MATH/STAT 355: Statistical Theory

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Welcome to Statistical Theory!

This book contains the course notes for *MATH/STAT 355: Statistical Theory** at Macalester College, as taught by Prof. Taylor Okonek. These notes draw from reading guides created by Prof. Kelsey Grinde, a little bit from the textbook, *An Introduction to Mathematical Statistics and Its Applications* by Richard Larsen and Morris Marx (6th Edition), and the STAT 512/513 Course Notes developed by Dr. Michael Perlman at the University of Washington. As of Spring 2025, this course no longer requires a textbook, and relies heavily on these course notes instead.

Each chapter of the course notes will contain (at a minimum):

1. Topic Introduction
2. Learning Objectives
3. Concept Questions
4. Definitions
5. Theorems
6. Worked Examples

I will be editing and adding to these notes throughout Spring 2025, so please check consistently for updates!

If you find any typos or have other questions, please email tokonek@macalester.edu.

* *MATH/STAT 355: Statistical Theory* went under the title *MATH/STAT 455: Mathematical Statistics* prior to Spring 2025. The course content is largely similar, the differences primarily being the structure of the course and not the content itself.

1 Probability: A Brief Review

MATH/STAT 355 builds directly on topics covered in *MATH/STAT 354: Probability*. You're not expected to perfectly remember everything from *Probability*, but you will need to have sufficient facility with the following topics covered in this review Chapter in order to grasp the majority of concepts covered in *MATH/STAT 355*.

1.1 Learning Objectives

By the end of this chapter, you should be able to…

- Distinguish between important probability models (e.g., Normal, Binomial)
- Derive the expectation and variance of a single random variable or a sum of random variables
- Define the moment generating function and use it to find moments or identify pdfs
- Derive pdfs of transformations of continuous random variables

1.2 Concept Questions

1. Which probability distributions are appropriate for *quantitative* (continuous) random variables?
2. Which probability distributions are appropriate for *categorical* random variables?
3. *Independently and Identically Distributed (iid)* random variables are an incredibly important assumption involved in many statistical methods. Why do you think it might be important/useful for random variables to have this property?
4. Why might we want to be able to derive distribution functions for transformations of random variables? In what scenarios can you imagine this being useful?

1.3 Definitions

You are expected to know the following definitions:

Random Variable

A random variable is a function that takes inputs from a sample space of all possible outcomes, and outputs real values or probabilities. As an example, consider a coin flip. The sample space of all possible outcomes consists of "heads" and "tails", and each outcome is associated with a probability (50% each, for a fair coin). For our purposes, you should know that random variables have probability density (or mass) functions, and are either discrete or continuous based on the number of possible outcomes a random variable may take. Random variables are often denoted with capital Roman letters, like X, Y, Z, etc.

Probability density function (discrete, continuous)

- Note: I don't care if you call a pmf a pdf... I will probably do this continuously throughout the semester. We don't need to be picky about this in *MATH/STAT 355*.

There are many different accepted ways to write the notation for a pdf of a random variables. Any of the following are perfectly appropriate for this class: $f(x)$, $\pi(x)$, $p(x)$, $f_X(x)$. I typically use either π or p, but might mix it up occasionally.

Key things I want you to know about probability density functions:

- $\pi(x) \geq 0$, everywhere. This should make sense (hopefully) because probabilities cannot be negative!
- $\int_{-\infty}^{\infty} \pi(x) = 1$. This should also (hopefully) makes sense. Probabilities can't be *greater* than one, and the probability of event occurring *at all (ever)* should be equal to one, if the event x is a random variable.

Cumulative distribution function (discrete, continuous)

Cumulative distribution functions we'll typically write as $F_X(x)$. or $F(x)$, for short. It is important to know that

$$F_X(x) = \Pr(X \leq x),$$

or in words, "the cumulative distribution function is the probability that a random variable lies before x." If you write $\Pr(X < x)$ instead of $\leq$, you're fine. The probability that a random variable is exactly one number (for an RV with a continuous pdf) is zero anyway, so these are the same thing. Key things I want you to know about cumulative distribution functions:

- $F(x)$ is non-decreasing. This is in part where the "cumulative" piece comes in to play. Recall that probabilities are basically integrals or sums. If we're integrating over something positive, and our upper bound for our integral *increases*, the area under the curve (cumulative probability) will increase as well.
- $0 \leq F(x) \leq 1$ (since probabilities have to be between zero and one!)
- $\Pr(a < X \leq b) = F(a) - F(b)$ (because algebra)

Joint probability density function

A joint probability density function is a probability distribution defined for more than one random variable at a time. For two random variables, X and Z, we could write their joint density function as $f_{X,Z}(x, z)$, or $f(x, z)$ for short. The joint density function encodes all sorts of fun information, including *marginal* distributions for X and Z, and conditional distributions (see next **bold** definition). We can think of the joint pdf as listing all possible pairs of outputs from the density function $f(x, z)$, for varying values of x and z. Key things I want you to know about joint pdfs:

- How to get a marginal pdf from a joint pdf:

  Suppose I want to know $f_X(x)$, and I know $f_{X,Z}(x, z)$. Then I can integrate or "average over" Z to get

$$f_X(x) = \int f_{X,Z}(x, z)dz$$

- The relationship between conditional pdfs, marginal pdfs, joint pdfs, and Bayes' theorem/rule
- How to obtain a joint pdf for *independent* random variables: just multiply their marginal pdfs together! This is how we will (typically) think about likelihoods!
- How to obtain a marginal pdf from a joint pdf when random variables are independent *without integrating* (think, "separability")

Conditional probability density function

A conditional pdf denotes the probability distribution for a (set of) random variable(s), *given that* the value for another (set of) random variable(s) is known. For two random variables, X and Z, we could write the conditional distribution of X "given" Z as $f_{X|Z}(x \mid z)$, where the "conditioning" is denoted by a vertical bar (in LaTeX, this is typeset using "\mid"). Key things I want you to know about conditional pdfs:

- The relationship between conditional pdfs, marginal pdfs, joint pdfs, and Bayes' theorem/rule
- How to obtain a conditional pdf from a joint pdf (again, think Bayes' rule)

- Relationship between conditional pdfs and independence (see next **bold** definition)

Independence

Two random variables X and Z are *independent* if and only if:

- $f_{X,Z}(x,z) = f_X(x)f_Z(z)$ (their joint pdf is "separable")
- $f_{X|Z}(x \mid z) = f_X(x)$ (the pdf for X does not depend on Z in any way)

  Note that the "opposite" is also true: $f_{Z|X}(z \mid x) = f_Z(z)$

In notation, we denote that two variables are independent as $X \perp\!\!\!\perp Z$, or $X \perp Z$. In LaTeX, the *latter* is typeset as "\perp", and the former is typeset as "\perp\!\!\!\perp". As a matter of personal preference, I (Taylor) prefer $\perp\!\!\!\perp$, but I don't like typing it out every time. Consider using the "\newcommand" functionality in LaTeX to create a shorthand for this for your documents!

Jacobian Matrix

Let f be a 1-1 and onto function, where $f(x_i) = y_i$ for $i = 1, \ldots, n$. Then the Jacobian matrix of f is the matrix of partial derivatives,

$$J_f(x) = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_n}{\partial x_1} \\ \vdots & & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_n}{\partial x_n} \end{pmatrix}$$

The Jacobian matrix is sometimes simply referred to as the "Jacobian", but be careful when simply calling it the Jacobian, since this can sometimes refer to the *determinant* of the Jacobian matrix as well. For this course, we'll always refer to the Jacobian matrix as a matrix, and the "Jacobian" as its determinant.

Jacobian

The Jacobian is the determinant of the Jacobian matrix, denoted by $|J_f(x)|$. Recall from linear algebra that $Det(A) = Det(A^\top)$. This is convenient, because it means we won't have worry too much about remembering which order our partial derivatives go in our matrix, for 2x2 matrices (which is all we'll be working with for this course).

Expected Value / Expectation

The expectation (or expected value) of a random variable is defined as:

$$E[X] = \int_{-\infty}^{\infty} x f(x) dx$$

Expected value is a weighted average, where the average is over all possible values a random variable can take, weighted by the probability that those values occur. Key things I want you to know about expectation:

- The relationship between expectation, variance, and moments (specifically, that $E[X]$ is the 1st moment!)
- The "law of the unconscious statistician" (see the Theorems section of this chapter)
- Expectation of linear transformations of random variables (see **Theorems** section of this chapter)

Variance

The variance of a random variable is defined as:

$$Var[X] = E[(X - E[X])^2] = E[X^2] - E[X]^2$$

In words, we can read this as "the expected value of the squared deviation from the mean" of a random variable X. Key things I want you to know about variance:

- The relationship between expectation, variance, and moments (hopefully clear, given the formula for variance)
- The relationship between variance and standard deviation: $Var(X) = sd(X)^2$
- The relationship between variance and covariance: $Var(X) = Cov(X, X)$
- $Var(X) \geq 0$. This should make sense, given that we're taking the expectation of something "squared" in order to calculate it!
- $Var(c) = 0$ for any constant, c.
- Variance of linear transformations of random variables (see **Theorems** section of this chapter)

r^{th} moment

The r^{th} moment of a probability distribution is given by $E[X^r]$. For example, when $r = 1$, the r^{th} moment is just the expectation of the random variable X. Key things I want you to know about moments:

- The relationship between moments, expectation, and variance
  - For example, if you know the first and second moments of a distribution, you should be able to calculate the variance of a random variable with that distribution!
- The relationship between moments and *moment generating functions* (see **Theorems** section of this chapter)

Covariance

The covariance of two random variables is a measure of their *joint* variability. We denote the covariance of two random variables X and Z as $Cov(X, Z)$, and

$$Cov(X, Z) = E[(X - E[X])(Y - E[Y])] = E[XY] - E[X]E[Y]$$

Some things I want you to know about covariance:

- $Cov(X, X) = Var(X)$
- $Cov(X, Y) = Cov(Y, X)$ (order doesn't matter)

Moment Generating Function (MGF)

The moment generating function of a random variable X is defined as

$$M_X(t) = E[e^{tX}]$$

A few things to note:

- $M_X(0) = 1$, always.
- If two random variables have the same MGF, they have the same probability distribution!
- MGFs are sometimes useful for showing how different random variables are related to each other

1.3.1 Distributions Table

You are also expected to know the probability distributions contained in Table 1, below. Note that you *do not* need to memorize the pdfs for these distributions, but you *should* be familiar with what types of random variables (continuous/quantitative, categorical, integer-valued, etc.) may take on different distributions. The more familiar you are with the forms of the pdfs, the easier/faster it will be to work through problem sets and quizzes.

Table 1.1: *Table 1.* Table of main probability distributions we will work with for *MATH/STAT 355*.

Distribution	PDF/PMF	Parameters	Support
Uniform	$\pi(x) = \frac{1}{\beta - \alpha}$	$\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}$	$x \in [\alpha, \beta]$
Normal	$\pi(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2\sigma^2}(x - \mu)^2)$	$\mu \in \mathbb{R}$, $\sigma > 0$	$x \in \mathbb{R}$

Distribution	PDF/PMF	Parameters	Support
Multivariate Normal	$\pi(\mathbf{x}) = (2\pi)^{-k/2}\lvert\Sigma\rvert^{-1/2}\exp(-\frac{1}{2}(\mathbf{x}-\mu)^\top\Sigma^{-1}(\mathbf{x}-\mu)))$	$\mu \in \mathbb{R}^k$, $\Sigma \in \mathbb{R}^{k\times k}$, positive semi-definite (in practice, almost always positive definite)	$x \in \mathbb{R}^k$
Gamma	$\pi(x) = \frac{\beta^\alpha}{\Gamma(\alpha)}x^{\alpha-1}e^{-\beta x}$	α (shape), β (rate) > 0	$x \in (0,\infty)$
Chi-squared	$\pi(x) = \frac{2^{-\nu/2}}{\Gamma(\nu/2)}x^{\nu/2-1}e^{-x/2}$	$\nu > 0$	$x \in [0,\infty)$
F	$\pi(x) = \frac{\Gamma(\frac{\nu_1+\nu_2}{2})}{\Gamma(\frac{\nu_1}{2})\Gamma(\frac{\nu_2}{2})}\left(\frac{\nu_1}{\nu_2}\right)^{\nu_1/2}\left(\frac{x^{(\nu_1-2)/2}}{\left(1+\left(\frac{\nu_1}{\nu_2}\right)x\right)^{(\nu_1+\nu_2)/2}}\right)$	$\nu_1, \nu_2 > 0$	$x \in [0,\infty)$
Exponential	$\pi(x) = \beta e^{-\beta x}$	$\beta > 0$	$x \in [0,\infty)$
Laplace (Double Exponential)	$\pi(x) = \frac{1}{2b}\exp(-\frac{\lvert x-\mu\rvert}{b})$	$\mu \in \mathbb{R}$, $b > 0$	$x \in \mathbb{R}$
Student-t	$\pi(x) = \frac{\Gamma((\nu+1)/2)}{\Gamma(\nu/2)\sqrt{\nu\pi}}(1+\frac{x^2}{\nu})^{-(\nu+1)/2}$	$\nu > 0$	$x \in \mathbb{R}$
Beta	$\pi(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}x^{\alpha-1}(1-x)^{\beta-1}$	$\alpha, \beta > 0$	$x \in [0,1]$
Poisson	$\pi(x) = \frac{\lambda^x e^{-\lambda}}{x!}$	$\lambda > 0$	$x \in \mathbb{N}$
Binomial	$\pi(x) = \binom{n}{x}p^x(1-p)^{n-x}$	$p \in [0,1], n = \{0,1,2,\dots\}$	$x \in \{0,1,\dots,n\}$
Multinomial	$\pi(\mathbf{x}) = \frac{n!}{x_1!\dots x_k!}p_1^{x_1}\dots p_k^{x_k}$	$p_i > 0$, $p_1+\dots+p_k = 1$, $n = \{0,1,2,\dots\}$	$\{x_1,\dots,x_k \mid \sum_{i=1}^k x_i = n, x_i \geq 0(i=1,\dots,k)\}$
Negative Binomial	$\pi(x) = \binom{x+r-1}{x}(1-p)^x p^r$	$r > 0$, $p \in [0,1]$	$x \in \{0,1,\dots\}$

1.4 Theorems

- Law of Total Probability

$$P(A) = \sum_n P(A \cap B_n),$$

or

$$P(A) = \sum_n P(A \mid B_n)P(B_n)$$

- Bayes' Theorem

$$\pi(A \mid B) = \frac{\pi(B \mid A)\pi(A)}{\pi(B)}$$

- Relationship between pdf and cdf

$$F_Y(y) = \int_{-\infty}^{y} f_Y(t)dt$$

$$\frac{\partial}{\partial y}F_Y(y) = f_Y(y)$$

- Expectation of random variables

$$E[X] = \int_{-\infty}^{\infty} xf(x)dx$$

$$E[X^2] = \int_{-\infty}^{\infty} x^2 f(x)dx$$

  - "Law of the Unconscious Statistician"

$$E[g(X)] = \int_{-\infty}^{\infty} g(x)f(x)dx$$

- Expectation and variance of linear transformations of random variables

$$E[cX + b] = cE[X] + b$$

$$Var[cX + b] = c^2 Var[X]$$

- Relationship between mean and variance

$$Var[X] = E[(X - E[X])^2] = E[X^2] - E[X]^2$$

  Also, recall that $Cov[X, X] = Var[X]$.

- Iterated Things

$$E[X] = E[E[X \mid Y]]$$

and

$$Var(X) = E[Var(X \mid Y)] + Var(E[X \mid Y])$$

- Finding a marginal pdf from a joint pdf

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x, y)dy$$

- Independence of random variables and joint pdfs

  If two random variables are independent, their joint pdf will be *separable*. For example, if X and Y are independent, we could write

$$f_{X,Y}(x, y) = f_X(x)f_Y(y)$$

- Expected value of a product of independent random variables

  Suppose random variables $X_1, \ldots, X_n$ are independent. Then we can write,

$$E\left[\prod_{i=1}^{n} X_i\right] = \prod_{i=1}^{n} E[X_i]$$

- Covariance of independent random variables

  If X and Y are independent, then $Cov(X, Y) = 0$. We can show this by noting that

$$\begin{aligned} Cov(X, Y) &= E[(X - E[X])(Y - E[Y])] && (1.1)\\ &= E[XY - XE[Y] - YE[X] + E[X]E[Y]] && (1.2)\\ &= E[XY] - E[XE[Y]] - E[YE[X]] + E[X]E[Y] && (1.3)\\ &= 2E[X]E[Y] - 2E[X]E[Y] && (1.4)\\ &= 0 && (1.5) \end{aligned}$$

- Using MGFs to find moments

  Recall that the moment generating function of a random variable X, denoted by $M_X(t)$ is

  $$M_X(t) = E[e^{tX}]$$

  Then the nth moment of the probability distribution for X , $E[X^n]$, is given by

  $$\left.\frac{\partial M_X}{\partial t^n}\right|_{t=0}$$

  where the above reads as "the nth derivative of the moment generating function, evaluated at $t = 0$."

- Using MGFs to identify pdfs

  MGFs uniquely identify probability density functions. If X and Y are two random variables where for all values of t, $M_X(t) = M_Y(t)$, then $F_X(x) = F_Y(y)$.

- Central Limit Theorem

  The classical CLT states that for independent and identically distributed (iid) random variables $X_1, \ldots, X_n$, with expected value $E[X_i] = \mu$ and $Var[X_i] = \sigma^2 < \infty$, the sample average (centered and standardized) converges in distribution to a standard normal distribution at a root-n rate. Notationally, this is written as

  $$\sqrt{n}(\bar{X} - \mu) \xrightarrow{d} N(0, \sigma^2)$$

  🌶 A fun aside: this is only *one* CLT, often referred to as the Levy CLT. There are other CLTs, such as the Lyapunov CLT and Lindeberg-Feller CLT!

1.4.1 Transforming Continuous Random Variables

We will *often* take at face value previously proven *relationships* between random variables. What I mean by this, as an example, is that it is a nice (convenient) fact that a sum of two independent normal random variables is *still* normally distributed, with a nice form for the mean and variance. In particular, if $X \sim N(\mu, \sigma^2)$ and $Y \sim N(\theta, \nu^2)$, then $X + Y \sim N(\mu + \theta, \sigma^2 + \nu^2)$. Most frequently used examples of these sorts of relationships can be found in the "Related Distributions" section of the Wikipedia page for a given probability distribution. Unless I explicitly ask you to derive/show how certain variables are related to each other, you can just state the known relationship, use it, and move on!

If I *do* ask you to derive/show these things, there a few different ways we can go about this. For this course, I expect you to know the "CDF method" for *one function* of *one random variable*, **and** the "Jacobian method" for a function of *more than one* random variable.

1.4.1.1 CDF Method: One random variable

Theorem. Let X be a continuous random variable with pdf $f_X(x)$. Define a new random variable $Y = g(X)$, for nice* functions g. Then $f_Y(y) = f_X(g^{-1}(y)) \times \frac{1}{g'(g^{-1}(y))}$.

🌶 *By *nice* functions we mean functions that are strictly increasing and smooth *on the required range*. As an example, $exp(x)$ is a smooth, strictly increasing function; $|x|$ is not on the *whole real line*, but *is* from $(0, \infty)$ (where a lot of useful pdfs are defined). For the purposes of this class, every function that you will need to do this for will be "nice." Note that there are also considerations that need to be taken regarding the *range* of continuous random variables when considering transforming them. We will mostly ignore these considerations in this class, but a technically complete derivation (or proof) must consider them.

Proof.

We can write

$$\begin{aligned} f_Y(y) &= \frac{\partial}{\partial y} F_Y(y) \\ &= \frac{\partial}{\partial y} \Pr(Y \leq y) \\ &= \frac{\partial}{\partial y} \Pr(g(X) \leq y) \\ &= \frac{\partial}{\partial y} \Pr(X \leq g^{-1}(y)) \\ &= \frac{\partial}{\partial y} F_X(g^{-1}(y)) \\ &= f_X(g^{-1}(y)) \times \frac{\partial}{\partial y} g^{-1}(y) \end{aligned}$$

where to obtain the last equality we use chain rule! Now we require some statistical trickery to continue… (note that this method is called the "CDF method" because we go *through* the CDF to derive the distribution for Y)

You will *especially* see this in the Bayes chapter of our course notes, but it is often true that our lives are made easier as statisticians if we multiply things by one, or add zero. What exactly do I mean? Rearranging gross looking formulas into things we are familiar with (like pdfs, for

example) often makes our lives easier and allows us to avoid dealing with such grossness. Here, the grossness is less obvious, but nonetheless relevant. Note that we can write

$$\begin{aligned} y &= y \\ y &= g(g^{-1}(y)) \\ \frac{\partial}{\partial y} y &= \frac{\partial}{\partial y} g(g^{-1}(y)) \\ 1 &= g'(g^{-1}(y)) \frac{\partial}{\partial y} g^{-1}(y) \qquad \text{(chain rule again!)} \\ \frac{1}{g'(g^{-1}(y))} &= \frac{\partial}{\partial y} g^{-1}(y) \end{aligned}$$

The right-hand side should look familiar: it is exactly what we needed to "deal with" in our proof! Returning to that proof, we have

$$\begin{aligned} f_Y(y) &= f_X(g^{-1}(y)) \times \frac{\partial}{\partial y} g^{-1}(y) \\ &= f_X(g^{-1}(y)) \times \frac{1}{g'(g^{-1}(y))} \end{aligned}$$

as desired.

1.4.1.2 Jacobian Method: More than one random variable

Transformations of single random variables are great, but we'll need to work with transformations of *more than one* random variable if we want to be able to manipulate joint pdfs. Suppose, for example, we have $X \sim Gamma(\alpha, \lambda)$ and $Y \sim Gamma(\beta, \lambda)$, where $X \perp\!\!\!\perp Y$. Let $U = X+Y$ and $W = \frac{X}{X+Y}$. How do we show that U and W are independent? Through finding the joint pdf! Which means we need a method for transforming more than one, continuous random variable. Enter the Jacobian Method.

Theorem. Let $X = (x_1, \ldots, x_n)$ be a vector of random variables (a random vector) with pdf $\pi_X(x)$. Suppose that $f(x) = y$ is a smooth, 1-1 and onto function, and that $|J_f(x)| > 0$ almost everywhere. Then $\pi_Y(y)$ is given by

$$\pi_Y(y) = \pi_X(f^{-1}(y)) \times \left| \frac{\partial x}{\partial y} \right| \times I_Y\{y\}$$

where $I_Y\{y\}$ denotes the support of Y.

NOTE: $|J_f(y)| = |\frac{\partial x}{\partial y}|$, above, where $f(x) = y$. This means that the numerators and denominators in the Jacobian Matrix in the definition in the Course Notes are *flipped* here. The reason for this becomes clear in the proof sketched below, noting that $|\frac{\partial x}{\partial y}|^{-1} = |\frac{\partial y}{\partial x}|$, for the supposed functions f.

Proof.

Note that if f is both 1-1 and onto, then f is *either* monotone increasing or monotone decreasing. We'll prove the case where f is increasing, and we'll note (but not show) how the decreasing case follows directly.

Let f be a smooth, monotone increasing function. For some subset $C \subseteq \mathbb{R}^n$,

$$\begin{aligned}\int_C \pi_Y(y)dy &= \Pr(Y \in C) \\ &= \Pr(f(X) \in C) \\ &= \Pr(X \in f^{-1}(C)) \\ &= \int_{f^{-1}(C)} \pi_X(x)dx\end{aligned}$$

Now we'll use a (convoluted) u-substitution to make this look like what we want it to look like. Let $u = f^{-1}(y)$. Note that this also means $u = x$. Then $du = (f^{-1}(y))'dy = dx$. Proceeding with u-substitution, we have

$$\begin{aligned}\int_C \pi_Y(y)dy &= \int_{f^{-1}(C)} \pi_X(x)dx \\ &= \int_C \pi_X(u)du \\ &= \int_C \pi_X(f^{-1}(y))(f^{-1}(y))'dy \\ &= \int_C \pi_X(f^{-1}(y))\left|\frac{dx}{dy}\right|dy\end{aligned}$$

which implies $\pi_Y(y) = \pi_X(f^{-1}(y))\left|\frac{dx}{dy}\right|$, as desired. The absolute value signs (the Jacobian piece) come into play to help us deal with the decreasing case.

1.5 Worked Examples

Problem 1: Suppose $X \sim Exponential(\lambda)$. Calculate $E[X]$ and $Var[X]$.

Solution:

We know that $f(x) = \lambda e^{-\lambda x}$. If we can calculate $E[X]$ and $E[X^2]$, then we're basically done! We can write

$$\begin{aligned} E[X] &= \int_0^\infty x\lambda e^{-\lambda x} dx \\ &= \lambda \int_0^\infty x e^{-\lambda x} dx \end{aligned}$$

And now we need integration by parts! Set $u = x$, $dv = e^{-\lambda x}dx$. Then $du = 1dx$ and $v = \frac{-1}{\lambda}e^{-\lambda x}$. Since $\int udv = uv - \int vdu$, we can continue

$$\begin{aligned} E[X] &= \lambda \int_0^\infty x e^{-\lambda x} dx \\ &= \lambda \left(-\frac{x}{\lambda} e^{-\lambda x} \Big|_0^\infty - \int_0^\infty \frac{-1}{\lambda} e^{-\lambda x} dx \right) \\ &= \lambda \left(- \int_0^\infty \frac{-1}{\lambda} e^{-\lambda x} dx \right) \\ &= \lambda \left(\frac{-1}{\lambda^2} e^{-\lambda x} \Big|_0^\infty \right) \\ &= \frac{-1}{\lambda} e^{-\lambda x} \Big|_0^\infty \\ &= \frac{1}{\lambda} e^{-0} \\ &= \frac{1}{\lambda} \end{aligned}$$

We can follow a similar process to get $E[X^2]$ (using the law of the unconscious statistician!). We can write

$$E[X^2] = \int_0^\infty x^2 \lambda e^{-\lambda x} dx$$
$$= \lambda \int_0^\infty x^2 e^{-\lambda x} dx$$

And now we need integration by parts again! Set $u = x^2$, $dv = e^{-\lambda x} dx$. Then $du = 2xdx$ and $v = \frac{-1}{\lambda} e^{-\lambda x}$. Since $\int udv = uv - \int vdu$, we can continue

$$\begin{aligned}
E[X] &= \lambda \int_0^\infty x^2 e^{-\lambda x} dx \\
&= \lambda \left(-\frac{x^2}{\lambda} e^{-\lambda x} \Big|_0^\infty - \int_0^\infty \frac{-2}{\lambda} x e^{-\lambda x} dx \right) \\
&= \lambda \left(-\frac{x^2}{\lambda} e^{-\lambda x} \Big|_0^\infty + \frac{2}{\lambda} \int_0^\infty x e^{-\lambda x} dx \right) \\
&= \lambda \left(-\frac{x^2}{\lambda} e^{-\lambda x} \Big|_0^\infty + \frac{2}{\lambda^3} \right) \\
&= \lambda \left(0 + \frac{2}{\lambda^3} \right) \\
&= \frac{2}{\lambda^2}
\end{aligned}$$

Now we can calculate $Var[X] = E[X^2] - E[X]^2$ as

$$Var[X] = E[X^2] - E[X]^2 = \frac{2}{\lambda^2} - \frac{1}{\lambda^2} = \frac{1}{\lambda^2}$$

And so we have $E[X] = \frac{1}{\lambda}$ and $Var[X] = \frac{1}{\lambda^2}$.

