# STAT 111: Mathematical Statistics II

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### Abstract

These notes arise from my studies in STAT 111: Mathematical Statistics II, taught by Professor Phil Everson, at Swarthmore College. I am responsible for all faults in this document, mathematical or otherwise. Feel free to message me with any suggestions or corrections at dyang5@swarthmore.edu.

# Contents

# 1 Discrete Probability Distributions

## 1.2 Indicator Variables

a) **Define $I(A)$ to be an indicator variable for the event $A$, meaning $I_{(A)} = 1$ if $A$ occurs and $I_{(A)} = 1$ if $A^c$ occurs. Relate this to a Bernoulli random variable. Show how an indicator variable is the _fundamental bridge_ between probability and expected value, in that $P(A) = E(I_{(A)})$. Use this to prove Boole's inequality: $P(A_1 \cup A_2 \cup \cdots \cup A_n) \leq P(A_1) + P(A_2) + \cdots + P(A_n)$. Try to think of a non-trivial example.**

We can write $I(A)$ as

$$I(A) = \begin{cases} 1 & \text{if } A \\ 0 & \text{if } A^c \end{cases}$$

where $A$ occurs with probability of $P(A)$, and $A^c$ occurs with probability $1 - P(A)$. This is equivalent to a $\text{Bern}(P(A))$ random variable.

For the fundamental bridge, note that $E[I(A)] = P(A) \cdot 1 + (1 - P(A)) \cdot 0 = P(A)$.

To prove Boole's Inequality, we will show that $P(A_1 \cup A_2 \cup \cdots \cup A_n) \leq P(A_1) + P(A_2) + \cdots + P(A_n)$. Rewriting the probability values on the left and right hand sides as expected values of indicator variables, we know that

$$P(A_1 \cup A_2 \cup \cdots \cup A_n) = E[I_{A_1 \cup A_2 \cup \cdots \cup A_n}].$$

On the other hand,

$$P(A_1) + P(A_2) + \cdots + P(A_n) = E[I_{A_1}] + E[I_{A_2}] + \cdots + E[I_{A_n}] = E[I_{A_1} + I_{A_2} + \cdots + I_{A_n}]$$

Thus, to prove Boole's inequality, it suffices to show that

$$E[I_{A_1 \cup A_2 \cup \cdots \cup A_n}] \leq E[I_{A_1} + I_{A_2} + \cdots + I_{A_n}].$$

Note that $I_{A_1 \cup A_2 \cup \cdots \cup A_n}$ can only be either 0 or 1, since it is an indicator. In the former case, none of $A_1$ to $A_n$ have occurred, so $I_{A_1} + I_{A_2} + \cdots + I_{A_n} = 0$. In the latter case, if $I_{A_1 \cup A_2 \cup \cdots \cup A_n} = 1$, then at least one of $A_1$ to $A_n$ has occurred, so $I_{A_1} + I_{A_2} + \cdots + I_{A_n} \geq 1$.

It follows that

$$I_{A_1 \cup A_2 \cup \cdots \cup A_n} \leq I_{A_1} + I_{A_2} + \cdots + I_{A_n}.$$

Taking the expected value of both sides, we arrive at Boole's Inequality.

_Example of Boole's Inequality_: Let $A$ represent the event of a fair coin flip; $A_i = 1$ if flip $i$ is heads, and $A_i = 0$ if it is tails. Boole's Inequality tells us that if we flip the coin 5 times, the probability we flip at least one heads is less than or equal to 5 times the probability we flip a heads on any single coin flip. Thus, the probability we flip at least one heads is at most $5 \cdot \frac{1}{2} = \frac{5}{2}$; this is trivial as this is greater than 1.

b) **A special case of Boole's inequality occurs when the events all have the same probability. Suppose $n$ graduates all throw their caps in the air and then retrieve a cap at random. Find an expression for the probability that none of the students retrieve their own cap (a derangement). Find the limit of this probability if the number of caps $n \to \infty$. *Hint: For $i = 1, ..., n$, let $A_i$ represent the event that person $i$ retrieves their own cap. Then $(A_1 \cup A_2 \cup ... \cup A_n)^c$ is the event that nobody ends up with their own cap.***

The probability of a derangement is

$$P(A_1 \cup A_2 \cup ... \cup A_n)^c = 1 - P(A_1 \cup A_2 \cup ... \cup A_n).$$

Taking the limit of this expression as $n \to \infty$ and using the Principle of Inclusion Exclusion, we know that this

$$\lim_{n \to \infty} 1 - P(A_1 \cup A_2 \cup ... \cup A_n) = 1 - \left[ \sum_{k=1}^{n} P(A_i) - \sum_{i<j} P(A_i \cap A_j) + \sum_{i<j<k} P(A_i \cap A_j \cap A_k) - ... \right]$$

$$= \lim_{n \to \infty} 1 - \left[ n \cdot \frac{1}{n} - \binom{n}{2}\left(\frac{1}{n} \cdot \frac{1}{n-1}\right) + \binom{n}{3}\left(\frac{1}{n} \cdot \frac{1}{n-1} \cdot \frac{1}{n-2}\right) \right]$$

Simplifying, this becomes

$$\lim_{n \to \infty} 1 - \left[ 1 - \frac{1}{2!} + \frac{1}{3!} - \frac{1}{4!} + ... \right] = \lim_{n \to \infty} \frac{1}{2!} - \frac{1}{3!} + \frac{1}{4!} - ...$$

Recall the Taylor Expansion of $e^x$: $e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$. We recognize the above expression as $e^{-1}$:

$$e^{-1} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} = \lim_{n \to \infty} \left( 1 - 1 + \frac{1}{2!} - \frac{1}{3!} + \frac{1}{4!} - ... \right)$$

$$= \lim_{n \to \infty} \frac{1}{2!} - \frac{1}{3!} + \frac{1}{4!} - ...$$

Thus,

$$\lim_{n \to \infty} P(A_1 \cup A_2 \cup ... \cup A_n)^c = \boxed{\frac{1}{e}}.$$

c) **In the caps example, let $X$ represent the number of graduates who retrieve their own cap. Explain why the distribution of $X$ is approximately Poisson(1) when $n$ is large (see 1(c)). Compare the exact probabilities of $X = 0$ and $X = 1$ to the corresponding Poisson probabilities when $n = 5$.**

Note that the probability that a given graduate receives their own cap (assuming nothing about all other graduate cap arrangements) is $p = \frac{1}{n}$. Though we are essentially sampling without replacement when throwing all the graduate caps in the air and retrieving them at random, we know from problem 1(b) that the distribution $X$ for the number of graduates who receive their own cap converges to Binom$(n, p)$ when $n$ is large.

Furthermore, note that $\lambda = np = n\frac{1}{n} = 1$ is fixed. Consequently, the limit of $P(X = x)$ as $n$ is large, by problem 1(c), is simply Poisson($\lambda$) = Poisson(1). We conclude that the distribution of $X$ is approximately Poisson(1) when $n$ is large.

Using the approximation $X \sim$ Poisson(1) for large $n$, we can approximate the probability of a derangement

$$f_x(x = 0, \lambda = 1) = \frac{1^0 e^{-1}}{0!} = \frac{1}{e}$$

and the probability that exactly one graduate gets their own cap:

$$f_x(x = 1, \lambda = 1) = \frac{1^1 e^{-1}}{1!} = \frac{1}{e}.$$

We can also compare these approximations with the exact probabilities of $X = 0$ and $X = 1$ for $n = 5$. Note that the probability of a derangement for $n = 5$ can be calculated using the formula from 2(b):

$$P(X = 0) = 1 - \left[ 5 \cdot \frac{1}{5} - \binom{5}{2}\frac{1}{5} \cdot \frac{1}{4} + \binom{5}{3}\frac{1}{5} \cdot \frac{1}{4} \cdot \frac{1}{3} - \binom{5}{4}\frac{1}{5} \cdot \frac{1}{4} \cdot \frac{1}{3} \cdot \frac{1}{2} + \binom{5}{5}\frac{1}{5} \cdot \frac{1}{4} \cdot \frac{1}{3} \cdot \frac{1}{2} \cdot \frac{1}{1} \right]$$

$$= \frac{11}{30} \approx 0.3\overline{6}$$

Note that the probability that $X = 1$ can be calculated by "picking" the graduate to get their own cap (of which there are 5 possibilites), multiplying this by the probability that the chosen graduate gets their own hat ($\frac{1}{5}$), and then multiplying this by the probability of a derangement with $n = 4$ (each of the remaining four graduates does not get their own cap):

$$P(X = 1) = 5 \cdot \frac{1}{5} \cdot P(\text{derangement for } n = 4 \text{ students})$$

$$= 1 - \left[ 4 \cdot \frac{1}{4} - \binom{4}{2}\frac{1}{4} \cdot \frac{1}{3} + \binom{4}{3}\frac{1}{4} \cdot \frac{1}{3} \cdot \frac{1}{2} - \binom{4}{4}\frac{1}{4} \cdot \frac{1}{3} \cdot \frac{1}{2}\frac{1}{1} \right]$$

$$= \frac{3}{8} = 0.375$$

We can see that even for small $n$ (in our case, $n = 5$), the expected probabilities approach $\frac{1}{e} \approx 0.36788$.

# 2 Continuous Random Variables

## 2.1 Intro to Continuous Random Variables

Assumptions for a Poisson process in time include

- Events are independent

- Rate of events through time is constant

- Events are not simultaneous

Suppose that $T_1, \ldots, T_n$ are i.i.d. Expo$(\lambda)$ random variables.

> **Definition 2.1**
>
> The **first order statistic**, defined to be the smallest of these, is $T_{(1)}$ follows the Expo$(n\lambda)$ distribution.

**Proof.** Consider the CDF of $T_{(1)}, P(T_{(1)} \leq t)$. Note that

$$P(T_{(1)} \leq t) = 1 - P(T_{(1)} > t)$$
$$= 1 - \left( e^{-\lambda t} \right)^n$$
$$= 1 - e^{-n\lambda t}$$

which is the CDF for an Expo$(n\lambda)$ distribution. $\square$

## 2.2 The Differential Argument and the Gamma Distribution

a) By definition,

$$P(X \in [x, x + dx)) = \int_x^{x+dx} f_x(y)\, dy.$$

For small deviation $dx$, we can approximate the integral as $f_x(x)\left[(x + dx) - x\right] = f_x(x)\, dx$.

