where we have

$$\begin{aligned}
(\star\star) &= P\left[\max\left(\frac{S^2}{\sigma_0^2} - 1, 0\right) \geq \underbrace{\frac{s^2}{\sigma_0^2} - 1}_{>0} \,\middle|\, H_0\right] \\
&= P\left[\frac{S^2}{\sigma_0^2} - 1 \geq \frac{s^2}{\sigma_0^2} - 1 \,\middle|\, H_0\right] \\
&= P\left[\frac{S^2}{\sigma_0^2} \geq \frac{s^2}{\sigma_0^2} \,\middle|\, H_0\right] \\
&= P\left[\frac{(n-1)S^2}{\sigma_0^2} \geq \frac{(n-1)s^2}{\sigma_0^2} \,\middle|\, H_0\right] \\
&= P\left[\chi^2(n-1) \geq \frac{(n-1)s^2}{\sigma_0^2}\right].
\end{aligned}$$

REMARK 8.8. The test statistics in the previous example are derived from the likelihood ratio test. In general, we can derive test statistics with the Neyman-Pearson lemma and the likelihood ratio test, which we will cover in the next section.

9 The Neyman-Pearson lemma and the likelihood ratio test

Definition 9.1. **Type I error probability** is the probability of a false positive, given by

$$\alpha = P[H_0 \text{ is rejected} \mid H_0].$$

In other words, it the probability of rejecting H_0 when H_0 is true.

Definition 9.2. **Type II error probability** is the probability of a false negative, given by

$$\beta = P[\text{fail to reject } H_0 \mid H_1].$$

In other words, it is the probability of failing to reject H_0 when H_0 is false.

Recall that the p-value is given by

$$p\text{-value} = P[D(\mathbf{X}) \geq D(\mathbf{x}) \mid H_0],$$

and if α is a given significance level, then we reject H_0 if we have p-value $\leq \alpha$. Let d_α be such that

$$P[D(\mathbf{X}) \geq d_\alpha \mid H_0] = \alpha,$$

which can always be found in the continuous case for any $0 \leq \alpha \leq 1$. Then, we reject H_0 at significance level α as long as $D(\mathbf{x}) \geq d_\alpha$ since there is a smaller tail probability compared to the tail probability of d_α, namely α. This motivates the following definition.

Definition 9.3. At a given significance level α, we reject H_0 if we have p-value $\leq \alpha$. The **rejection region** is defined to be the set

$$R := \{\mathbf{x} : D(\mathbf{x}) \text{ would lead us to reject } H_0\}.$$

In this continuous case, the rejection region turns out to be

$$R = \{\mathbf{x} : D(\mathbf{x}) \geq d_\alpha\}.$$

Given the rejection region R, notice that the type I error probability is given by

$$P[x \in R \mid H_0],$$

whereas the type II error probability is

$$P[x \in R^c \mid H_1].$$

Definition 9.4. **Power** is the probability of rejecting H_0 when H_0 is false; that is,

$$P[\text{rejecting } H_0 \mid H_1] = 1 - \beta.$$

Observe that this is the probability of the correct decision being made. Thus, a more powerful test is desirable. This is equivalent to minimizing the type II error probability.

Recall that if $X_1, \ldots, X_n$ is a random sample from $\mathrm{N}(\mu, \sigma^2)$ and we want to test $H_0 : \mu = \mu_0$ versus $H_1 : \mu \neq \mu_0$, we had the test statistic

$$D(\mathbf{X}) = \frac{|\overline{X} - \mu_0|}{S/\sqrt{n}}$$

with $D(\mathbf{X}) \sim t(n-1)$ under H_0. At the significance level $\alpha = 0.05$, we have

$$\begin{aligned} 0.05 &= P[D(\mathbf{X}) \geq d_{0.05} \mid H_0] \\ &= P[t(n-1) \geq d_{0.05}] \end{aligned}$$

so that $d_{0.05} = t_{0.95}(n-1)$. Thus, the rejection region is the set

$$R = \{\mathbf{x} : D(\mathbf{x}) \geq d_{0.05}\} = \{\mathbf{x} : D(\mathbf{x}) \geq t_{0.95}(n-1)\}.$$

Now, the type I error probability is given by

$$\begin{aligned} P[\text{rejecting } H_0 \mid H_0] &= P[D(\mathbf{X}) \geq t_{0.95}(n-1) \mid H_0] \\ &= P[t(n-1) \geq t_{0.95}(n-1)] \\ &= 0.05, \end{aligned}$$

which turns out to be equal to the significance level $\alpha = 0.05$. For the type II error probability

$$P[D(\mathbf{X}) < t_{0.95}(n-1) \mid H_1],$$

we obtain a non-central t-distribution, which is beyond the scope of the course, so we will not compute it.

In the legal court example at the beginning of Week 8, we see that the type I error probability corresponds to an innocent defendant being declared guilty, and the type II error probability corresponds to a guilty defendant failing to be convicted. The type I error is much more serious than the type II error.

Our goal now will be to control the type I error probability, while having the smallest possible type II error probability to maximize the power of the test.

LEMMA 9.5 (Neyman-Pearson lemma). Suppose that $X_1, \ldots, X_n$ is a random sample, and suppose we want to test $H_0 : \theta = \theta_0$ versus $H_1 : \theta = \theta_1$. For some constant c, suppose that the rejection region

$$R = \left\{\mathbf{x} : \frac{L(\theta_1; \mathbf{x})}{L(\theta_0; \mathbf{x})} > c\right\}$$

corresponds to a test with a type I error probability of α. Then this test is a most powerful test among all tests with a type I error probability of at most α for the test $H_0 : \theta = \theta_0$ versus $H_1 : \theta = \theta_1$.

In particular, the Neyman-Pearson lemma gives us a way of finding a most powerful test among a collection of tests with type I error probability $\leq \alpha$.

EXAMPLE 9.6. Let $X_1, \ldots, X_n$ be a random sample from $\mathrm{N}(\theta, 1)$. At a type I error probability of $\alpha = 0.05$, find a most powerful test for $H_0 : \theta = 0$ versus $H_1 : \theta = \theta_1$ for some fixed constant $\theta_1 > 0$.