Problem 2: Show that an exponentially distributed random variable is "memoryless", i.e. show that $\Pr(X > s + x \mid X > s) = \Pr(X > x)$, $\forall s$.

Solution:

Recall that the CDF of an exponential distribution is given by $F(x) = 1 - e^{-\lambda x}$. Thanks to Bayes rule, we can write

$$\begin{aligned}
\Pr(X > s + x \mid X > s) &= \frac{\Pr(X > s + x, X > s)}{\Pr(X > s)} \\
&= \frac{\Pr(X > s + x)}{\Pr(X > s)} \\
&= \frac{1 - \Pr(X < s + x)}{1 - \Pr(X < s)} \\
&= \frac{1 - F(s + x)}{1 - F(s)}
\end{aligned}$$

where the second equality is true because $x > 0$. Then we can write

$$\begin{aligned}
\Pr(X > s + x \mid X > s) &= \frac{1 - F(s + x)}{1 - F(s)} \\
&= \frac{1 - \left(1 - e^{-\lambda(s+x)}\right)}{1 - (1 - e^{-\lambda s})} \\
&= \frac{e^{-\lambda(s+x)}}{e^{-\lambda s}} \\
&= \frac{e^{-\lambda s - \lambda x}}{e^{-\lambda s}} \\
&= e^{-\lambda x} \\
&= 1 - F(x) \\
&= \Pr(X > x)
\end{aligned}$$

and we're done!

Problem 3: Suppose $X \sim \mathit{Exponential}(1/\lambda)$, and $Y \mid X \sim \mathit{Poisson}(X)$. Show that $Y \sim \mathit{Geometric}(1/(1 + \lambda))$.

Solution:

Note that we can write $f(x, y) = f(y \mid x)f(x)$, and $f(y) = \int f(x, y)dx$. Then

$$f(x, y) = \left(\frac{1}{\lambda} e^{-x/\lambda}\right)\left(\frac{x^y e^{-x}}{y!}\right)$$

And so,

$$\begin{aligned} f(y) &= \int f(x,y)dx \\ &= \int \left(\frac{1}{\lambda}e^{-x/\lambda}\right)\left(\frac{x^y e^{-x}}{y!}\right)dx \\ &= \frac{1}{\lambda y!}\int x^y e^{-x(1+\lambda)/\lambda}dx \end{aligned}$$

And we can again use integration by parts! Let $u = x^y$ and $dv = e^{-x(1+\lambda)/\lambda}dx$. Then we have $du = yx^{y-1}dx$ and $v = -\frac{\lambda}{1+\lambda}e^{-x(1+\lambda)/\lambda}$, and we can write

$$\begin{aligned} f(y) &= \frac{1}{\lambda y!}\int x^y e^{-x(1+\lambda)/\lambda}dx \\ &= \frac{1}{\lambda y!}\left(-x^y\frac{\lambda}{1+\lambda}e^{-x(1+\lambda)/\lambda}\Big|_{x=0}^{x=\infty} + \int \frac{\lambda}{1+\lambda}e^{-x(1+\lambda)/\lambda}yx^{y-1}dx\right) \\ &= \frac{1}{\lambda y!}\left(\int \frac{\lambda}{1+\lambda}e^{-x(1+\lambda)/\lambda}yx^{y-1}dx\right) \\ &= \frac{1}{\lambda y!}\left(\frac{\lambda}{1+\lambda}\right)y\left(\int e^{-x(1+\lambda)/\lambda}x^{y-1}dx\right) \end{aligned}$$

This *looks* gross, but it's actually not so bad. Note that, since Y is Poisson, it can only take integer values beginning at 1! Then we can *repeat* the process of integration by parts y *times* in order to get rid of $x^{y\cdots}$ term on the inside of the integral. Specifically, each time we do this process we will pull out a $\left(\frac{\lambda}{1+\lambda}\right)$, and a $y-i$ for the ith integration by parts step (try this one or two steps for yourself to see how it will simplify if you find this unintuitive!). We end up with,

$$\begin{aligned} f(y) &= \frac{1}{\lambda y!}\left(\frac{\lambda}{1+\lambda}\right)^y y! \\ &= \frac{1}{\lambda}\left(\frac{\lambda}{1+\lambda}\right)^y \end{aligned}$$

Now let $p = \frac{1}{1+\lambda}$. If we can show that $f(y) \sim Geometric(p)$ then we're done. Note that $1-p = \lambda/(1+\lambda)$. We have

$$
\begin{aligned}
f(y) &= \frac{1}{\lambda}(1-p)^y \\
&= \frac{1}{\lambda}(1-p)^{y-1}(1-p) \\
&= (1-p)^{y-1}\frac{1}{\lambda}\left(\frac{\lambda}{1+\lambda}\right) \\
&= (1-p)^{y-1}\left(\frac{1}{1+\lambda}\right) \\
&= (1-p)^{y-1}p
\end{aligned}
$$

which is exactly the pdf of a geometric random variable with parameter p and trials that begin at 1.

An *alternative* solution (which perhaps embodies the phrase "work smarter, not harder") actually doesn't involve integration by parts at all! As statisticians, we typically like to avoid actually integrating anything whenever possible, and this is often achieved by manipulating algebra enough to essentially "create" a pdf out of what we see (since pdfs integrate to 1!). Massive props to a student for solving this problem in a much "easier" way, answer below:

$$
\begin{aligned}
f(y) &= \int_0^\infty f(y \mid x) f(x) dx \\
&= \int_0^\infty (\frac{1}{\lambda} e^{-\frac{x}{\lambda}})(\frac{x^y}{y!} e^{-x}) dx \\
&= \frac{1}{\lambda y!} \int_0^\infty x^y e^{-\frac{x}{\lambda}(1+\lambda)} dx \\
&= \frac{1}{\lambda y!} \int_0^\infty \frac{(\frac{1+\lambda}{\lambda})^{y+1}}{(\frac{1+\lambda}{\lambda})^{y+1}} \frac{\Gamma(y+1)}{\Gamma(y+1)} x^{(y+1)-1} e^{-\frac{x}{\lambda}(1+\lambda)} dx \\
&= \frac{\Gamma(y+1)}{\lambda y! (\frac{1+\lambda}{\lambda})^{y+1}} \int_0^\infty \frac{(\frac{1+\lambda}{\lambda})^{y+1}}{\Gamma(y+1)} x^{(y+1)-1} e^{-\frac{x}{\lambda}(1+\lambda)} dx \\
&= \frac{\Gamma(y+1)}{\lambda y! (\frac{1+\lambda}{\lambda})^{y+1}} (1) \\
&= \frac{y!}{\lambda y! (\frac{1+\lambda}{\lambda})^{y+1}} \\
&= \frac{\lambda^{-1}}{(\frac{1+\lambda}{\lambda})^{y+1}} \\
&= \frac{\lambda^y}{(1+\lambda)^{y+1}} \\
&= \frac{1}{(1+\lambda)} \frac{\lambda^y}{(1+\lambda)^y} \\
&= \frac{1}{(1+\lambda)} (1 - \frac{1}{(1+\lambda)})^y \\
&= p(1-p)^y \qquad (\text{where } p = \frac{1}{1+\lambda})
\end{aligned}
$$

Note that we arrive at a slightly different answer with this approach. Specifically, we arrive at the pdf of a geometric random variable with parameter p and trials that begin at 0, as opposed to 1. There's some subtlety here that we're going to choose to ignore.

Problem 4: Suppose that $X \sim N(\mu, \sigma^2)$, and let $Y = \frac{X-\mu}{\sigma}$. Find the distribution of Y (simplifying all of your math will be useful for this problem).

Solution:

To solve this problem, we can use the theorem on transforming continuous random variables. We must first define our function g that relates X and Y. In this case, we have $g(a) = \frac{a-\mu}{\sigma}$. Now all we need to do is collect the mathematical "pieces" we need to use theorem: $g^{-1}(a)$, and $g'(a)$, and finally, the pdf of a normal random variable. We have

$$
\begin{aligned}
f_X(x) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2\sigma^2}(x-\mu)^2) \\
g^{-1}(a) &= \sigma a + \mu \\
g'(a) &= \frac{\partial}{\partial a}\left(\frac{a-\mu}{\sigma}\right) = \frac{1}{\sigma}
\end{aligned}
$$

Putting it all together, we have

$$
\begin{aligned}
f_Y(y) &= f_X(g^{-1}(y)) \times \frac{1}{g'(g^{-1}(y))} \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2\sigma^2}(\sigma y + \mu - \mu)^2) \times \sigma \\
&= \frac{1}{\sqrt{2\pi}\sigma} \exp(-\frac{1}{2\sigma^2}(\sigma y)^2) \times \sigma \\
&= \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2\sigma^2}\sigma^2 y^2) \\
&= \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2} y^2)
\end{aligned}
$$

and note that this is the pdf of a normally distributed random variable with mean 0 and variance 1! Thus, we have shown that $\frac{X-\mu}{\sigma} \sim N(0,1)$. **Fun Fact:** If this random variable reminds you of a Z-score, *it should*!

Problem 5: Suppose the joint pdf of two random variables X and Y is given by $f_{X,Y}(x,y) = \lambda\beta e^{-x\lambda - y\beta}$. Determine if X and Y are independent, showing why or why not.

Solution:

To determine whether X and Y are independent (or not), we need to determine if their joint pdf is "separable." Doing some algebra, we can see that

$$
\begin{aligned}
f_{X,Y}(x,y) &= \lambda\beta e^{-x\lambda - y\beta} \\
&= \lambda\beta e^{-x\lambda} e^{-y\beta} \\
&= \left(\lambda e^{-x\lambda}\right)\left(\beta e^{-y\beta}\right)
\end{aligned}
$$

and so since we can write the joint distribution as a function of X multiplied by a function of Y, X and Y are independent (and in this case, both have exponential distributions).

Problem 6: Suppose the joint pdf of two random variables X and Y is given by $f_{X,Y}(x,y) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\binom{n}{y}x^{y+\alpha-1}(1-x)^{n-y+\beta-1}$. Determine if X and Y are independent, showing why or why not.

Solution:

To determine whether X and Y are independent (or not), we need to determine if their joint pdf is "separable." Right away, we should note that a piece of the pdf contains x^y, and therefore we are *never* going to be able to fully separate out this joint pdf into a function of x times a function y. Therefore, X and Y are *not* independent. In this case, we actually have $X \sim Beta(\alpha, \beta)$, and $Y \mid X \sim Binomial(n, y)$ (we'll return to this example in the Bayes chapter!).

Problem 7: Let X and Y be independent random variables with $X \sim Exponential(1)$ and $Y \sim Exponential(1)$. Find the joint distribution of $Z = X - Y$ and $W = X + Y$, and use this joint distribution to show that $Z \sim Laplace(0, 1)$.

Solution:

Let X and Y be independent random variables with $X \sim Exponential(1)$ and $Y \sim Exponential(1)$. Find the joint distribution of $Z = X - Y$ and $W = X + Y$, and use this joint distribution to show that $Z \sim Laplace(0, 1)$.

We'll need a couple things before we can directly apply the Jacobian method:

- The joint distribution, $\pi_{X,Y}(x, y)$
- Our function $f(x, y)$ and its inverse
- Our Jacobian matrix, given by $J_f(z, w) = \begin{pmatrix} \frac{\partial x}{\partial z} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial z} & \frac{\partial y}{\partial w} \end{pmatrix}$
- Our Jacobian, given by $\left| J_f(z, w) \right|$
- The support of the joint distribution $\pi_{Z,W}(z, w)$ (we'll do this step at the end).

Since X and Y are independent, we have

$$\pi_{X,Y}(x, y) = e^{-x}e^{-y} = e^{-x-y}$$

Now we must determine what our function f is, and its inverse. From the problem set-up, we have $f(x, y) \longmapsto (x - y, x + y)$. To find the inverse function, we can rearrange these outputs

to define x and y solely in terms of z and w. Some algebra included below:

$$\begin{aligned}
x &= z + y \\
y &= w - x \\
x &= z + w - x \\
2x &= z + w \\
x &= \frac{z+w}{2} \quad \text{(Our first equation)!} \\
y &= w - \frac{z+w}{2} \\
y &= \frac{2w - z - w}{2} \\
y &= \frac{w-z}{2} \quad \text{(Our second equation!)}
\end{aligned}$$

Which gives us $f^{-1}(z,w) \longmapsto (\frac{z+w}{2}, \frac{w-z}{2})$. The Jacobian matrix is then given by

$$J_f(z,w) = \begin{pmatrix} \frac{\partial(\frac{z+w}{2})}{\partial z} & \frac{\partial(\frac{z+w}{2})}{\partial w} \\ \frac{\partial(\frac{w-z}{2})}{\partial z} & \frac{\partial(\frac{w-z}{2})}{\partial w} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{-1}{2} & \frac{1}{2} \end{pmatrix}$$

and the Jacobian is given by $|J_f(z,w)| = (1/2)(1/2) - (1/2)(-1/2) = 1/2$.

Now we determine the support of the distribution $\pi_{Z,W}(z,w)$. Since X and Y are exponential, we know that

$$\begin{aligned}
0 \leq x < \infty \\
0 \leq y < \infty
\end{aligned}$$

Plugging in some things and rearranging, we get

$$\begin{aligned}
0 &\leq \frac{z+w}{2} < \infty \\
0 &\leq z + w < \infty \\
-z &\leq w < \infty \quad \text{(or)} - w \leq z < \infty
\end{aligned}$$

and

$$\begin{aligned}
0 &\leq \frac{w-z}{2} < \infty \\
0 &\leq w - z < \infty \\
z &\leq w < \infty
\end{aligned}$$

Putting these together, we have $-w \leq z \leq w < \infty$, so the support for z, marginally is given by $[-w, w]$. The support for w, marginally, is given by $[0, \infty)$, since it is a sum of two random

variables that have that same support. Note that this therefore means z can range from $(-\infty, \infty)$, depending on the value of w.

We can now finally apply the Jacobian method to obtain $\pi_{Z,W}(z,w)$ using the separate pieces we have calculated, obtaining:

$$\begin{aligned}
\pi_{Z,W}(z,w) &= \pi_{X,Y}(f^{-1}(z,w)) \times |J_f(z,w)| \times I\{-w \leq z \leq w, 0 \leq w < \infty\} \\
&= \exp(-\frac{z+w}{2} - \frac{w-z}{2}) \times \frac{1}{2} \times I\{-w \leq z \leq w, 0 \leq w < \infty\} \\
&= \frac{1}{2}\exp(\frac{-z-w-w+z}{2}) \times I\{-w \leq z \leq w, 0 \leq w < \infty\} \\
&= \frac{1}{2}e^{-w} \times I\{-w \leq z \leq w, 0 \leq w < \infty\}
\end{aligned}$$

Now that we have the joint distribution $\pi_{Z,W}(z,w)$, we must integrate with respect to W to get the marginal distribution of Z. Recall that we have both $-z \leq w < \infty$ and $z \leq w < \infty$, so we consider these two cases separately. We have

$$\pi_Z(z) = \begin{cases} \int_z^\infty \frac{1}{2}e^{-w}dw = -\frac{1}{2}e^{-w}\Big|_z^\infty = \frac{1}{2}e^{-z} & 0 \leq z < \infty \\ \int_{-z}^\infty \frac{1}{2}e^{-w}dw = -\frac{1}{2}e^{-w}\Big|_{-z}^\infty = \frac{1}{2}e^{z} & -\infty < z \leq 0 \end{cases}$$

which can equivalently be written as

$$\pi_Z(z) = \frac{1}{2}e^{-|z|} \quad -\infty < z < \infty$$

which implies $Z \sim Laplace(0,1)$.

2 Maximum Likelihood Estimation

In *Probability*, you calculated probabilities of events by assuming a probability model for data and then *assuming you knew the value of the parameters* in that model. In *Mathematical Statistics*, we will similarly write down a probability model but then we will use observed data to *estimate the value of the parameters* in that model.

There is more than one technique that you can use to estimate the value of an unknown parameter. You're already familiar with one technique—**least squares estimation**—from *STAT 155*. We'll review the ideas behind that approach later in the course. To start, we'll explore two other widely used estimation techniques: **maximum likelihood estimation** (this chapter) and the **method of moments** (next chapter).

Introduction to MLE

To understand maximum likelihood estimation, we can first break down each individual word in that phrase: (1) maximum, (2) likelihood, (3) estimation. We'll start in reverse order.

Recall from your introductory statistics course that we are (often) interested in estimating *true, unknown* ***parameters*** in statistics, using some data. Our best guess at the truth, based on the data we observe / sample that we have, is an ***estimate*** of the truth (given some modeling assumptions). This is all the "estimation" piece is getting at here. We're going to be learning about a method that produces estimates!

The likelihood piece may be less familiar to you. A likelihood is essentially a fancy form of a function (see the Definitions section for an *exact* definition), that combines an assumed probability distribution for your data, with some unknown parameters.* The key here is that a likelihood is a *function*. It may *look* more complicated than a function like $y = mx + b$, but we can often manipulate them in a similar fashion, which comes in handy when trying to find the…

Maximum! We've maximized functions before, and we can do it again! There are ways to maximize functions numerically (using certain algorithms, such as Newton-Raphson for example, which we'll cover in a later chapter), but we will primarily focus on maximizing likelihoods *analytically* in this course to help us build intuition.

Recall from calculus: To maximize a function we…

1. Take the derivative of the function

2. Set the derivative equal to zero
3. Solve!
4. (double check that the second derivative is negative, so that it's actually a maximum as opposed to a minimum)
5. (also check the endpoints)

The last two steps we'll often skip in this class, since things have a tendency to work out nicely with most likelihood functions. If we are trying to maximize a likelihood with *multiple* parameters, there a few different ways we can go about this. One way (which is nice for distributions like the multivariate normal) is to place all of the parameters in a vector, write the distribution in terms of matrices and vectors, and then use matrix algebra to obtain all of the MLEs for each parameter at once! An alternative way is to take *partial* derivatives of the likelihood function with respect to each parameter, and solve a *system* of equations to obtain MLEs for each parameter. We'll see an example of this in Problem Set 1 as well as Worked Example 2!

One final thing to note (before checking out worked examples and making sure you have a grasp on definitions and theorems) is that it is often *easier* to maximize the *log-likelihood* as opposed to the the likelihood… un-logged. This is for a variety of reasons, one of which is that many common probability density functions contain some sort of e^x term, and logging (*natural* logging) simplifies that for us. Another one is that log rules sometimes make taking derivatives easier. The value of a parameter that maximizes the log-likelihood is the same value that maximizes the likelihood, un-logged (since log is a monotone, increasing function). This is truly just a convenience thing!

When maximizing the "usual" way doesn't work…

To maximize a function what I'm calling the "usual" way involves the five steps listed above. Unfortunately, sometimes this doesn't work. We typically recognize that the process won't work once we get to step 3, and realize that "solving" ends up giving us an MLE that doesn't depend at all on our data. When this happens, it's usually because the MLE is an *order statistic* (see Definitions section of this chapter), and usually because the distribution of our random variable has a range that depends on our unknown parameter. An example of this (that will appear on your homework) occurs when $X_1, \ldots, X_n \sim \text{Uniform}(0, \theta)$. In this case, the range of X_i depends directly on θ, since it cannot be any *greater than* θ.

In these cases, the process of finding the MLE for our unknown parameter usually involves plotting the likelihood as a function of the unknown parameter. We then look at where that function achieves its maximum (usually at one of the endpoints), and determine which observation (again, typically the minimum or maximum) will maximize our likelihood.

Maximum Likelihood: Does it make sense? Is it even "good"?

Let's think for a minute about why maximum likelihood, as a procedure for producing estimates of parameters, might make sense. Given a distributional assumption* (a probability density function) for *independent* random variables, we define a "likelihood" as a product of their densities. We can think of this intuitively as just the "likelihood" or "chance" that our data occurs, given a specific distribution. Maximum likelihood estimators then tell us, given that assumed likelihood, **what parameter values make our observed data *most likely*** to have occurred.

So. Does it make sense? I would argue, intuitively, yes! Yes, it does. Is it good? That's perhaps a different question with a more complicated answer. It's a good baseline, certainly, and foundational to *much* of statistical theory. We'll see in a later chapter that maximum likelihood estimates have good properties related to having minimal variance among a larger class of estimators (yay!), but the maximum likelihood estimators we will consider in this course rely on *parametric* assumptions (i.e. we assume that the data follows a specific probability distribution in order to calculate MLEs). There are ways around these assumptions, but they are outside the scope of our course.

*🌶️ Note that distributions are only involved in *parametric* methods, as opposed to non-parametric and semi-parametric methods, the latter of which are for independent study or a graduate course in statistics!

Relation to Least-Squares

Recall that we typically write a simple linear regression model in one of two ways. For n observations $X_1, \dots, X_n$ with outcomes $Y_1, \dots, Y_n$, we can write

$$E[Y_i \mid X_i] = \beta_0 + \beta_1 X_i$$

or we can write

$$Y_i = \beta_0 + \beta_1 X_i + \epsilon_i$$

where $E[\epsilon_i] = 0$. The latter equation makes it more clear where residuals come into play (they are just given by ϵ_i), and the former perhaps makes it more clear why the word "average" usually finds its way into our interpretations of regression coefficients. The second form, however, allows us to make it more clear how we would write up a "least-squares" equation.

Recall that the least-squares line (or, line of "best" fit) is the line that minimizes the *sum of squared residuals*. Parsing these words out, note that our residuals can be written as

$$\epsilon_i = Y_i - \beta_0 - \beta_1 X_i.$$

Squared residuals are then written as

$$\epsilon_i^2 = (Y_i - \beta_0 - \beta_1 X_i)^2,$$

and finally, the *sum* of squared residuals is given by

$$\sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 X_i)^2$$

We can find what values of β_0 and β_1 minimize this sum by taking partial derivatives, setting equations equal to zero, and solving. It turns out that if let $\epsilon_i \overset{iid}{\sim} N(0, \sigma^2)$ where σ^2 is *known*, then the MLE for β_0 and β_1 are equivalent to the values of β_0 and β_1 that minimize the sum of squared residuals!

2.1 Learning Objectives

By the end of this chapter, you should be able to…

- Derive maximum likelihood estimators for parameters of common probability density functions
- Calculate maximum likelihood estimators "by hand" for common probability density functions
- Explain (in plain English) why maximum likelihood estimation is an intuitive approach to estimating unknown parameters using a combination of (1) observed data, and (2) a distributional assumption

2.2 Concept Questions

1. What is the intuition behind the maximum likelihood estimation (MLE) approach?
2. What are the typical steps to find a MLE?
3. Are there ever situations when the typical steps to finding a MLE don't work? If so, what can we do instead to find the MLE?
4. How do the steps to finding a MLE change when we have more than one unknown parameter?

2.3 Definitions

You are expected to know the following definitions:

Parameter

In a frequentist* framework, a parameter is a *fixed*, unknown truth (very philosophical). By fixed, I mean "not random". We assume that there is some true unknown value, governing the generation of all possible random observations of all possible people and things *in the whole world*. We sometimes call this unknown governing process the "superpopulation" (think: all who ever have been, all who are, and all who ever will be).

Practically speaking, parameters are things that we want to estimate, and we will estimate them using observed data!

*Two main schools of thought in statistics are: (1) Frequentist (everything you've ever learned so far in statistics, realistically), and (2) Bayesian. We'll cover the latter, and differences between the two, in a later chapter. There's also technically Fiducial inference as a third school of thought, but that one's never been widely accepted.

Statistic/Estimator

A statistic (or "estimator") is a function of your data, used to "estimate" an unknown parameter. Often, statistics/estimators will be functions of *means* or averages, as we'll see in the worked examples for this chapter!

Likelihood Function

Let $x_1, \ldots, x_n$ be a sample of size n of independent observations from the probability density function $f_X(x \mid \theta)$, where θ is a set of unknown parameters that define the pdf. Then the likelihood function $L(\theta)$ is the product of the pdf evaluated at each x_i,

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

Note that this *looks* exactly like the joint pdf for n independent random variables, but it is *interpreted* differently. A likelihood is a function of *parameters*, given a set of observations (random variables). A joint pdf is a function of random variables.

Note: The likelihood function is one of the reasons why we like independent observations so much! If observations aren't independent, we can't simply multiply all of their pdfs together to get a likelihood function.

Maximum Likelihood Estimate (MLE)

Let $L(\theta) = \prod_{i=1}^{n} f_X(x_i \mid \theta)$ be the likelihood function corresponding to a random sample of observations $x_1, \ldots, x_n$. If θ_e is such that $L(\theta_e) \geq L(\theta)$ for all possible values θ, then θ_e is called a *maximum likelihood estimate* for θ.