Note that this expression becomes exact when $dx$ approaches 0: formally, we have

$$\lim_{dx \to 0} \frac{P(X \in [x, x + dx))}{dx} = \lim_{dx \to 0} \frac{F(x + dx) - F(x)}{dx} = f_x(x)$$

because the second expression is the limit form of the derivative of the CDF at $x$, which is precisely the value of the PDF at $x$: $f_x(x)$.

We can use the Differential argument to derive the Exponential density function. Since the CDF of an Exponential variable at time $t$ measures the probability that an event has occured

by time $t$, we can measure the probability that the first Poisson event occurs in the time interval $[t, t + dt)$ by subtracting the CDF at times $t + dt$ and time $t$:

$$P(\text{first occurence in } [t, t + dt)) = \left(1 - e^{-\lambda(t+dt)}\right) - \left(1 - e^{-\lambda t}\right)$$

$$= e^{-\lambda t} - e^{-\lambda(t+dt)}$$

Dividing this expression by $dt$ and taking the limit as $dt$ approaches 0, we derive the Exponential variable density at time $t$:

$$f_t(t) = \lim_{dt \to 0} \frac{e^{-\lambda t} - e^{-\lambda(t+dt)}}{dt}.$$

Using L'Hopital's Rule, this becomes

$$f_t(t) = \lim_{dt \to 0} \frac{e^{-\lambda t} - e^{-\lambda(t+dt)}}{dt}$$

$$= \lim_{dt \to 0} \frac{\lambda e^{-\lambda(t+dt)}}{1}$$

$$= \lambda e^{-\lambda t}.$$

b) We can similarly use the differential argument to derive the Gamma$(k, \lambda)$ density; let $X$ be the time of the $k$th event for a Poisson process with rate $\lambda$. We can model the probability of $k - 1$ events occurring before time $x$ using Pois$(\lambda x)$, where $\lambda x$ represents the expected number of events to occur in $x$ units of time. Similarly, we can model the probability of 1 event occurring in the interval $[x, x + dx)$ using Pois$(\lambda dx)$.

Thus, the probability of $k - 1$ events occurring before time $x$ and a $k$th event occurring in $[x, x + dx)$ is

$$P(k - 1 \text{ events before time } x)P(1 \text{ event before time } t)$$

$$= \frac{(\lambda x)^{k-1} e^{-\lambda x}}{(k-1)!} \frac{(\lambda dx)^1 e^{-\lambda dx}}{1!}$$

$$= \frac{\lambda^k e^{-\lambda(x+dx)} dx}{(k-1)!} x^{k-1}$$

Dividing this probability by $dx$ and taking the limit as $dx$ approaches 0, we find that

$$f_x(k, \lambda) = \lim_{dx \to 0} \frac{\left(\frac{\lambda^k e^{-\lambda(x+dx)} dx}{(k-1)!} x^{k-1}\right)}{dx}$$

$$= \lim_{dx \to 0} \frac{\lambda^k e^{-\lambda(x+dx)}}{(k-1)!} x^{k-1}$$

$$= \frac{\lambda^k e^{-\lambda x}}{(k-1)!} x^{k-1}$$

which matches the Gamma$(k, \lambda)$ density we expect.

Note that if $X_1 \sim$ Gamma$(k_1, \lambda)$ and $X_2 \sim$ Gamma$(k_2, \lambda)$ are independent, intuitively, $X_1 + X_2 \sim$ Gamma$(k_1 + k_2, \lambda)$, as we can think of $X_1$ and $X_2$ representing the sum for waiting times in two non-overlapping time intervals. We will reserve discussion for why the sum of two independent Gamma variables with different $\lambda$ values is not Gamma for part (d).

c) Recall the form of the Gamma PDF derived in part (b):

$$f_x(k, \lambda) = \frac{\lambda^k e^{-\lambda x}}{(k-1)!} x^{k-1}.$$

Note that our derivation measures the average wait time for $k$ events to occur, where $k$ is an integer. However, the Gamma Distribution also extends to values of $k$ which are not necessarily integers – all positive real $k$, in fact. To understand the extension and subsequent definition of the Gamma Distribution, we introduce the notion of a Gamma Function, an extension of the factorial function for real numbers. For integer $k$, $\Gamma(k) = (k-1)!$, which matches with the normalizing constant in our present PDF.

In general, if $\alpha$ is a positive real value replacing our $k$ parameter, we define the PDF of $X \sim$ Gamma$(\alpha, \lambda)$ to be

$$f_x(\alpha, \lambda) = \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha-1}.$$

We can derive the definition of Gamma Function by forcing this PDF to integrate to 1 as $x$ ranges from 0 to $\infty$. Note that

$$\int_0^\infty \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha-1} \, dx = \frac{\lambda^\alpha}{\Gamma(\alpha)} \int_0^\infty e^{-\lambda x} x^{\alpha-1} \, dx.$$

Apply the change of variables $y = \lambda x$. It follows that $x = \frac{y}{\lambda}$ so $dx = \frac{1}{\lambda} dy$. Our integral now becomes

$$\frac{\lambda^\alpha}{\Gamma(\alpha)} \int_0^\infty e^{-\lambda x} x^{\alpha-1} \, dx = \frac{\lambda^\alpha}{\Gamma(\alpha)} \int_0^\infty e^{-y} \left(\frac{y}{\lambda}\right)^{\alpha-1} \left(\frac{1}{\lambda} dy\right).$$

Simplifying and setting the resulting expression to 1 (since our PDF should integrate to 1), we find that

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

This inspires our definition of the **Gamma Function**:

$$\boxed{\Gamma(\alpha) = \int_0^\infty e^{-y} y^{\alpha-1} \, dy}$$

which is defined for any positive real values of the parameter $\alpha$.

With the above definition of the Gamma Function, we can derive a nice recursive definition of the Gamma Function, one which will illuminate its relationship with the factorial function.

Note that by definition, $\Gamma(\alpha + 1) = \int_0^\infty e^{-y} y^\alpha \, dy$.

Using Integration by Parts, we find that

$$\Gamma(\alpha + 1) = \left[y^\alpha(-e^{-y})\right]_0^\infty - \int_0^\infty (-e^{-y})\alpha y^\alpha \, dy$$

$$= 0 + \alpha \int_0^\infty (e^{-y}) y^\alpha \, dy$$

$$= \alpha\Gamma(\alpha).$$

Since $\Gamma(1) = \int_0^\infty e^{-y} y^{1-1} \, dy = 1$ by definition, it follows recursively that $\Gamma(\alpha) = (\alpha - 1)!$.

d) A final powerful property of the Gamma distribution is that for any constant $c > 0$, if $X \sim \text{Gamma}(\alpha, \lambda)$, then $Y = cX \sim \text{Gamma}\left(\alpha, \frac{\lambda}{c}\right)$. This property can be thought of as a changing in the units for the $\lambda$ parameter: intuitively, if $X$ measures the waiting time for $\alpha$ events to occur given a rate of $\lambda$ in some unit of time (e.g seconds), $Y = cX$ may measure the waiting time for $\alpha$ events to occur given a rate of $\lambda$ in a new unit of time (e.g. minutes, where $c = \frac{1}{60}$).

*Note: This intuition, which relates the $\lambda$ parameter to a given unit of time, also gives us an idea of why the sum of two Gamma variables with different $\lambda$ values is not itself Gamma: we cannot sum the waiting times for events of processes measured in different units of time.*

Suppose that $Y = cX$. Comparing the CDFs of $X$ and $Y$, we find that

$$F_Y(y) = P(cX < y) = P\left(X < \frac{y}{c}\right) = F_X\left(\frac{y}{c}\right).$$

Taking the derivative of both sides, we find a relationship between the PDFs. Since $y = cx$, we have

$$f_Y(y) = \frac{1}{c} f_X\left(\frac{y}{c}\right) = \frac{1}{c} f_X(x).$$

The scaling property itself can be proved by comparing the PDFs for $X$ and $Y$. Note that

$$f_x(\alpha, \lambda) = \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha - 1}.$$

Consider $\frac{1}{c} f_x(\alpha, \lambda) = \frac{1}{c} \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha-1}$. We can rewrite this expression in a few equivalent forms:

$$
\begin{aligned}
\frac{1}{c} f_x(\alpha, \lambda) &= \frac{1}{c} \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha-1} \\
&= \left(\frac{1}{c}\right)^\alpha c^{\alpha-1} \frac{\lambda^\alpha e^{-\lambda x}}{\Gamma(\alpha)} x^{\alpha-1} \\
&= \left[\left(\frac{1}{c}\right)^\alpha \lambda^\alpha\right] \left(c^{\alpha-1} x^{\alpha-1}\right) \frac{\lambda^\alpha e^{-\frac{\lambda}{x}(cx)}}{\Gamma(\alpha)} \\
&= \left(\frac{\lambda}{c}\right)^\alpha (cx)^{\alpha-1} \frac{e^{-\frac{\lambda}{c}(cx)}}{\Gamma(\alpha)}
\end{aligned}
$$

Note that the resulting expression is precisely the PDF for a Gamma $\left(\alpha, \frac{\lambda}{c}\right)$ RV, so

$$
Y = cX \sim \text{Gamma}\left(\alpha, \frac{\lambda}{c}\right)
$$

as desired.

## 2.3  The Uniform Distribution

> **Definition 2.2**
>
> Let $F$ be the CDF for a continuous random variable. The **inverse function** $G(u)$ is defined to satisfy $G(u) = x$ if $F(x) = u$.
>
> Suppose that $U \sim \text{Unif}(0,1)$. Then $X = G(U)$ has CDF $F$.

> **Remark.** Let $U \sim \text{Unif}(0,1)$. Then $X = G(U) \sim \text{Expo}(\lambda)$.