Solution: By the Neyman-Pearson lemma, a most powerful test with type I error probability 0.05 has rejection region

$$R = \left\{\mathbf{x} : \frac{L(\theta_1; \mathbf{x})}{L(\theta_0; \mathbf{x})} > c\right\}$$

for some constant c. In particular, we have

$$P\left[\frac{L(\theta_1; \mathbf{x})}{L(\theta_0; \mathbf{x})} > c \,\middle|\, H_0\right] = \alpha.$$

Now, we only need to find the constant c. First, we have

$$\begin{aligned} L(\theta; \mathbf{x}) &= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{(x_i - \theta)^2}{2}\right) \\ &= \left(\frac{1}{\sqrt{2\pi}}\right)^n \exp\left(-\frac{1}{2}\sum_{i=1}^{n}(x_i - \theta)^2\right). \end{aligned}$$

Hence, we see that

$$\begin{aligned}\frac{L(\theta_1;\mathbf{x})}{L(\theta_0;\mathbf{x})} &= \frac{\exp(-\frac{1}{2}\sum_{i=1}^n (x_i-\theta_1)^2)}{\exp(-\frac{1}{2}\sum_{i=1}^n (x_i-\theta_0)^2)} \\ &= \frac{\exp(-\frac{1}{2}\sum_{i=1}^n (x_i^2-2\theta_1 x_i+\theta_1^2))}{\exp(-\frac{1}{2}\sum_{i=1}^n (x_i^2-2\theta_0 x_i+\theta_0^2))} \\ &= \exp\left(-\frac{1}{2}\left(-2\theta_1\sum_{i=1}^n x_i + n\theta_1^2\right)+\frac{1}{2}\left(-2\theta_0\sum_{i=1}^n x_i+n\theta_0^2\right)\right) \\ &= \exp\left((\theta_1-\theta_0)\sum_{i=1}^n x_i - \frac{n}{2}\theta_1^2+\frac{n}{2}\theta_0^2\right).\end{aligned}$$

It follows that

$$\begin{aligned}0.05 &= P\left[\frac{L(\theta_1;\mathbf{x})}{L(\theta_0;\mathbf{x})} > c \,\middle|\, H_0\right] \\ &= P\left[\exp\left((\theta_1-\theta_0)\sum_{i=1}^n x_i - \frac{n}{2}\theta_1^2+\frac{n}{2}\theta_0^2\right) > c \,\middle|\, H_0\right] \\ &= P\left[\exp\left(\theta_1\sum_{i=1}^n x_i - \frac{n}{2}\theta_1^2\right) > c \,\middle|\, H_0\right],\end{aligned}$$

where the last equality follows since $\theta_0 = 0$. Observe that $\exp(\theta_1\sum_{i=1}^n x_i - \frac{n}{2}\theta_1^2)$ is strictly increasing with respect to $\sum_{i=1}^n x_i$ since $\theta_1 > 0$. Therefore, we have

$$\exp\left(\theta_1\sum_{i=1}^n x_i - \frac{n}{2}\theta_1^2\right) > c \iff \sum_{i=1}^n x_i > c^*$$

for some other constant c^*. Then we have

$$0.05 = P\left[\sum_{i=1}^n x_i > c^* \,\middle|\, H_0\right],$$

and since $X_1,\dots,X_n$ are a random sample from $\mathrm{N}(\theta,1)$, we get $\sum_{i=1}^n X_i \sim \mathrm{N}(n\theta,n)$. In particular, under $H_0:\theta=0$, we have $\sum_{i=1}^n X_i\sim\mathrm{N}(0,n)$, which implies that

$$P\left[\frac{\sum_{i=1}^n X_i}{\sqrt{n}} > \frac{c^*}{\sqrt{n}} \,\middle|\, H_0\right] = P\left[Z > \frac{c^*}{\sqrt{n}}\right],$$

where $Z\sim\mathrm{N}(0,1)$. Then $c^*/\sqrt{n} = Z_{0.95} = 1.645$ so that $c^* = 1.645\sqrt{n}$. Finally, the rejection region is given by the set

$$R = \left\{\mathbf{x} : \frac{L(\theta_1;\mathbf{x})}{L(\theta_0;\mathbf{x})} > c\right\} = \left\{\mathbf{x} : \sum_{i=1}^n x_i > 1.645\sqrt{n}\right\}.$$

Likelihood ratio test. Suppose that we want to test $H_0:\theta\in\Omega_0$ versus $H_1:\theta\in\Omega\setminus\Omega_0$ where Ω is the parameter space containing all possible values of the unknown parameter θ, and Ω_0 is a subset of Ω. The **likelihood ratio test** of $H_0:\theta\in\Omega_0$ versus $H_1:\theta\in\Omega\setminus\Omega_0$ then has rejection region

$$R = \left\{\mathbf{x} : \Lambda(\mathbf{x}) = \frac{\max_{\theta\in\Omega} L(\theta;\mathbf{x})}{\max_{\theta\in\Omega_0} L(\theta;\mathbf{x})} > c\right\},$$

where the constant c is determined by the type I error probability.

REMARK 9.7. The constant c cannot be cannot always be found exactly. In such a case, we can find an approximation for c based on the asymptotic distribution

$$2\log[\Lambda(\mathbf{X})] \sim \chi^2(k)$$

under H_0, where k is the difference in the number of free parameters in Ω and Ω_0.

Notice that

$$\max_{\theta\in\Omega} L(\theta;\mathbf{x}) = \max\left(\max_{\theta\in\Omega_0} L(\theta;\mathbf{x}),\ \max_{\theta\in\Omega\setminus\Omega_0} L(\theta;\mathbf{x})\right).$$

If the maximum of $L(\theta;\mathbf{x})$ is achieved in the null parameter space Ω_0, then $\Lambda(\mathbf{x}) = 1$. Otherwise, the maximum of $L(\theta;\mathbf{x})$ is achieved in $\Omega\setminus\Omega_0$, in which case we have $\Lambda(\mathbf{x}) \geq 1$. In particular, we see that we must have $c > 1$.

We will denote

$$L(\hat{\theta};\mathbf{x}) := \max_{\theta\in\Omega} L(\theta;\mathbf{x})$$

where $\hat{\theta} = \operatorname{argmax}_{\theta\in\Omega} L(\theta;\mathbf{x})$, which we call the **unconstrained MLE**. On the other hand, we denote

$$L(\tilde{\theta};\mathbf{x}) := \max_{\theta\in\Omega_0} L(\theta;\mathbf{x})$$

where $\tilde{\theta} = \operatorname{argmax}_{\theta\in\Omega_0} L(\theta;\mathbf{x})$, which is known as the **constrained MLE**.

EXAMPLE 9.8. Suppose that $X_1,\ldots,X_n$ is a random sample from $\mathrm{N}(\mu,\sigma^2)$ where σ^2 is known. Consider the test $H_0: \mu=\mu_0$ versus $H_1: \mu\neq\mu_0$. Find the likelihood ratio test with type I error probability α.