Log-likelihood

In statistics, when we say "log," we essentially always mean "ln" (or, natural log). The log-likelihood is then, hopefully unsurprisingly, given by $\log(L(\theta))$. One thing that's useful to note (and will come in handy when calculating MLEs, is that the log of a product is equal to a sum of logs. For likelihoods, that means

$$\log(L(\theta)) = \log\left(\prod_{i=1}^{n} f_X(x_i \mid \theta)\right) = \sum_{i=1}^{n} \log(f_X(x_i \mid \theta))$$

This will end up making it *much* easier to take derivatives than needing to deal with products!

Order Statistic

The kth order statistic is equal to a sample's kth smallest value. Practically speaking, there are essentially three order statistics we typically care about: the minimum, the median, and the maximum. We denote the minimum (or, first order statistic) in a sample of random variables $X_1, \ldots, X_n$ as $X_{(1)}$, the maximum as $X_{(n)}$, and the median $X_{(m+1)}$ where $n = 2m + 1$ *when* n *is odd*. Note that median is in fact not an order statistic if n is even (since the median is an average of two values, $X_{(m)}$ and $X_{(m+1)}$, in this case.

2.4 Theorems

None for this chapter!

2.5 Worked Examples

Problem 1: Suppose we observe n independent observations $X_1, \ldots, X_n \sim Bernoulli(p)$, where $f_X(x) = p^x(1-p)^{1-x}$. Find the MLE of p.

Solution:

We can write the likelihood function as

$$L(p) = \prod_{i=1}^{n} p^{x_i}(1-p)^{1-x_i}$$

Then the log-likelihood is given by

$$
\begin{aligned}
\log(L(p)) &= \log\left[\prod_{i=1}^{n} p^{x_i}(1-p)^{1-x_i}\right] \\
&= \sum_{i=1}^{n} \log\left[p^{x_i}(1-p)^{1-x_i}\right] \\
&= \sum_{i=1}^{n} \left[\log(p^{x_i}) + \log((1-p)^{1-x_i})\right] \\
&= \sum_{i=1}^{n} \left[x_i \log(p) + (1-x_i)\log(1-p)\right] \\
&= \log(p)\sum_{i=1}^{n} x_i + \log(1-p)\sum_{i=1}^{n}(1-x_i) \\
&= \log(p)\sum_{i=1}^{n} x_i + \log(1-p)(n-\sum_{i=1}^{n} x_i)
\end{aligned}
$$

We can take the derivative of the log-likelihood with respect to p, and set it equal to zero…

$$
\begin{aligned}
\frac{\partial}{\partial p}\log(L(p)) &= \frac{\partial}{\partial p}\left[\log(p)\sum_{i=1}^{n} x_i + \log(1-p)(n-\sum_{i=1}^{n} x_i)\right] \\
&= \frac{\sum_{i=1}^{n} x_i}{p} - \frac{n-\sum_{i=1}^{n} x_i}{1-p} \\
0 &\equiv \frac{\sum_{i=1}^{n} x_i}{p} - \frac{n-\sum_{i=1}^{n} x_i}{1-p} \\
\frac{\sum_{i=1}^{n} x_i}{p} &= \frac{n-\sum_{i=1}^{n} x_i}{1-p} \\
(1-p)\sum_{i=1}^{n} x_i &= p(n-\sum_{i=1}^{n} x_i) \\
\sum_{i=1}^{n} x_i - p\sum_{i=1}^{n} x_i &= pn - p\sum_{i=1}^{n} x_i \\
\sum_{i=1}^{n} x_i &= pn \\
\frac{1}{n}\sum_{i=1}^{n} x_i &= p
\end{aligned}
$$

and by solving for p, we get that the MLE of p is equal to $\frac{1}{n}\sum_{i=1}^{n} x_i$. We will *often* see

that the MLEs of parameters are functions of sample averages (in this case, just the identity function!).

Problem 2: Suppose $X_1, X_2, \ldots, X_n$ are a random sample from the Normal pdf with parameters μ and σ^2:

$$f_X(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2},$$

for $-\infty < x < \infty$, $-\infty < \mu < \infty$, and $\sigma^2 > 0$. Find the MLEs of μ and σ^2. (Note that this is Question 5 on the MLE section of Problem Set 1! For your HW, try your best to do this problem from scratch, without looking at the course notes!)

Solution:

Since we are dealing with a likelihood with two parameters, we'll need to solve a *system* of equations to obtain the MLEs for μ and σ^2.

$$\begin{aligned}
\log(L(\mu, \sigma^2)) &= \log(\prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp(-\frac{1}{2\sigma^2}(x_i - \mu)^2)) \\
&= \sum_{i=1}^{n} \left[\log(\frac{1}{\sqrt{2\pi\sigma^2}}) - \frac{1}{2\sigma^2}(x_i - \mu)^2 \right] \\
&= \sum_{i=1}^{n} \left[-\frac{1}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(x_i - \mu)^2 \right] \\
&= \frac{-n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i - \mu)^2
\end{aligned}$$

Now we need to find $\frac{\partial}{\partial\sigma^2}\log(L(\mu, \sigma^2))$ and $\frac{\partial}{\partial\mu}\log(L(\mu, \sigma^2))$. Let's make our lives a little bit easier by setting $\sigma^2 \equiv \theta$ (so we don't trip ourselves up with the exponent). We get

$$\begin{aligned}
\frac{\partial}{\partial\theta}\log(L(\mu, \theta)) &= \frac{\partial}{\partial\theta}\left(\frac{-n}{2}\log(2\pi\theta) - \frac{1}{2\theta}\sum_{i=1}^{n}(x_i - \mu)^2 \right) \\
&= \frac{-2\pi n}{4\pi\theta} + \frac{\sum_{i=1}^{n}(x_i - \mu)^2}{2\theta^2} \\
&= \frac{-n}{2\theta} + \frac{\sum_{i=1}^{n}(x_i - \mu)^2}{2\theta^2}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial}{\partial \mu}\log(L(\mu,\theta)) &= \frac{\partial}{\partial \mu}\left(\frac{-n}{2}\log(2\pi\theta) - \frac{1}{2\theta}\sum_{i=1}^{n}(x_i-\mu)^2\right) \\
&= \frac{\partial}{\partial \mu}\left(-\frac{1}{2\theta}\sum_{i=1}^{n}(x_i^2 - 2\mu x_i + \mu^2)\right) \\
&= \frac{\partial}{\partial \mu}\left(-\frac{1}{2\theta}(\sum_{i=1}^{n}x_i^2 - 2\mu\sum_{i=1}^{n}x_i + n\mu^2)\right) \\
&= \frac{\partial}{\partial \mu}\left(-\frac{1}{2\theta}(-2\mu\sum_{i=1}^{n}x_i + n\mu^2)\right) \\
&= \frac{\partial}{\partial \mu}\left(\frac{\sum_{i=1}^{n}x_i}{\theta}\mu - \frac{n}{2\theta}\mu^2\right) \\
&= \frac{\sum_{i=1}^{n}x_i}{\theta} - \frac{n}{\theta}\mu
\end{aligned}$$

We now have the following system of equations to solve:

$$\begin{aligned}
0 &\equiv \frac{-n}{2\theta} + \frac{\sum_{i=1}^{n}(x_i-\mu)^2}{2\theta^2} \\
0 &\equiv \frac{\sum_{i=1}^{n}x_i}{\theta} - \frac{n}{\theta}\mu
\end{aligned}$$

Typically, we solve one of the equations for *one* of the parameters, plug that into the other equation, and then go from there. We'll start by solving the second equation for μ.

$$\begin{aligned}
0 &= \frac{\sum_{i=1}^{n}x_i}{\theta} - \frac{n}{\theta}\mu \\
\frac{n}{\theta}\mu &= \frac{\sum_{i=1}^{n}x_i}{\theta} \\
\mu &= \frac{1}{n}\sum_{i=1}^{n}x_i
\end{aligned}$$

Well that's convenient! We already have the MLE for μ as being just the sample average. Plugging this into the first equation in our system we obtain

$$
\begin{aligned}
0 &= \frac{-n}{2\theta} + \frac{\sum_{i=1}^{n}(x_i - \mu)^2}{2\theta^2} \\
0 &= \frac{-n}{2\theta} + \frac{\sum_{i=1}^{n}(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)^2}{2\theta^2} \\
\frac{n}{2\theta} &= \frac{\sum_{i=1}^{n}(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)^2}{2\theta^2} \\
n &= \frac{\sum_{i=1}^{n}(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)^2}{\theta} \\
\theta &= \frac{1}{n}\sum_{i=1}^{n}(x_i - \frac{1}{n}\sum_{i=1}^{n} x_i)^2] \\
\theta &= \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2
\end{aligned}
$$

where $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$. And so finally, we have that the MLE for σ^2 is given by $\frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2$, and the MLE for μ is given by $\bar{x}$!

3 Method of Moments

At this point in the course, we've now seen one (hopefully intuitive) way to obtain estimators for unknown parameters in probability distributions: maximum likelihood estimation. An alternative approach to producing a "reasonable" estimator for an unknown parameter is called the "Method of Moments." As the name implies, this method uses moments to derive estimators! Recall from probability theory that the rth moment of a probability distribution for X is given by $E[X^r]$. We can make use of relationships that between *theoretical* moments and *sample* moments to derive reasonable estimators!

In general, the steps involved in obtaining a MOM estimator are:

1. Determine how many equations are in the system we need to solve
2. Find the theoretical moments
3. Set theoretical moments equal to sample moments
4. Solve!

Why do we need more than one approach to obtain estimators?

We already have maximum likelihood estimation, and it seems reasonable, so why might we want another approach to obtaining estimates? A few reasons!

One is that estimators vary with regards their theoretical "properties" (as we'll see in the following chapters). These properties are one way to define how "good" an estimator is, and we ideally want our estimators to be the best of the best.

Another reason why we might sometimes want another approach to obtaining estimators, quite frankly, is that maximum likelihood estimators are sometimes a pain to calculate. In some cases, there isn't even a closed form solution for the parameter we're trying to estimate. In these scenarios, we need numerical optimization in order to obtain maximum likelihood estimators. While numerical optimization isn't the end of the world (it's actually often quite easy to implement), it can be *very* computationally intensive for more complex likelihoods. In general, if we can obtain a closed form estimator *analytically* (via calculus/algebra, for example), we'll be better off in the long run.* With the method of moments approach, it is often much easier to obtain a closed form estimator analytically.

* This is mostly a function the fact that much statistics research focuses on developing new methods for solving problems and analyzing data (think: linear regression but fancier, linear regression but *new* somehow, etc.). Statistics is inherently practical. You (probably) want any methods that you develop to be practically usable by people who are perhaps not statisticians. No one is going to use your method if it takes an unreasonably long time to compute an estimator. Imagine how irritating it would be if it took your machine two days to compute linear regression coefficients in R, for example.

3.1 Learning Objectives

By the end of this chapter, you should be able to…

- Derive method of moments estimators for parameters of common probability density functions
- Explain (in plain English) why method of moments estimation is an intuitive approach to estimating unknown parameters

3.2 Concept Questions

1. What is the intuition behind the method of moments (MOM) procedure for estimating unknown parameters?
2. What are the typical steps to find a MOM estimator?
3. What advantages does the MOM approach offer compared to MLE?
4. Do the MOM and MLE approaches always yield the same estimate?

3.3 Definitions

You are expected to know the following definitions:

Theoretical Moment

The r^{th} *theoretical* moment of a probability distribution is given by $E[X^r]$. For example, when $r = 1$, the r^{th} moment is just the expectation of the random variable X.

Sample Moment

The r^{th} *sample* moment of a probability distribution is given by $\frac{1}{n}\sum_{i=1}^{n} x_i^r$, for a random sample of observations $x_1, \ldots, x_n$.

Method of Moments Estimates

Let $x_1, \ldots, x_n$ be a random sample of observations from the pdf $f_X(x \mid \theta)$. The method of moments estimates are then the solutions to the set of s equations given by

$$\begin{aligned} E[X] &= \frac{1}{n}\sum_{i=1}^{n} x_i \\ E[X^2] &= \frac{1}{n}\sum_{i=1}^{n} x_i^2 \\ &\vdots \\ E[X^s] &= \frac{1}{n}\sum_{i=1}^{n} x_i^s \end{aligned}$$

If our pdf depends on only a single unknown parameter, we only need to solve the first equation. If we have two unknown parameters, we need to solve the system of the first two equations. So on and so forth.

3.4 Theorems

None for this chapter!

3.5 Worked Examples

In general (for these worked examples *as well as the problem sets*), I do not expect you to calculate theoretical moments by hand. We practiced that in the probability review chapter, and now we can use those known theoretical moments to make our lives easier.

Problem 1: Suppose $X_1, \ldots, X_n \sim Poisson(\lambda)$. Find the MLE of λ *and* the MOM estimator of λ.

Solution:

To obtain the MLE, note that we can write the likelihood as

$$L(\lambda) = \prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}$$

and the log-likelihood as

$$\log(L(\lambda)) = \sum_{i=1}^{n} [x_i \log(\lambda) - \lambda - \log(x_i!)]$$

where I've used one "log rule" in the above to simplify: $\log(a^b) = b \times log(a)$. Taking the derivative of the log-likelihood and setting it equal to zero, we obtain

$$\begin{aligned}
\frac{\partial}{\partial \lambda} \log(L(\lambda)) &= \frac{1}{\lambda} \sum_{i=1}^{n} x_i - n \\
0 &\equiv \frac{1}{\lambda} \sum_{i=1}^{n} x_i - n \\
n &= \frac{1}{\lambda} \sum_{i=1}^{n} x_i \\
\lambda &= \frac{1}{n} \sum_{i=1}^{n} x_i
\end{aligned}$$

and so the MLE for λ is the sample average. To obtain the MOM estimator for λ, first note that the pdf contains only one parameter. Therefore, we only need to set the first theoretical moment equal to the first sample moment, and solve. Note that the first theoretical moment of a Poisson distribution is $E[X] = \lambda$, and so equating this to the first sample moment, we obtain that the MOM estimator for λ is again, just the sample average! Much "easier" to compute than the MLE, in this case.

Problem 2: Suppose $X_1, ..., X_n \sim Bernoulli(\theta)$. Find the MOM estimator for θ.

Solution:

Note that our pdf contains only one parameter. Then we only need to solve a "system" of one equation. We have

$$\begin{aligned}
E[X] &= \frac{1}{n} \sum_{i=1}^{n} x_i \\
\theta &= \frac{1}{n} \sum_{i=1}^{n} x_i
\end{aligned}$$

and we're done! The system is pretty easy to "solve" when the theoretical moment is exactly the parameter we're interested in.

Problem 3: Suppose $Y_1, ..., Y_n \sim Uniform(0, \theta)$. Find the MOM estimator for θ.

Solution:

Note that our pdf contains only one parameter. Then we only need to solve a "system" of one equation. We have

$$\begin{aligned} E[Y] &= \frac{1}{n}\sum_{i=1}^{n} y_i \\ \frac{\theta}{2} &= \frac{1}{n}\sum_{i=1}^{n} y_i \\ \theta &= 2\bar{y} \end{aligned}$$

And so the MOM estimator for θ is 2 times the sample mean. Note that this is an example where the MOM estimator and MLE are not the same (you derived the MLE on your first problem set)!

4 Properties of Estimators

Now that we've developed the tools for deriving estimators of unknown parameters, we can start thinking about different metrics for determining how "good" our estimators actually are. In general, we like our estimators to be:

- **Unbiased**: Our estimate should be estimating *what it's supposed to be estimating*, for lack of a better phrase. Bias (or, unbiased-ness, in this case) is related to accuracy. In introductory statistics, you likely discussed sample bias (or, whether or not the data you collect is representative of the population you are trying to make inference on) and information bias (or, whether the values of the data you collect are representative of the people who report them). If you have a biased sample or biased information, your estimates (think, regression coefficients) are likely going to misrepresent true relationships in the population.

  Bias of *estimates* has a very specific definition in statistical theory that is *distinct* from sample bias and information bias. Questions of sample bias and information bias are important to consider when collecting and analyzing data, and questions of whether or not our estimates are biased are important to consider *prior* to analyzing data.

- **Precise:** In short, if our estimates are wildly uncertain (think, gigantic confidence intervals), they'll essentially be of no use to us from a practical perspective. As an extreme example, consider how you would feel if a new cancer drug was released with *very* severe side-effects, but scientists noted that the drug would increase cancer patients expected survival time by somewhere between 1 and 700 days. Are we really certain enough, in this case, that the benefits of the drug outweigh the potential costs? What if instead, the expected survival time would increase between 650 and 700 days? Would that change your answer?

  These types of questions are precisely (ha!) why precision is important. Again, you've likely discussed precision (colloquially) in an introductory statistics course. In statistical theory, precision (similar to bias) has a very specific definition. So long as our estimates are unbiased, we want to minimize variance (and therefore increase precision) as much as we possibly can. Even at the same sample size, some estimates are more precise than others, which we'll explore in this chapter.

The Bias-Variance Trade-off

If you are familiar with machine learning techniques or models for prediction purposes more generally (as opposed to inference), you may have stumbled upon the phrase "bias-variance trade-off." In scenarios where we want to make good predictions for new observations using a statistical model, one way to measure how "well" our model is predicting new observations is through minimizing **mean squared error**. Intuitively, this is something we should *want* to minimize: "errors" (the difference between a predicted value and an observed value) are bad, we square them because the direction of the error (above or below) shouldn't matter too much, and average over them because we need a summary measure of all our errors combined, and an average seems reasonable. In statistical terms, mean squared error has a very specific definition (see below) as the expected value of what is sometimes called a *loss function* (where in this case, loss is defined as squared error loss). We'll return to this in the decision theory chapter of our course notes.

It just so happens that we can decompose mean squared error into a sum of two terms: the variance of our estimator + the bias of our estimator (squared). What this means for us is that two estimators may have the *exact same* MSE, but *very* different variances or biases (potentially). In general, if we hold MSE constant and imagine *increasing* the variance of our estimator, the bias would need to decrease accordingly to maintain the same MSE. This is where the "trade-off" comes from. MSE is an *incredibly* commonly used metric for assessing prediction models, but as we will see, doesn't necessarily paint a full picture in terms of how "good" an estimator is. Smaller MSE does not automatically imply "better estimator," just as smaller bias (in some cases) does not automatically imply "better estimator."

Sufficiency

Another property we like to have in an estimator (sometimes) is called *sufficiency*. I like to think about sufficiency in terms of minimizing the amount of information we need to retain in order to get a "complete picture" of what's going on. Suppose, for example, someone is allergic to tomatoes. Rather than listing *every food* that contains tomatoes and saying that they're allergic to each of them individually, they could just say that they're allergic to tomatoes and call it a day. Stating "tomatoes" is **sufficient** information in this case for us to get the whole picture of their allergies!

A similar concept applies to estimators. Recall from the MLE chapter of the notes that we previously showed that the MLE of a sample proportion is given by $\bar{X}$. If I want someone to be able to obtain the MLE for a sample proportion, I then have a few options. I could give them:

- Every observation I know, $x_1, \ldots, x_n$
- Just one number, the sample mean, $\frac{1}{n}\sum_{i=1}^{n} x_i$
- All my observations plus some extra information, just for fun!

It should hopefully be obvious that you don't need extra information for fun, but we *also* don't need to know the value of each individual observation. The sample mean is sufficient! Formal definitions and a relevant theorem to follow.

4.1 Learning Objectives

By the end of this chapter, you should be able to…

- Calculate bias and variance of various estimators for unknown parameters
- Explain the distinction between bias and variance colloquially in terms of precision and accuracy, and why these properties are important
- Compare estimators in terms of their relative efficiency
- Justify why there exists a bias-variance trade-off, and explain what consequences this may have when comparing estimators

4.2 Concept Questions

1. Intuitively, what is the difference between bias and precision?
2. What are the typical steps to checking if an estimator is unbiased?
3. How can we construct unbiased estimators?
4. If an estimator is unbiased, is it also *asymptotically* unbiased? If an estimator is asymptotically unbiased, is it necessarily unbiased?
5. When comparing estimators, how can we determine which estimator is more efficient?
6. Why might we care about sufficiency, particularly when thinking about the variance of unbiased estimators?
7. Describe, in your own words, what the Cramér-Rao inequality tells us.
8. What is the difference between a UMVUE and an efficient estimator? Does one imply the other?

4.3 Definitions

You are expected to know the following definitions:

Unbiased

An estimator $\hat{\theta} = g(X_1, \dots, X_n)$ is an unbiased estimator for θ if $E[\hat{\theta}] = \theta$, for all θ.

Asymptotically Unbiased

An estimator $\hat{\theta} = g(X_1, \dots, X_n)$ is an *asymptotically* unbiased estimator for θ if $\lim_{n\to\infty} E[\hat{\theta}] = \theta$.

Precision

The precision of a random variable X is given by $\frac{1}{Var(X)}$.

Mean Squared Error (MSE)

The mean squared error of an estimator is given by

$$MSE(\hat{\theta}) = E[(\hat{\theta} - \theta)^2] = Var(\hat{\theta}) + Bias(\hat{\theta})^2$$

Sufficient

For some function T, $T(X)$ is a sufficient statistic for an unknown parameter θ if the conditional distribution of X given $T(X)$ does not depend on θ. A "looser" definition is that the distribution of X must depend on θ *only through* $T(X)$.

Minimal Sufficiency

For some function T^*, $T^*(X)$ is a minimal sufficient statistic for an unknown parameter θ if $T^*(X)$ is sufficient, *and* for every other sufficient statistic $T(X)$. $T^*(X) = f(T(X))$ for some function f.

Complete

A statistic $T(X)$ is *complete* for an unknown parameter θ if

$$E[g(T(x))] \text{ is } \theta - \text{free} \implies g(T(x)) \text{ is constant, almost everywhere}$$

for a nice function g.

Importantly, it is *equivalent* to say that $T(X)$ is *complete* for an unknown parameter θ if

$$E[g(T(x))] = 0 \implies g(T(x)) = 0 \quad \text{almost everywhere}$$

Relative Efficiency

The relative efficiency of an estimator $\hat{\theta}_1$ with respect to an estimator $\hat{\theta}_2$ is the ratio $Var(\hat{\theta}_2)/Var(\hat{\theta}_1)$.

Uniformly Minimum-Variance Unbiased Estimator (UMVUE)

An estimator $\hat{\theta}^*$ is the UMVUE if, for all estimators $\hat{\theta}$ in the class of unbiased estimators Θ,

$$Var(\hat{\theta}^*) \leq Var(\hat{\theta})$$

Score

The score is defined as the first partial derivative with respect to θ of the log-likelihood function, given by

$$\frac{\partial}{\partial\theta} \log L(\theta \mid x)$$

Information Matrix

The information matrix* $I(\theta)$ for a collection of iid random variables $X_1, \ldots, X_n$ is the variance of the score, given by

$$I(\theta) = E\left[\left(\frac{\partial}{\partial\theta} \log L(\theta \mid x)\right)^2\right] = -E\left[\frac{\partial^2}{\partial\theta^2} \log L(\theta \mid x)\right]$$

Note that the above formula *is* in fact the variance of the score, since we can show that the *expectation* of the score is 0 (under some regularity conditions). This is shown as part of the proof of the C-R lower bound in the Theorems section of this chapter.

The information matrix is sometimes written in terms of a pdf for a single random variable as opposed to a likelihood. In this case, we have $I(\theta) = nI_1(\theta)$, where the $I_1(\theta)$ on the right-hand side is defined as $E\left[\left(\frac{\partial}{\partial\theta} \log f_X(x \mid \theta)\right)^2\right]$. Sometimes $I_1(\theta)$ is written without the subscript 1 which is a slight abuse of notation that is endlessly confusing (to me, at least). For this set of course notes, we'll always specify the information matrix in terms of a pdf for a single random variable with the subscript 1, for clarity.

*The information matrix is often referred to as the Fisher Information matrix, as it was developed by Sir Ronald Fisher. Fisher developed *much* of the core, statistical theory that we use today. He was also the founding chairman of the University of Cambridge Eugenics Society, and contributed to a large body of scientific work and public policy that promoted racist and classist ideals.

4.4 Theorems

Covariance Inequality (based on the Cauchy-Schwarz inequality)

Let X and Y be random variables. Then,

$$Var(X) \geq \frac{Cov(X,Y)^2}{Var(Y)}$$

The proof is quite clear on Wikipedia.

The Factorization Criterion for sufficiency

Consider a pdf for a random variable X that depends on an unknown parameter θ, given by $\pi(x \mid \theta)$. The statistic $T(x)$ is sufficient for θ if and only if $\pi(x \mid \theta)$ factors as:

$$\pi(x \mid \theta) = g(T(x) \mid \theta)h(x)$$

where $g(T(x) \mid \theta)$ depends on x only through $T(x)$, and $h(x)$ does not depend on θ.

Note that in the statistics literature this criterion is sometimes referred to as the Fisher-Neyman Factorization Criterion.

Two proofs available on Wikipedia. The one for the discrete-only case is more intuitive, if you'd like to look through one of them.

Lehmann-Scheffe Theorem

Suppose that a random variable X has pdf given by $f(x \mid \theta)$, and that $T^*(X)$ is such that for every* pair of points (x, y), the ratio of pdfs

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

does not depend on θ **if and only if** $T^*(x) = T^*(y)$. Then $T^*(X)$ is a minimal sufficient statistic for θ.

*every pair of points that have the same support as X.

Proof.

We'll utilize something called a likelihood ratio (literally a ratio of likelihoods) to prove this theorem. We'll also come back to likelihood ratios later in the Hypothesis Testing chapter!

Let θ_1 and θ_2 be two possible values of our unknown parameter θ. Then a likelihood ratio comparing densities evaluated at these two values is defined as

$$L_{\theta_1,\theta_2}(x) \equiv \frac{f(x \mid \theta_2)}{f(x \mid \theta_1)}$$

Our proof will proceed as follows:

1. We'll show that if $T(X)$ is sufficient, then $L_{\theta_1,\theta_2}(X)$ is a function of $T(X)$ $\forall$ θ_1, θ_2.
2. We'll show the converse: If $L_{\theta_1,\theta_2}(X)$ is a function of $T(X)$ $\forall$ θ_1, θ_2, then $T(X)$ is sufficient. This combined with (1) will show that $L_{\theta_1,\theta_2}(X)$ is a minimal sufficient statistic.
3. We'll use the above two statements to prove the theorem!