## 2.4  The Normal and Chi-Square Distributions

> **Definition 2.3** (Chi-Square)
>
> The sum of $k$ independent squared standard normal variables follows a Chi-square distribution with $k$ degrees of freedom, denoted $\chi^2_{(}k)$.

> **Remark.** $\chi^2_{(}1) \sim \text{Gamma}\left(\frac{1}{2}, \frac{1}{2}\right)$.

> In general, $\chi^2_{(}\nu) \sim \text{Gamma}\left(\frac{\nu}{2}, \frac{1}{2}\right)$ due to the properties of a sum Gamma RVs.

> Furthermore, due to the scaling property of Gamma RVs, if $X \sim \text{Gamma}(\alpha, \lambda)$, then $Y = 2\lambda X \sim \text{Gamma}\left(\alpha, \frac{1}{2}\right)$ which is equivalent to a $\chi^2_{2\alpha}$ random variable.

## 2.5   The Beta Distribution

**Definition 2.4**

The **Beta Distribution** is the conjugate prior of the binomial distribution; if we assume a coin flip has a probability of success following a Beta distribution, the posterior distribution, after accounting for new data, is also a Beta distribution.

**Remark.** Let $V_1 \sim \text{Gamma}(a, \lambda)$ and $V_2 \sim \text{Gamma}(b, \lambda)$. Then

$$X = \frac{V_1}{V_1 + V_2} \sim \text{Beta}(a, b).$$

**Remark.** Let $U_1, \ldots, U_n$ be i.i.d. $\text{Unif}(0, 1)$ random variables. Then the $k$th order statistic $U_k$ follows a $\text{Beta}(k, n - k + 1)$ distribution for $k = 1, \ldots, n$.

## 2.6   The Beta, $F$, and $t$ distributions

**Definition 2.5** (Relationships between Gamma, Beta, and $F^*$ Distributions)

Let $V_1 \sim \text{Gamma}(a, \lambda)$, $V_2 \sim \text{Gamma}(b, \lambda)$.

Then $X = \frac{V_1}{V_1 + V_2} \sim \text{Beta}(a, b)$.

Then $R = \frac{V_1}{V_2} = \frac{X}{1-X}$ has PDF

$$f_R(r) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)} r^{a-1} \left(\frac{1}{1+r}\right)^{a+b}.$$

Furthermore, $Y = c\frac{V_1}{V_2} = cR \sim F^*(a, b, c)$ has PDF

$$f_Y(y) = \frac{\Gamma(a + b)}{\Gamma(a)\Gamma(b)} \frac{y^{a-1}c^b}{(c + y)^{a+b}} I(y > 0)$$

$$\propto \frac{y^{a-1}c^b}{(c + y)^{a+b}} I(y > 0)$$

for $a > 0$, $b > 0$, $c > 0$. This is known as the $F^*(a, b, c)$ **density.**

**Definition 2.6** (F-distribution)

The $F$**-distribution** is defined in terms of Chi-Square random variables: if $V_1 \sim \chi_{(m_1)}^2$ is independent of $V_2 \sim \chi_{(m_2)}^2$, then

$$F_{(m_1, m_2)} \sim \frac{\left(\frac{V_1}{m_1}\right)}{\left(\frac{V_2}{m_2}\right)}.$$

**Remark.** $F_{(n,m)} = F^* \left( \frac{n}{2}, \frac{m}{2}, \frac{m}{n} \right).$

**Definition 2.7**

If $Z \sim N(0,1)$ is independent of $V \sim \chi^2_{(m)}$, then

$$T = \frac{Z}{\sqrt{\frac{V}{m}}} \sim t_{(m)},$$

the **t-distribution** with $m$ degrees of freedom. Furthermore, $T^2 \sim F_{(1,m)}$.

# 3 Expected Value

## 3.1 Definition of Expected Value

**Definition 3.1**

For a discrete RV $X$, the **expected value of** $X$ is $\mathbb{E}[X] = \sum_i x_i P(x_i)$.

For a continuous RV $X$, $\mathbb{E}[X] = \int_{-\infty}^{\infty} x f(x) \, dx$.

**Remark.** The expected value of a random variable may not always be defined – the integral may be unbounded, the integrand may be nonintegrable, or the random variable could be both discrete and continuous.

**Example.** $X \sim \text{Cauchy}(1)$ has pdf $f_X(x) = \frac{1}{\pi} \frac{1}{1+x^2}$ has undefined expected value, as the absolute integral diverges.

## 3.2 Linearity of Expectation

**Definition 3.2** (Linearity of Expectation)

If $X_1, X_2, \ldots, X_n$ are random variables, then

$$\mathbb{E}[X_1 + X_2 + \cdots + X_n] = \mathbb{E}[X_1] + \mathbb{E}[X_2] + \cdots + \mathbb{E}[X_n]$$

*regardless of whether* $X_1, X_2, \ldots, X_n$ *are independent or not.*

**Example.** Suppose that $n$ missiles are targeted independent by $n$ intercepts, each choosing a target at random. Find the expected number of missiles targets.

**Answer.** Define an indicator variable $I_k$ for each $k \in \{1, \ldots, n\}$ such that

$$I_k = \begin{cases} 1 & \text{if missile } k \text{ is targeted} \\ 0 & \text{otherwise} \end{cases}$$

Define $X$ to be the number of missiles targeted. Note that

$$\mathbb{E}[X] = \mathbb{E}[I_1] + \cdots + \mathbb{E}[I_n].$$

Note that $\mathbb{E}[I_k]$ for any $k$ is $1 - \left(\frac{n-1}{n}\right)^n$, so $\mathbb{E}[X] = n(1 - \left(\frac{n-1}{n}\right)^n)$.
As $n \to \infty$, it follows that

$$\mathbb{E}[X] = \lim_{n \to \infty} n \left[ 1 - \left( \frac{n-1}{n} \right)^n \right] = n \left( \frac{e-1}{e} \right).$$

⊛

## 3.3 LOTUS and Variance

**Theorem 3.1** (LOTUS (Law of the Unconscious Statistician)). For a random variable $X$, and a fixed function $g$ then $Y = g(x)$ has

$$\mathbb{E}[Y] = \begin{cases} \sum_x g(x)p(x) & \text{if X is discrete} \\ \int_{-\infty}^{\infty} g(x)f(x)\,dx & \text{if X is continuous} \end{cases}$$

where $p(x)$ and $f(x)$ are the pmf and pdf of $X$, respectively.

This holds only if $\sum_x |g(x)|p(x)$ or $\int_{-\infty}^{\infty} |g(x)|f(x)\,dx$ converge.

**Theorem 3.2** (Markov's Inequality). For a random variable $X$,

$$P(X \geq t) \leq \frac{\mathbb{E}[X]}{t}.$$

**Theorem 3.3** (Chebyshev's Inequality). For a random variable $X$ with mean $\mu$ and variance $\sigma^2$ and for $t > 0$,

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

## 3.4 Moment Generating Functions

**Definition 3.3** (Moment Generating Function)

The **Moment Generating Function** of a random variable $X$ is

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

The $k$th derivative of $M_x(t)$ at $t = 0$ is $\mathbb{E}\left[X^k\right]$, the $k$th moment of the distribution of $X$.

**Theorem 3.4** (Uniqueness Property of MGFs). If two random variables $X$ and $Y$ have the same MGFs for all $t$ in an interval containing 0, then $F_X(x) = F_Y(x)$ i.e. they must have the same distribution for all $x$.

**Remark.** $M_{a+bX}(t) = e^{at}M_X(bt)$.

Furthermore, for independent random variables $X_1, \ldots, X_n$, each with MGF $M_{X_i}$, the MGF for $Y = \sum X_i$ is

$$M_Y(t) = \prod M_{X_i}(t).$$

## 3.5 Inequalities and Approximate Methods

**Theorem 3.5** (Jensen's Inequality). If $g$ is a convex function, then

$$\mathbb{E}\left[g(X)\right] \geq g(\mathbb{E}\left[X\right]).$$

If $g$ is concave, then

$$\mathbb{E}\left[g(X)\right] \leq g(\mathbb{E}\left[X\right]).$$

Using Taylor approximations, we can derive approximations for the mean and variance of a random variable under a transformation $g$.

**Lemma 3.1.** If $X$ is a random variable with mean $\mu_X$ and variance $\sigma_X^2$ and the transformed variable $Y = g(X)$,

$$\mathbb{E}\left[y\right] \approx g(\mu_x) + \frac{1}{2}\sigma_X^2 g''(\mu_X)$$

and

$$\text{Var}\left[Y\right] \approx g'(\mu_X)^2 \text{Var}\left[X\right].$$

## 3.6 Conditional Expectation

**Remark.** Intuitively (without working with the definitions), conditional expectations given events and random variables are different: conditional expectation given an event is a value whereas conditional expectation given a random variable yields a random variable.

**Theorem 3.6** (Law of Total Expectation: Adam's Law). $\mathbb{E}\left[Y\right] = \mathbb{E}\left[\mathbb{E}\left[Y \mid X\right]\right]$

**Theorem 3.7** (Law of Total Variance: Eve's Law).

$$\text{Var}\left[Y\right] = \mathbb{E}\left[\text{Var}\left[Y \mid X\right]\right] + \text{Var}\left[\mathbb{E}\left[Y \mid X\right]\right]$$

# 4 Joint and Conditional Distributions

## 4.1 Joint, Marginal, and Conditional Distributions

> **Definition 4.1** (Joint, Marginal, and Conditional)
>
> The **joint pdf** describes the probability density of observing both $X = x$ and $Y = y$ simultaneously.
>
> The **marginal pdf of** $Y$ represents the probability density of observing $Y = y$, irrespective of the value of $X$.
>
> The **conditional pdf of** $Y$ given $X = x$ represents the probability density of observing $X = x$, given that $Y = y$.