Solution: We have $\Omega=\mathbb{R}$ and $\Omega_0=\{\mu_0\}$ in this case. It is easy to see that $\tilde{\mu}=\mu_0$, so we only need to find $\hat{\mu}$. Indeed, we have

$$L(\mu;\mathbf{x}) = \prod_{i=1}^n \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(x_i-\mu)^2}{2\sigma^2}\right),$$

and we leave it as an exercise to show that $\hat{\mu} = \operatorname{argmax}_{\mu\in\mathbb{R}} L(\mu;\mathbf{x}) = \bar{x}$. Then we have

$$\begin{aligned}
\Lambda(\mathbf{x}) &= \frac{L(\hat{\mu};\mathbf{x})}{L(\tilde{\mu};\mathbf{x})} \\
&= \frac{(1/\sqrt{2\pi\sigma^2})^n \exp(-\frac{1}{2\sigma^2}\sum_{i=1}^n (x_i-\bar{x})^2)}{(1/\sqrt{2\pi\sigma^2})^n \exp(-\frac{1}{2\sigma^2}\sum_{i=1}^n (x_i-\mu_0)^2)} \\
&= \exp\left(-\frac{\sum_{i=1}^n x_i^2 - n\bar{x}^2}{2\sigma^2} + \frac{\sum_{i=1}^n x_i^2 - 2\mu_0\sum_{i=1}^n x_i + n\mu_0^2}{2\sigma^2}\right) \\
&= \exp\left(\frac{n(\bar{x}-\mu_0)^2}{2\sigma^2}\right).
\end{aligned}$$

Notice that $\Lambda(\mathbf{x})$ is increasing with respect to $(\bar{x}-\mu_0)^2/(\sigma^2/n)$, so we reject μ_0 if

$$\Lambda(\mathbf{x}) > c \iff \frac{(\bar{x}-\mu_0)^2}{\sigma^2/n} > c^*$$

for some other constant c^*. Under $H_0: \mu=\mu_0$, we have $X_i \sim \mathrm{N}(\mu_0,\sigma^2)$ so that $\overline{X} \sim \mathrm{N}(\mu_0,\sigma^2/n)$. Then

$$\frac{\overline{X}-\mu_0}{\sqrt{\sigma^2/n}} \sim \mathrm{N}(0,1) \implies \frac{(\overline{X}-\mu_0)^2}{\sigma^2/n} \sim \chi^2(1).$$

under H_0. Finally, we have

$$\alpha = P[\Lambda(\mathbf{x}) > c \mid H_0] = P\left[\frac{(\overline{X}-\mu_0)^2}{\sigma^2/n} > c^* \,\middle|\, H_0\right] = P[\chi^2(1) > c^*],$$

which gives us $c^* = \chi^2_{1-\alpha}(1)$.

10 Asymptotic likelihood ratio test, goodness of fit tests

Suppose that $Y_1, \ldots, Y_n$ is a random sample with PDF $f(y;\theta)$, where the unknown parameter θ has parameter space Ω. Under some regularity conditions, the likelihood ratio test for $H_0 : \theta \in \Omega_0$ versus $H_1 : \theta \in \Omega \setminus \Omega_0$ based on

$$\Lambda(\mathbf{Y}) = \frac{L(\hat{\theta};\mathbf{Y})}{L(\tilde{\theta};\mathbf{Y})}$$

is such that, under the null hypothesis $H_0 : \theta \in \Omega_0$ for sufficiently large n, we have

$$2\log\Lambda(\mathbf{Y}) \sim \chi^2(k-q),$$

where

- q is the number of unknown/free parameters under the constraint of the null hypothesis (that is, within Ω_0), and
- k is the number of unknown/free parameters without any constraint (that is, within Ω).

Example 10.1. Suppose that $(Y_1, Y_2, Y_3) \sim \text{Multi}(n; \theta_1, \theta_2, \theta_3)$ where $\theta_1 + \theta_2 + \theta_3 = 1$. Find the asymptotic likelihood ratio test for the test $H_0 : \theta_1 = \theta_2 = \theta_3$ versus $H_1 : \neg H_0$ with a type I error probability of 0.05.

Solution: We have the likelihood function

$$L(\theta_1, \theta_2, \theta_3) = \frac{n!}{y_1!y_2!y_3!}\theta_1^{y_1}\theta^{y_2}\theta^{y_3}.$$

Note that the unconstrained MLEs are given by $\hat{\theta}_1 = y_1/n$, $\hat{\theta}_2 = y_2/n$, and $\hat{\theta}_3 = y_3/n$. There are $k = 2$ unknown parameters here since once two of the parameters are known, the third is fixed. On the other hand, since $\theta_1 + \theta_2 + \theta_3 = 1$, the constrained MLEs are $\tilde{\theta}_1 = \tilde{\theta}_2 = \tilde{\theta}_3 = 1/3$, and there are $q = 0$ unknown parameters in this case. Hence, we obtain

$$\Lambda(y_1, y_2, y_3) = \frac{L(\hat{\theta}_1, \hat{\theta}_2, \hat{\theta}_3)}{L(\tilde{\theta}_1, \tilde{\theta}_2, \tilde{\theta}_3)} = \frac{\frac{n!}{y_1!y_2!y_3!}(\frac{y_1}{n})^{y_1}(\frac{y_2}{n})^{y_2}(\frac{y_3}{n})^{y_3}}{\frac{n!}{y_1!y_2!y_3!}(\frac{1}{3})^{y_1}(\frac{1}{3})^{y_2}(\frac{1}{3})^{y_3}} = \left(\frac{3y_1}{n}\right)^{y_1}\left(\frac{3y_2}{n}\right)^{y_2}\left(\frac{3y_3}{n}\right)^{y_3}.$$

Under H_0 for large n, we have

$$2\log\Lambda(Y_1, Y_2, Y_3) \sim \chi^2(k-q) = \chi^2(2-0) = \chi^2(2).$$

Thus, the rejection region is the set

$$R = \{(y_1, y_2, y_3) : 2\log\Lambda(y_1, y_2, y_3) > c^*\},$$

where we have

$$0.05 = P[2\log\Lambda(Y_1, Y_2, Y_3) > c^* \mid H_0] = P[\chi^2(2) > c^*]$$

so that $c^* = \chi^2_{0.95}(2)$

Suppose the multinomial probabilities $\theta_1, \ldots, \theta_k$ satisfy $0 < \theta_j < 1$ for all $1 \le j \le k$ and $\sum_{j=1}^k \theta_j = 1$. Then

$$(Y_1, \ldots, Y_k) \sim f(y_1, \ldots, y_k; \theta_1, \ldots, \theta_k) = \frac{n!}{y_1! \cdots y_k!}\theta_1^{y_1} \cdots \theta_k^{y_k}.$$

We wish to test the hypothesis that the probabilities $\theta_1, \ldots, \theta_k$ are related in some way, say they are all functions of a parameter α such that

$$H_0 : \theta_j = \theta_j(\alpha),\ 1 \le j \le k$$

where $\alpha = (\alpha_1, \ldots, \alpha_p)$ and $p < k-1$. Then an asymptotic likelihood ratio test is based on

$$\Lambda(\mathbf{Y}) = \frac{L(\hat{\theta}; \mathbf{Y})}{L(\tilde{\theta}; \mathbf{Y})}$$

where the unconstrained MLE is

$$\hat{\theta} = (\hat{\theta}_1, \ldots, \hat{\theta}_k) = \left(\frac{Y_1}{n}, \ldots, \frac{Y_k}{n}\right),$$

and the constrained MLE is $\tilde{\theta} = (\theta_1(\tilde{\alpha}), \ldots, \theta_k(\tilde{\alpha}))$ with $\tilde{\alpha}$ being the MLE of α.