First, suppose that $T(X)$ is sufficient for θ. Then, by definition we can write

$$L_{\theta_1,\theta_2}(x) = \frac{f(x \mid \theta_2)}{f(x \mid \theta_1)} = \frac{g(T(x) \mid \theta_1)h(x)}{g(T(x) \mid \theta_2)h(x)} = \frac{g(T(x) \mid \theta_1)}{g(T(x) \mid \theta_2)}$$

and so $L_{\theta_1,\theta_2}(X)$ is a function of $T(x)$ $\forall$ θ_1, θ_2.

Second, assume WLOG that θ_1 is fixed, and denote our unknown parameter $\theta_2 = \theta$. We can rearrange our likelihood ratio as

$$\begin{aligned} L_{\theta_1,\theta}(x) &= \frac{f(x \mid \theta)}{f(x \mid \theta_1)} \\ f(x \mid \theta) &= L_{\theta_1,\theta}(x) f(x \mid \theta_1) \end{aligned}$$

and note that $L_{\theta_1,\theta}(x)$ is a function of $T(X)$ by assumption, and $f(x \mid \theta_1)$ is a function of x that does not depend on our unknown parameter θ. Then $T(X)$ satisfies the factorization criterion, and is therefore sufficient.

Let $T^{**}(X) \equiv L_{\theta_1,\theta_2}(X)$. Then the first two statements we have shown give us that

$$T(X) \text{ is sufficient} \iff T^{**}(X) \text{ is a function of } T(X)$$

and therefore $T^{**}(X)$ is a minimal sufficient statistic, by definition.

We'll now (officially) prove our theorem. By hypothesis of the theorem,

$$
\begin{aligned}
T^*(x) = T^*(y) &\iff \frac{f(y \mid \theta)}{f(x \mid \theta)} \text{ is } \theta - free \\
&\iff \frac{f(y \mid \theta_1)}{f(x \mid \theta_1)} = \frac{f(y \mid \theta_2)}{f(x \mid \theta_2)} \quad \forall \theta_1, \theta_2 \\
&\iff \frac{f(y \mid \theta_2)}{f(y \mid \theta_1)} = \frac{f(x \mid \theta_2)}{f(x \mid \theta_1)} \quad \forall \theta_1, \theta_2 \\
&\iff L_{\theta_1,\theta_2}(y) = L_{\theta_1,\theta_2}(x) \quad \forall \theta_1, \theta_2 \\
&\iff T^{**}(y) = T^{**}(x)
\end{aligned}
$$

Therefore $T^*(X)$ and $T^{**}(X)$ are equivalent. Since $T^{**}(X)$ is a minimal sufficient statistic, $T^*(X)$ is therefore also minimal sufficient.

Complete, Sufficient, Minimal

If $T(X)$ is complete and sufficient, then $T(X)$ is minimal sufficient.

Proof.

Just kidding! Prove it on your own and show it to me, if you want bonus points in my heart :)

Rao-Blackwell-Lehmann-Scheffe (RBLS)

Let $T(X)$ be a complete and sufficient statistic for unknown parameter θ, and let $\tau(\theta)$ be some function of θ. If there exists at least one unbiased estimator $\tilde{\tau}(X)$ for $\tau(\theta)$, then there exists a *unique* UMVUE $\hat{\tau}(T(X))$ for $\tau(\theta)$ given by

$$\hat{\tau}(T(X)) = E[\tilde{\tau}(X) \mid T(X)]$$

Why do we care? An important consequence of the RBLS Theorem is that if $T(X)$ is a complete and sufficient statistic for θ, then any function $\phi(T(X))$ is the UMVUE of its expectation $E[\phi(T(X))]$ (so long as the expectation is finite for all θ). This Theorem is therefore a *very* convenient way to find UMVUEs: (1) Find a complete and sufficient statistic for an unknown parameter, and (2) functions of that statistic are then the UMVUE for their expectation!

Proof.

To prove RBLS, we first must prove an Improvement Lemma and a Uniqueness Lemma.

Improvement Lemma. Suppose that $T(X)$ is a sufficient statistic for θ. If $\tilde{\tau}(X)$ is an unbiased estimator of $\tau(\theta)$, then $E[\tilde{\tau}(X) \mid T(X)]$ does not depend on θ (by sufficiency) and is also an estimator of $\tau(\theta)$, which (importantly) has smaller variance than $\tilde{\tau}(X)$.

Proof of Lemma. First, note that $E[\tilde{\tau}(X) \mid T(X)]$ is an unbiased estimator for $\tau(\theta)$, since

$$\begin{aligned} E[E[\tilde{\tau}(X) \mid T(X)]] &= E[\tilde{\tau}(X)] \qquad \text{(Law of Iterated Expectation)} \\ &= \tau(\theta) \qquad (\tilde{\tau}(X) \text{ is unbiased}) \end{aligned}$$

Then,

$$\begin{aligned} Var(\tilde{\tau}(X)) &= E[Var(\tilde{\tau}(X) \mid T(X))] + Var(E[\tilde{\tau}(X) \mid T(X)]) \\ &\geq Var(E[\tilde{\tau}(X) \mid T(X)]) \end{aligned}$$

and we're done! $E[\tilde{\tau}(X) \mid T(X)]$ has a smaller variance than $\tau(\tilde{X})$. Since both are unbiased, this is considered an "improvement" (hence the name of the Lemma).

Uniqueness Lemma. If $T(X)$ is complete, then for some unknown parameter θ and function of it $\tau(\theta)$, $\tau(\theta)$ has at most *one* unbiased estimator $\hat{\tau}(T(X))$ *that depends on* $T(X)$.

Proof of Lemma. Suppose, toward contradiction, that $\tau(\theta)$ has more than one unbiased estimator that depends on $T(X)$, given by $\tilde{\tau}(T(X))$ and $\hat{\tau}(T(X))$, $\tilde{\tau}(T(X)) \neq \hat{\tau}(T(X))$. Then

$$E[\tilde{\tau}(T(X)) - \hat{\tau}(T(X))] = \tau(\theta) - \tau(\theta) = 0 \quad \forall \theta$$

Let $g(T(X)) = \tilde{\tau}(T(X)) - \hat{\tau}(T(X))$. Since $T(X)$ is complete, and $E[g(T(X))] = 0$, this implies $\tilde{\tau}(T(X)) - \hat{\tau}(T(X)) = 0$, which means $\tilde{\tau}(T(X)) = \hat{\tau}(T(X))$. Contradiction.

Back to the proof of RBLS.

We've shown previously that $\hat{\tau}(T(X))$ is an unbiased estimator for $\tau\theta$ (law of iterated expectation). Let $\tau_1(X)$ be any other unbiased estimator for $\tau(\theta)$, and let $\tau_2(T(X)) = E[\tau_1(X) \mid T(X)]$. Then $\tau_2(T(X))$ is also unbiased for $\tau(\theta)$ (again, iterated expectation), and by the Uniqueness Lemma (since T is complete by supposition), $\hat{\tau}(T(X)) = \tau_2(T(X))$. But,

$$\begin{aligned} Var(\hat{\tau}(T(X))) &= Var(\tau_2(T(X))) \qquad (\hat{\tau} = \tau_2) \\ &\leq Var(\tau_1(T(X))) \qquad \text{(Improvement Lemma)} \end{aligned}$$

so $\hat{\tau}(T(X))$ is the UMVUE for $\tau(\theta)$, as desired.

Cramér-Rao Lower Bound

Let $f_Y(y \mid \theta)$ be a pdf with nice* conditions, and let $Y_1, \ldots, Y_n$ be a random sample from $f_Y(y \mid \theta)$. Let $\hat{\theta}$ be *any* unbiased estimator of θ. Then

$$
\begin{aligned}
Var(\hat{\theta}) &\geq \left\{ E\left[\left(\frac{\partial \log(L(\theta \mid y))}{\partial \theta} \right)^2 \right] \right\}^{-1} \\
&= -\left\{ E\left[\frac{\partial^2 \log(L(\theta \mid y))}{\partial \theta^2} \right] \right\}^{-1} \\
&= \frac{1}{I(\theta)}
\end{aligned}
$$

*our nice conditions that we need are that $f_Y(y \mid \theta)$ has continuous first- and second-order derivatives, which would quickly discover we need by looking at the form for the C-R lower bound, and that the set of values y where $f_Y(y \mid \theta) \neq 0$ does not depend on θ. If you are familiar with the concept of the "support" of a function, that is where this second condition comes from. The key here is that this condition allows to interchange derivatives and integrals, in particular, $\frac{\partial}{\partial \theta} \int f(x)dx = \int \frac{\partial}{\partial \theta} f(x)dx$, which we'll need to complete the proof.

Proof.

Let $X = \frac{\partial \log L(\theta|\mathbf{y})}{\partial \theta}$. By the Covariance Inequality,

$$
Var(\hat{\theta}) \geq \frac{Cov(\hat{\theta}, X)^2}{Var(X)}
$$

and so if we can show

$$
\begin{aligned}
\frac{Cov(\hat{\theta}, X)^2}{Var(X)} &= \left\{ E\left[\left(\frac{\partial \log(L(\theta \mid \mathbf{y}))}{\partial \theta} \right)^2 \right] \right\}^{-1} \\
&= \frac{1}{I(\theta)}
\end{aligned}
$$

then we're done, as this is the C-R lower bound. Note first that

$$
\begin{aligned}
E[X] &= \int x f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \left(\frac{\partial \log L(\theta \mid \mathbf{y})}{\partial \theta} \right) f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \left(\frac{\partial \log f_Y(\mathbf{y} \mid \theta)}{\partial \theta} \right) f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \frac{\frac{\partial}{\partial \theta} f_Y(\mathbf{y} \mid \theta)}{f_Y(\mathbf{y} \mid \theta)} f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \frac{\partial}{\partial \theta} f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \frac{\partial}{\partial \theta} \int f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \frac{\partial}{\partial \theta} 1 \\
&= 0
\end{aligned}
$$

This means that

$$
\begin{aligned}
Var[X] &= E[X^2] - E[X]^2 \\
&= E[X^2] \\
&= E\left[\left(\frac{\partial \log L(\theta \mid \mathbf{y})}{\partial \theta} \right)^2 \right]
\end{aligned}
$$

and

$$
\begin{aligned}
Cov(\hat{\theta}, X) &= E[\hat{\theta}X] - E[\hat{\theta}]E[X] \\
&= E[\hat{\theta}X] \\
&= \int \hat{\theta} x f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \hat{\theta} \left(\frac{\partial \log L(\theta \mid \mathbf{y})}{\partial \theta} \right) f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \hat{\theta} \left(\frac{\partial \log f_Y(\mathbf{y} \mid \theta)}{\partial \theta} \right) f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \hat{\theta} \frac{\frac{\partial}{\partial \theta} f_Y(\mathbf{y} \mid \theta)}{f_Y(\mathbf{y} \mid \theta)} f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \int \hat{\theta} \frac{\partial}{\partial \theta} f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \frac{\partial}{\partial \theta} \int \hat{\theta} f_Y(\mathbf{y} \mid \theta) d\mathbf{y} \\
&= \frac{\partial}{\partial \theta} E[\hat{\theta}] \\
&= \frac{\partial}{\partial \theta} \theta \\
&= 1
\end{aligned}
$$

where $E[\hat{\theta}] = \theta$ since our estimator is unbiased. Putting this all together, we have

$$
\begin{aligned}
Var[\hat{\theta}] &\geq \frac{Cov(\hat{\theta}, X)^2}{Var(X)} \\
&= \frac{1^2}{E\left[\left(\frac{\partial \log L(\theta | \mathbf{y})}{\partial \theta} \right)^2 \right]} \\
&= \frac{1}{I(\theta)}
\end{aligned}
$$

as desired.

Comment: Note that what the Cramér-Rao lower bound tells us is that, if the variance of an unbiased estimator is *equal* to the Cramér-Rao lower bound, then that estimator has the *minimum possible variance* among all unbiased estimators there could possibly be. This allows us to *prove*, for example, whether or not an unbiased estimator is the UMVUE: If an unbiased estimator's variance achieves the C-R lower bound, then it is *optimal* according to the UMVUE criterion.

4.5 Worked Examples

Problem 1: Suppose $X_1, \ldots, X_n \overset{iid}{\sim} Exponential(1/\theta)$. Compute the MLE of θ, and show that it is an unbiased estimator of θ.

Solution:

Note that we can write

$$\begin{aligned}
L(\theta) &= \prod_{i=1}^{n} \frac{1}{\theta} e^{-x_i/\theta} \\
\log L(\theta) &= \sum_{i=1}^{n} \log(\frac{1}{\theta} e^{-x_i/\theta}) \\
&= \sum_{i=1}^{n} \log(\frac{1}{\theta}) - \sum_{i=1}^{n} x_i/\theta \\
&= -n\log(\theta) - \frac{1}{\theta}\sum_{i=1}^{n} x_i \\
\frac{\partial}{\partial\theta} \log L(\theta) &= \frac{\partial}{\partial\theta}\left(-n\log(\theta) - \frac{1}{\theta}\sum_{i=1}^{n} x_i\right) \\
&= -\frac{n}{\theta} + \frac{\sum_{i=1}^{n} x_i}{\theta^2}
\end{aligned}$$

Setting this equal to 0 and solving for θ we obtain

$$\begin{aligned}
0 &\equiv -\frac{n}{\theta} + \frac{\sum_{i=1}^{n} x_i}{\theta^2} \\
\frac{n}{\theta} &= \frac{\sum_{i=1}^{n} x_i}{\theta^2} \\
n &= \frac{\sum_{i=1}^{n} x_i}{\theta} \\
\theta &= \frac{1}{n}\sum_{i=1}^{n} x_i
\end{aligned}$$

and so the MLE for θ is the sample mean. To show that the MLE is unbiased, we note that

$$E\left[\frac{1}{n}\sum_{i=1}^{n}X_i\right] = \frac{1}{n}\sum_{i=1}^{n}E[X_i] = \frac{1}{n}\sum_{i=1}^{n}\theta = \theta$$

as desired.

Problem 2: Suppose again that $X_1, \ldots, X_n \overset{iid}{\sim} Exponential(1/\theta)$. Let $\hat{\theta}_2 = Y_1$, and $\hat{\theta}_3 = nY_{(1)}$. Show that $\hat{\theta}_2$ and $\hat{\theta}_3$ are unbiased estimators of θ. Hint: use the fact that $Y_{(1)} \sim Exponential(n/\theta)$

Solution:

Note that the mean of a random variable $Y \sim Exponential(\lambda)$ is given by $1/\lambda$. Then we can write

$$E[\hat{\theta}_2] = E[Y_1] = \frac{1}{1/\theta} = \theta$$

and

$$E[\hat{\theta}_3] = E[nY_{(1)}] = \frac{n}{n/\theta} = \theta$$

as desired.

Problem 3: Compare the variance of the estimators from Problems 1 and 2. Which is most efficient?

Solution:

Recall that the variance of a random variable $Y \sim Exponential(\lambda)$ is given by $1/\lambda^2$. Let the MLE from Problem 1 be denoted $\hat{\theta}_1 = \bar{X}$. Then we can write

$$Var\left[\hat{\theta}_1\right] = Var\left[\frac{1}{n}\sum_{i=1}^{n}X_i\right] = \frac{1}{n^2}\sum_{i=1}^{n}Var[X_i] = \frac{1}{n^2}\left(\frac{n}{(1/\theta)^2}\right) = \frac{\theta^2}{n}$$

and

$$Var\left[\hat{\theta}_2\right] = Var[Y_1] = \frac{1}{(1/\theta)^2} = \theta^2$$

and

$$Var\left[\hat{\theta}_3\right] = Var[nY_{(1)}] = n^2Var[Y_{(1)}] = \frac{n^2}{(n/\theta)^2} = \theta^2$$

Thus, the variance of the MLE, $\hat{\theta}_1$, is most efficient, and is n times smaller than the variance of both $\hat{\theta}_2$ and $\hat{\theta}_3$.

Problem 4: Suppose $X_1, \ldots, X_n \overset{iid}{\sim} N(\mu, \sigma^2)$. Show that the estimator $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} X_i$ *and* the estimator $\hat{\mu}_w = \sum_{i=1}^{n} w_i X_i$ are both unbiased estimators of μ, where $\sum_{i=1}^{n} w_i = 1$.

Solution:

We can write

$$E[\hat{\mu}] = E\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] = \frac{1}{n}\sum_{i=1}^{n} E[X_i] = \frac{1}{n}\sum_{i=1}^{n} \mu = \mu$$

and

$$E[\hat{\mu}_w] = E\left[\sum_{i=1}^{n} w_i X_i\right] = \sum_{i=1}^{n} w_i E\left[X_i\right] = \sum_{i=1}^{n} w_i \mu = \mu \sum_{i=1}^{n} w_i = \mu$$

as desired.

Problem 5: Determine whether the estimator $\hat{\mu}$ or $\hat{\mu}_w$ is more efficient, in Problem 5, if we additionally impose the constraint $w_i \geq 0 \ \forall i$. (Note that this is a more "general" example based on Example 5.4.5 in Larsen & Marx) (Hint: use the Cauchy-Schwarz inequality)

Solution:

To determine relative efficiency, we must compute the variance of each estimator. We have

$$Var[\hat{\mu}] = Var\left[\frac{1}{n}\sum_{i=1}^{n} X_i\right] = \frac{1}{n^2}\sum_{i=1}^{n} Var[X_i] = \frac{1}{n^2}\sum_{i=1}^{n} \sigma^2 = \sigma^2/n$$

and

$$
\begin{aligned}
Var[\hat{\mu}_w] &= Var\left[\sum_{i=1}^{n} w_i X_i\right] \\
&= \sum_{i=1}^{n} Var[w_i X_i] \\
&= \sum_{i=1}^{n} w_i^2 Var[X_i] \\
&= \sum_{i=1}^{n} w_i^2 \sigma^2 \\
&= \sigma^2 \sum_{i=1}^{n} w_i^2
\end{aligned}
$$

And so to determine which estimator is more efficient, we need to determine if $\frac{1}{n}$ is less than $\sum_{i=1}^{n} w_i^2$ (or not). The Cauchy-Schwarz inequality tells us that

$$
\begin{aligned}
\left(\sum_{i=1}^{n} w_i \cdot 1\right)^2 &\leq \left(\sum_{i=1}^{n} w_i^2\right)\left(\sum_{i=1}^{n} 1^2\right) \\
\left(\sum_{i=1}^{n} w_i\right)^2 &\leq \left(\sum_{i=1}^{n} w_i^2\right) n \\
1 &\leq \left(\sum_{i=1}^{n} w_i^2\right) n \\
\frac{1}{n} &\leq \sum_{i=1}^{n} w_i^2
\end{aligned}
$$

and therefore, $\hat{\mu}$ is more efficient than $\hat{\mu}_w$.

Problem 6: Suppose $X_1, \ldots, X_n \overset{iid}{\sim} N(\mu, \sigma^2)$. Show that the MLE for σ^2 is *biased*, and suggest a modified variance estimator for σ^2 that is *unbiased*. (This is Example 5.4.4 in Larsen & Marx)

Solution:

Recall that the MLE for σ^2 is given by $\frac{1}{n}\sum_{i=1}^{n}(X_i - \bar{X})^2$. Then

$$
\begin{aligned}
E\left[\frac{1}{n}\sum_{i=1}^{n}(X_i-\bar{X})^2\right] &= \frac{1}{n}\sum_{i=1}^{n}E\left[(X_i-\bar{X})^2\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}E\left[X_i^2-2X_i\bar{X}+\bar{X}^2\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}E[X_i^2]-2E\left[\frac{1}{n}\sum_{i=1}^{n}X_i\bar{X}\right]+E[\bar{X}^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}E[X_i^2]-2E\left[\bar{X}\frac{1}{n}\sum_{i=1}^{n}X_i\right]+E[\bar{X}^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}E[X_i^2]-2E\left[\bar{X}^2\right]+E[\bar{X}^2] \\
&= \frac{1}{n}\sum_{i=1}^{n}E[X_i^2]-E\left[\bar{X}^2\right]
\end{aligned}
$$

Recall that since $X_i \overset{iid}{\sim} N(\mu,\sigma^2)$, $\bar{X}\sim N(\mu,\sigma^2/n)$, and that we can write $Var[Y]+E[Y]^2 = E[Y^2]$ (definition of variance). Then we can write

$$
\begin{aligned}
E\left[\frac{1}{n}\sum_{i=1}^{n}(X_i-\bar{X})^2\right] &= \frac{1}{n}\sum_{i=1}^{n}E[X_i^2]-E\left[\bar{X}^2\right] \\
&= \frac{1}{n}\sum_{i=1}^{n}(\sigma^2+\mu^2)-\left(\frac{\sigma^2}{n}+\mu^2\right) \\
&= \sigma^2+\mu^2-\frac{\sigma^2}{n}-\mu^2 \\
&= \sigma^2-\frac{\sigma^2}{n} \\
&= \sigma^2\left(1-\frac{1}{n}\right) \\
&= \sigma^2\left(\frac{n-1}{n}\right)
\end{aligned}
$$

Therefore, since $E[\hat{\sigma}^2_{MLE}]\neq\sigma^2$, the MLE is unbiased. Note that

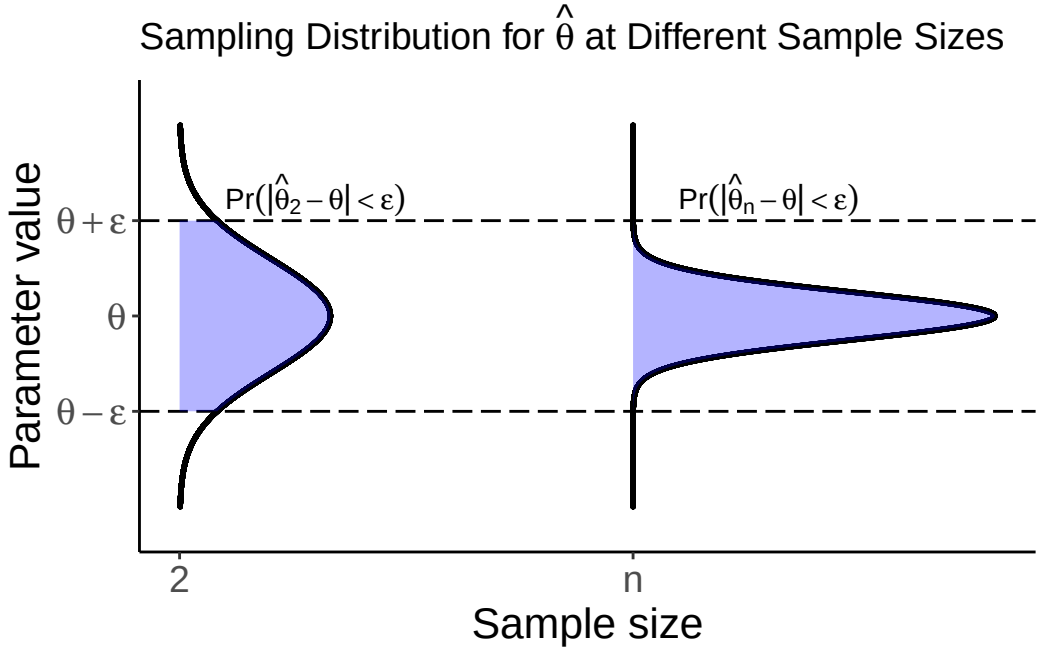
$$
\begin{aligned}
E\left[\left(\frac{n}{n-1}\right)\frac{1}{n}\sum_{i=1}^{n}(X_i-\bar{X})^2\right] &= \left(\frac{n}{n-1}\right)\left(\frac{n-1}{n}\right)\sigma^2 \\
&= \sigma^2
\end{aligned}
$$

and so the estimator $\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \bar{X})^2$ is an unbiased estimator for σ^2. This estimator is often called the "sample variance", and is denoted by S^2.

5 Consistency

The properties of estimators that we've covered thus far (with the exception of asymptotic unbiasedness) have all been what are called *finite sample* properties. All we mean by this is that our sample size (n) is less than infinity (hence: finite). In practice of course, our sample size will always be less than infinity; however, it is still nice to know what happens to our estimators (in terms of bias, variance, etc.) as our sample size gets *really really large*. Much of Frequentist statistics relies on asymptotic (read: infinite sample size) theory to quantify our uncertainty via confidence intervals, for example.

Consistency is one such asymptotic property that we care about. As opposed to asymptotic unbiasedness, consistency tells us something about the *entire shape* of a distribution, as opposed to just the *center* of our distribution. Prof. Brianna Heggeseth and Prof. Kelsey Grinde have a great visual for this below:



The idea here is that as our sample size gets large (as we move to the right on the x-axis), consistency tells us something about the entire *distribution* of our estimator being within some boundary. Asymptotic unbiasedness, on the other hand, only tells us about whether the center of our distribution (a single point!) lies where it "should" (at the truth).

Why do we care about consistency? Because we care about uncertainty! It would be really unfortunate if, in collecting more and more data, we didn't get any more certain about the true parameter we're trying to estimate. Intuitively, we want to be *more confident* (less uncertain) in our estimators when we have larger sample sizes. This is exactly what consistency is concerned with. How do we prove whether or not an estimator is consistent? (Typically) Chebyshev's Inequality, which we state and prove below.

5.1 Learning Objectives

By the end of this chapter, you should be able to…

- Distinguish between finite sample properties and asymptotic properties of estimators
- Prove (using Chebyshev's inequality) whether or not an estimator is consistent

5.2 Concept Questions

1. What is the distinction between a fixed sample property and an asymptotic property of an estimator?
2. Describe, in your own words, what it means for an estimator to be consistent.
3. How can we use Chebyshev's inequality to show that an estimator is consistent?
4. Which of the estimation techniques we've seen so far yield consistent estimators?

5.3 Definitions

You are expected to know the following definitions:

Asymptotically Unbiased

An estimator $\hat{\theta} = g(X_1, \dots, X_n)$ is an *asymptotically* unbiased estimator for θ if $\lim_{n\to\infty} E[\hat{\theta}] = \theta$.