## 4.2 Covariance

> **Definition 4.2** (Covariance and Correlation)
>
> The **covariance of** $X$ **and** $Y$ is defined as
>
> $$\text{Cov}\left[X, Y\right] = \mathbb{E}\left[(X - \mathbb{E}\left[X\right])\left(Y - \mathbb{E}\left[Y\right]\right)\right]$$
> $$= \mathbb{E}\left[XY\right] - \mathbb{E}\left[X\right]\mathbb{E}\left[Y\right]$$
>
> The **correlation of** $X$ **and** $Y$ is
>
> $$\rho = \frac{\text{Cov}\left[X, Y\right]}{\sigma_X \sigma_Y}.$$
>
> where $-1 \leq \rho \leq 1$.

## 4.3 Multivariate Normal

a) A random vector $\mathbf{X} = (X_1, \ldots, X_k)$ is said to have a Multivariate Normal (MVN) distribution if every linear combination of the $X_j$ follows a Normal distribution. That is,

$$t_1 X_1 + \cdots + t_k X_k$$

follows a Normal distribution for any choice of constants $t_1, \ldots, t_k$.

This definition may allow for vectors that do not have a proper joint density function: this is more clear with the definition of the joint density function below (the covariance matrix for a vector with correlated entries will not be invertible).

b) If $\mathbf{Y} \sim N_n(\mu, \mathbf{V})$, then the joint PDF for $\mathbf{y} = (y_1, \ldots, y_n)$ is

$$f_{\mathbf{Y}}(\mathbf{y}) = \frac{\exp\left[-\frac{1}{2}(\mathbf{y} - \mu)^T \mathbf{V}^{-1}(\mathbf{y} - \mu)\right]}{\sqrt{(2\pi)^n |\det \mathbf{V}|}}$$

It follows that this is an extension of the bivariate Normal density to larger dimensions. Note that the bivariate case is a specific case of the Multivariate Normal where $n = 2$. If $\mathbf{Y} \sim N_2(\mu, \mathbf{V})$, then $\mu = \begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}$ and $\mathbf{V} = \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}$.

One can check that indeed, the expression

$$
\begin{aligned}
f_{\mathbf{Y}}(\mathbf{y}) &= \frac{\exp\left[-\frac{1}{2}(\mathbf{y} - \mu)^T \mathbf{V}^{-1}(\mathbf{y} - \mu)\right]}{\sqrt{(2\pi)^n |\det \mathbf{V}|}} \\
&= \frac{\exp\left[-\frac{1}{2}\begin{pmatrix} y_1 - \mu_1 \\ y_2 - \mu_2 \end{pmatrix}^T \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix}^{-1} \begin{pmatrix} y_1 - \mu_1 \\ y_2 - \mu_2 \end{pmatrix}\right]}{\sqrt{(2\pi)^n |\sigma_1^2\sigma_2^2(1 - p^2)|}},
\end{aligned}
$$

obtained by plugging in the respective expressions for the bivariate case, matches the bivariate Normal density. The calculation/algebra is left as an exercise to the reader.

c) Suppose that $V$ is block diagonal; without loss of generality, we can assume that

$$
\mathbf{V} = \begin{bmatrix} \mathbf{V}_1 & 0 \\ 0 & \mathbf{V}_2 \end{bmatrix}.
$$

By properties of block matrices, we know that $\det \mathbf{V} = (\det \mathbf{V}_1)(\det \mathbf{V}_2)$. Furthermore,

$$
\mathbf{V}^{-1} = \begin{bmatrix} \mathbf{V}_1 & 0 \\ 0 & \mathbf{V}_2 \end{bmatrix}^{-1} = \begin{bmatrix} \mathbf{V}_1^{-1} & 0 \\ 0 & \mathbf{V}_2^{-1} \end{bmatrix}
$$

Suppose that $Y_1 \sim N_{n_1}(\mu_1, \mathbf{V}_1)$ and $Y_2 \sim N_{n_2}(\mu_2, \mathbf{V}_2)$, where $n_1 + n_2 = n$, $\mu_1$ and $\mu_2$ form $\mu$ of $Y$, and similarly, $\mathbf{V}_1$ and $\mathbf{V}_2$ form $\mathbf{V}$. Note that

$$
\exp\left[-\frac{1}{2}(\mathbf{y} - \mu)^T \mathbf{V}^{-1}(\mathbf{y} - \mu)\right] = \exp\left[-\frac{1}{2}(\mathbf{y}_1 - \mu_1)^T \mathbf{V_1}^{-1}(\mathbf{y}_1 - \mu_1)\right] \exp\left[-\frac{1}{2}(\mathbf{y}_2 - \mu_2)^T \mathbf{V_2}^{-1}(\mathbf{y}_2 - \mu_2)\right].
$$

Furthermore,

$$
\sqrt{(2\pi)^n |\det \mathbf{V}|} = \sqrt{(2\pi)^{n_1 + n_2} |\det \mathbf{V_1} \det \mathbf{V_2}|}.
$$

It follows that

$$
\begin{aligned}
f_{\mathbf{Y}}(\mathbf{y}) &= \frac{\exp\left[-\frac{1}{2}(\mathbf{y} - \mu)^T \mathbf{V}^{-1}(\mathbf{y} - \mu)\right]}{\sqrt{(2\pi)^n |\det \mathbf{V}|}} \\
&= \frac{\exp\left[-\frac{1}{2}(\mathbf{y}_1 - \mu_1)^T \mathbf{V_1}^{-1}(\mathbf{y}_1 - \mu_1)\right]}{\sqrt{(2\pi)^{n_1} |\det \mathbf{V_1}|}} \frac{\exp\left[-\frac{1}{2}(\mathbf{y}_2 - \mu_2)^T \mathbf{V_2}^{-1}(\mathbf{y}_2 - \mu_2)\right]}{\sqrt{(2\pi)^{n_2} |\det \mathbf{V_2}|}} \\
&= f_{\mathbf{Y}_1}(\mathbf{y}_1) f_{\mathbf{Y}_2}(\mathbf{y}_2)
\end{aligned}
$$

where $\mathbf{Y}_1$ and $\mathbf{Y}_2$ are two independent sub-vectors of $\mathbf{Y}$.

d) Consider the covariance between $\overline{Y}$ and $Y_i - \overline{Y}$ for any $i$ from 1 to $n$. Note that

$$
\text{Cov}\left[\overline{Y}, Y_i - \overline{Y}\right] = \text{Cov}\left[\overline{Y}, Y_i\right] - \text{Cov}\left[\overline{Y}, \overline{Y}\right]
$$

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by the linearity property of covariance. Since $\overline{Y} = \sum_{i=1}^{n} Y_i$, it follows that

$$
\begin{aligned}
\mathrm{Cov}\left[\overline{Y}, Y_i - \overline{Y}\right] &= \mathrm{Cov}\left[\overline{Y}, Y_i\right] - \mathrm{Cov}\left[\overline{Y}, \overline{Y}\right] \\
&= \mathrm{Cov}\left[\frac{1}{n}Y_i + \frac{1}{n}\sum_{j|i\neq j\,\&\,j\geq 1}^{n} Y_j, Y_i\right] - \frac{\sigma^2}{n} \\
&= \frac{1}{n}\mathrm{Cov}\left[Y_i, Y_i\right] - \frac{\sigma^2}{n} \\
&= \frac{\sigma^2}{n} - \frac{\sigma^2}{n} = 0.
\end{aligned}
$$

Thus, we find that $\mathrm{Cov}\left[\overline{Y}, Y_i - \overline{Y}\right] = 0$ for $i = 1, \ldots, n$, so $\overline{Y}$ is uncorrelated with each $Y_i - \overline{Y}$.

Since

$$
s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2
$$

by definition, and $\overline{Y}$ is independent from each $Y_i - \overline{Y}$, it follows that $\overline{Y}$ is independent of $s^2$.

# 6 Tests of Hypotheses

You can generalize Neyman-Pearson Lemma to one-sided hypotheses tests, which will give a UMP (Uniformly Most Powerful) Test.

## 6.6 GLR Test for Multinomial Distribution

a) **Let $X_j$ be the count of dice rolls equal to $j$ (for $j \in \{1,\ldots,6\}$) for $n$ iid rolls of a six-sided die. Use these to define the joint likelihood function $L(\theta_1,\ldots,\theta_6)$ for the probabilities of the six faces ($\sum \theta_j = 1$). Use Lagrange multipliers to show the MLE's are $\hat{\theta}_j = X_j/n$, for $j \in \{1,\ldots 6\}$.**

For $X_j$ the count of dice rolls equal to $j$ (for $j \in \{1,\ldots,6\}$), the joint likelihood function for the $L(\theta_1,\ldots,\theta_6)$ is

$$L(\theta_1,\ldots,\theta_6) = \frac{n!}{x_1!\ldots x_6!}\theta_1^{x_1}\ldots\theta_6^{x_6}.$$

Equivalently, the log-likelihood is

$$l(\theta_1,\ldots,\theta_6) = \log\left(\frac{n!}{x_1!\ldots x_6!}\right) + \sum_{i=1}^{6} x_i \log(\theta_i)$$

where $\sum \theta_i = 1$.

To determine the MLE's $\hat{\theta}_i$, we use Lagrange Multipliers and work to maximize

$$l(\theta_1,\ldots,\theta_6,\lambda) = \log\left(\frac{n!}{x_1!\ldots x_6!}\right) + \sum_{i=1}^{6} x_i \log(\theta_i) + \lambda\left(\sum_{i=1}^{6} \theta_i - 1\right)$$

where the extra $\lambda(\sum_{i=1}^{6} \theta_i - 1)$ term comes from the Lagrange multiplier $\lambda$ and the constraint $\sum \theta_i = 1$.

To maximize $l(\theta_1,\ldots,\theta_6,\lambda)$, we need the partials with respect to each $\theta_i$ and $\lambda$ to be equal to 0:

$$\frac{\partial l}{\partial \theta_i} = \frac{x_i}{\theta_i} + \lambda = 0 \text{ and } \frac{\partial l}{\partial \lambda} = \left(\sum \theta_i\right) - 1 = 0.$$

The former condition $\frac{x_i}{\theta_i} + \lambda = 0$ tells us that $\hat{\theta}_i = -\frac{x_i}{\lambda}$.