Now, under H_0 for large n, we have

$$2\log\Lambda(\mathbf{Y}) \sim \chi^2(k-1-p).$$

Notice that

$$2\log\Lambda(\mathbf{Y}) = 2\sum_{j=1}^{k} Y_j \log\left[\frac{\hat{\theta}_j}{\theta_j(\tilde{\alpha})}\right] = 2\sum_{j=1}^{k} Y_j \log\left(\frac{Y_j}{E_j}\right),$$

where $\hat{\theta}_j = Y_j/n$ and the expected frequencies under H_0 are $E_j = n\theta_j(\tilde{\alpha})$ for all $1 \le j \le k$.

Example 10.2. Suppose that $(Y_1, Y_2, Y_3) \sim \text{Multi}(n; \theta_1, \theta_2, \theta_3)$ so that $k = 3$ here. Consider an asymptotic likelihood ratio test for the null hypothesis

$$H_0 : \theta_1 = \alpha^2,\ \theta_2 = 2\alpha(1-\alpha),\ \theta_3 = (1-\alpha)^2, \quad \alpha \in (0,1).$$

Since this only depends on the parameter α, we have $p = 1$. Compute the p-value for $n = 100$, $y_1 = 17$, $y_2 = 46$, and $y_3 = 37$.

Solution: First, note that under H_0 for large n, we have

$$2\log\Lambda(Y_1, Y_2, Y_3) = 2\sum_{j=1}^{3} Y_j \log\left(\frac{Y_j}{E_j}\right) \sim \chi^2(k-1-p) = \chi^2(3-1-1) = \chi^2(1).$$

It follows that

$$\begin{aligned} p\text{-value} &= P[2\log\Lambda(Y_1, Y_2, Y_3) > 2\log\Lambda(y_1, y_2, y_3) \mid H_0] \\ &\approx P[\chi^2(1) > 2\log\Lambda(y_1, y_2, y_3)]. \end{aligned}$$

Now, note that

$$2\log\Lambda(y_1, y_2, y_3) = 2\sum_{j=1}^{3} y_j \log\left(\frac{y_j}{e_j}\right)$$

where $e_j = n\theta_j(\tilde{\alpha})$ for all $1 \le j \le 3$ and $\tilde{\alpha} = \text{argmax}_{\alpha\in(0,1)} L(\alpha)$. We see that

$$L(\alpha) = \frac{n!}{y_1!y_2!y_3!}(\alpha^2)^{y_1}(2\alpha(1-\alpha))^{y_2}((1-\alpha)^2)^{y_3} = \frac{n!}{y_1!y_2!y_3!}2^{y_2}\alpha^{2y_1+y_2}(1-\alpha)^{y_2+2y_3}.$$

Using the usual method of finding $\ell(\alpha)$ and solving for $\partial\ell(\alpha)/\partial\alpha = 0$, we find that

$$\tilde{\alpha} = \frac{2y_1 + y_2}{2n} = \frac{2\cdot 17 + 46}{2\cdot 100} = \frac{2}{5}.$$

From here, we obtain $e_1 = 100(\frac{2}{5})^2 = 16$, $e_2 = 100(2\cdot\frac{2}{5}\cdot\frac{3}{5}) = 48$, and $e_3 = 100(\frac{3}{5})^2 = 36$. This then yields

$$2\log\Lambda(y_1, y_2, y_3) \approx 0.173$$

and finally, we get p-value $\approx 0.917 > 0.1$.

EXAMPLE 10.3. The number of service interruptions in a communications system over 200 separate days is summarized in the following table.

Number of interruptions	0	1	2	3	4	5	> 5	Total
Observed frequency	64	71	42	18	4	1	0	200

Among these 200 days, let Y_j be the number of days with j interruptions. Then we see that

$$(Y_0, Y_1, Y_2, Y_3, \dots) \sim \text{Multi}(200; \theta_0, \theta_1, \theta_2, \theta_3, \dots),$$

where each θ_j is the probability of j interruptions occurring in a single day. Determine whether a Poisson model for the number of interruptions in a single day is consistent with these data.

Solution: Notice that if $X_1, \dots, X_{200} \sim \text{Poi}(\theta)$, then

$$\theta_j = P[X_1 = j] = \frac{\theta^j e^{-\theta}}{j!}, \quad j = 0, 1, 2, \dots.$$

We note that $Y_j = \sum_{i=1}^{200} I[X_i = j]$ for all $j = 0, 1, 2, \dots$, where I denotes the indicator function.

Therefore, if a Poisson model is a good fit for these data, then we should fail to reject the null hypothesis

$$H_0 : \theta_j = \frac{\theta^j e^{-\theta}}{j!}, \quad j = 0, 1, 2, \dots.$$

Recall that θ_j is the number of interruptions in a single day and

$$(Y_0, Y_1, Y_2, Y_3, \dots) \sim \text{Multi}(200; \theta_0, \theta_1, \theta_2, \theta_3, \dots),$$

so we have

$$L(\theta) = \frac{n!}{y_0! y_1! \cdots y_5!} \left(\prod_{j=0}^{5} [\theta_j(\theta)]^{y_j} \right) \left(\prod_{j=6}^{\infty} [\theta_j(\theta)]^{y_j} \right),$$

where we note that the last product is simply 1 since $y_j = 0$ for all $j \geq 6$. Finding $\ell(\theta)$ and solving for $\partial \ell(\theta)/\partial \theta = 0$, one can find that

$$\hat{\theta} = \frac{1}{n} \sum_{j=0}^{5} j \cdot y_j = 1.15.$$

Now, consider

$$2 \log \Lambda(y_0, y_1, y_2, \dots) = 2 \sum_{j=0}^{\infty} y_j \log \left(\frac{y_j}{e_j} \right).$$

The logarithm is not well-defined here in the case that $j \geq 6$ since $y_j = 0$. However, we can alternatively consider the following table.