Consistent

An estimator $\hat{\theta}_n = h(X_1, \dots, X_n)$ is consistent for θ if it converges in probability to θ. That is, for all $\epsilon > 0$,

$$\lim_{n\to\infty} \Pr(|\hat{\theta}_n - \theta| < \epsilon) = 1$$

Note that we write our estimator with a subscript n here to clarify that our estimator depends on our sample size. There is an alternative $\epsilon - \delta$ definition of consistency, but we won't focus on it for this course.

Weak Law of Large Numbers

For independent and identically distributed random variables $X_1, \ldots, X_n$ with finite expectation $\mu < \infty$,

$$\lim_{n \to \infty} \Pr(|\overline{X} - \mu| < \epsilon) = 1$$

Alternatively, we can write that as $n \to \infty$, $\overline{X} \xrightarrow{p} \mu$, where "$\xrightarrow{p}$" denotes convergence in probability.

5.4 Theorems

Chebyshev's Inequality

Let W be a random variable with mean μ and variance σ^2. Then for any $\epsilon > 0$,

$$\Pr(|W - \mu| < \epsilon) \geq 1 - \frac{\sigma^2}{\epsilon^2},$$

or, equivalently,

$$\Pr(|W - \mu| \geq \epsilon) \leq \frac{\sigma^2}{\epsilon^2}.$$

Proof.

Let $\epsilon > 0$. Then

$$
\begin{aligned}
\sigma^2 &= \mathrm{Var}(W) \\
&= \int_{-\infty}^{\infty} (w-\mu)^2 f_W(w) dw \\
&= \int_{-\infty}^{\mu-\epsilon} (w-\mu)^2 f_W(w) dw + \int_{\mu-\epsilon}^{\mu+\epsilon} (w-\mu)^2 f_W(w) dw + \int_{\mu+\epsilon}^{\infty} (w-\mu)^2 f_W(w) dw \\
&\geq \int_{-\infty}^{\mu-\epsilon} (w-\mu)^2 f_W(w) dw + 0 + \int_{\mu+\epsilon}^{\infty} (w-\mu)^2 f_W(w) dw \\
&= \int_{|w-\mu|\geq\epsilon} (w-\mu)^2 f_W(w) dw \\
&\geq \int_{|w-\mu|\geq\epsilon} \epsilon^2 f_W(w) dw \\
&= \epsilon^2 \int_{|w-\mu|\geq\epsilon} f_W(w) dw \\
&= \epsilon^2 P(|W-\mu| \geq \epsilon)
\end{aligned}
$$

and rearranging yields

$$
\begin{aligned}
\sigma^2 &\geq \epsilon^2 P(|W-\mu| \geq \epsilon) \\
P(|W-\mu| \geq \epsilon) &\leq \frac{\sigma^2}{\epsilon^2}
\end{aligned}
$$

as desired.

Corollary 1: If $\hat{\theta}_n$ is an unbiased estimator for θ and $\lim_{n\to\infty} Var(\hat{\theta}_n) = 0$, then $\hat{\theta}_n$ is consistent for θ. (You'll prove this corollary on a problem set!)

Corollary 2: If $\hat{\theta}_n$ is an asymptotically unbiased estimator for θ and $\lim_{n\to\infty} Var(\hat{\theta}_n) = 0$, then $\hat{\theta}_n$ is consistent for θ.

Note that the second corollary is a bit stronger than the first one, in that the first corollary actually *implies* the second. If an estimator is unbiased, then it is certainly asymptotically unbiased as well.

5.5 Worked Examples

Problem 1: Suppose $X_1, \ldots, X_n \overset{iid}{\sim} N(\mu, \sigma^2)$. Show that the MLE for σ^2 is *asymptotically* unbiased.

Solution:

The MLE for σ^2 is given by $\frac{1}{n}\sum_{i=1}^{n}(X_i - \overline{X})^2$ (see the MLE section of the course notes, worked example problem 2), and has expectation $\left(\frac{n-1}{n}\right)\sigma^2$ (see the Properties section of the course notes, worked example problem 6). To show that this estimator is asymptotically unbiased, note that we have

$$\begin{aligned}\lim_{n\to\infty} E[\hat{\sigma^2}_{MLE}] &= \lim_{n\to\infty}\left(\frac{n-1}{n}\right)\sigma^2 \\ &= (1)\,\sigma^2 \\ &= \sigma^2\end{aligned}$$

and therefore, the MLE for σ^2 is asymptotically unbiased.

Problem 2: Suppose $Y_1, \ldots, Y_n \overset{iid}{\sim} Uniform(0, \theta)$, and recall that $\hat{\theta}_{MLE} = Y_{(n)}$ with $f_{Y_{(n)}}(y \mid \theta) = \frac{n}{\theta^n}y^{n-1}$, $0 \le y \le \theta$. Prove that $\hat{\theta}_{MLE}$ is a consistent estimator for θ.

Solution:

To prove that $\hat{\theta}_{MLE}$ is consistent, we must first show that $\hat{\theta}_{MLE}$ is (either) unbiased or asymptotically unbiased, and then we must show that the variance of $\hat{\theta}_{MLE}$ tends to zero as $n \to \infty$. To begin, note that

$$\begin{aligned}E\left[\hat{\theta}_{MLE}\right] &= \int_0^\theta y f_{Y_{(n)}}(y \mid \theta)dy \\ &= \int_0^\theta y\left(\frac{n}{\theta^n}y^{n-1}\right)dy \\ &= \frac{n}{\theta^n}\int_0^\theta y^n dy \\ &= \frac{n}{\theta^n}\left(\frac{y^{n+1}}{n+1}\Bigg|_0^\theta\right) \\ &= \frac{n}{\theta^n}\left(\frac{\theta^{n+1}}{n+1}\right) \\ &= \left(\frac{n}{n+1}\right)\theta\end{aligned}$$

and so $\hat{\theta}_{MLE}$ is biased. It is, however, asymptotically *unbiased*. Note that $\left(\frac{n}{n+1}\right) \overset{n\to\infty}{\to} 1$, and therefore $E\left[\hat{\theta}_{MLE}\right] \overset{n\to\infty}{\to} \theta$.

All that's left is to show that $Var\left[\hat{\theta}_{MLE}\right] \overset{n\to\infty}{\to} 0$. We can write

$$\begin{aligned}
E\left[Y_{(n)}^2\right] &= \int_0^\theta y^2 \frac{ny^{n-1}}{\theta^n} dy \\
&= \frac{n}{\theta^n} \int_0^\theta y^{n+1} dy \\
&= \frac{n}{\theta^n} \left(\frac{y^{n+2}}{n+2} \Big|_0^\theta \right) \\
&= \frac{n}{\theta^n} \left(\frac{\theta^{n+2}}{n+2} \right) \\
&= \left(\frac{n}{n+2} \right) \theta^2
\end{aligned}$$

and therefore

$$\begin{aligned}
\lim_{n\to\infty} Var\left[\hat{\theta}_{MLE}\right] &= \lim_{n\to\infty} \left[E\left[Y_{(n)}^2\right] - E\left[Y_{(n)}\right]^2 \right] \\
&= \lim_{n\to\infty} \left[\left(\frac{n}{n+2} \right) \theta^2 - \left(\frac{n}{n+1} \right)^2 \theta^2 \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\left(\frac{n}{n+2} \right) - \left(\frac{n}{n+1} \right)^2 \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\frac{n}{n+2} - \frac{n^2}{(n+1)^2} \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\frac{n(n+1)^2 - n^2(n+2)}{(n+2)(n+1)^2} \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\frac{n(n^2+2n+1) - n^3 - 2n^2}{(n+2)(n^2+2n+1)} \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\frac{n^3+2n^2+n-n^3-2n^2}{n^3+2n^2+2n^2+5n+2} \right] \\
&= \theta^2 \lim_{n\to\infty} \left[\frac{n}{n^3+4n^2+5n+2} \right] \\
&= 0
\end{aligned}$$

where the last term goes to zero because $\frac{n}{n^3} \to 0$ as $n \to \infty$. Therefore, $\hat{\theta}_{MLE}$ is a consistent estimator for θ.

6 Asymptotics & the Central Limit Theorem

Asymptotic unbiasedness and consistency allow us to assess the behavior of estimators when sample sizes get large. Thus far, however, we've only discussed what happens to *point estimates* as n goes to infinity. Point estimates are great, but they don't tell the whole story. In order to truly quantify uncertainty (which is arguably one of the main goals of statistics, if not *the* main goal), we need to be able to estimate a range of plausible values for our estimators: we need to be able to construct confidence intervals. This is made possible primarily by asymptotic normality, the Central Limit Theorem, and properties of the normal distribution.

Confidence Intervals

Confidence intervals are one of the most difficult concepts for a budding statistician to grasp, because they don't have the intuitive, probabilistic definition we often want them to have (aka the probability that the truth lies within the interval). As with Frequentist statistics more generally, the definition of a confidence interval relies on the concept of *repeated sampling* from a population.

A confidence interval either contains the true parameter, or it does not. There is no probability involved in that statement. Probability comes into play when considering that, under repeated sampling, if we construct confidence intervals each time we take a new sample and construct an estimator, a given percentage *of those intervals* will contain the true parameter.

Confidence Intervals - The CLT

The primary way that we construct confidence intervals is by "rearranging" the CLT so that a quantity's asymptotic distribution does not depend on the data nor the parameter of interest. This process is sometimes called establishing an *approximate pivotal quantity.*

As an example, consider an iid random sample $X_1, \dots, X_n$ where $E[X_i] = \mu$ and $Var[X_i] = \sigma^2$, where σ^2 is known. The CLT tells us that

$$\sqrt{n}(\bar{X} - \mu) \xrightarrow{d} N(0, \sigma^2).$$

We can use this to construct a confidence interval for μ. By Slutsky's theorem we can write

$$\frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \xrightarrow{d} N(0,1).$$

and note now that we *know* the asymptotic distribution for the (pivotal) quantity on the left, and can therefore use the *quantiles* of this distribution to construct confidence intervals. For a standard normal distribution (as is the case here) we can note that 95% of the distribution is contained within 1.96 standard deviations of the mean, and therefore

$$\Pr\left(-1.96 \leq \frac{\bar{X} - \mu}{\sigma/\sqrt{n}} \leq 1.96\right) = 0.95$$

We can rearrange the probability statement on the left hand side to get

$$\Pr\left(\bar{X} - 1.96\sigma/\sqrt{n} \leq \mu \leq \bar{X} + 1.96\sigma/\sqrt{n}\right) = 0.95$$

and therefore, our 95% confidence interval for μ is given by $\left(\bar{X} - 1.96\sigma/\sqrt{n}, \bar{X} + 1.96\sigma/\sqrt{n}\right)$.

Confidence Intervals - "Exact"

A second way that we construct confidence intervals is through a concrete distributional assumption, and known quantiles of those distributions. Note that the confidence interval constructed above involves the Central Limit Theorem, and *no finite sample* distributional assumption. All we assume are that the data are iid observations with finite means and variances. The "distribution" only comes into play as our sample size gets large.

When sample sizes *aren't* large, applying the CLT might not make a whole lot of sense. In these scenarios, it can be useful to use an alternative confidence interval construction, aided by assuming a specific distribution for our random variables. In some scenarios these assumptions may make more sense than others: in short, we're *always* making some sort of assumption, regardless of what we do. It's part of our job as statisticians to ensure that the assumptions we make, make sense for the application we're working with!

One example of a commonly used "exact" confidence interval is the Clopper-Pearson interval for a binomial proportion. Consider an iid random sample $X_1, \ldots, X_n$, where $\sum_{i=1}^{n} X_i \sim Binomial(n, p)$. Intuitively, the interval is constructed by the following steps:

1. Find the *largest* p such that $\Pr(X \leq k) \geq \alpha/2$, where k is the observed number of successes. Call this largest value p_U.
2. Find the *smallest* p such that $\Pr(X \geq k) \geq \alpha/2$, where k is again the observed number of successes. Call this smallest value p_L.
3. Define the $100(1-\alpha)\%$ confidence interval for p to be (p_U, p_L).

This construction process allows us to determine all possible values of p that are compatible with our observed number of successes (which is exactly what a confidence interval should do).

In more math-y terms, We can show that if $\sum_{i=1}^{n} X_i \sim Binomial(n, p)$, then $\Pr(\sum_{i=1}^{n} X_i \geq x) = \Pr(Y \leq p)$, where $Y \sim Beta(\sum_{i=1}^{n} x_i, n - \sum_{i=1}^{n} x_i + 1)$. The point of doing this is that we can rewrite our probability statements (involved in our confidence interval construction) in terms of a random variable that *does not depend* on p. We can then compute the Clopper-Pearson interval for p as

$$\Phi_{\frac{\alpha}{2};x,n-x+1} < p < \Phi_{1-\frac{\alpha}{2};x+1,n-x}$$

where $\Phi_{a;v,w}$ is the ath quantile from a Beta distribution with shape parameters v and w. Alternatively, you can even write the Clopper-Pearson in terms of quantiles of the F-distribution, but the Beta format is enough to emphasize the main point: If we can determine the distribution of some function of our data and unknown parameter, and manipulate that distribution enough so that it depends on neither the data nor unknown parameter, we can use quantiles and probability statements to construct confidence intervals.

Convergence

If an estimator $\hat{\theta}_n$ is a consistent estimator for θ, we also say that $\hat{\theta}_n$ converges in probability to θ (i.e., $\hat{\theta}_n \xrightarrow{p} \theta$). There are three different types of convergence: almost sure convergence, convergence in probability, and convergence in distribution (in order from "strongest" to "weakest"). The main two that we'll care about for this course are convergence in probability and convergence in distribution. Mathematical details about convergence are for a more advanced statistical theory course (or perhaps a more advanced course in analysis). For our purposes, it will suffice to know that (1) convergence in probability *implies* convergence in distribution, (2) the Central Limit Theorem, delta-method, and Slutsky's Theorem are tools we can use to determine (and manipulate) asymptotic distributions of random variables, and (3) the Continuous Mapping Theorem (defined below).

Asymptotic Properties of MLEs

In addition to the nice intuition behind maximum likelihood estimation (finding the parameters that make our data the most likely to have occurred), most* MLEs also have incredibly convenient asymptotic properties, including:

- Asymptotic unbiasedness
- Consistency

- Asymptotic normality
- Asymptotic efficiency

The definitions of the latter two properties are included below (and the former in the previous chapters).

*the MLEs that do not have all of these properties are the ones that don't have certain "regularity conditions." For the MLEs we consider in this class, these are the MLEs that are on the boundary of the support of the pdf (such as the maximum or minimum order statistic).

6.1 Learning Objectives

By the end of this chapter, you should be able to…

- Explain the usefulness of the Central Limit Theorem for Frequentist statistical theory
- Manipulate asymptotic distributions to remove their dependence on unknown parameters using the delta-method and Slutsky's theorem
  - …and explain why such manipulation is important for confidence interval construction
- Derive confidence intervals for unknown parameters based on asymptotic or exact distributions

6.2 Concept Questions

1. What feature of a confidence interval tells us about the precision of our estimator?
2. Why is "removing" unknown parameters from the asymptotic distribution of our estimators important when constructing confidence intervals?

6.3 Definitions

Asymptotic Normality

An estimator $\hat{\theta}_n$ is asymptotically normal if $\hat{\theta}_n$ converges in distribution to a normally distributed random variable.

Asymptotic Efficiency

An estimator $\hat{\theta}_n$ is asymptotically efficient if it's asymptotic variance attains the C-R Lower Bound. Note that this is the C-R Lower Bound for a *single* observation, and therefore the asymptotic distribution of an MLE looks something like this:

$$\sqrt{n}(\hat{\theta}_n - \theta) \xrightarrow{d} N\left(0, \frac{1}{I_1(\theta)}\right)$$

Confidence Interval

A 100(1 - α)% confidence interval for a parameter θ is given by (a, b), where $\Pr(a \leq \theta \leq b) = 1 - \alpha$.

6.4 Theorems

Central Limit Theorem (CLT)

For iid random variables $X_1, \ldots, X_n$ with mean μ and variance σ^2,

$$\sqrt{n}(\bar{X}_n - \mu) \xrightarrow{d} N(0, \sigma^2)$$

where "$\xrightarrow{d}$" denotes convergence in distribution.

Proof.

Note that this proof is not completely rigorous, in that we will use the following theorem (without proof) in order to prove the CLT:

Theorem: Let $W_1, \ldots, W_n$ be a sequence of random variables with MGF of the sequence W_n given by $M_{W_n}(t)$. Also, let V denote another random variable with MGF $M_V(t)$. Then if $\lim_{n\to\infty} M_{W_n}(t) = M_V(t)$, for all values of t in some interval around $t = 0$, then the sequence $W_1, \ldots, W_n$ converges in distribution to V.

Suppose $X_1, \ldots, X_n$ with mean μ and variance σ^2, and let $Y_i = (X_i - \mu)/\sigma$. Then $E[Y_i] = 0$, and $Var[Y_i] = 1$ since

$$E[Y_i] = E\left[(X_i - \mu)/\sigma\right] = \frac{1}{\sigma}(E[X_i] - \mu) = \frac{1}{\sigma}(\mu - \mu) = 0$$

and

$$Var[Y_i] = Var\left[(X_i - \mu)/\sigma\right] = \frac{1}{\sigma^2}Var[X_i - \mu] = \frac{1}{\sigma^2}Var[X_i] = \frac{\sigma^2}{\sigma^2} = 1$$

Further, let

$$Z_n = \frac{\sqrt{n}(\bar{X} - \mu)}{\sigma} = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} Y_i$$

where the last two terms are equal since

$$\begin{aligned}
\frac{1}{\sqrt{n}} \sum_{i=1}^{n} Y_i &= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \left(\frac{X_i - \mu}{\sigma} \right) \\
&= \frac{1}{\sigma\sqrt{n}} \sum_{i=1}^{n} (X_i - \mu) \\
&= \frac{1}{\sigma\sqrt{n}} (n\bar{X} - n\mu) \\
&= \frac{\sqrt{n}(\bar{X} - \mu)}{\sigma}
\end{aligned}$$

We'll show that $Z_n \xrightarrow{d} N(0,1)$ by showing that the MGF of Z_n converges to the MGF of a standard normal distribution. Let $M_Y(t)$ denote the MGF of each Y_i. Then the MGF of $\sum_{i=1}^{n} Y_i$ is given by

$$E[e^{t\sum_{i=1}^{n} Y_i}] = E[e^{tY_1} e^{tY_2} \dots e^{tY_n}] = E[e^{tY_1}] E[e^{tY_2}] \dots E[e^{tY_n}] = M_Y(t)^n$$

and the MGF of Z_n is

$$M_{Z_n}(t) = E[e^{tZ_n}] = E[e^{t\frac{1}{\sqrt{n}}\sum_{i=1}^{n} Y_i}] = M_Y\left(\frac{t}{\sqrt{n}}\right)^n$$

Now note that the Taylor expansion of the function e^{tY} about 0 is given by

$$e^{tY} = 1 + tY + \frac{t^2Y^2}{2!} + \frac{t^3Y^3}{3!} + \dots$$

Taking the expectation of both sides, we obtain

$$E[e^{tY}] = 1 + tE[Y] + \frac{t^2E[Y^2]}{2!} + \frac{t^3E[Y^3]}{3!} + \dots$$

and note now that the left hand side is the MGF for Y. Recalling that $E[Y] = 0$ and $Var[Y] = 1$, we have

$$E[e^{tY}] = 1 + \frac{t^2}{2!} + \frac{t^3 E[Y^3]}{3!} + ...$$

And therefore

$$E[e^{tZ_n}] = \left[1 + \frac{t^2}{2n} + \frac{t^3 E[Y^3]}{3! n^{3/2}} + ...\right]^n$$

We'll now make use of a theorem regarding sequences of real numbers (without proof): Let a_n and c_n be sequences of real numbers such that $a_n \overset{n\to\infty}{\to} 0$ and $c_n a_n^2 \overset{n\to\infty}{\to} 0$. Then if $a_n c_n \overset{n\to\infty}{\to} b$, $(1 + a_n)^{c_n} \overset{n\to\infty}{\to} e^b$.

Let $a_n = \frac{t^2}{2n} + \frac{t^3 E[Y^3]}{3! n^{3/2}} + ...$ and $c_n = n$. Note that both $a_n \overset{n\to\infty}{\to} 0$ and $c_n a_n^2 \overset{n\to\infty}{\to} 0$. Then

$$\lim_{n\to\infty} a_n c_n = \lim_{n\to\infty} \left[\frac{t^2}{2} + \frac{t^3 E[Y^3]}{3! n^{1/2}} + ...\right] = \frac{t^2}{2}$$

and therefore

$$M_{Z_n}(t) = (1 + a_n)^{c_n} \overset{n\to\infty}{\to} e^{t^2/2}$$

where we note that the right hand side is the MGF of a standard normal distribution. Then finally, we have proved that

$$\sqrt{n}(\bar{X} - \mu) \overset{d}{\to} N(0, \sigma^2)$$

as desired.

Continuous Mapping Theorem

If $X_n \overset{p}{\to} X$, and g is a continuous function, then $g(X_n) \overset{p}{\to} g(X)$. Similarly for convergence almost surely and convergence in distribution.

Proof. Left to the reader, but also on Wikipedia.

Slutsky's Theorem

If $g(X, Y)$ is a jointly continuous function at every point (X, a) for some fixed a, and if $X_n \overset{d}{\to} X$ and $Y_n \overset{p}{\to} a$, then $g(X_n, Y_n) \overset{d}{\to} g(X, a)$.

Proof. Beyond the scope of the course, unfortunately, but here's a link to the Wikipedia page if you want to go down that rabbit hole in your spare time.

Delta-method

Let $\sqrt{n}(Y-\mu) \xrightarrow{d} N(0,\sigma^2)$. If $g(Y)$ is differentiable at μ and $g'(\mu) \neq 0$, then

$$\sqrt{n}\left(g(Y)-g(\mu)\right) \xrightarrow{d} N(0,[g'(\mu)]^2\sigma^2)$$

Proof.

Since g is differentiable at μ, it's first-order Taylor expansion is given by

$$g(Y) = g(\mu) + (Y-\mu)g'(\mu) + O(|Y-\mu|^2)$$

where $O(f(x))$, referred to as "Big O," describes the limiting behavior of the function $f(x)$. In this case, we use it to note that every term in the Taylor expansion after the first derivative evaluated at μ is growing no faster than $|Y-\mu|^2$ as $n \to \infty$.

Rearranging, note that

$$g(Y) - g(\mu) = (Y-\mu)g'(\mu) + O(|Y-\mu|^2)$$

and so

$$\sqrt{n}\left(g(Y)-g(\mu)\right) = \sqrt{n}(Y-\mu)g'(\mu) + O(\sqrt{n}|Y-\mu|^2)$$

Then note that $\sqrt{n}(Y-\mu) \xrightarrow{d} N(0,\sigma^2)$, $g'(\mu) \xrightarrow{p} g'(\mu)$ since it's just a constant, and $O(\sqrt{n}|Y-\mu|^2) \xrightarrow{p} 0$ (due to the $\sqrt{n}$ term). Then using two applications of Slutsky's theorem, we can write that

$$\sqrt{n}(Y-\mu)g'(\mu) \xrightarrow{d} N(0,\sigma^2)g'(\mu) = \xrightarrow{d} N(0,[g'(\mu)]^2\sigma^2)$$

and

$$\begin{aligned}\sqrt{n}(Y-\mu)g'(\mu) + O(\sqrt{n}|Y-\mu|^2) &\xrightarrow{d} N(0,\sigma^2)g'(\mu) + 0 \\ &\stackrel{d}{=} N(0,[g'(\mu)]^2\sigma^2)\end{aligned}$$

and so finally we have shown that

$$\sqrt{n}\left(g(Y)-g(\mu)\right) \xrightarrow{d} N(0,[g'(\mu)]^2\sigma^2)$$

as desired.

6.5 Worked Examples

Problem 1: Suppose $\sqrt{n}(Y_n - \mu) \xrightarrow{d} N(0, \sigma^2)$. Find the asymptotic distribution of $\sqrt{n}(Y_n^2 - \mu^2)$ when $\mu \neq 0$.

Solution:

We can apply the delta-method with the function $g(x) = x^2$. Note that $g'(x) = 2x$, and therefore we can write

$$\begin{aligned}
\sqrt{n}(Y_n - \mu) &\xrightarrow{d} N(0, \sigma^2) \\
\sqrt{n}(g(Y_n) - g(\mu)) &\xrightarrow{d} N(0, [g'(\mu)]^2\sigma^2) \\
\sqrt{n}(Y_n^2 - \mu^2) &\xrightarrow{d} N(0, [2\mu]^2\sigma^2) \\
\sqrt{n}(Y_n^2 - \mu^2) &\xrightarrow{d} N(0, 4\mu^2\sigma^2)
\end{aligned}$$

Problem 2: Suppose $X_1, \ldots, X_n \overset{iid}{\sim} Bernoulli(p)$, and recall that the MLE for p is given by $\hat{p}_{MLE} = \frac{1}{n}\sum_{i=1}^{n} X_i$. Find the asymptotic distribution of $\hat{p}_{MLE}$ using the CLT and known properties of the Bernoulli distribution (expectation and variance, for example), and construct a 95% confidence interval for p based on this asymptotic distribution.