Now, the latter condition $(\sum \theta_i) - 1 = 0$ tells us that

$$\sum \hat{\theta}_i = -\frac{\sum x_i}{\lambda} = 1,$$

and solving for $\lambda$ gives us $\hat{\lambda} = -\sum x_i$. Thus, for each $\hat{\theta}_i$, we know that

$$\hat{\theta}_i = -\frac{x_i}{\lambda} = \frac{-x_i}{-\sum x_i} = \frac{x_i}{n}$$

as desired.

b) **Derive the GLR test of $H_0: \theta_1 = \cdots = \theta_6$ vs $H_1$: not $H_0$. Suppose $n = 24$ rolls gave counts of $X_1 = 8$, $X_2 = X_3 = X_4 = X_5 = 4$, and $X_6 = 0$. Show how simulation may be used to compute an exact $p$-value. Compare to using the Chi-square approximation for $-2 \log \Lambda$.**

As we saw previously,

$$L(\theta_1, \ldots, \theta_6) = \frac{n!}{x_1! \ldots x_6!} \theta_1^{x_1} \ldots \theta_6^{x_6}$$

Our null hypothesis is $H_0: \theta_1 = \cdots = \theta_6 = \frac{1}{6}$ and alternative hypothesis is $H_1$: not $H_0$, so

$$
\begin{aligned}
\Lambda &= \frac{\max\limits_{H_0} \frac{n!}{x_1! \ldots x_6!} \theta_1^{x_1} \ldots \theta_6^{x_6}}{\max\limits_{H_0 \cup H_1} \frac{n!}{x_1! \ldots x_6!} \theta_1^{x_1} \ldots \theta_6^{x_6}} \\
&= \frac{\left(\frac{1}{6}\right)^{x_1 + \cdots + x_6}}{\left(\frac{x_1}{n}\right)^{x_1} \ldots \left(\frac{x_6}{n}\right)^{x_6}}
\end{aligned}
$$

where the denominator is from the fact that $\hat{\theta}_i = \frac{x_i}{n}$, which we derived in part (a). Note that

$$
\begin{aligned}
-2\log(\Lambda) &= -2 \sum_{i=1}^{6} x_i \log \left( \frac{\frac{1}{6}}{\frac{x_i}{n}} \right) \\
&= -2 \left( \sum x_i \log \frac{1}{6} - \sum x_i \log \left( \frac{x_i}{n} \right) \right) \\
&= -2 \left( n \log \left( \frac{1}{6} \right) - \sum \log \left( \left( \frac{x_i}{n} \right)^{x_i} \right) \right)
\end{aligned}
$$

The Chi-square approximation for $-2 \log \Lambda \overset{\cdot}{\sim} \chi_\nu^2$ where $\nu$ is the difference in the dimensions of the null and alternative parameter spaces; in this case, $\nu = 6 - 1 = 5$.

For the given data, we find that

$$\Lambda = \frac{\left(\frac{1}{6}\right)^{24}}{\left(\frac{8}{24}\right)^8 \left(\frac{4}{24}\right)^{16}} = \frac{1}{256}$$

so $-2 \log \Lambda \approx 11.1$. Using the Chi-Square approximation $\chi_5^2$, we find the associated p-value using the R command $1 - pchisq(11.1, 5) = 0.049$. We can compare this approximation to the exact p-value which we can acquire through simulation (see attached R Code).

Note that the interpretation of the p-value is the probability of achieving such an extreme value of $-2 \log \Lambda$ in $n$ rolls, assuming $H_0$ is true.

c) **For a 2-way table of counts, derive the GLR test for independence of the row and column variables. Show that the Chi-square approximation for $-2\log\Lambda$ is asymptotically equivalent to the Pearson Chi-square test of independence (See Rice 9.5, 13.4).**

See the image below for the GLR test for independence of the row and column variables in a two-way table of counts.



To show the asymptotic equivalence of the Chi-square approximation for $-2\log\Lambda$ with the Pearson Chi-square test of independence, we will manipulate the expression for $-2\log\Lambda$.

Note that

$$\Lambda = \prod_{i=1}^{2}\prod_{j=1}^{2}\frac{\theta_{ij}^{x_{ij}}}{\hat{\theta}_{ij}^{x_{ij}}} = \prod_{i=1}^{2}\prod_{j=1}^{2}\left(\frac{\theta_{ij}}{\hat{\theta}_{ij}}\right)^{x_{ij}}.$$

It follows that

$$-2\log\Lambda = 2\sum_{i=1}^{2}\sum_{j=1}^{2}x_{ij}\log\left(\frac{\hat{\theta}_{ij}}{\theta_{ij}}\right)$$

$$= 2n\sum_{i=1}^{2}\sum_{j=1}^{2}\hat{\theta}_{ij}\log\left(\frac{\hat{\theta}_{ij}}{\theta_{ij}}\right)$$

where the second step follows from the fact that $x_i = n\hat{\theta}_{ij}$.

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Note furthermore that for large $n$, we should expect $\hat{\theta}_{ij} \approx \theta_{ij}$. Since the Taylor Series expansion of the function

$$f(x) = x \log\left(\frac{x}{x_0}\right)$$

about $x_0$ is $f(x) = (x - x_0) + \frac{1}{2}(x - x_0)^2 \frac{1}{x_0} + \ldots$, we find that

$$-2 \log \Lambda = 2n \sum_{i=1}^{2} \sum_{j=1}^{2} \hat{\theta}_{ij} \log\left(\frac{\hat{\theta}_{ij}}{\theta_{ij}}\right)$$

$$\approx 2n \left[ \sum_{i=1}^{2} \sum_{j=1}^{2} \left(\hat{\theta}_{ij} - \theta_{ij}\right) + \frac{1}{2} \frac{(\hat{\theta}_{ij} - \theta_{ij})^2}{\hat{\theta}_{ij}} \right]$$

$$\approx 2n \sum_{i=1}^{2} \sum_{j=1}^{2} \left(\hat{\theta}_{ij} - \theta_{ij}\right) + n \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{(\hat{\theta}_{ij} - \theta_{ij})^2}{\hat{\theta}_{ij}}$$

Note that by definition,

$$\sum_{i=1}^{2} \sum_{j=1}^{2} \hat{\theta}_{ij} = \sum_{i=1}^{2} \sum_{j=1}^{2} \theta_{ij} = 1$$

so the first term in the approximation is 0. Thus, we find that

$$-2 \log \Lambda \approx n \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{(\hat{\theta}_{ij} - \theta_{ij})^2}{\hat{\theta}_{ij}}$$

$$\approx \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{(n\hat{\theta}_{ij} - n\theta_{ij})^2}{n\hat{\theta}_{ij}}$$

$$\approx \sum_{i=1}^{2} \sum_{j=1}^{2} \frac{(x_{ij} - n\theta_{ij})^2}{n\hat{\theta}_{ij}}$$

where once again the final step follows from the fact that $x_{ij} = n\hat{\theta}_{ij}$.

This is simply the test statistic for the Pearson Chi-Square test for independence, so we conclude that the Chi-square approximation for $-2 \log \Lambda$ is asymptotically equivalent to the Pearson Chi-square test of independence, as desired.

# 8 Multiple Comparisons

## 8.3 Stein's Paradox

a) **Describe the conclusions you might make after carrying out a one-way ANOVA F test, and how you would estimate the $\theta_i$'s when the null hypothesis is rejected or not rejected.**

A one-way ANOVA F Test works to check whether there are statistically significant differences in the means of 3 or more groups of data. The null hypothesis is of the form

$$H_0 : \theta_1 = \cdots = \theta_k$$

and the alternative hypothesis is that are at least two group means that are significantly different from each other.

When the null hypothesis is not rejected, we conclude that there is no statistically significant between the group means; consequently, a good estimate for each $\theta_i$ is the overall group mean for the observed data. On the other hand, when the null hypothesis is rejected, we know that the group means are not all equal. The MLE's for each group are individually the group averages, so we can use those as estimates for each $\theta_i$.

b) **Charles Stein proved in 1962 that, for any values $\theta_1, \ldots, \theta_k$, with $k \geq 3$, if $Y_i \sim N(\theta_i, V)$ are independent for $i = 1, \ldots, k$, the vector $\{Y_1, \ldots, Y_k\}$ is *inadmissible* as a joint estimate of $\{\theta_1, \ldots, \theta_k\}$ with respect to squared error loss. That is, there is another estimate $\{\hat{\theta}_1, \ldots, \hat{\theta}_k\}$ such that**

$$\mathbb{E}\left[\sum (\hat{\theta}_i - \theta_i)^2\right] \leq \mathbb{E}\left[\sum (Y_i - \theta_i)^2\right] = nV$$

**and the inequality is strict for some $\{\theta_1, \ldots, \theta_k\}$. Explain why this theorem may be in conflict with part of your answer to (a).**

Stein's Theorem tells us that our above estimate for the $\theta_i$'s (taking the averages of each of the groups) is *inadmissible*, in the sense that there is another estimate that has smaller mean square error. But we anticipated from part (a) that the observed $Y_i$ is the MLE for each group – these seem to be in conflict with each other.

The subtlety relies in the fact that we are no longer estimating each group mean individually (in which case the MLE is simply the observed averages). Rather, when we are dealing with a group of different means, Stein's estimate says that there are estimation rules with smaller total squared error (summing across all groups) than simply estimating the averages for each individual group. Equivalently, "no matter what the values of the true means, there are estimation rules with smaller total risk."

c) **Stein, along with Willard James, provide an alternative joint estimator (the James-Stein estimate) that has a smaller expected sum of squares error:**

$$k = 3: \quad \hat{\theta}_i = \hat{B}\mu + (1 - \hat{B})Y_i, \quad \hat{B} = \frac{V}{\sum (Y_i - \mu)^2}, \quad \mu = \text{any fixed constant (e.g. 0)}$$

$$k > 3: \quad \hat{\theta}_i = \hat{B}\overline{Y} + (1 - \hat{B})Y_i, \quad \hat{B} = \frac{(k - 3)V}{\sum (Y_i - \mu)^2}.$$

For $k > 3$, shrinkage is done towards the average value, and for $k = 3$, shrinkage is done towards an arbitrary constant that does not depend on the data. The common variance is known. Describe how the Stein estimate "shrinks" the $Y_i$'s together, and how this can reduce the mean square error by introducing directional bias that anticipates regression towards the mean (an improved version requires $\hat{B} \leq 1$.) Note that the $Y_i$'s are typically more variable than the $\theta_i$'s. Use simulation to test a $k = 3$ case based on the Wordle example. Use $\mu = 3.5$ and $V = 1$ and try various values of $\theta_1$, $\theta_2$, and $\theta_3$.