Number of interruptions	0	1	2	3	≥ 4	Total
Observed frequency	64	71	42	18	5	200

Notice that there are $k = 5$ parameters here whereas H_0 only depends on the one parameter θ, so $p = 1$. Hence, we obtain

$$2 \log \Lambda(Y_0, Y_1, Y_2, Y_3, Y_{\geq 4}) = 2 \sum_j Y_j \log \left(\frac{Y_j}{E_j} \right) \sim \chi^2(k - 1 - p) = \chi^2(5 - 1 - 1) = \chi^2(3).$$

Now, we get

$$e_j = 200 \cdot \frac{(1.15)^j e^{-1.15}}{j!}$$

so that $e_0 = 63.33$, $e_1 = 72.83$, $e_2 = 41.88$, $e_3 = 16.05$, and $e_{\geq 4} = 5.91$. Then

$$2 \log \Lambda(y_0, y_1, y_2, y_3, y_{\geq 4}) = 2\left[64 \log\left(\frac{64}{63.33}\right) + \cdots + 5 \log\left(\frac{5}{5.91}\right)\right] = 0.43.$$

Finally, we have

$$p\text{-value} \approx P[\chi^2(3) > 0.43] = 0.93.$$

Since p-value > 0.1, there is no evidence against the hypothesis that the Poisson model fits these data.

Example 10.4. Suppose that a random sample $t_1, t_2, \ldots, t_{100}$ is collected, and we wish to test that the data comes from an EXP(θ) distribution. We partition the range of T into k intervals, and we count the number of observations y_j that fall into the j-th interval for each $1 \leq j \leq k$. Assuming an EXP(θ) model, the probability that an observation lies in the j-th interval $I_j = (a_{j-1}, a_j)$ is

$$p_j(\theta) = \int_{a_{j-1}}^{a_j} f(t;\theta)\,\mathrm{d}t = e^{-a_{j-1}/\theta} - e^{-a_j/\theta}, \quad 1 \leq j \leq k. \tag{$*$}$$

Suppose that the observed data is as in the following table. Here, we have $k = 7$ intervals. To calculate

Interval	0 to 100	100 to 200	200 to 300	300 to 400	400 to 600	600 to 800	> 800
y_j	29	22	12	10	10	9	8
e_j	27.6	20.0	14.4	10.5	13.1	6.9	7.6

the expected frequencies under the null hypothesis ($*$), we need an estimate of θ which can be obtained by maximizing the likelihood function

$$L(\theta) = \prod_{j=1}^{7} [p_j(\theta)]^{y_j} = \prod_{j=1}^{7} (e^{-a_{j-1}/\theta} - e^{-a_j/\theta})^{y_j}.$$

Note that $p = 1$ since there is only one unknown parameter under ($*$), namely θ. This is a case that requires numerical methods such as Newton's method to solve for the MLE, so we note that one can find that $\hat{\theta} = 310.0$. The expected frequences $e_j = 100 p_j(\hat{\theta})$ are then given in the above table. It follows that

$$2 \log \Lambda(\mathbf{y}) = 2 \sum_{j=1}^{7} y_j \log\left(\frac{y_j}{e_j}\right) = 2\left[29 \log\left(\frac{29}{27.6}\right) + \cdots + 8 \log\left(\frac{8}{7.6}\right)\right] = 1.91.$$

The number of degrees of freedom is $k - 1 - p = 7 - 1 - 1 = 5$, so

$$p\text{-value} = P[2 \log \Lambda(\mathbf{Y}) \geq 1.91 \mid H_0] \approx P[\chi^2(5) \geq 1.91] = 0.86.$$

Thus, there is no evidence against the model ($*$).

11 Two-way contingency tables, independence between two factors

We often want to assess whether two factors are related to each other. One approach to do this is to test the hypothesis that the factors are independent. More precisely, for a random sample of individuals, suppose that the individuals can be classified according to two factors, say A and B.

- For factor A, an individual can be any of a mutually exclusive types or levels $A_1, \ldots, A_a$, where $a \geq 2$.
- For factor B, an individual can be any of b mutually exclusive types or levels $B_1, \ldots, B_b$, where $b \geq 2$.

For a random sample of n individuals, let y_{ij} denote the number of individuals that have A-type A_i and B-type B_j. The observed data are arranged in a **two-way contingency table**, as seen below.

	B_1	B_2	$\cdots$	B_b	Total (rows)
A_1	y_{11}	y_{12}	$\cdots$	y_{1b}	r_1
A_2	y_{21}	y_{22}	$\cdots$	y_{2b}	r_2
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
A_a	y_{a1}	y_{a2}	$\cdots$	y_{ab}	r_a
Total (columns)	c_1	c_2	$\cdots$	c_b	n

Let θ_{ij} be the probability that a random selected individual has combined type (A_i, B_j), and note that

$$\sum_{i=1}^{a} \sum_{j=1}^{b} \theta_{ij} = 1.$$

Thus, we can adopt a multinomial model for this problem, namely

$$(Y_{11}, Y_{12}, \ldots, Y_{ab}) \sim \text{Multi}(n; \theta_{11}, \theta_{12}, \ldots, \theta_{ab}).$$

Now, denote α_i to be the probability that an individual is of type A_i, where $0 < \alpha_i < 1$ and $\sum_{i=1}^{a} \alpha_i = 1$. Similarly, let β_j be the probability that an individual is of type B_j, with $0 < \beta_j < 1$ and $\sum_{j=1}^{b} \beta_j = 1$.

To test the independence of the classifications A and B, we test the null hypothesis

$$H_0 : \theta_{ij} = \alpha_i \beta_j, \quad 1 \leq i \leq a, \quad 1 \leq j \leq b.$$

Under H_0 for large n, it can be shown that the likelihood ratio test is based on

$$2 \sum_{i=1}^{a} \sum_{j=1}^{b} Y_{ij} \log\left(\frac{Y_{ij}}{E_{ij}}\right) \sim \chi^2((a-1)(b-1)),$$

where for all $1 \leq i \leq a$ and $1 \leq j \leq b$, we have $e_{ij} = n\tilde{\alpha}_i \tilde{\beta}_j = r_i c_j / n$ with $\tilde{\alpha}_i = r_i/n$ and $\tilde{\beta}_j = c_j/n$.

Example 11.1. Consider two blood type classification systems given in the below two-way contingency table.

	O	A	B	AB	Total (rows)
Rh+	82	89	54	19	244
Rh−	13	27	7	9	56
Total (columns)	95	116	61	28	300

Let H_0 be the hypothesis that these two blood type classification systems are independent. Under H_0 for large n, we have

$$2 \sum_{i=1}^{2} \sum_{j=1}^{3} Y_{ij} \log\left(\frac{Y_{ij}}{E_{ij}}\right) \sim \chi^2((2-1)(4-1)) = \chi^2(3).$$

For a given significance level α, the rejection region for the test is

$$R = \left\{ (y_{11}, y_{12}, \ldots, y_{23}) : 2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right) > \chi^2_{1-\alpha}(3) \right\},$$

or alternatively, the p-value is given by

$$p\text{-value} = P\left[\chi^2(3) > 2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right)\right].$$

We have the expected frequencies

$$e_{11} = \frac{244\cdot 95}{300} = 77.27, \qquad e_{12} = \frac{244\cdot 116}{300} = 94.35, \qquad e_{13} = \frac{244\cdot 61}{300} = 49.61.$$

The remaining expected frequencies can be obtained with subtraction, namely

$$e_{14} = r_1 - e_{11} - e_{12} - e_{13},$$

and for all $1 \le j \le 4$, we have $e_{2j} = c_j - e_{1j}$ as there are only two rows.