Solution:

We know that $E[X_i] = p$ and $Var[X_i] = p(1-p)$. Then the CLT tell us that

$$\sqrt{n}(\hat{p}_{MLE} - p) \xrightarrow{d} N(0, p(1-p))$$

The WLLN gives us that $\hat{p}_{MLE} \xrightarrow{p} p$, since $\hat{p}_{MLE}$ is a sample mean. We can then use the continuous mapping theorem to show that $\frac{1}{\sqrt{\hat{p}_{MLE}(1-\hat{p}_{MLE})}} \xrightarrow{p} \frac{1}{\sqrt{p(1-p)}}$. Applying Slutsky's theorem, we then have

$$\sqrt{n}\left(\frac{\hat{p}_{MLE} - p}{\sqrt{\hat{p}_{MLE}(1-\hat{p}_{MLE})}}\right) \xrightarrow{d} N(0, 1)$$

and finally, (letting $\hat{p} = \hat{p}_{MLE}$ for ease of notation)

$$
\begin{aligned}
0.95 &= \Pr\left(-1.96 < \frac{\hat{p}-p}{\sqrt{\hat{p}(1-\hat{p})/n}} < 1.96\right) \\
&= \Pr\left(-1.96\sqrt{\hat{p}(1-\hat{p})/n} < \hat{p}-p < 1.96\sqrt{\hat{p}(1-\hat{p})/n}\right) \\
&= \Pr\left(\hat{p}-1.96\sqrt{\hat{p}(1-\hat{p})/n} < p < \hat{p}+1.96\sqrt{\hat{p}(1-\hat{p})/n}\right)
\end{aligned}
$$

7 Hypothesis Testing

The goal of hypothesis testing is to make a decision between two conflicting theories, or "hypotheses." The process of hypothesis testing involves the following steps:

1. State the hypotheses: H_0 (null hypothesis) vs H_1 (alternative hypothesis)
2. Investigate: are data compatible with H_0? assuming H_0 were true, are data extreme?
3. Make a decision: reject H_0 or fail to reject H_0

The first step is relatively straightforward. For the purposes of this course, our null hypothesis will always be that some unknown parameter we are interested in (θ) is equal to a fixed point (θ_0). We'll consider two possible alternatives hypothesis:

- $H_1 : \theta = \theta_1$ ("simple" alternative)
- $H_1 : \theta \neq \theta_0$ (two-sided alternative)

The former is the simplest, non-trivial alternative hypothesis we can consider, and we can prove some nice things in this setting (and hence build intuition for hypothesis testing broadly). The latter is perhaps more relevant, particularly in linear regression.

If you recall from introductory statistics, the latter alternative provides the set-up we have when testing if the linear relationship between a predictor X and outcome Y are "statistically significantly" associated; we test the null hypothesis $H_0 : \beta_1 = 0$ against the alternative, $H_1 : \beta_1 \neq 0$, where $E[Y \mid X] = \beta_0 + \beta_1 X$. In this example, we'd have the unknown parameter β_1, and the fixed point of our null hypothesis as $\theta_0 = 0$.

The second step of hypothesis testing is the investigation. In determining whether the data are compatible with the null hypothesis, we must first derive a *test statistic*. Test statistics are typically functions of (1) our estimators and (2) the distribution of our estimator *under the null hypothesis*. Intuitively, if we can determine the distribution of our estimator under the null hypothesis, we can then observe whether or not the data we actually have is "extreme" or not, given a certain threshold, α, for our hypothesis test. This threshold α is directly related to a $100(1-\alpha)\%$ confidence interval, where anything observed outside the confidence interval bounds is considered to lie in the "rejection region" (where you would thus reject the null hypothesis).

There are three classical forms of test statistics that have varying finite-sample properties, and can be shown to be asymptotically equivalent: the Wald test, the likelihood ratio test

(LRT), and the score test (also sometimes called the Lagrange multiplier test). Each of these is explained in further detail below.

Wald Tests

Suppose we are interested in testing the hypotheses $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$. The Wald test is the hypothesis test that uses the Wald test statistic λ_W, where

$$\lambda_W = \left(\frac{\hat{\theta}_{MLE} - \theta_0}{se(\hat{\theta}_{MLE})} \right)^2.$$

Intuitively, the Wald test measures the difference between the estimated value for θ and the null value for θ, standardized by the variation of your estimator. If this reminds you (once again) of a z-score, it should! In linear regression, with normally distributed standard errors, it turns out that $\sqrt{W}$ follows a t distribution (we'll show this on your problem set!).

Wald tests statistics are extremely straightforward to compute from the Central Limit Theorem. The CLT states that, for iid $X_1, \ldots, X_n$ with expectation μ and variance σ,

$$\sqrt{n}(\overline{X} - \mu) \xrightarrow{d} N(0, \sigma^2).$$

Slutsky's theorem allows us to write

$$\left(\frac{\overline{X} - \mu}{\sigma/\sqrt{n}} \right) \xrightarrow{d} N(0, 1),$$

and note that the left-hand side is an estimator minus it's expectation, divided by it's standard error. When $\overline{X}$ is the MLE for μ, this is the square root of the Wald test statistic! The final thing to note is that the right-hand side tells us this quantity converges in distribution to a standard normal distribution. Think about what we've previously shown about standard normals "squared" to intuit the asymptotic distribution of a Wald test statistic: a χ^2_ν random variable, where the degrees of freedom ν in this case is one! For a single parameter restriction (i.e. one hypothesis for one unknown parameter), the asymptotic distribution of a Wald test statistic will always be χ^2_1.

Wald Tests for Multiple Hypotheses

Note that there is also a multivariate version of the Wald test, used to jointly test *multiple* hypotheses on multiple parameters. In this case, we can write our null and alternative hypotheses using matrices and vectors.

As a simple example, consider a linear regression model where we have a single, categorical predictor with three categories. Our regression model looks something like this:

$$E[Y \mid X] = \beta_0 + \beta_1 X_{Cat2} + \beta_2 X_{Cat3}$$

If we want to test if there is a significant association between Y and X, we can't look at $\hat{\beta}_1$ and $\hat{\beta}_2$ separately. Rather, we need to test the joint null hypothesis $\beta_1 = \beta_2 = 0$, vs. the alternative where *at least one* of our coefficients is *not* equal to zero. In introductory statistics, we did this using the `anova` function in R. In matrix form, we can write our null and alternative hypotheses as:

- $H_0 : R\beta = \mathbf{r}$
- $H_1 : R\beta \neq \mathbf{r}$

where R in this case is the identity matrix, $\beta = (\beta_0, \beta_1)^\top$, and $\mathbf{r} = (0, 0)^\top$. The Wald test statistic in this multi-hypothesis, multi-parameter case can then be written as

$$(R\hat{\theta} - \mathbf{r})^\top [R(\hat{V}/n)R^\top]^{-1}(R\hat{\theta} - \mathbf{r})$$

where $\hat{V}$ is an estimator of the covariance matrix for $\hat{\theta}$. We won't focus on multi-hypothesis, multi-parameter tests in this course, but I *do* want you to be able to draw connections between statistical theory and things you learned way back in your introductory statistics course, hence why this is included in the notes.

Likelihood Ratio Tests

Suppose we are interested in testing the hypotheses $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$. The likelihood ratio test is the hypothesis test that uses the likelihood ratio test statistic λ_{LRT}, where

$$\lambda_{LRT} = -2 \log \left(\frac{\sup\limits_{\theta = \theta_0} L(\theta)}{\sup\limits_{\theta \in \Theta} L(\theta)} \right).$$

Since the ratio of the likelihoods is bounded between 0 and 1 (since the denominator will always be at least as large as the numerator), the LRT statistic is always positive. When

λ_{LRT} is large, it suggests that the data are not compatible with H_0, and values of λ_{LRT} close to 0 suggest the data *are* compatible with H_0. Therefore, we'll reject H_0 for large values of λ_{LRT} and fail to reject H_0 if λ_{LRT} is small. The likelihood ratio test is the most "powerful" of all level α tests when we have a simple alternative hypothesis, and we can prove this using the Neyman-Pearson Lemma. For the simple null hypothesis on a single parameter that we consider, it can be shown that $\lambda_{LRT} \xrightarrow{d} \chi^2_1$, just as with the Wald test statistic.

Score Tests

Suppose we are interested in testing the hypotheses $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$. The score test is the hypothesis test that uses the score test statistic λ_S,

$$\lambda_S = \frac{\left(\frac{\partial}{\partial \theta_0} \log L(\theta_0 \mid x)\right)^2}{I(\theta_0)}$$

as its test statistic. Note that the score test statistic depends *only* on the distribution of the estimator under the null hypothesis, rather than the maximum likelihood estimator. This is sometimes referred to as a test that requires only computation of a *restricted* estimator (where θ_0 is "restricted" by the null distribution). The score test statistic is particularly useful when the MLE is on the boundary of the parameter space (think: order statistics).

Intuitively, if θ_0 is near the estimator that maximizes the log likelihood function, the derivative of the log likelihood function should be close to 0. The score statistic "standardizes" this derivative by a measure of the variation of the estimator, contained in the information matrix. Values of λ_S that are closer to zero are then more compatible with H_0, since because it suggests θ_0 is close to the estimator that maximizes the log likelihood function. We'll reject H_0 for large values of λ_S. For the simple null hypothesis on a single parameter that we consider, it can be shown that $\lambda_S \xrightarrow{d} \chi^2_1$, just as with the Wald test statistic and LRT statistic.

7.1 Learning Objectives

By the end of this chapter, you should be able to…

- Derive and implement a hypothesis test using each of the three classical test statistics to distinguish between two conflicting hypotheses
- Describe the differences and relationships between Type I Error, Type II Error, and power, as well as the factors that influence each of them
- Calculate the power or Type II error for a given hypothesis test

7.2 Concept Questions

1. What is the goal of hypothesis testing?
2. What are the typical steps to deriving a hypothesis test?
3. What is the difference between a one-sided and a two-sided alternative hypothesis? How does this impact our hypothesis testing procedure? How does this impact our p-value?
4. How are test statistics and p-values related?
5. How is type I error related to the choice of significance level?
6. What are the typical steps to calculating the probability of a type II error?
7. How is type II error related to the power of a hypothesis test?
8. What factors influence the power of a test? In practice, which of these factors can we control?

7.3 Definitions

Wald Test Statistic

The Wald test statistic λ_W for testing the hypothesis $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$ is given by

$$\lambda_W = \left(\frac{\hat{\theta}_{MLE} - \theta_0}{se(\hat{\theta}_{MLE})} \right)^2,$$

where $\hat{\theta}_{MLE}$ is a maximum likelihood estimator.

Likelihood Ratio Test (LRT) Statistic

The likelihood ratio test statistic λ_{LRT} for testing the hypothesis $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$ is given by

$$\lambda_{LRT} = -2 \log \left(\frac{\sup\limits_{\theta=\theta_0} L(\theta)}{\sup\limits_{\theta \in \Theta} L(\theta)} \right),$$

where we note that the denominator, $\sup\limits_{\theta \in \Theta} L(\theta)$, is the likelihood evaluated at the maximum likelihood estimator.

Score Test Statistic

The score test statistic λ_S for testing the hypothesis $H_0 : \theta = \theta_0$ vs. $H_1 : \theta \neq \theta_0$ is given by

$$\lambda_S = \frac{\left(\frac{\partial}{\partial \theta_0} \log L(\theta_0 \mid x)\right)^2}{I(\theta_0)}.$$

Power

Power is the probability that we *correctly* reject the null hypothesis; aka, the probability that we reject the null hypothesis, when the null hypothesis is actually false. As a conditional probability statement: Pr(Reject $H_0 \mid H_0$ False). Note that

$$\text{Power} = 1 - \text{Type II Error}$$

Type I Error ("False positive")

Type I Error is the probability that the null hypothesis is rejected, when the null hypothesis is actually true. As a conditional probability statement: Pr(Reject $H_0 \mid H_0$ True)

Type II Error ("False negative")

Type II Error is the probability that we fail to reject the null hypothesis, given that the null hypothesis is actually false. As a conditional probability statement: Pr(Fail to reject $H_0 \mid H_0$ False)

Critical Region / Rejection Region

The critical/rejection region is defined as the set of values for which the null hypothesis would be rejected. This set is often denoted with a capital R.

Critical Value

The critical value is the point that separates the rejection region from the "acceptance" region (i.e., the value at which the decision for your hypothesis test would change). Acceptance is in quotes because we should never "accept" the null hypothesis… but we still call the "fail-to-reject" region the acceptance region for short.

Significance Level

The significance level, denoted α, is the probability that, under the null hypothesis, the test statistic lies in the critical/rejection region.

P-value

The p-value associated with a test statistic is the probability of obtaining a value *as or more extreme* than the observed test statistic, under the null hypothesis.

Uniformly Most Powerful (UMP) Test

A "most powerful" test is a hypothesis test that has the *greatest* power among all possible tests of a given significance threshold α. A *uniformly* most powerful (UMP) test is a test that is most powerful for all possible values of parameters in the restricted parameter space, Θ_0.

More formally, let the set R denote the rejection region of a hypothesis test. Let

$$\phi(x) = \begin{cases} 1 & \text{if } x \in R \\ 0 & \text{if } x \in R^c \end{cases}$$

Then $\phi(x)$ is an indicator function. Recalling that expectations of indicator functions are probabilities, note that $E[\phi(x)] = \Pr(\text{Reject } H_0)$. $\phi(x)$ then represents our hypothesis test. A hypothesis test $\phi(x)$ is UMP of size α if, for any other hypothesis test $\phi'(x)$ of size (*at most*) α,

$$\sup_{\theta \in \Theta_0} E[\phi'(X) \mid \theta] \leq \sup_{\theta \in \Theta_0} E[\phi(X) \mid \theta]$$

we have that $\forall \theta \in \Theta_1$,

$$E[\phi'(X) \mid \theta] \leq E[\phi(X) \mid \theta],$$

where Θ_0 is the set of all values for θ that align with the null hypothesis (sometimes just a single point, sometimes a region), and Θ_1 is the set of all values for θ that align with the alternative hypothesis (sometimes just a single point, sometimes a region). **Note:** In general, UMP tests *do not exist* for two-sided alternative hypotheses. The Neyman-Pearson lemma tells us about UMP tests for simple null and alternative hypotheses, and the Karlin-Rubin theorem extends this to one-sided null and alternative hypotheses.

7.4 Theorems

Neyman-Pearson Lemma

Consider a hypothesis test with $H_0 : \theta = \theta_0$ and $H_1 : \theta = \theta_1$. Let ϕ be a *likelihood ratio test* of level α, where $\alpha = E[\phi(X) \mid \theta_0]$. Then ϕ is a UMP level α test for thee hypotheses $H_0 : \theta = \theta_0$ and $H_1 : \theta = \theta_1$.

Proof.

Let $\alpha = E[\phi(X) \mid \theta_0]$. Note that the LRT statistic is simplified in the case of these simple hypotheses, and can be written just as $\frac{f(x|\theta_1)}{f(x|\theta_0)}$.* If the likelihood under the alternative is greater than some constant c (which depends on α), then we reject the null in favor of the alternative, and vice versa. Then the hypothesis testing function ϕ can be written as

$$\phi(x) = \begin{cases} 0 & \text{if } \lambda_{LRT} = \frac{f(x|\theta_1)}{f(x|\theta_0)} < c \\ 1 & \text{if } \lambda_{LRT} = \frac{f(x|\theta_1)}{f(x|\theta_0)} > c \\ \text{Flip a coin} & \text{if } \lambda_{LRT} = \frac{f(x|\theta_1)}{f(x|\theta_0)} = c \end{cases}$$

Suppose ϕ' is any other test such that $E[\phi'(X) \mid \theta_0] \leq \alpha$ (another level α test). Then we must show that $E[\phi'(X) \mid \theta_1] \leq E[\phi(X) \mid \theta_1]$.

By assumption, we have

$$E[\phi(X) \mid \theta_0] = \int \phi(x) f_X(x \mid \theta_0) dx = \alpha$$
$$E[\phi'(X) \mid \theta_0] = \int \phi'(x) f_X(x \mid \theta_0) dx \leq \alpha$$

Therefore we can write

$$\begin{aligned}
&E[\phi(X) \mid \theta_1] - E[\phi'(X) \mid \theta_1] \\
&\quad = \int \phi(x) f_X(x \mid \theta_1) dx - \int \phi'(x) f_X(x \mid \theta_1) dx \\
&\quad = \int [\phi(x) - \phi'(x)] f_X(x \mid \theta_1) dx \\
&\quad = \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} > c\right\}} \underbrace{[\phi(x) - \phi'(x)]}_{\geq 0} f_X(x \mid \theta_1) dx + \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} < c\right\}} \underbrace{[\phi(x) - \phi'(x)]}_{\leq 0} f_X(x \mid \theta_1) dx + \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} = c\right\}} [\phi(x) - \phi' \\
&\quad \geq \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} > c\right\}} [\phi(x) - \phi'(x)] c f_X(x \mid \theta_0) dx + \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} < c\right\}} [\phi(x) - \phi'(x)] c f_X(x \mid \theta_0) dx + \int_{\left\{\frac{f(x|\theta_1)}{f(x|\theta_0)} = c\right\}} [\phi(x) - \phi \\
&\quad = c \int [\phi(x) - \phi'(x)] f_X(x \mid \theta_0) dx \\
&\quad = c \int \phi(x) f_X(x \mid \theta_0) dx - c \int \phi'(x) f_X(x \mid \theta_0) dx \\
&\quad \geq c(\alpha - \alpha) \\
&\quad = 0
\end{aligned}$$

And rearranging yields

$$\begin{aligned}
E[\phi(X) \mid \theta_1] - E[\phi'(X) \mid \theta_1] &\geq 0 \\
E[\phi(X) \mid \theta_1] &\geq E[\phi'(X) \mid \theta_1]
\end{aligned}$$

as desired.

*Note: The $-2\log(...)$ piece comes into play for the LRT statistic to ensure that the test statistic converges in distribution to a χ^2 random variable. When we're just comparing the LRT statistic to another LRT test statistic, we can (more simply) just compare the ratio of likelihoods. Think: comparing X vs. Y is equivalent to comparing $\log(X)$ vs. $\log(Y)$ if we are only interested in the direction of the difference between them, since log is a monotone function.

7.5 Worked Examples

Problem 1: Let $Y_i \overset{iid}{\sim} N(\mu, \sigma^2)$, where $\sigma^2 = 25$ is *known*. Suppose we want to test the hypotheses $H_0 : \mu = 8$ vs. $H_1 : \mu \neq 8$ and we observe $\overline{Y} = 10$ across $n = 64$ observations. Can we reject H_0, with a significance threshold of $\alpha = 0.05$? (Use a Wald test statistic)

Solution:

Our hypotheses are already stated in the problem set-up. The next thing we should do is derive a Wald test statistic. We know that the MLE for μ is given by $\hat{\mu}_{MLE} = \overline{Y}$ (we have shown this is previous problem sets/worked examples). Then the Wald test statistic can be written as

$$\lambda_W = \left(\frac{\hat{\mu}_{MLE} - \mu_0}{\sigma/\sqrt{n}}\right)^2 = \left(\frac{10-8}{5/\sqrt{64}}\right)^2 = 10.24$$

We can compare this test statistic to the critical value from a χ^2_1 distribution since, by properties of normal distributions and recalling that standard normal distributions squared are χ^2_1,

$$\begin{aligned} \overline{Y} &\sim N(\mu, \sigma^2/n) \\ \frac{\overline{Y} - \mu}{\sigma/\sqrt{n}} &\sim N(0,1) \\ \left(\frac{\overline{Y} - \mu}{\sigma/\sqrt{n}}\right)^2 &\sim \chi^2_1 \end{aligned}$$

To calculate the critical value when $\alpha = 0.05$, we turn to R.

```r
# The quantile function for a given distribution gives us the value at which
# a given percentage of the distributions lies ahead of that value, which
# is exactly what we want in this case!

qchisq(1 - 0.05, df = 1)
```

```
[1] 3.841459
```

Finally, noting that our test statistic is greater than the critical value, we reject H_0.

Problem 2: Suppose we wanted to use a different significance level α. How would the procedure in Problem 1 change if we let $\alpha = 0.001$? How would the procedure in Problem 1 change if we let $\alpha = 0.1$?

Solution:

Changing the significance level changes the *critical value*, and may change whether or not we reject H_0, depending on the difference between our critical value and the test statistic. We can calculate what the critical value would be if we let $\alpha = 0.01$ and $\alpha = 0.1$ again in R:

```r
# alpha = 0.01
qchisq(1 - 0.001, df = 1)
```

```
[1] 10.82757
```

```r
# alpha = 0.1
qchisq(1 - 0.1, df = 1)
```

```
[1] 2.705543
```

Note that when $\alpha = 0.1$, we still reject H_0. This should make intuitive sense, since increasing α only can only increase our rejection region. However, when $\alpha = 0.001$, we would *fail to reject* H_0, as our test statistic is not "more extreme" (greater) than the critical value.

Problem 3: Suppose we have a random sample $X_1, \ldots, X_n \sim Bernoulli(p)$, and we want to test the hypotheses $H_0 : p = 0.5$, $H_1 : p \neq 0.5$. Suppose we calculate an estimator for p as $\hat{p} = \frac{1}{n}\sum_{i=1}^{n} X_i$. Derive a Wald test statistic for this hypothesis testing scenario (simplifying as much as you can).

Solution:

Recall that $\hat{p}$ as defined in the problem set-up is the MLE for p. Then the Wald test statistic can be written as

$$\lambda_W = \left(\frac{\hat{p} - p_0}{se(\hat{p})} \right)^2.$$

We can simplify a little further by calculating $se(\hat{p})$ and plugging in p_0. Recall from the CLT (and Slutsky) that we have

$$\left(\frac{\hat{p} - p_0}{\sqrt{\hat{p}(1-\hat{p})/n}} \right) \xrightarrow{d} N(0,1)$$

Then the standard error of $\hat{p}$ is given by $\sqrt{\hat{p}(1-\hat{p})/n}$, and our Walt test statistic simplifies to

$$\lambda_W = \left(\frac{\hat{p} - 0.5}{\sqrt{\hat{p}(1-\hat{p})/n}} \right)^2.$$

(Note that this is as "simplified" as we can get without knowing $\hat{p}$ or n)

Problem 4: Derive a LRT statistic for the hypothesis testing scenario described in Problem 3 (simplifying as much as you can).

Solution:

The LRT statistic is given by

$$\lambda_{LRT} = -2 \log \left(\frac{\sup\limits_{p=p_0} L(p)}{\sup\limits_{p \in \Theta} L(p)} \right) = -2 \log \left(\frac{L(0.5)}{L(\hat{p}_{MLE})} \right)$$

The likelihood for our observations can be written as

$$L(p) = \prod_{i=1}^{n} p^{x_i} (1-p)^{(1-x_i)}$$

And so our LRT statistic simplifies to

$$
\begin{aligned}
\lambda_{LRT} &= -2\log\left(\frac{L(0.5)}{L(\hat{p})}\right) \\
&= -2\left[\log L(0.5) - \log L(\hat{p})\right] \\
&= -2\left[\log(0.5)\sum_{i=1}^{n} X_i + \log(1-0.5)\sum_{i=1}^{n}(1-X_i) - \log(\hat{p})\sum_{i=1}^{n} X_i - \log(1-\hat{p})\sum_{i=1}^{n}(1-X_i)\right] \\
&= -2\left[\log(0.5)\left(\sum_{i=1}^{n} X_i + \sum_{i=1}^{n}(1-X_i)\right) - \log(\hat{p})\sum_{i=1}^{n} X_i - \log(1-\hat{p})\sum_{i=1}^{n}(1-X_i)\right] \\
&= -2\left[n\log(0.5) - \log(\hat{p})\sum_{i=1}^{n} X_i - \log(1-\hat{p})\sum_{i=1}^{n}(1-X_i)\right] \\
&= -2\left[n\log(0.5) - \log(\hat{p})n\overline{X} - \log(1-\hat{p})(n-n\overline{X})\right] \\
&= -2n\left[\log(0.5) - \log(\hat{p})\hat{p} - \log(1-\hat{p})(1-\hat{p})\right]
\end{aligned}
$$

(Note that this is as "simplified" as we can get without knowing $\hat{p}$ or n)

Problem 5: Derive a score test statistic for the hypothesis testing scenario described in Problem 3 (simplifying as much as you can).

Solution:

The score test statistic is given by

$$\lambda_S = \frac{\left(\frac{\partial}{\partial p_0}\log L(p_0 \mid x)\right)^2}{I(p_0)}.$$

We can simplify by deriving the score and information matrix, and then plugging in $p_0 = 0.5$. We have,

$$
\begin{aligned}
\frac{\partial}{\partial p_0}\log L(p_0 \mid x) &= \frac{\partial}{\partial p_0}\left[\log(p_0)\sum_{i=1}^{n} X_i + \log(1-p_0)\sum_{i=1}^{n}(1-X_i)\right] \\
&= \frac{\sum_{i=1}^{n} X_i}{p_0} - \frac{n-\sum_{i=1}^{n} X_i}{1-p_0} \\
\left(\frac{\partial}{\partial p_0}\log L(p_0 \mid x)\right)^2 &= \left(\frac{\sum_{i=1}^{n} X_i}{p_0} - \frac{n-\sum_{i=1}^{n} X_i}{1-p_0}\right)^2
\end{aligned}
$$

and plugging in $p_0 = 0.5$, we have,

$$\left(\frac{\partial}{\partial p_0}\log L(p_0 \mid x)\right)^2 = \left(\frac{\sum_{i=1}^n X_i}{0.5} - \frac{n-\sum_{i=1}^n X_i}{1-0.5}\right)^2 = \left(\frac{-n+2\sum_{i=1}^n X_i}{0.5}\right)^2 = \left(-2n+4\sum_{i=1}^n X_i\right)^2.$$

The information matrix is given by $-E\left[\frac{\partial^2}{\partial p_0^2}\log L(p_0 \mid x)\right]$. Piecing this together,

$$\begin{aligned}\frac{\partial^2}{\partial p_0^2}\log L(p_0 \mid x) &= \frac{\partial}{\partial p_0}\left[\frac{\sum_{i=1}^n X_i}{p_0} - \frac{n-\sum_{i=1}^n X_i}{1-p_0}\right] \\ &= \frac{-\sum_{i=1}^n X_i}{p_0^2} - \frac{n-\sum_{i=1}^n X_i}{(1-p_0)^2}\end{aligned}$$

And to get $I(p_0)$, we take the negative expectation of the above quantity under the null hypothesis (that is, where $E[X] = p_0$) to obtain

$$\begin{aligned}I(p_0) &= -E\left[\frac{-\sum_{i=1}^n X_i}{p_0^2} - \frac{n-\sum_{i=1}^n X_i}{(1-p_0)^2}\right] \\ &= \frac{1}{p_0^2}\sum_{i=1}^n E[X_i] + \frac{1}{(1-p_0)^2}\left(n - \sum_{i=1}^n E[X_i]\right) \\ &= \frac{1}{p_0^2}\sum_{i=1}^n p_0 + \frac{1}{(1-p_0)^2}\left(n - \sum_{i=1}^n p_0\right) \\ &= \frac{n}{p_0} + \frac{n}{(1-p_0)^2}(1-p_0) \\ &= \frac{n}{p_0} + \frac{n}{(1-p_0)}\end{aligned}$$

And plugging in $p_0 = 0.5$ we have

$$I(0.5) = \frac{n}{0.5} + \frac{n}{(1-0.5)} = 2n + 2n = 4n.$$

Then, finally, the score test statistic (simplified as much as possible) is given by

$$
\begin{aligned}
\lambda_S &= \frac{\left(\frac{\partial}{\partial p_0} \log L(p_0 \mid x)\right)^2}{I(p_0)} \\
&= \frac{\left(-2n + 4\sum_{i=1}^{n} X_i\right)^2}{4n} \\
&= \frac{\left(-2n + 4n\hat{p}\right)^2}{4n} \\
&= \frac{4n^2\left(-1 + 2\hat{p}\right)^2}{4n} \\
&= n\left(-1 + 2\hat{p}\right)^2
\end{aligned}
$$

Problem 6: For each of Problems 3, 4, and 5, calculate the p-values from each test when $\hat{p} = 0.4$ and $n = 300$.