As per the formulas, we can think of the Stein estimate as a weighted average between $\mu$ or $\overline{Y}$ and the $Y_i$'s. This introduces what can be understood as a "shrinkage to the grand average", i.e. shrinking the $Y_i$'s to be closer together.

Since the MSE is the sum of the bias squared and the variance, by shrinking the $Y_i$'s together, even if we are introducing some directional bias, we are also working to regress towards the mean, so the decrease in the variance will outweigh the effect of the increase in bias. By this logic, Stein's estimate actually decreases the MSE.

The Stein estimate makes sense because the $Y_i$'s vary about their underlying $\theta_i$'s, so the overall variability in the $Y_i$'s will typically be larger than the variability in the $\theta_i$'s. To anticipate this, each $Y_i$ is shrunk toward some common value, and the most obvious value to shrink toward is $\overline{Y}$, the average of the $Y_i$'s. The following example illustrates this well:
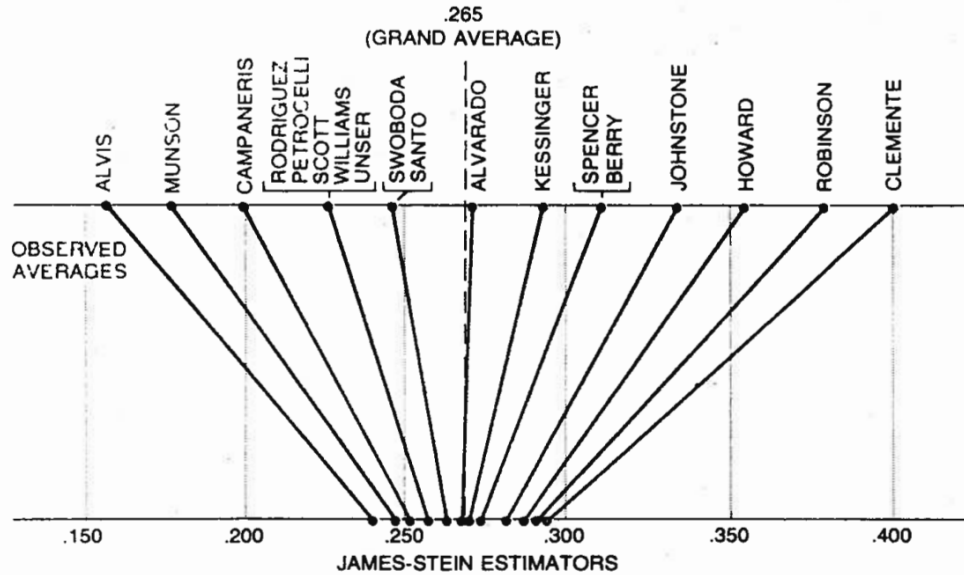


JAMES-STEIN ESTIMATORS for the 18 baseball players were calculated by "shrinking" the individual batting averages toward the overall "average of the averages." In this case the grand average is .265 and each of the averages is shrunk about 80 percent of the distance to this value. Thus the theorem on which Stein's method is based asserts that the true batting abilities are more tightly clustered than the preliminary batting averages would seem to suggest they are.

Mathematically, note that since $Y_i \sim N(\theta_i, V)$ by assumption, it follows that

$$Y_i = \theta_i + \sqrt{V} Z_i.$$

It makes sense, then, that $\text{Var}[Y_i] > \text{Var}[\theta_i]$.

Finally, see the R Code for simulations to test a $k = 3$ case based on the Wordle example in previous problems. The code uses $\mu = 3.5$ and $V = 1$, along with various values of $\theta_1$, $\theta_2$, and $\theta_3$.

d) **Use data from the 2004 WNBA season to demonstrate the Stein estimate for $k = 13$. Let $y$ represent the average points scored for each team in their first $n = 5$ games, and $\theta$ represent the average for the remaining games in that season (a less noisy estimate of the underlying mean value). Imagine trying to predict the $\theta_i$'s based on the $Y_i$'s. Estimate a common variance $V$ based on the team sample standard deviations and treat this as known for constructing the James-Stein estimates. Make a graph of $\theta$ vs $Y$, and draw in lines corresponding to using the $Y$ and $\hat{\theta}_i$'s. Add in the least squares line for fitting a straight line to estimate the $\theta_i$'s from the $Y_i$'s. Compare to the slope and intercept for the Stein estimate, along with the sums of squares about the $Y_i$'s, the $\hat{\theta}_i$'s, and about $\bar{Y}$.**

See R Code.

e) **Explain why shrinking the $Y_i$'s together seems like a sensible thing to do for the WNBA example, but may seem paradoxical in other situations. Use the Efron and Morris example of predicting batting averages, along with a proportion of foreign made cars. Argue that using total squared error as a loss function means you are acting as if you have $k$ related problems, and that this helps explain the apparent paradox.[1]**

Efron and Morris often say the Stein estimate "anticipates regression to the mean" and improves the estimates by "borrowing strength from the ensemble." In the context of the baseball players, the ensemble (the collection of 18 players with 45 at-bats on a specific date in 1970) provides information about the distribution of batting averages in Major League Baseball that year. If we observed only one player's average, it would be equally likely to be an overestimate or an under-estimate of the player's true probability of getting a hit. But in the context of other similar players, we might reasonably judge a particular batting average is more likely to be an over-estimate or under-estimate. For example, Clemente's .400 was the largest of a sample of 18 batting averages. Without any outside knowledge that .400 is an unusually high average for a professional player, one could still judge that this was likely to be an over-estimate of Clemente's true probability. A classical confidence interval for Clemente's mean would be symmetric about .400, allowing for the possibility that he had

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[1]Details/wording taken from Phil's article on Stein's Paradox. Examples from Efron and Morris's Stein's Paradox article.

a true probability larger than .400 and was in a batting slump for those first 45 at-bats. The Stein estimate predicts Clemente to bat closer to the overall average $y = .265$, but still to be above average. Similarly, the Stein estimate predicts Max Alvis' final average to be higher than .156, but still below average.

Similarly, shrinking the $Y_i$'s together in the WNBA example is essentially the idea of "regressing to the mean" and/or "borrowing strength from the ensemble."

What makes Stein's result more paradoxical is his general statement that when estimating a collection of $k$ (possibly unrelated) means using a set of independent sample averages, the averages are inadmissible. That is, there is another estimate that does better (in terms of minimizing the sum of squares) for every possible set of means. The Stein estimate was shown to be such an estimate. Efron and Morris illustrate the paradoxical nature of this fact by including a nineteenth average in their collection: the percentage of a random sample of 45 foreign-made automobiles. Now, they consider estimating the 18 player means and the overall percent of foreign-made cars. Applying Stein's estimate seems to imply that the percentage of foreign-made cars is influenced by the batting performances of Clemente and the others.

*But this is in fact not as paradoxical as one may think. With a simple regression model (to minimize the sum of squares), the fitted value for the percent of foreign cars would be influenced by the batting averages. The Stein estimate essentially attempts to fit this regression model without having observed the responses, but assuming that they will be centered about the same mean as the predictors. Consequently, the loss function (total squared error) supposes that the problems are related, in which case Stein's estimate is not paradoxical.*

# 11  Simple Linear Regression

## 11.5  Matrix Representation

The linear model becomes much easier to manage when represented in matrix and vector form. Let $Y$ be the $n \times 1$ vector of $Y_1, \dots, Y_n$, and let $X$ be an $n \times 2$ matrix with a column of 1's and a column with the values $x_1, \dots, x_n$. Define $\boldsymbol{\beta}$ to be the $2 \times 1$ vector of $\beta_0$ and $\beta_1$.

a) **Show that the simple regression model can be written as $Y = X\boldsymbol{\beta} + \varepsilon$, for $\varepsilon \sim N_n(\mathbf{0}, \sigma^2 I)$.**

   Note that the typical simple linear regression model assumes $Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$. Extending this to the matrix representation is simple, and works as expected: we get that

   $$Y = X\boldsymbol{\beta} + \varepsilon.$$

   Indeed, we see that

   $$\begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{bmatrix}$$

   is precisely the matrix representation of SLR.

b) **Explain why we can't solve $Y = X\boldsymbol{\beta}$ to get $\boldsymbol{\beta} = X^{-1}Y$, but we can solve $X^T Y = X^T X \boldsymbol{\beta}$ to get $\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T Y$.**

   Note that $X$ is a $n \times 2$ matrix, so its inverse does not exist. Consequently, instead of solving $Y = X\boldsymbol{\beta}$ to get $\boldsymbol{\beta} = X^{-1}Y$, we can solve

   $$X^T Y = X^T X \boldsymbol{\beta}$$

   Note now that $X^T X$ is a $2 \times 2$ matrix, so we can solve by multiplying by $(X^T X)^{-1}$ to get

   $$\boxed{\hat{\boldsymbol{\beta}} = (X^T X)^{-1} X^T Y}.$$

c) **Show the generalization of the expansion in 4b, and explain how it shows that $\hat{\boldsymbol{\beta}}$ is the MLE.**

   $$(Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta}) = (Y - X\hat{\boldsymbol{\beta}})^T (Y - X\hat{\boldsymbol{\beta}}) + (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}) X^T X (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}).$$

   We use our trick of adding and subtracting by the same constant in our left hand side expression, and then expanding. Note that

   $$(Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta}) = ((Y - X\hat{\boldsymbol{\beta}}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta}))^T ((Y - X\hat{\boldsymbol{\beta}}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta}))$$