	O	A	B	AB	Total (rows)
Rh+	82 (77.27)	89 (94.35)	54 (49.61)	19 (22.77)	244
Rh−	13 (17.73)	27 (21.65)	7 (11.39)	9 (5.23)	56
Total (columns)	95	116	61	28	300

We then find that

$$2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right) = 8.447,$$

in which case it follows that

$$p\text{-value} = P[\chi^2(3) \ge 8.447] = 0.0376.$$

Since this is small, there is evidence against the hypothesis based on the data, so the blood type classification systems are dependent in this case. However, note that by comparing the y_{ij}'s and the e_{ij}'s, the degree of dependence does not appear to be large.

A similar problem arises when individuals can be one of the b types $B_1, \ldots, B_b$, but the individuals can be divided into a groups $A_1, \ldots, A_a$. In this case, we might be interested in whether the proportions of the types $B_1, \ldots, B_b$ within each of the groups $A_1, \ldots, A_a$ are the same.

To be precise, we want to know whether the probability θ_{ij} that an individual in group A_i is also B-type B_j is the same for all $1 \le i \le a$. Note that $\sum_{j=1}^{b}\theta_{ij} = 1$ for all $1 \le i \le a$, and we test the null hypothesis

$$H_0 : \theta_1 = \theta_2 = \cdots = \theta_a, \quad \theta_i = (\theta_{i1}, \ldots, \theta_{ib}), \quad 1 \le i \le a.$$

Under H_0 for large n, it can be shown that

$$2\sum_{i=1}^{a}\sum_{j=1}^{b} Y_{ij}\log\left(\frac{Y_{ij}}{E_{ij}}\right) \sim \chi^2((a-1)(b-1)),$$

where for all $1 \le i \le a$ and $1 \le j \le b$, we have $e_{ij} = n_i(y_{+j}/n)$ where $y_{+j} = \sum_{i=1}^{a} y_{ij}$.

EXAMPLE 11.2. Suppose there are three hospitals A, B, and C. During a certain period, they all performed a number of risky surgical procedures, and their successes and failures were recorded.

	A	B	C
Successes	23	43	85
Failures	2	7	15

We wish to test if there is a statistically significant difference between the three hospitals. Let H_0 be the hypothesis that the proportions between their successes and failures are the same. Then under H_0 for large n, we have

$$2\sum_{i=1}^{2}\sum_{j=1}^{3} Y_{ij}\log\left(\frac{Y_{ij}}{E_{ij}}\right) \sim \chi^2((2-1)(3-1)) = \chi^2(2).$$

Now, for a given significance level α, the rejection region is given by

$$R = \left\{(y_{11}, y_{12}, \ldots, y_{23}) : 2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right) > \chi^2_{1-\alpha}(2)\right\}.$$

In particular, we have

$$p\text{-value} = P\left[\chi^2(2) > 2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right)\right].$$

Then we have $e_{ij} = r_i c_j/n$ for all $1 \le i \le 2$ and $1 \le j \le 3$, so we obtain the following table.

	A	B	C
Successes	23 (21.57)	43 (43.14)	85 (86.29)
Failures	2 (3.43)	7 (6.86)	15 (13.71)

Finally, we have

$$2\sum_{i=1}^{2}\sum_{j=1}^{3} y_{ij}\log\left(\frac{y_{ij}}{e_{ij}}\right) = 0.936$$

so it follows that

$$p\text{-value} = P[\chi^2(2) > 0.936] = 0.626.$$

Since this is large, we fail to reject the null hypothesis $H_0 : \theta_1 = \theta_2$.

12 Bayesian inference

So far, we have considered a parameter to be a fixed unknown constant. We assumed that only the random sample and statistics derived from the sample were random.

However, in the Bayesian setup, we assume that the parameter is also random. We begin by asserting that the parameter θ has been generated by some distribution π, which is called the **prior distribution**. The observations obtained from the corresponding probability (density) function $f(x;\theta)$ can then be interpreted as the conditional probability (density) function, given the value of θ.

The prior distribution $\pi(\theta)$ quantifies information about θ prior to any real data $\mathbf{x}$ being collected. It can be

- constructed on the basis of past data, or
- chosen to incorporate subjective information based on an expert's experience and personal judgement.

The purpose of the data is then to adjust the distribution of θ in light of the data, resulting in the **posterior distribution** for the parameter. Any conclusions about the plausible value of parameter are to be drawn from the posterior distribution.

Suppose that $\theta \sim \pi(\theta)$, the prior distribution. Moreover, suppose we are given the value of the parameter resulting from the random sample $X_1, \ldots, X_n$. Each X_i comes from the conditional probability (density) function $f(x;\theta)$ (alternatively denoted by $f(x \mid \theta)$).

Definition 12.1. The **posterior distribution** of the parameter θ is the conditional probability (density) function of θ given the data $\mathbf{x} = (x_1, \ldots, x_n)$. It is given by

$$\pi(\theta \mid \mathbf{x}) = \frac{\pi(\theta)L(\theta;\mathbf{x})}{\int \pi(\theta)L(\theta;\mathbf{x})\,\mathrm{d}\theta} \propto \pi(\theta)L(\theta;\mathbf{x}).$$

Notice that the denominator is the marginal probability (density) function of the sample, and it is free of the parameter θ. We can effectively treat it as a constant, which is why we can say that $\pi(\theta \mid \mathbf{x})$ is proportional to the numerator.

Remark 12.2. Since Bayesian inference is based on the posterior distribution, it depends only on the data through the likelihood function.

Example 12.3. Suppose that a coin is tossed n times with probability of heads θ. Suppose that it is known from previous experience that the probability of heads is not always $1/2$, but follows a $\text{BETA}(10,10)$ distribution. If the n tosses result in x heads, find the posterior PDF of θ.

Solution: We know that $\pi(\theta \mid x) \propto \pi(\theta)L(\theta;x)$. We have likelihood function

$$L(\theta;x) = f(x \mid \theta) = \frac{n!}{x!(n-x)!}\theta^x(1-\theta)^{n-x}$$

and prior distribution $\text{BETA}(10,10)$ so that

$$\pi(\theta) = \frac{\Gamma(10+10)}{\Gamma(10)\Gamma(10)}\theta^{10-1}(1-\theta)^{10-1}, \quad 0 < \theta < 1.$$

Consequently, we have

$$\begin{aligned}\pi(\theta \mid x) &\propto \frac{\Gamma(10+10)}{\Gamma(10)\Gamma(10)}\theta^{10-1}(1-\theta)^{10-1} \cdot \frac{n!}{x!(n-x)!}\theta^x(1-\theta)^{n-x} \\ &\propto \theta^{10+x-1}(1-\theta)^{10+n-x-1}.\end{aligned}$$

Notice that if $Z \sim \text{BETA}(a,b)$ with $a, b > 0$, then its PDF is given by

$$f(z) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}z^{a-1}(1-z)^{b-1}, \quad 0 < z < 1.$$

In particular, we see that $\pi(\theta \mid x) \sim \text{BETA}(10+x, 10+n-x)$.