Solution:

We'll again use R to obtain the critical values for these hypothesis tests, noting that in each case, the test statistic follows a χ^2_1 distribution asymptotically:

```
p_hat <- 0.4
n <- 300

# Wald test statistic
lambda_w <- ((p_hat - 0.5)/(sqrt(p_hat * (1 - p_hat) / n)))^2

# LRT statistic
lambda_lrt <- -2 * n * (log(0.5) - log(p_hat) * p_hat - log(1 - p_hat) * (1 - p_hat))

# Score test statistic
lambda_s <- n * (-1 + 2 * p_hat)^2

# Compare statistics
lambda_w
```

```
[1] 12.5
```

```
lambda_lrt
```

```
[1] 12.08131
```

```r
lambda_s
```

```
[1] 12
```

```r
# Calculate p-values
# Recall: probability that we observe something *as or more extreme*
1 - pchisq(lambda_w, df = 1)
```

```
[1] 0.000406952
```

```r
1 - pchisq(lambda_lrt, df = 1)
```

```
[1] 0.0005092985
```

```r
1 - pchisq(lambda_s, df = 1)
```

```
[1] 0.0005320055
```

Things to note:

- When n is large (300, in this case), each of the three classical test statistics are approximately equal! This makes sense, as they all converge in distribution to the same random variable, asymptotically.
- P-values are the probability that we would observe something *as or more extreme* than what we actually did observe, under the null hypothesis. In R, we can use the `p` function (for a given pdf) to calculate this.

Problem 7: Repeat Problem 6 but with $\hat{p} = 0.4$ and $n = 95$. If your significance threshold were $\alpha = 0.05$, would your conclusion to the hypothesis test be the same regardless of which test statistic you chose?

Solution:

To answer this question, we can again calculate p-values, and compare them to 0.05 (note that we could have also calculated a critical value, and compared our test statistics to the critical value, as these are equivalent).

```r
p_hat <- 0.4
n <- 95

# Wald test statistic
lambda_w <- ((p_hat - 0.5)/(sqrt(p_hat * (1 - p_hat) / n)))^2

# LRT statistic
lambda_lrt <- -2 * n * (log(0.5) - log(p_hat) * p_hat - log(1 - p_hat) * (1 - p_hat))

# Score test statistic
lambda_s <- n * (-1 + 2 * p_hat)^2

# Compare statistics
lambda_w
```

```
[1] 3.958333
```

```r
lambda_lrt
```

```
[1] 3.825748
```

```r
lambda_s
```

```
[1] 3.8
```

```r
# Calculate p-values
# Recall: probability that we observe something *as or more extreme*
1 - pchisq(lambda_w, df = 1)
```

```
[1] 0.04663986
```

```r
1 - pchisq(lambda_lrt, df = 1)
```

```
[1] 0.05047083
```

```r
1 - pchisq(lambda_s, df = 1)
```

```
[1] 0.05125258
```

In this case, we would reject H_0 using the Wald test statistic, but *fail to reject* using the LRT statistic and score test statistic, since the only p-value that was below our significance threshold was the one calculated from the Wald test statistic. Finite-sample distributions of the three classical test statistics are generally unknown; only asymptotically have they been shown to be equivalent, and therefore, can provide *different* answers to hypothesis tests when sample sizes are relatively small.

8 Bayesian Statistics

Everything that we have covered so far in this course (and likely what you have covered in your entire statistics education thus far) has been from a *Frequentist* perspective. Frequentist statistics relies on the underlying belief that, in reality, there is some *fixed, unknown* truth (parameter) that we attempt to estimate by sampling from a population, computing an estimate, and quantifying our uncertainty. Uncertainty quantification typically takes the form of a confidence interval, and relies on the idea of repeated sampling from a population. The term "Frequentist" comes from the idea of a probability being related to the "frequency" at which an event occurs.

Bayesian statistics is named for Thomas Bayes, who coined **Bayes' Theorem** in 1763. At around a similar time, Pierre-Simon Laplace worked on very similar ideas, though all credit to Bayesian statistics is typically given to Thomas Bayes. While Bayes' Theorem itself is not inherently Bayesian (it is quite literally just a probability rule), it provides us with a mathematical foundation for Bayesian philosophy.

Philosophy

While Frequentists treat parameters as unknown, fixed constants, Bayesians instead treat parameters as random variables, such that parameters follow probability distributions. This distinction may seem subtle, but has large consequences on the interpretation of uncertainty in each paradigm, as well as the properties of Frequentist and Bayesian estimators (particularly in finite samples).

Rather than think of probability as being related to the frequency at which events occur, Bayesians instead think of probabilities in the more colloquial way: the *plausibility* that an event were to occur. In order to calculate the latter, we incorporate prior information or beliefs about the event *and* the data we observe to *update* our beliefs.

Note that this is inherently subjective, as prior information / beliefs are involved in our estimation framework. This subjectivity is one of the main reasons why Bayesian statistics was historically rejected and frowned upon in the statistics community, in addition to computational challenges that have really only been alleviated with computational advances made in the last 50 or so years. From a purely philosophical standpoint, Frequentist and Bayesian inference provide an interesting case study of the Enlightenment period, and modern thinking more broadly, compared with *post*-modern thinking. Back in the day, Frequentists and Bayesians were distinct. Nowadays, most reasonable statisticians will agree that both Frequentist and

Bayesian methods have a place in statistics, are subjective in their own ways, and are both useful in different circumstances.

Prior and Posterior Distributions

Suppose we collect data $\mathbf{X}$ (a random vector), and are interested in estimating some parameter θ. If we treat θ as a random variable, like Bayesians do, Bayes' theorem (again, really more of a probability rule than a theorem) states that,

$$\pi(\theta \mid \mathbf{X}) = \frac{\pi(\mathbf{X} \mid \theta)\pi(\theta)}{\pi(\mathbf{X})}.$$

The *marginal* distribution $\pi(\theta)$ is called the prior distribution for our parameter, and represents our initial beliefs. The *conditional* distribution $\pi(\mathbf{X} \mid \theta)$ is called the *likelihood*, and is exactly the same as the likelihoods we've been considering all throughout the semester thus far! Finally, $\pi(\theta \mid \mathbf{X})$ is called the *posterior* distribution for our parameter (our updated beliefs based on our prior beliefs and the data we observe), and $\pi(\mathbf{X})$ is called a normalizing constant (since it is constant in terms of θ, and is the term needed to ensure that the posterior distribution is a valid pdf, i.e., integrates to one).

In words, Bayesian statistics revolves around the following construct:

$$\text{Posterior} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Normalizing Constant}}$$

Prior distributions can be more or less informative, depending on context and modeling choice. Bayesian philosophy can be categorized roughly into two groups: "subjective" Bayes, and "objective" Bayes. Subjective Bayesians believe that prior information should be based on real-world, prior knowledge, and should typically be informative. Objective Bayesians use Bayesian inference as a tool to obtain reasonable estimates, but do not always incorporate *actual* prior knowledge into their prior distributions. Just as with the Frequentist vs. Bayesian debate, nowadaws, both subjective and objective Bayesian philosophies are generally accepted to have their time and place.

When choosing a prior distribution without actual prior knowledge of the unknown parameter, people sometimes opt for less informative priors (often called "uninformative" priors, though this is a misnomer). An example of a less informative prior would be something like a Uniform distribution on a large, non-infinite parameter space. People also sometimes choose to use *improper* priors, such as a Uniform distribution on an *infinite* parameter space. Such priors are called "improper" because they do not integrate to one, as pdfs must in order to be, by definition, pdfs. The use of improper priors can still, in many cases, lead to proper posterior distributions, but their use is still much less accepted in the broader statistical community.

Uncertainty

In Frequentist statistics, our estimate of an unknown parameter is a single point, and we quantify uncertainty with confidence intervals (based on the concept of repeated sampling). In Bayesian statistics, rather than a single point, we instead obtain an *entire distribution* for our unknown parameter. We can calculate single points from this distribution if we choose to (the mean of the posterior distribution, median, etc.), and some of these points have nice interpretations with regards to decision theory as we'll see in the next chapter. We can also make direct probability statements about the unknown parameter using this distribution, *without* the need for repeated sampling!

Rather than confidence intervals, we instead construct *credible* intervals using the quantiles of the posterior distribution. The interpretation of a credible interval is exactly the probability that the parameter lies between two values, given our prior beliefs and the data that we observe. Note that this is the interpretation that every student in introductory statistics wants *confidence* intervals to have! This is an exceedingly natural interpretation of a measure of uncertainty, and is much more easily understood by non-statisticians than the interpretation of a confidence interval.

Computation

While Bayesian computation is not the focus of this course, it should be noted that in most practical applications of Bayesian statistics, the computational "lift" of a Bayesian analysis is generally higher than that of a Frequentist analysis. In some cases, such as when we have conjugate priors (as defined below), computation is not a significant issue when doing a Bayesian analysis. However, conjugate priors are relatively rare in the "real world," and so more advanced computational techniques are required to estimate posterior distributions. There are two primary modes of estimating posterior distributions, with various computation programmes that have been developed to assist with model-fitting:

1. Markov-chain Monte Carlo methods (MCMC)
2. Laplace approximations

MCMC methods are more classical, and include Gibbs samplers, Hamiltonian Monte Carlo methods such as Stan, and more. These methods provide exact posterior distributions, but rely on tuning parameters and convergence diagnostics that can potentially be difficult to work with correctly. Laplace approximation techniques are newer, and include programmes such as Integrated Nested Laplace Approximations (INLA) and Template Model Builder (TMB). These methods provide *approximate* posterior distributions, but do not rely on tuning parameters nor do they require convergence diagnostics. They are often *significantly* faster than MCMC methods to run, but do not provide accurate approximations to posterior distributions in all cases.

To learn more, take a look at Bayes Rules! (co-authored by Mac's very own Alicia Johnson), or take STAT 454.

8.1 Learning Objectives

By the end of this chapter, you should be able to…

- Articulate the differences in Frequentist and Bayesian philosophy
- Derive the posterior distribution for an unknown parameter based on a specified prior and likelihood
- Evaluate the properties of posterior means, medians, etc.
- Articulate the impact of the choice of prior distribution on Bayesian estimation

8.2 Concept Questions

1. What is the difference between the Bayesian and Frequentist philosophies?
2. What are the typical steps to deriving a posterior distribution?
3. How is the posterior distribution impacted by the observed data and our choice of prior? What sorts of considerations should we keep in mind in choosing a prior?
4. How are Bayes and maximum likelihood estimators typically related?
5. What are typical Frequentist properties (e.g., bias, asymptotic bias, consistency) of Bayesian estimators (posterior means, for example)?

8.3 Definitions

Bayes' Theorem, Prior distribution, Posterior distribution

For two random variables θ and $\mathbf{X}$, Bayes' theorem states that,

$$\pi(\theta \mid \mathbf{X}) = \frac{\pi(\mathbf{X} \mid \theta)\pi(\theta)}{\pi(\mathbf{X})},$$

where $\pi(\theta)$ denotes the **prior distribution** of θ, $\pi(\mathbf{X} \mid \theta)$ denotes the likelihood, $\pi(\theta \mid \mathbf{X})$ denotes the **posterior distribution** of θ, and $\pi(\mathbf{X})$ denotes the normalizing constant.

Improper prior

An improper prior is a prior distribution that *does not integrate to 1*. This means that the prior is not a probability density function, since all pdfs must integrate to 1. In practice, some improper priors can still lead to proper posterior distributions, and as such, they are

occasionally used as one type of non-informative prior. The most commonly used improper proper is the uniform distribution from $-\infty$ to ∞.

Conjugate prior

A conjugate prior is a prior distribution that is in the same probability density family as the posterior distribution. Conjugate priors primarily used for computational convenience (as the posterior distributions then have closed form solutions), or when conjugacy makes sense in the context of the modeling problem. For examples of conjugate priors, the Wikipedia page linked here is quite complete.

Posterior mode

The posterior mode is, as the name implies, the mode of the posterior distribution. In math, the posterior mode is the estimate $\hat{\theta}$ that satisfies,

$$\frac{\partial}{\partial\theta}\pi(\theta \mid \mathbf{X}) = 0.$$

Posterior median

The posterior median is, as the name implies, the median of the posterior distribution. In math, the posterior median is the estimate $\hat{\theta}$ that satisfies,

$$\int_{-\infty}^{\hat{\theta}} \pi(\theta \mid \mathbf{X})d\theta = 0.5$$

Posterior mean

The posterior mean is, as the name implies, the mean of the posterior distribution. In math, the posterior mean is the estimate

$$\hat{\theta} = E[\theta \mid \mathbf{X}] = \int \theta\pi(\theta \mid \mathbf{X})d\theta$$

Credible interval

A 100(1 - α)% credible interval is an interval $(\Phi_{\alpha/2}, \Phi_{1-\alpha/2})$ for a parameter θ is given by

$$\int_{\Phi_{\alpha/2}}^{\Phi_{1-\alpha/2}} \pi(\theta \mid \mathbf{X})d\theta = 1 - \alpha,$$

where Φ_p denotes the pth quantile of the posterior distribution.

8.4 Theorems

None for this chapter, other than Bayes' theorem, which doesn't really count as a theorem cause it's just a probability rule!

8.5 Worked Examples

Problem 1: Suppose we have a random sample $X_1, \dots, X_n \overset{iid}{\sim} Bernoulli(\theta)$, and choose a $Beta(\alpha, \beta)$ prior for θ. Derive the posterior distribution, $\pi(\theta \mid X_1, \dots, X_n)$.

Solution:

We can write,

$$\begin{aligned}
\pi(\theta \mid X_1, \dots, X_n) &\propto \left(\prod_{i=1}^{n} f(x_i) \right) \pi(\theta) \\
&= \left(\prod_{i=1}^{n} \theta^{x_i} (1-\theta)^{1-x_i} \right) \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1} \\
&= \theta^{\sum_{i=1}^{n} x_i} (1-\theta)^{n-\sum_{i=1}^{n} x_i} \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1-\theta)^{\beta-1} \\
&\propto \theta^{\sum_{i=1}^{n} x_i + \alpha - 1} (1-\theta)^{n-\sum_{i=1}^{n} x_i + \beta - 1}
\end{aligned}$$

where we recognize the kernel of a $Beta(\sum_{i=1}^{n} X_i + \alpha, n - \sum_{i=1}^{n} X_i + \beta)$ distribution, and therefore this is the posterior distribution for θ.

Problem 2: Derive the posterior mean for θ in Problem 1.

Solution:

We know that the expectation of a $Beta(a, b)$ distribution is given by $\frac{a}{a+b}$, and so we have

$$\hat{\theta} = \frac{\sum_{i=1}^{n} X_i + \alpha}{\sum_{i=1}^{n} X_i + \alpha + n - \sum_{i=1}^{n} X_i + \beta} = \frac{\sum_{i=1}^{n} X_i + \alpha}{\alpha + \beta + n}$$

Problem 3: Write the posterior mean from Problem 2 as a function of the MLE, $\hat{\theta}_{MLE} = \overline{X}$, and the *prior* mean for θ. What do you notice?

Solution:

We can write,

$$
\begin{aligned}
\hat{\theta} &= \frac{\sum_{i=1}^{n} X_i + \alpha}{\alpha + \beta + n} \\
&= \frac{\sum_{i=1}^{n} X_i}{\alpha + \beta + n} + \frac{\alpha}{\alpha + \beta + n} \\
&= \frac{\frac{n}{n}\sum_{i=1}^{n} X_i}{\alpha + \beta + n} + \frac{\frac{\alpha(\alpha+\beta)}{\alpha+\beta}}{\alpha + \beta + n} \\
&= \left(\frac{n}{\alpha + \beta + n}\right)\overline{X} + \left(\frac{\alpha + \beta}{\alpha + \beta + n}\right)\left(\frac{\alpha}{\alpha + \beta}\right)
\end{aligned}
$$

and so we can see that the posterior mean is a *weighted average* of the prior mean and the MLE (in this case, the sample mean)!

Problem 4: Suppose we have a random sample $X_1, \ldots, X_n \overset{iid}{\sim} Poisson(\lambda)$, and choose a $Gamma(\alpha, \beta)$ prior for λ. Derive the posterior distribution, $\pi(\lambda \mid X_1, \ldots, X_n)$.

Solution:

We can write,

$$
\begin{aligned}
\pi(\lambda \mid X_1, \ldots, X_n) & \\
&\propto \left(\prod_{i=1}^{n} f(x_i)\right) \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda} \\
&= \left(\prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}\right) \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda} \\
&= \frac{\lambda^{\sum_{i=1}^{n} x_i} e^{-n\lambda}}{\prod_{i=1}^{n} x_i!} \frac{\beta^\alpha}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda} \\
&\propto \lambda^{\sum_{i=1}^{n} x_i + \alpha - 1} e^{-n\lambda - \beta\lambda} \\
&= \lambda^{\sum_{i=1}^{n} x_i + \alpha - 1} e^{-(n+\beta)\lambda}
\end{aligned}
$$

where we recognize the kernel of a $Gamma(\sum_{i=1}^{n} X_i + \alpha, n + \beta)$ distribution, and therefore this is the posterior distribution for λ.

Problem 5: Derive the posterior mean for λ in Problem 4.

Solution:

We know that the expectation of a $Gamma(a, b)$ distribution is given by $\frac{a}{b}$, and so we have

$$\hat{\lambda} = \frac{\sum_{i=1}^{n} X_i + \alpha}{n + \beta}$$

Problem 6: Write the posterior mean from Problem 5 as a function of the MLE, $\hat{\lambda}_{MLE} = \overline{X}$, and the *prior* mean for λ. What do you notice?

Solution:

We can write,

$$\begin{aligned}
\hat{\lambda} &= \frac{\sum_{i=1}^{n} X_i + \alpha}{n + \beta} \\
&= \frac{\sum_{i=1}^{n} X_i}{n + \beta} + \frac{\alpha}{n + \beta} \\
&= \frac{n\overline{X}}{n + \beta} + \frac{\frac{\beta\alpha}{\beta}}{n + \beta} \\
&= \left(\frac{n}{n + \beta}\right)\overline{X} + \left(\frac{\beta}{n + \beta}\right)\frac{\alpha}{\beta}
\end{aligned}$$

and so we can see (again) that the posterior mean is a *weighted average* of the prior mean and the MLE (in this case, the sample mean)!

Problem 7: What is the asymptotic behavior of the posterior means calculated in Problems 2 and 5?

Solution:

In both cases, as $n \to \infty$, the posterior mean will approach the MLE! This is easiest to note after we observe that the posterior mean is a weighted average of the MLE and the prior mean. The weight on the prior mean will approach zero, as the weight on the MLE will approach 1, as n goes to infinity.

9 Decision Theory

Statistical decision theory is the branch of statistics that concerns itself with figuring out the best possible choice to make in a given situation using probability theory. Colloquially, decisions often have pros and cons. We can quantify these pros and cons using a *loss function*, and calculate the expected loss of a given decision (formally called *risk*). As you might guess, risk is something we want to *minimize*. We can minimize risk (after formally defining it) using the same calculus techniques we've been using all semester!

For the purposes of this class, the "decisions" we make are our choice of estimator for an unknown parameters. This is one type of *deterministic* decision rule. At the beginning of this course, we learned about two different intuitive approaches to defining estimators (or "decisions"): maximum likelihood estimation and the method of moments. In this chapter, we'll find estimators that minimize risk!

While decision theory is not inherently Bayesian, it is one way to "justify" point estimates from posterior distributions. **Bayes estimates** are posterior point estimates that minimize a certain loss function. The posterior mean, median, and mode are all such point estimates, for example.

Admissibility

An important concept in decision theory is the idea of *admissibility*. An admissible decision rule is one that has the lowest possible risk out of all decision rules, for all possible parameter values. It is easier to define (in math) an *inadmissible* decision rule, and then note that an admissible decision rule is *not* inadmissible (double negative).

An decision rule D (think, $\hat{\theta}$) is inadmissible if there exists a rule D' (think, some other estimator) such that

$$\begin{aligned} R(D,\theta) &\leq R(D,\theta) \quad \forall\theta \\ R(D',\theta) &< R(D,\theta) \quad \text{for some } \theta \end{aligned}$$

where $R(D,\theta)$ is the risk of a decision D for a paramater θ. If D is not inadmissible, it is *admissible*. In words, in order for a decision rule to be admissible, it must have risk *at least*

as small as every other possible decision rule everywhere in the parameter space, *and* it must have strictly lower risk for at least one parameter value.

One of the most fascinating results to come out of decision theory (in my personal opinion) is that the sample mean is *not* an admissible decision rule for the mean of a Multivariate Normal distribution under MSE loss when the mean has greater than or equal to three dimensions! Relating this to what you know from introductory statistics, this means that (from a decision theory perspective) *least squares* is not an admissible approach to estimating the regression coefficients in a linear regression model with *at least two* covariates. The specific (biased) estimator of the mean that provides a lower MSE in this case is called the James-Stein estimator.

Minimaxity

One other "property" of a decision rule in addition to admissibility is called *minimaxity*. Think once more about pros and cons of decisions. Some cons are worse than others (consider extreme side effects of drugs, for example). A **minimax** decision rule is one that the *lowest possible maximal* risk, out of a set of decision rules. It "minimizes" the "maximum"!

Bayes and minimax decision rules are generally related through the concept of a *least favorable prior sequence*. Intuitively, a "least favorable" prior is one that leads to higher risk than other priors. The theory involved in minimax problems requires a pretty solid understanding of analysis techniques, and are beyond the scope of this course (but are interesting to look into on your own time!).

9.1 Learning Objectives

By the end of this chapter, you should be able to…

- Derive a Bayes estimate for a common loss function
- Distinguish between admissible and inadmissible decision rules

9.2 Concept Questions

9.2.1 Reading Questions

1. What are some examples of commonly-used loss functions?
2. What are the typical steps to finding a Bayes estimate?
3. What are the Bayes estimates for absolute error loss and squared error loss?
4. What does it mean for a decision rule to be admissible (in colloquial language)?
5. What does it mean for a decision rule to be minimax (in colloquial language)?

9.3 Definitions

Loss Function

Let $\hat{\theta}$ be an estimator for θ. A loss function associated with $\hat{\theta}$ is denoted $L(\hat{\theta}, \theta)$, where $L(\hat{\theta}, \theta) \geq 0$ and $L(\theta, \theta) = 0$. A reasonable loss function will increase the further away $\hat{\theta}$ and θ are from each other.

Decision Rule

For the purposes of this class, an estimator! In the statistics literature, you will often see this denoted D, but we can also denote the decision rule $\hat{\theta}$ for this class.

Risk

In words, risk is the expected loss of our decision, given our data. In math,

$$R(\hat{\theta}, \theta) = E[L(\hat{\theta}, \theta) \mid \mathbf{Y}] = \int L(\hat{\theta}, \theta)\pi(\theta \mid \mathbf{Y})d\theta$$

Bayes Estimate

A Bayes estimate is the estimate or decision rule that minimizes risk (expected posterior loss). This is sometimes called a "Bayes rule" in the literature.

Unique Bayes Rule

For a given prior $\pi(\theta)$, a decision rule D_π is a *unique Bayes rule* (estimate) if, for all θ, a decision rule is a Bayes rule if and only if it is equal to D_π. Bayes rules are unique when:

- The loss function used is MSE loss
- The risk of the Bayes rule is finite
- A σ-field condition is satisfied (well beyond the scope of this course)

For what we consider in this course, whenever we use MSE loss in this course, the other two conditions will be satisfied.

Admissibility

An decision rule D is inadmissible if there exists a rule D' such that

$$\begin{aligned} R(D', \theta) &\leq R(D, \theta) \quad \forall \theta \\ R(D', \theta) &< R(D, \theta) \quad \text{for some } \theta \end{aligned}$$

where $R(D, \theta)$ is the risk of a decision D for a paramater θ. If D is not inadmissible, it is *admissible*.

9.4 Theorems

Theorem (Unique Bayes rules are admissible). Any unique Bayes rule is admissible.

Proof. We'll prove this by contradiction!

Suppose that D_π is a unique Bayes rule with respect to some prior $\pi(\theta)$, and that D_π is *inadmissible*. Then there exists some other decision rule D' such that $R(D', \theta) \leq R(D_\pi, \theta)$, for all θ. Then,

$$\begin{aligned} R(D', \theta) &\leq R(D_\pi, \theta) \qquad \text{(inadmissibility)} \\ &= \inf_D R(D, \pi) \qquad (D_\pi \text{ is Bayes}) \end{aligned}$$

and since $R(D', \theta) \leq \inf_D R(D, \pi)$, D' is Bayes. But D_π is *unique* Bayes by assumption, so this is a contradiction.

Therefore, D_π is admissible.

9.5 Worked Examples

Problem 1: Show that the posterior median is the decision rule that minimizes risk with respect to absolute loss, $L(\widehat{\theta}, \theta) = |\widehat{\theta} - \theta|$.