   Expanding, we find that

   $$\begin{aligned} (Y - X\boldsymbol{\beta})^T (Y - X\boldsymbol{\beta}) &= ((Y - X\hat{\boldsymbol{\beta}}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta}))^T ((Y - X\hat{\boldsymbol{\beta}}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta})) \\ &= (Y - X\hat{\boldsymbol{\beta}})^T (Y - X\hat{\boldsymbol{\beta}}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta})^T (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta}) \\ &\quad + (Y - X\hat{\boldsymbol{\beta}})^T (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta}) + (X\hat{\boldsymbol{\beta}} - X\boldsymbol{\beta})^T (Y - X\hat{\boldsymbol{\beta}}) \end{aligned}$$

Note that the latter two terms are both $1 \times 1$, so $(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{X}\hat{\boldsymbol{\beta}} - \boldsymbol{X}\boldsymbol{\beta}) = (\boldsymbol{X}\hat{\boldsymbol{\beta}} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})$. To simplify the above expression, we work with the term

$$
\begin{aligned}
(\boldsymbol{X}\hat{\boldsymbol{\beta}} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) &= (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \boldsymbol{X}^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) \\
&= (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T(\boldsymbol{X}^T\boldsymbol{Y} - \boldsymbol{X}^T\boldsymbol{X}\hat{\boldsymbol{\beta}}) \\
&= (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T(\boldsymbol{X}^T\boldsymbol{Y} - \boldsymbol{X}^T\boldsymbol{X}((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y})) \\
&= (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T(\boldsymbol{X}^T\boldsymbol{Y} - \boldsymbol{X}^T\boldsymbol{Y}) \\
&= 0.
\end{aligned}
$$

Thus, our latter two terms are both 0 and we are left with the generalized expansion in 4b:

$$
(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) = (\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) + (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})\boldsymbol{X}^T\boldsymbol{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}).
$$

Note that for $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, we have that $\boldsymbol{Y} \sim (\boldsymbol{X}\boldsymbol{\beta}, \sigma^2\boldsymbol{I})$. As we've seen previously (presentation 3), maximizing the likelihood is a matter of minimizing the least squares error expression $(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})$, which appears as the negative exponent of an exponential. The expression $(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})$, which can be written using the generalized expression above:

$$
(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) = (\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) + (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta})\boldsymbol{X}^T\boldsymbol{X}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}).
$$

is minimized when the latter term is 0, meaning $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}$. Thus, the MLE is simply $\hat{\boldsymbol{\beta}}$.

d) **Recall that, for an $n \times 1$ vector random variable Y with mean vector $\mu$ and covariance matrix V, if M is an $m \times n$ matrix of constants, then MY has mean $\mathbf{M}\mu$ and covariance $\mathbf{MVM^T}$. Show that $\hat{\beta}$ has mean vector $\beta$ and covariance matrix $\sigma^2(\mathbf{X^TX})^{-1}$. Verify the variance and covariance results from presentation 3.**

Recall that $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}$ and $\boldsymbol{Y} \sim (\boldsymbol{X}\boldsymbol{\beta}, \sigma^2\boldsymbol{I})$. It follows that

$$
\begin{aligned}
\mathbb{E}\left[\hat{\boldsymbol{\beta}}\right] &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\mathbb{E}\left[\boldsymbol{Y}\right] \\
&= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{\beta} \\
&= \boldsymbol{\beta}.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\mathrm{Var}\left[\hat{\boldsymbol{\beta}}\right] &= \mathrm{Var}\left[(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{Y}\right] \\
&= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\mathrm{Var}\left[Y\right]((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T)^T \\
&= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\sigma^2\boldsymbol{I}((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T)^T \\
&= \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}((\boldsymbol{X}^T\boldsymbol{X})^{-1})^T \\
&= \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}.
\end{aligned}
$$

To verify the variance and covariance results from presentation 3, one can check using the fact that

$$
\mathbf{X^TX} = \begin{bmatrix} n & n\bar{x} \\ n\bar{x} & \sum x_i^2 \end{bmatrix}
$$

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that indeed,

$$\sigma^2(\mathbf{X}^T\mathbf{X})^{-1} = \begin{bmatrix} \text{Var}\left[\hat{\beta}_0\right] & \text{Cov}\left[\hat{\beta}_0, \hat{\beta}_1\right] \\ \text{Cov}\left[\hat{\beta}_0, \hat{\beta}_1\right] & \text{Var}\left[\hat{\beta}_1\right] \end{bmatrix}$$

*(Some manipulation and use of the fact that $\sum(x_i - \bar{x})^2 = \sum x_i^2 - n\bar{x}^2$ is needed – see presentation 3 notes for more details.)*

e) **A matrix M is a projection matrix if and only if $\mathbf{M}^T = \mathbf{M}$ and $\mathbf{MM} = \mathbf{M}$. The vector of fitted mean values is $\hat{\mathbf{Y}} = \mathbf{X}\hat{\beta} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} = \mathbf{HY}$, and the vector of fitted residuals is $\hat{\varepsilon} = \mathbf{Y} - \hat{\mathbf{Y}} = (\mathbf{I} - \mathbf{H})\mathbf{Y}$, where I is the $n \times n$ identity matrix. Show that $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ and $\mathbf{I} - \mathbf{H}$ are orthogonal projection matrices. Note that $\mathbf{Y} = \mathbf{HY} + (\mathbf{I} - \mathbf{H})\mathbf{Y} = \hat{\mathbf{Y}} + \hat{\varepsilon}$.**

Note that if $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$, then

$$\mathbf{H}^T = (\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)^T = ((\mathbf{X})^T)^T((\mathbf{X}^T\mathbf{X})^{-1})^T\mathbf{X}^T.$$

Since $\mathbf{X}^T\mathbf{X}$ is symmetric, its inverse is also symmetric, so $((\mathbf{X}^T\mathbf{X})^{-1})^T = (\mathbf{X}^T\mathbf{X})^{-1}$. Thus,

$$\mathbf{H}^T = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T = \mathbf{H}.$$

Similarly,

$$\begin{aligned} \mathbf{H}^2 &= (\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T)(\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T) \\ &= (\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T) \\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T \\ &= \mathbf{H} \end{aligned}$$

as desired. Consequently, $\mathbf{H}$ is a projection matrix.

On the other hand, note that

$$(\mathbf{I} - \mathbf{H})^T = \mathbf{I}^T - \mathbf{H}^T = \mathbf{I} - \mathbf{H}.$$

Furthermore,

$$\begin{aligned} (\mathbf{I} - \mathbf{H})(\mathbf{I} - \mathbf{H}) &= \mathbf{I}^2 - 2\mathbf{IH} + \mathbf{H}^2 \\ &= \mathbf{I} - 2\mathbf{H} + \mathbf{H} \\ &= \mathbf{I} - \mathbf{H}. \end{aligned}$$

Thus, once again, $\mathbf{I} - \mathbf{H}$ is a projection matrix. Finally, they are orthogonal: note that

$$\mathbf{H}(\mathbf{I} - \mathbf{H}) = \mathbf{HI} - \mathbf{H}^2 = \mathbf{H} - \mathbf{H} = \mathbf{0}.$$

In the next presentation, we will see build some intuition behind what these matrices represent and how they are used.

# 13 Bayesian Inference

## 13.1 Bayesian Regression Model

a) **The Normal linear model implies $\hat{\boldsymbol{\beta}} \mid \boldsymbol{\beta}, \sigma^2 \sim N_p(\boldsymbol{\beta}, \boldsymbol{V})$, where $\boldsymbol{V} = \sigma^2(\mathbf{X^T X})^{-1}$. Assuming a prior distribution $\boldsymbol{\beta} \sim N_p(\boldsymbol{\gamma}, \boldsymbol{A})$, find the implied posterior distribution for $\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}, \sigma^2$.**

Recall that the setup for linear regression: $\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \sigma \boldsymbol{Z}$, where $\boldsymbol{Z} \sim N_n(0, \boldsymbol{I})$. It follows that the likelihood

$$
\begin{aligned}
L(\boldsymbol{Y} \mid \boldsymbol{\beta}) = f_{Y|\beta}(\boldsymbol{Y} \mid \boldsymbol{\beta}) &\propto \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})\right)\right] \\
&= \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right)\right] \\
&\propto \exp\left[-\frac{1}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\left(\sigma^2(\boldsymbol{X}^T\boldsymbol{X})\right)^{-1}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right].
\end{aligned}
$$

Note that this likelihood depends only on $\hat{\beta}$, so $\hat{\beta}$ is a sufficient statistic for $\beta$.

As for the posterior pdf, we have

$$
\begin{aligned}
f_{\beta|Y}(\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}, \sigma^2) &= f_{\boldsymbol{\beta}} L(\boldsymbol{Y} \mid \boldsymbol{\beta}) \\
&\propto \exp\left[-\frac{1}{2}(\boldsymbol{\beta} - \boldsymbol{\gamma})^T \boldsymbol{A}^{-1}(\boldsymbol{\beta} - \boldsymbol{\gamma})\right] \exp\left[-\frac{1}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\left(\sigma^2(\boldsymbol{X}^T\boldsymbol{X})\right)^{-1}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right] \\
&\propto \exp\left[-\frac{1}{2}\left((\boldsymbol{\beta} - \boldsymbol{\gamma})^T \boldsymbol{A}^{-1}(\boldsymbol{\beta} - \boldsymbol{\gamma}) + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\left(\sigma^2(\boldsymbol{X}^T\boldsymbol{X})\right)^{-1}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right)\right] \\
&= \exp\left[-\frac{1}{2}\left(\boldsymbol{\beta}^T(\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})\boldsymbol{\beta} - 2\boldsymbol{\beta}^T(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma}) + \boldsymbol{\beta}^T\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{\gamma}^T\boldsymbol{A}^{-1}\boldsymbol{\gamma}\right)\right] \\
&\propto \exp\left[-\frac{1}{2}\left(\boldsymbol{\beta} - \mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right]\right)^T (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}\left(\boldsymbol{\beta} - \mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right]\right)\right].
\end{aligned}
$$