We now discuss some commonly used priors.

- **Conjugate priors.** If a prior distribution has the property that the posterior distribution is in the same family of distributions as the prior, then the prior is called a **conjugate prior**.

- **Flat priors.** When there is no reason to prefer one value of θ over another, we can use a **flat prior**, which is given by
$$\pi(\theta) = c, \quad -\infty < \theta < \infty$$
for some positive constant $c \in \mathbb{R}^+$.

REMARK 12.4.

- The choice of the prior to be a conjugate prior is often motivated by mathematical convenience.

- Flat priors are the usual way of representing ignorance about the parameter, and they are frequently used in practice.

- It can be argued that flat priors are more objective since conjugate priors may contain personal bias as well as background knowledge so that some values of θ are more plausible than others.

- In some applications, the amount of prior information available is far less than the information contained in the data. In this case, there is little point in worrying about a precise specification of the prior distribution.

- Notice that $\pi(\theta) = c$ for $-\infty < \theta < \infty$ is an improper prior since we have
$$\int_{-\infty}^{\infty} \pi(\theta)\,\mathrm{d}\theta = \infty.$$

EXAMPLE 12.5. Suppose that $X_1, \ldots, X_n$ is a random sample drawn from $\mathrm{UNIF}(0, \theta)$. Show that the prior distribution $\theta \sim \mathrm{PAR}(a, b)$ is a conjugate prior.

Solution: First, note that the prior distribution is given by
$$\pi(\theta) = \frac{ba^b}{\theta^{b+1}}, \quad \theta \geq a.$$

The likelihood function is
$$L(\theta; \mathbf{x}) = \prod_{i=1}^{n} f(x_i \mid \theta) = \begin{cases} 1/\theta^n & \text{if } x_i \in [0, \theta] \text{ for all } 1 \leq i \leq n \\ 0 & \text{otherwise} \end{cases} = \frac{1}{\theta^n} I[x_{(n)} \leq \theta].$$

The posterior distribution is then
$$\begin{aligned} \pi(\theta \mid \mathbf{x}) &\propto \frac{ba^b}{\theta^{b+1}} I[\theta \geq a] \cdot \frac{1}{\theta^n} I[x_{(n)} \leq \theta] \\ &\propto \frac{1}{\theta^{b+n+1}} I[\theta \geq \max(a, x_{(n)})]. \end{aligned}$$

It follows that $(\theta \mid \mathbf{x}) \sim \mathrm{PAR}(\max(a, x_{(n)}), b+n)$, so the prior is a conjugate prior.

EXAMPLE 12.6. Suppose that $X_1, \ldots, X_n$ is a random sample drawn from $\mathrm{N}(\theta, 1)$. Show that the prior distribution $\theta \sim \mathrm{N}(0, \gamma^2)$ is a conjugate prior.

Solution: We have prior distribution
$$\pi(\theta) = \frac{1}{\sqrt{2\pi\gamma^2}} \exp\left(-\frac{(\theta - 0)^2}{2\gamma^2}\right)$$

and likelihood function

$$L(\theta;\mathbf{x}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\cdot 1}} \exp\left(-\frac{(x_i-\theta)^2}{2\cdot 1}\right) = (2\pi)^{-n/2}\exp\left(-\frac{1}{2}\sum_{i=1}^{n}(x_i-\theta)^2\right).$$

It follows that

$$\begin{aligned}
\pi(\theta \mid \mathbf{x}) &\propto \exp\left(-\frac{\theta^2}{2\gamma^2}\right)\exp\left(-\frac{1}{2}\sum_{i=1}^{n}(x_i-\theta)^2\right) \\
&= \exp\left[-\frac{1}{2}\left(\sum_{i=1}^{n}x_i^2 - 2\theta\sum_{i=1}^{n}x_i + n\theta^2 + \frac{\theta^2}{\gamma^2}\right)\right] \\
&= \exp\left(-\frac{1}{2}\sum_{i=1}^{n}x_i^2\right)\exp\left[-\frac{1}{2}\left(\theta^2\left(n+\frac{1}{\gamma^2}\right) - 2\theta\sum_{i=1}^{n}x_i\right)\right] \\
&\propto \exp\left[-\frac{n+1/\gamma^2}{2}\left(\theta^2 - \frac{2\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\theta\right)\right] \\
&= \exp\left[-\frac{n+1/\gamma^2}{2}\left(\left(\theta - \frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\right)^2 - \left(\frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\right)^2\right)\right] \\
&= \exp\left[-\frac{n+1/\gamma^2}{2}\left(\theta - \frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\right)^2\right]\exp\left[\frac{n+1/\gamma^2}{2}\left(\frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\right)^2\right] \\
&\propto \exp\left[-\frac{n+1/\gamma^2}{2}\left(\theta - \frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}\right)^2\right].
\end{aligned}$$

Therefore, we see that

$$(\theta \mid \mathbf{x}) \sim N\left(\frac{\sum_{i=1}^{n}x_i}{n+1/\gamma^2}, \frac{1}{n+1/\gamma^2}\right).$$

EXAMPLE 12.7. Suppose that $X \sim \mathrm{Bin}(n,\theta)$ with the flat prior $\theta \sim \mathrm{UNIF}(0,1)$. Find the posterior distribution of θ.

Solution: We have prior distribution

$$\pi(\theta) = 1, \quad 0 < \theta < 1$$

and likelihood function

$$L(\theta;x) = \frac{n!}{x!(n-x)!}\theta^x(1-\theta)^{n-x}.$$

Then, we have

$$\begin{aligned}
\pi(\theta \mid x) &\propto 1\cdot\frac{n!}{x!(n-x)!}\theta^x(1-\theta)^{n-x} \\
&\propto \theta^x(1-\theta)^{n-x}, \quad 0<\theta<1.
\end{aligned}$$

Recall that if $Z \sim \mathrm{BETA}(\alpha,\beta)$, then the PDF of Z is

$$f(z) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}z^{\alpha-1}(1-z)^{\beta 0-1}, \quad 0<z<1.$$

Therefore, we see that $(\theta \mid x) \sim \mathrm{BETA}(x+1, n-x+1)$.

EXERCISE 12.8. Suppose that $X_1,\dots,X_n$ is a random sample drawn from $\mathrm{N}(\theta,1)$. Find the posterior distribution of θ with a flat prior.

The mean of the posterior distribution $\pi(\theta \mid \mathbf{X})$ is the **Bayes point estimator** of θ. We state without proof that the Bayes point estimator minimizes the Bayes risk for the squared error loss with respect to the prior $\pi(\theta)$ given $\mathbf{X}$.

EXAMPLE 12.9. Find the Bayes point estimator for Example 12.3, and compare it to the MLE of θ.

Solution: Recall that we had $X \sim \text{Bin}(n, \theta)$ and $\theta \sim \text{BETA}(10, 10)$, and we showed that $(\theta \mid x) \sim \text{BETA}(x + 10, n - x + 10)$. Moreover, recall that if $Z \sim \text{BETA}(\alpha, \beta)$, then

$$E(Z) = \frac{\alpha}{\alpha + \beta}.$$

Therefore, the posterior mean

$$\frac{x + 10}{(x + 10) + (n - x + 10)} = \frac{x + 10}{n + 20}$$

is the Bayes point estimate. Then, the Bayes point estimator is given by

$$\frac{X + 10}{n + 20}.$$

On the other hand, the MLE of θ for $X \sim \text{Bin}(n, \theta)$ is simply $\hat{\theta} = X/n$. Notice that the 10 in the numerator and the 20 in the denominator of the Bayes point estimator occurs due to the prior distribution.

EXAMPLE 12.10. Find the Bayes point estimator for Example 12.5, and compare it to the MLE of θ.

Solution: We had a random sample $X_1, \ldots, X_n$ from $\text{UNIF}(0, \theta)$ and prior distribution $\theta \sim \text{PAR}(a, b)$. We showed that $(\theta \mid \mathbf{x}) \sim \text{PAR}(\max(a, x_{(n)}), b + n)$. If $Z \sim \text{PAR}(a, b)$, then it can be shown that

$$E(Z) = \frac{ab}{b^{-1}}$$

given that $b > 1$. The Bayes point estimator of θ is then

$$\frac{\max(a, X_{(n)}) \cdot (b + n)}{(b + n)^{-1}}$$

if $b + n > 1$. On the other hand, the MLE of θ is $X_{(n)}$.

EXERCISE 12.11. For Example 12.6, Example 12.7, and Exercise 12.8, find their Bayes point estimators and compare them with the MLEs.

A Bayesian can use the posterior distribution $\pi(\theta \mid \mathbf{x})$ to determine points $c_1(\mathbf{x})$ and $c_2(\mathbf{x})$ such that

$$\int_{c_1}^{c_2} \pi(\theta \mid \mathbf{x})\,\mathrm{d}\theta = 0.95, \qquad \int_{-\infty}^{c_1} \pi(\theta \mid \mathbf{x})\,\mathrm{d}\theta = \int_{c_2}^{\infty} \pi(\theta \mid \mathbf{x})\,\mathrm{d}\theta = 0.025.$$

This yields a 95% equal-tail **Bayesian credible interval** $[c_1(\mathbf{x}), c_2(\mathbf{x})]$ for the parameter θ. A Bayesian will then state that given the data, the conditional probability that the parameter falls within this interval is 0.95. No such probability can be ascribed to a confidence interval.

EXAMPLE 12.12. Find a 95% equal-tail Bayesian credible interval for Example 12.3.

Solution: We had posterior distribution $(\theta \mid x) \sim \text{BETA}(x + 10, n - x + 10)$. Denote $c_1(x)$ and $c_2(x)$ by the 2.5% and 97.5% quantiles of this distribution, respectively. Then we have

$$P[c_1(x) \leq \theta \leq c_2(x) \mid x] = 0.95.$$

Unfortunately, we cannot say much more in this example, as there is no explicit expression for the quantiles of the beta distribution. (However, given an explicit value for x, these can be computed using software.)

EXAMPLE 12.13. Find a 95% equal-tail Bayesian credible interval for Example 12.5.

Solution: We had a random sample $X_1, \ldots, X_n$ from $\text{UNIF}(0, \theta)$ with prior distribution $\theta \sim \text{PAR}(a, b)$. We then found the posterior distribution $(\theta \mid \mathbf{x}) \sim \text{PAR}(\max(a, x_{(n)}), b + n)$. Thus, a 95% equal-tail Bayesian credible interval is given by $[c_1(\mathbf{x}), c_2(\mathbf{x})]$ where

$$\begin{aligned} P[c_1(\mathbf{x}) \le \theta \le c_2(\mathbf{x}) \mid \mathbf{x}] &= 0.95, \\ P[\theta \le c_1(\mathbf{x}) \mid \mathbf{x}] &= 0.025. \end{aligned}$$

We first look at the general case. If $Z \sim \text{PAR}(\alpha, \beta)$, then the PDF of Z is

$$f(z) = \frac{\beta \alpha^\beta}{z^{\beta+1}}, \quad z \ge \alpha.$$

We want to find c_1 and c_2 such that

$$\int_{-\infty}^{c_1} \frac{\beta \alpha^\beta}{z^{\beta+1}} \, \mathrm{d}z = 0.025, \tag{1}$$

$$\int_{c_2}^{\infty} \frac{\beta \alpha^\beta}{z^{\beta+1}} \, \mathrm{d}z = 0.975, \tag{2}$$

From equation (1), we have

$$\begin{aligned} 0.025 &= \int_{-\infty}^{c_1} \frac{\beta \alpha^\beta}{z^{\beta+1}} \, \mathrm{d}z \\ &= \int_{\alpha}^{c_1} \frac{\beta \alpha^\beta}{z^{\beta+1}} \, \mathrm{d}z \\ &= \beta \alpha^\beta \left[-\frac{1}{\beta} z^{-\beta} \right]_{\alpha}^{c_1} \\ &= -\alpha^\beta (c_1^{-\beta} - \alpha^{-\beta}) = 1 - \left(\frac{\alpha}{c_1} \right)^\beta, \end{aligned}$$

where the second equality follows from the fact that the support set of the Pareto distribution is $z \ge \alpha$. In particular, we have $(\alpha/c_1)^\beta = 0.975$ so that

$$c_1 = \frac{\alpha}{(0.975)^{1/\beta}}.$$

Similarly, one can find that

$$c_2 = \frac{\alpha}{(0.025)^{1/\beta}}.$$

For our specific case, we have $\alpha = \max(a, x_{(n)})$ and $\beta = b + n$, so a 95% equal-tail Bayes credible interval for θ is $[c_1(\mathbf{x}), c_2(\mathbf{x})]$ where

$$\begin{aligned} c_1(\mathbf{x}) &= \frac{\max(a, x_{(n)})}{(0.975)^{\frac{1}{b+n}}}, \\ c_2(\mathbf{x}) &= \frac{\max(a, x_{(n)})}{(0.025)^{\frac{1}{b+n}}}. \end{aligned}$$

EXERCISE 12.14. For each of Example 12.6, Example 12.7, and Exercise 12.8, find a 95% equal-tail Bayesian credible interval.