Note that we have a quadratic term with respect to $\boldsymbol{\beta}$, so we can recognize this as a MVN density. Recall that for $\boldsymbol{Y} \sim N_n(\boldsymbol{\mu}, \tilde{\boldsymbol{V}})$, the density

$$
f_Y(\boldsymbol{Y}) \propto \exp\left[-\frac{1}{2}\left((\boldsymbol{Y} - \boldsymbol{\mu})^T\tilde{\boldsymbol{V}}^{-1}(\boldsymbol{Y} - \boldsymbol{\mu})\right)\right] \propto \exp\left[-\frac{1}{2}\left(\boldsymbol{Y}^T\tilde{\boldsymbol{V}}^{-1}\boldsymbol{Y} - 2\boldsymbol{Y}^T\tilde{\boldsymbol{V}}^{-1}\boldsymbol{\mu}\right)\right].
$$

Matching the respective terms, we see that

$$
\tilde{\boldsymbol{V}} = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}
$$

so the variance of the posterior distribution is

$$
\operatorname{Var}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right] = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}.
$$

On the other hand, we also have that

$$\tilde{\boldsymbol{V}}^{-1}\boldsymbol{\mu} = (\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma}),$$

so solving for $\boldsymbol{\mu}$ gives the mean of the posterior distribution

$$\mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right] = \tilde{\boldsymbol{V}}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma})$$
$$= (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma}).$$

b) **For symmetric, invertible $p \times p$ matrices $\boldsymbol{V}$ and $\boldsymbol{A}$, show that**

$$(\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1} = \boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{A}.$$

**Use this to express $\mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right]$ as a weighted average of the vectors $\boldsymbol{\gamma}$ and $\hat{\boldsymbol{\beta}}$.**

Note that

$$\left[\boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{V}\right]^{-1} = \boldsymbol{V}^{-1}(\boldsymbol{V} + \boldsymbol{A})\boldsymbol{A}^{-1}$$
$$= (\boldsymbol{I} + \boldsymbol{V}^{-1}\boldsymbol{A})\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1} + \boldsymbol{V}^{-1}$$

so

$$(\boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A}^{-1})\boldsymbol{V}) = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}.$$

Similarly,

$$\left[\boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{A}\right]^{-1} = \boldsymbol{A}^{-1}(\boldsymbol{V} + \boldsymbol{A})\boldsymbol{V}^{-1}$$
$$= \boldsymbol{A}^{-1}(\boldsymbol{I} + \boldsymbol{A}\boldsymbol{V}^{-1}) = \boldsymbol{A}^{-1} + \boldsymbol{V}^{-1}.$$

so

$$(\boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A}^{-1})\boldsymbol{A}) = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}.$$

We conclude that

$$\boxed{(\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1} = \boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{V} = \boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{A}}$$

From part (a), we have that

$$\mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right] = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma}).$$

Expanding and simplifying, we get that

$$\mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right] = (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{A}^{-1}\boldsymbol{\gamma})$$
$$= (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}}) + (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{A}^{-1}\boldsymbol{\gamma}).$$

We can substitute $\boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{V}$ and $\boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{A}$ for the first and second $(\boldsymbol{V} + \boldsymbol{A})^{-1}$ terms, respectively, to get

$$
\begin{aligned}
\mathbb{E}\left[\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}\right] &= (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}}) + (\boldsymbol{V}^{-1} + \boldsymbol{A}^{-1})^{-1}(\boldsymbol{A}^{-1}\boldsymbol{\gamma}) \\
&= \boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{V}(\boldsymbol{V}^{-1}\hat{\boldsymbol{\beta}}) + \boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{A}(\boldsymbol{A}^{-1}\boldsymbol{\gamma}) \\
&= \boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1}\hat{\boldsymbol{\beta}} + \boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1}\boldsymbol{\gamma}.
\end{aligned}
$$

We see that this is a weighted average of $\hat{\boldsymbol{\beta}}$ and $\boldsymbol{\gamma}$, as $\boldsymbol{A}(\boldsymbol{V} + \boldsymbol{A})^{-1} + \boldsymbol{V}(\boldsymbol{V} + \boldsymbol{A})^{-1} = 1$.

c) **Show that assuming $p(\boldsymbol{\beta}) \propto c$ leads to the posterior distribution $\boldsymbol{\beta} \mid y, \sigma^2 \sim N_p(\hat{\boldsymbol{\beta}}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1})$, which gives another Bayesian-Frequentist symmetry.**

For $p(\boldsymbol{\beta}) \propto c$, we have

$$
\begin{aligned}
f_{\beta \mid Y}(\boldsymbol{\beta} \mid \hat{\boldsymbol{\beta}}, \sigma^2) &= f_{\boldsymbol{\beta}} L(\boldsymbol{Y} \mid \boldsymbol{\beta}) \\
&= c\exp\left[-\frac{1}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\left(\sigma^2(\boldsymbol{X}^T\boldsymbol{X})\right)^{-1}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right] \\
&\propto \exp\left[-\frac{1}{2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\left(\sigma^2(\boldsymbol{X}^T\boldsymbol{X})\right)^{-1}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right]
\end{aligned}
$$

and so the posterior distribution is $\boldsymbol{\beta} \mid y, \sigma^2 \sim N_p(\hat{\boldsymbol{\beta}}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1})$.

This gives the Bayesian-frequentist symmetry:

$$
\hat{\boldsymbol{\beta}} - \boldsymbol{\beta} \mid y, \sigma^2 \sim N_p(0, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1})
$$

for Bayesian inference, and in the frequentist perspective, $\hat{\boldsymbol{\beta}} \sim N_p(\boldsymbol{\beta}, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1})$ so

$$
\hat{\boldsymbol{\beta}} - \boldsymbol{\beta} \mid \beta, \sigma^2 \sim N_p(0, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}).
$$

d) **The *restricted maximum likelihood* (REML) estimate for a variance is computed by first integrating the mean parameters out of the joint likelihood function and then maximizing with respect to $\sigma^2$ (as opposed to maximizing the joint likelihood function). Show that the REML estimate for a multiple regression is the mean squared error (MSE). Explain why this procedure is more coherent in the context of a constant prior density for $\beta$.**

From our previous work, we know that $\boldsymbol{Y} \sim N_n(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2\boldsymbol{I})$, so

$$
\begin{aligned}
L(\boldsymbol{\beta}, \sigma^2) &\propto (\sigma^2)^{-\frac{n}{2}}\exp\left[-\frac{1}{2\sigma^2}(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})\right] \\
&\propto (\sigma^2)^{-\frac{n}{2}}\exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) + (\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right)\right]
\end{aligned}
$$

To get the REML, we integrate out the mean parameter $\boldsymbol{\beta}$ to get

$$L^*(\sigma^2) = \int_{\mathbb{R}^p} f(\boldsymbol{Y} \mid \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta}) \, d\boldsymbol{\beta}$$

(where in the constant prior case, we have $p(\boldsymbol{\beta}) \propto c$), and so

$$L^*(\sigma^2) \propto (\sigma^2)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})\right)\right] \int_{\mathbb{R}^p} \exp\left[-\frac{1}{2\sigma^2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right] d\boldsymbol{\beta}$$

Recognizing the integral as a kernel of a MVN random variable with mean $\boldsymbol{\beta}$ and covariance matrix $\sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}$ (so that the respective pdf integrates to 1), we have that this simplifies to

$$L^*(\sigma^2) \propto (\sigma^2)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})\right)\right] \int_{\mathbb{R}^p} \exp\left[-\frac{1}{2\sigma^2}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{\beta} - \hat{\boldsymbol{\beta}})\right] d\boldsymbol{\beta}$$

$$= (\sigma^2)^{-\frac{n}{2}} \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})\right)\right] (2\pi)^{\frac{n}{2}} |\sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1}|^{\frac{1}{2}}$$

$$\propto (\sigma^2)^{-\frac{n-p}{2}} \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})\right)\right].$$

(Note that the last step follows from the fact that for a $p \times p$ matrix $\boldsymbol{A}$, $|c\boldsymbol{A}| = c^p|\boldsymbol{A}|$.)

Maximizing over $\sigma^2$ as we have done previously, we get the REML estimate

$$\hat{\sigma}^2 = \frac{(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})}{n - p} = \frac{1}{n - p}\sum(Y_i - \hat{\boldsymbol{Y}})^2 = \text{MSE}.$$

e) **Assuming the joint Jeffreys prior density $p(\beta, \sigma^2) \propto 1/\sigma^2, \sigma^2 > 0$, show that the marginal posterior density for $\sigma^2 \mid y$ is reciprocal-Gamma. Outline how to generate posterior draws for the $\beta'_j s$ or $\mu_i = \boldsymbol{X}_i^T\boldsymbol{\beta}$s, or for future $Y$ values.**

For the joint Jeffreys prior density $p(\beta, \sigma^2) \propto 1/\sigma^2$, we have that

$$L^*(\sigma^2) = \int_{\mathbb{R}^p} f(\boldsymbol{Y} \mid \boldsymbol{\beta}, \sigma^2) p(\boldsymbol{\beta}, \sigma^2) \, d\boldsymbol{\beta}$$

$$= \frac{1}{\sigma^2} \int_{\mathbb{R}^p} f(\boldsymbol{Y} \mid \boldsymbol{\beta}, \sigma^2) \, d\boldsymbol{\beta}$$

$$\propto (\sigma^2)^{-\left(\frac{n-p}{2}+1\right)} \exp\left[-\frac{1}{2\sigma^2}\left((\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})\right)\right].$$

Thus, the marginal posterior density $\sigma^2 \mid y \sim \text{InvGamma}\left(\frac{n-p}{2}, \frac{((\boldsymbol{Y}-\boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{Y}-\boldsymbol{X}\hat{\boldsymbol{\beta}}))}{2}\right)$, or

$$\boxed{\sigma^2 \mid y \sim \text{InvGamma}\left(\frac{n-p}{2}, \frac{SSE}{2}\right).}$$

We also have that
$$\boldsymbol{\beta} \mid y, \sigma^2 \sim N_p(\hat{\boldsymbol{\beta}}, \sigma^2 (\boldsymbol{X}^T \boldsymbol{X})^{-1}).$$

Thus, we can generate posterior draws or future $Y$ values. See R Code for real/simulated data.