Solution:

We can write the risk with respect to absolute loss as

$$\begin{aligned} R(\theta_0, \theta) &= E[L(\theta_0, \theta) \mid \mathbf{Y}] \\ &= \int L(\theta_0, \theta) \pi(\theta \mid \mathbf{y}) d\theta \\ &= \int |\theta_0 - \theta| \pi(\theta \mid \mathbf{y}) d\theta \\ &= \int_{I\{\theta_0 \geq \theta\}} (\theta_0 - \theta)\, \pi(\theta \mid \mathbf{y}) d\theta + \int_{I\{\theta_0 < \theta\}} (\theta - \theta_0)\, \pi(\theta \mid \mathbf{y}) d\theta \\ &= \int_{-\infty}^{\theta_0} (\theta_0 - \theta)\, \pi(\theta \mid \mathbf{y}) d\theta + \int_{\theta_0}^{\infty} (\theta - \theta_0)\, \pi(\theta \mid \mathbf{y}) d\theta \end{aligned}$$

Taking the derivative with respect to θ_0, and setting this equal to zero we get

$$
\begin{aligned}
0 &\equiv \frac{\partial}{\partial \theta_0} R(\theta_0, \theta) \\
&= \frac{\partial}{\partial \theta_0} \left(\int_{-\infty}^{\theta_0} (\theta_0 - \theta)\, \pi(\theta \mid \mathbf{y}) d\theta + \int_{\theta_0}^{\infty} (\theta - \theta_0)\, \pi(\theta \mid \mathbf{y}) d\theta \right) \\
&= (\theta_0 - \theta_0)\, \pi(\theta_0 \mid \mathbf{y}) - \int_{-\infty}^{\theta_0} \pi(\theta \mid \mathbf{y}) d\theta - (\theta_0 - \theta_0)\, \pi(\theta_0 \mid \mathbf{y}) + \int_{\theta_0}^{\infty} \pi(\theta \mid \mathbf{y}) d\theta \\
&= -\int_{-\infty}^{\theta_0} \pi(\theta \mid \mathbf{y}) d\theta + \int_{\theta_0}^{\infty} \pi(\theta \mid \mathbf{y}) d\theta \\
\int_{-\infty}^{\theta_0} \pi(\theta \mid \mathbf{y}) d\theta &= \int_{\theta_0}^{\infty} \pi(\theta \mid \mathbf{y}) d\theta
\end{aligned}
$$

(recalling that $\int_{-\infty}^{x} f(y)dy = f(x)$ and $\int_{x}^{\infty} f(y)dy = -f(x)$ and applying chain rule), and note that these two integrals are equal when θ_0 is the posterior median.

Problem 2: Show that the posterior mode is the decision rule that minimizes risk with respect to 0-1 loss,

$$
L(\hat{\theta}, \theta) = \begin{cases} 0 & \text{if } \hat{\theta} = \theta \\ 1 & \text{if } \hat{\theta} \neq \theta \end{cases}
$$

when θ is a *discrete* random variable.

Solution:

Note that we can rewrite the 0-1 loss function as $L(\hat{\theta}, \theta) = 1 - I\{\hat{\theta} = \theta\}$. Then we can write,

$$
\begin{aligned}
R(\theta_0, \theta) &= E[L(\theta_0, \theta) \mid \mathbf{Y}] \\
&= \sum_{\theta} L(\theta_0, \theta) \pi(\theta \mid \mathbf{y}) \\
&= \sum_{\theta} (1 - I\{\theta_0 = \theta\})\, \pi(\theta \mid \mathbf{y}) \\
&= \sum_{\theta} \pi(\theta \mid \mathbf{y}) - \sum_{\theta} I\{\theta_0 = \theta\} \pi(\theta \mid \mathbf{y}) \\
&= 1 - \pi(\theta_0 \mid \mathbf{y})
\end{aligned}
$$

since pmfs sum to 1. Then taking the derivative and setting this equal to zero gives

$$
\begin{aligned}
0 &\equiv \frac{\partial}{\partial \theta_0} R(\theta_0, \theta) \\
&= \frac{\partial}{\partial \theta_0} \left(1 - \pi(\theta_0 \mid \mathbf{y})\right) \\
&= \frac{\partial}{\partial \theta_0} \pi(\theta_0 \mid \mathbf{y})
\end{aligned}
$$

and the solution to this equation is, by definition, the posterior mode.

Note: For the case where θ is a continuous random variable, we need something called a Dirac delta function to prove this. The reasoning for *why* we need this (and the proof, which is similar to the discrete case) is given below.

Solution for continuous θ :

Note that we can rewrite the 0-1 loss function as $L(\hat{\theta}, \theta) = 1 - \delta\{\hat{\theta} - \theta\}$, where δ is the Dirac delta function. Then we can write,

$$
\begin{aligned}
R(\theta_0, \theta) &= E[L(\theta_0, \theta) \mid \mathbf{Y}] \\
&= \int L(\theta_0, \theta) \pi(\theta \mid \mathbf{y}) d\theta \\
&= \int \left(1 - \delta(\theta_0 - \theta)\right) \pi(\theta \mid \mathbf{y}) d\theta \\
&= \int \pi(\theta \mid \mathbf{y}) d\theta - \int \delta(\theta_0 - \theta) \pi(\theta \mid \mathbf{y}) d\theta \\
&= 1 - \pi(\theta_0 \mid \mathbf{y})
\end{aligned}
$$

since pdfs integrate to 1. The reason why we can't use the same indicator definition as for the discrete case is because the integral of an indicator that is only positive at a single observation is *zero*. The Dirac delta function, on the other hand, has positive mass (equal to 1) at $\theta_0 - \theta = 0$. Take Projects in Real Analysis to learn more! Taking the derivative and setting this equal to zero gives the same result as in the discrete case.

10 Computational Optimization

Welcome to the last chapter of the course notes! There are no worked examples or concept questions for this chapter, which is instead focused on practical implementation of a handful of useful algorithms, and useful computational techniques that you may come across in your future, statistical career. Go forth and compute!

10.1 Newton-Raphson

Recall from the second chapter of the course notes the typical procedure for finding an MLE:

1. Find the log likelihood
2. Take a derivative with respect to the unknown parameter(s)
3. Set it equal to zero, and solve

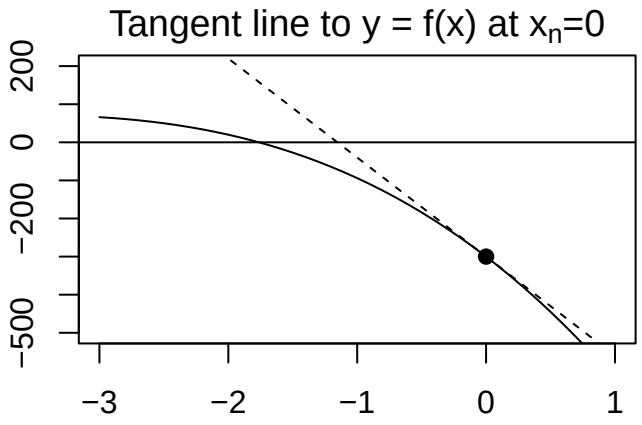
We previously saw that *sometimes* this procedure doesn't work, in particular, when the support of the density function depends on our unknown parameters. In these cases, we noted that the MLE would be an order statistic. There are *other* situations, however, where neither the MLE is neither readily found analytically nor is it an order statistic. In these cases, we turn to computational techniques, such as **Newton-Raphson**.

Newton-Raphson is a root-finding algorithm, and hence useful when trying to maximize a function (or a likelihood!). Suppose we want to find a root (i.e., the value of x such that $f(x) = 0$) of the function f with derivative denoted f'. Newton-Raphson takes the following steps:

1. Start with an initial guess x_0
2. Update your guess according to $x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$
3. Repeat step 2 according to $x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$ until your guesses have "converged" (i.e. are very very similar)

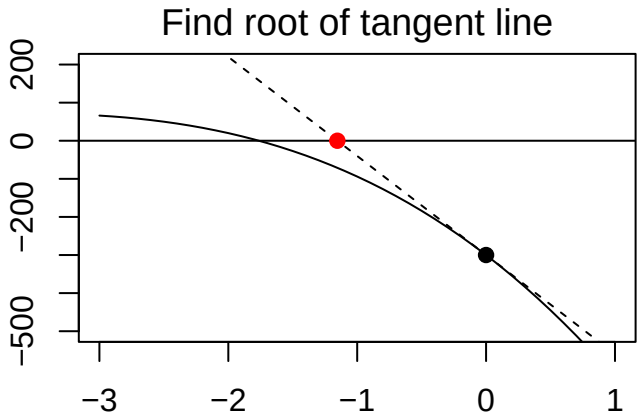
A maximum likelihood estimator is the root of the first derivative of the log-likelihood (a.k.a. the value at which the derivative of the log-likelihood crosses zero). This means that, for finding MLEs, the Newton-Raphson algorithm replaces $f = \frac{\partial}{\partial\theta} \log L(\theta)$.

We can visualize this process as follows:



The equation of the tangent line to the curve $y = f(x)$ at a point $x = x_n$ is

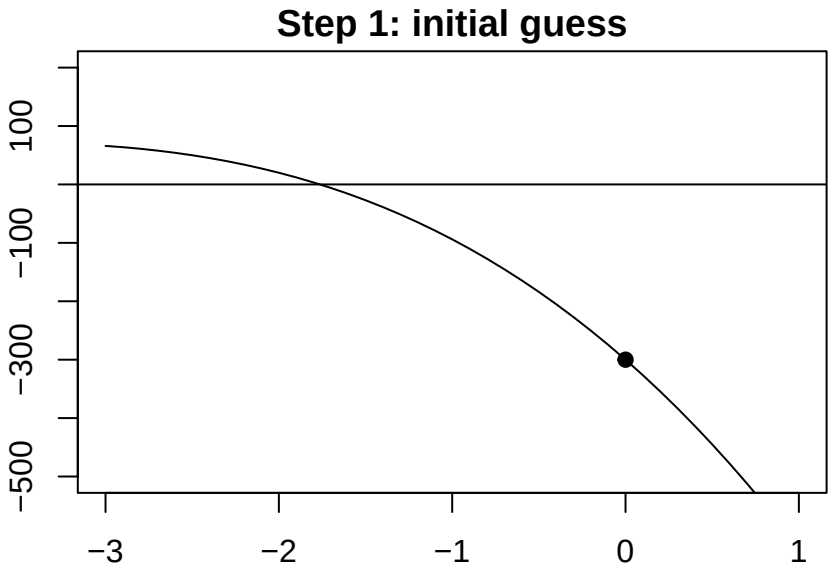
$$y = f'(x_n)(x - x_n) + f(x_n)$$



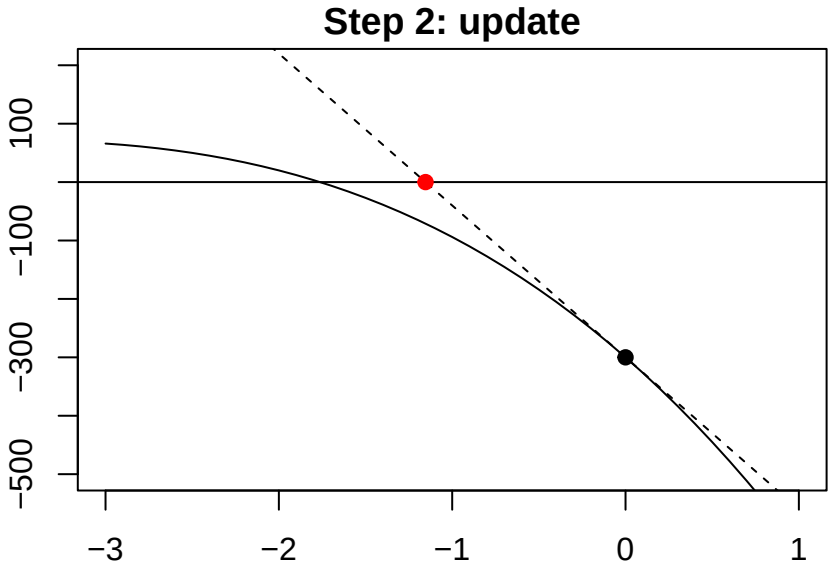
The root of this tangent line (i.e., the place where it crosses the x-axis) is easy to find:

$$0 = f'(x_n)(x - x_n) + f(x_n) \iff x = x_n - f(x_n)/f'(x_n)$$

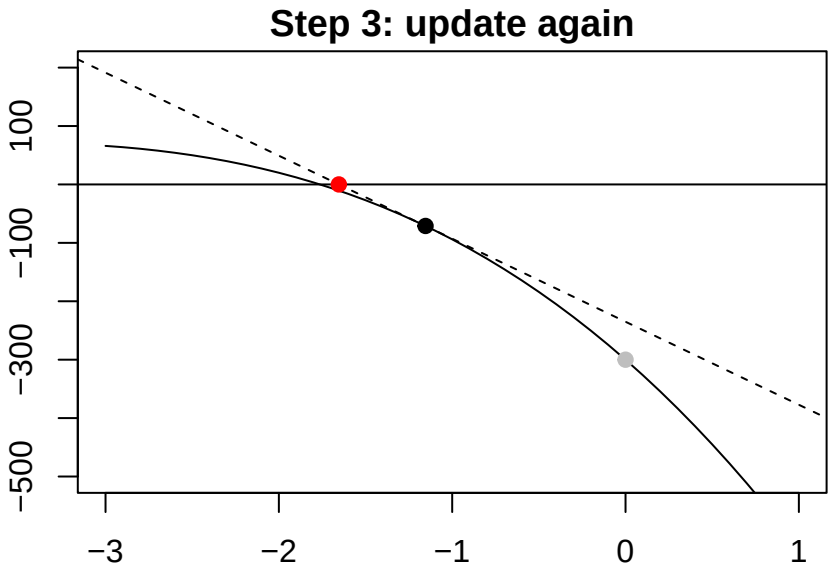
Take this root of the tangent line as our next guess, then repeat…



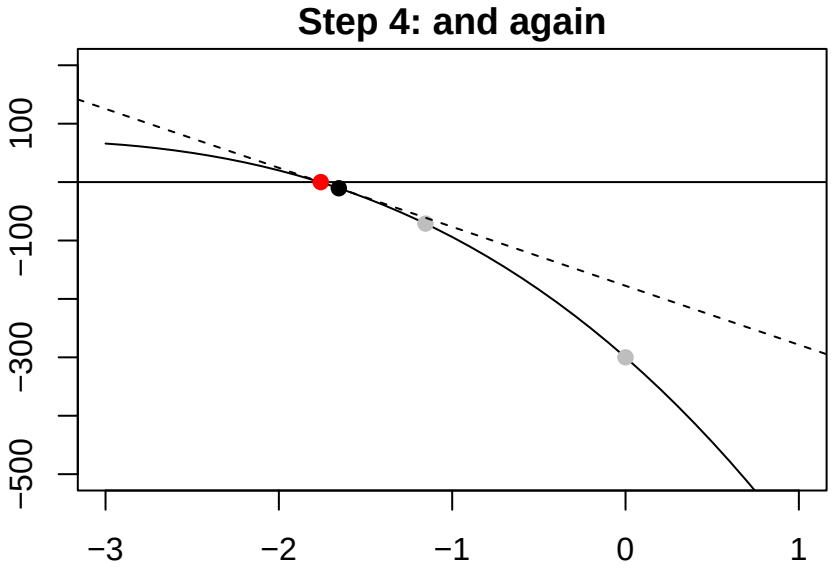
...and repeat...



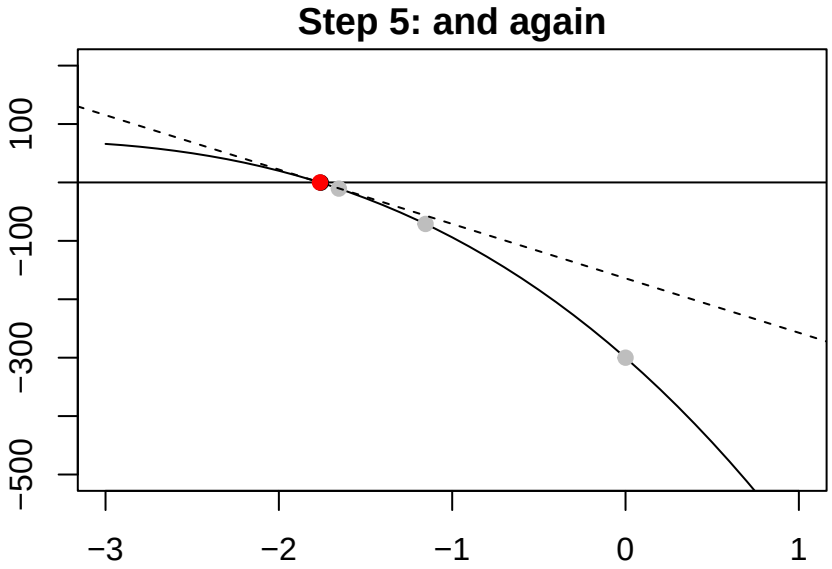
...and repeat...



...and repeat...



...and repeat...



…and keep repeating until you've converged!

The multivariate version of Newton-Raphson is called the Scoring algorithm (also sometimes called Fisher's scoring), and is used in `R` to obtain estimates of logistic regression coefficients.

Motivating Example: Logistic Regression

Suppose that we observe data (y_i, x_i) where the outcome y is binary. A natural model for these data is to assume the statistical model

$$\begin{aligned} y_i &\sim Bernoulli(p_i), \\ \log\left(\frac{p_i}{1-p_i}\right) &= \beta_0 + \beta_1 x_i. \end{aligned}$$

This is a simple logistic regression model, with unknown parameters given by the logistic regression coefficients β_0, β_1. Let's attempt to find MLEs for β_0 and β_1 analytically.

Note that $p_i = \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}$. Then the likelihood of our Bernoulli observations y_i can be written as

$$L(\beta_0, \beta_1) = \prod_{i=1}^{n} \left(\frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}\right)^{y_i} \left(\frac{1}{1+e^{\beta_0+\beta_1 x_i}}\right)^{1-y_i}$$

Following the typical procedure, we log the likelihood…

$$\begin{aligned}\log(L(\beta_0,\beta_1)) &= \sum_{i=1}^{n}\left[y_i\log(\frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}) + (1-y_i)\log(\frac{1}{1+e^{\beta_0+\beta_1 x_i}})\right] \\ &= \sum_{i=1}^{n}\left[y_i(\beta_0+\beta_1 x_i) - y_i\log(1+e^{\beta_0+\beta_1 x_i}) - \log(1+e^{\beta_0+\beta_1 x_i}) + y_i\log(1+e^{\beta_0+\beta_1 x_i})\right] \\ &= \sum_{i=1}^{n}\left[y_i(\beta_0+\beta_1 x_i) - \log(1+e^{\beta_0+\beta_1 x_i})\right]\end{aligned}$$

…taking the partial derivatives with respect to β_0 and β_1 we get…

$$\begin{aligned}\frac{\partial}{\partial\beta_0}\log(L(\beta_0,\beta_1)) &= \sum_{i=1}^{n}\left[y_i - \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}\right] \\ \frac{\partial}{\partial\beta_1}\log(L(\beta_0,\beta_1)) &= \sum_{i=1}^{n}\left[x_i\left(y_i - \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}\right)\right]\end{aligned}$$

…and if you try to solve the system of equations given by

$$\begin{aligned}0 &\equiv \sum_{i=1}^{n}\left[y_i - \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}\right] \\ 0 &\equiv \sum_{i=1}^{n}\left[x_i\left(y_i - \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}\right)\right]\end{aligned}$$

you'll get nowhere! There is no analytical (sometimes called "closed-form") solution. In this case, we'd need to use the Scoring algorithm to solve for the regression coefficient estimates, since we have more than one unknown parameter.

Why do anything analytically, if Newton-Raphson exists?

You may be wondering why you've been doing calculus/algebra the entire semester, when such an algorithm exists. The answer is two-fold.

1. Going through the steps of finding an MLE analytically helps build intuition. We saw that in the vast majority of cases, maximum likelihood estimators are functions of sample means. This is less obvious when doing everything numerically (using an algorithm). In addition to gaining insight from finding MLEs by hand, this practice also gave you the opportunity to learn/use common "tricks" in statistics, that will find their way into problems you complete down the road or research you may eventually conduct.

2. Numerical optimization is *slow*. For simple cases like the ones we've seen in class, numerical optimization would techniques like Newton-Raphson would run relatively quickly. However, for more complex likelihoods with many unknown parameters, various optimization techniques can be so slow as to be computationally prohibitive. Even with continual improvements in computational power (and improvements in the algorithms themselves), computational speed is an important consideration when conducting statistical research or developing new methodology. If it takes someone two weeks to fit their regression model using numerical optimization, for example, that person may never fit a regression model ever again, or give up entirely. Especially when considering *who* has access to computational power, this can become an equity issue. If you can solve something analytically, **do it**. It's significantly faster in the long-term, even it takes you some time to do the calculus/algebra.

10.2 Simulation Studies

Sometimes proofs are hard. In such cases (and more generally), it can often be useful to "test" or observe properties of estimators in a computational setting, rather than in a rigorous mathematical context. This is where simulation studies come into play, and if you eventually find yourself conducting statistical research, knowing how to conduct a well-designed, reproducible, simulation study is an incredibly important skill.

The general idea of simulation study is to generate realistic settings (data) that could be observed in the real world, in order to compare properties of various estimators and their behavior in scenarios where the "truth" is *known* (because *you* generated the truth!). Steps include:

1. Determine your simulation settings (different parameter values, sample sizes, etc.)
2. Generate *many* data sets for each setting
3. Compute your estimator / implement your method for each data set
4. Record the relevant property of that estimator / method for each data set
5. Summarize your results across data sets and simulation settings

This can be a *great* way to get a feel for how certain estimators/methods behave in different settings without needing to rigorously prove something. Additionally, it can be used to *inform* more rigorous proofs down the line; if we can better understand how estimators/methods behave, we may be able to relate that behavior to existing proofs and build upon them!

10.3 Gibbs Samplers

Not everything is conjugate. In cases where we don't have conjugate priors, posterior distributions may not have closed-form, analytical pdfs, and instead we rely on Markov-chain Monte-Carlo (MCMC) algorithms (or Laplace approximations) to generate samples from posteriors.

As noted in the Bayes chapter of our course notes, Bayes Rules! is a great place to go for an introduction to Bayesian statistics. Here, we'll talk through one (classical) example of an MCMC approach to posterior inference; Gibbs Samplers.

The gist of Gibbs Sampling is that, when we have more than one unknown parameter, we can obtain the *joint* posterior distribution for all parameters by updating our guesses about each parameter, one at a time. This involves working with what are typically called *full conditionals* (the distribution of each parameter *conditional on everything else*).

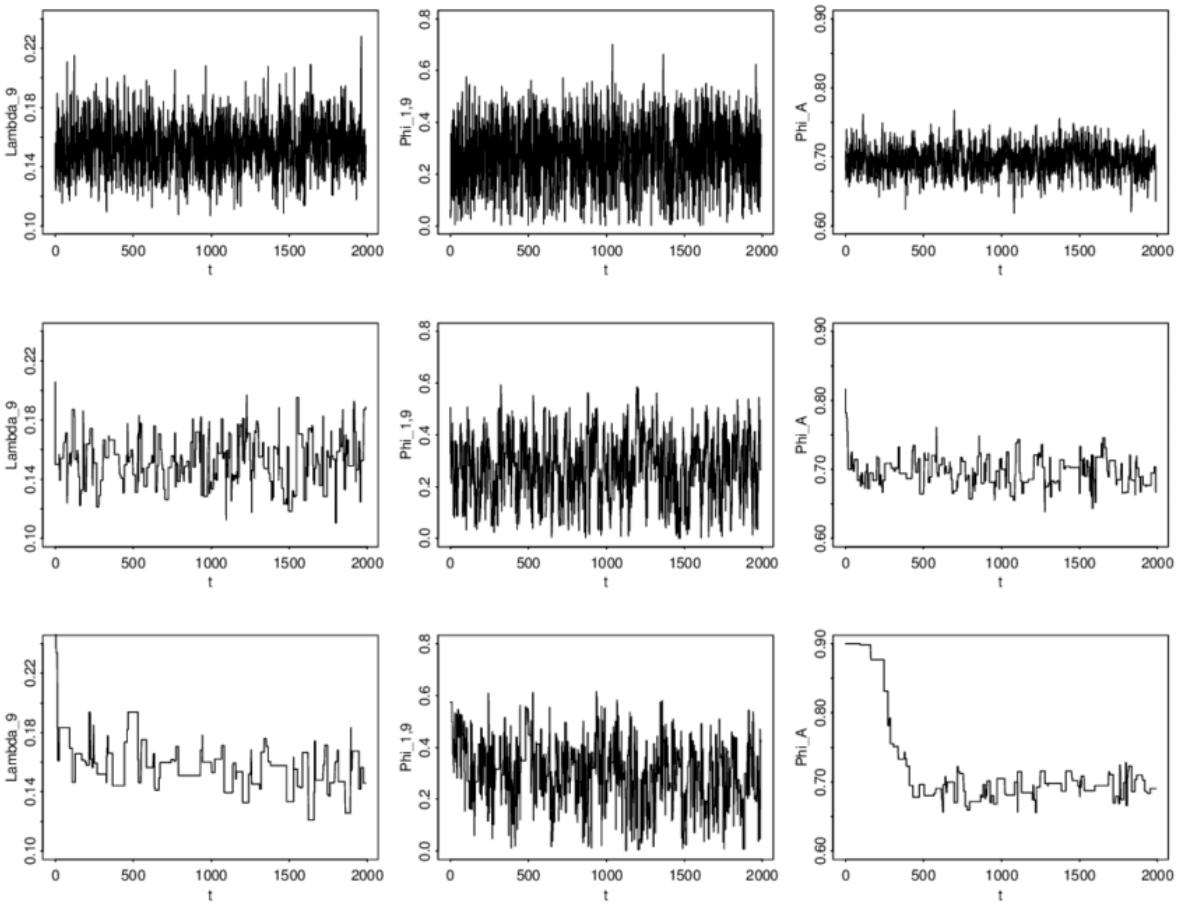
The Gibbs Sampling algorithm is as follows:

1. Choose initial values for each unknown parameter, $\theta_1^{(0)}$, $\theta_2^{(0)}$, ..., $\theta_p^{(0)}$
2. Sample $\theta_1^{(0)} \sim \pi(\theta_1^{(0)} \mid \theta_2^{(0)}, \dots, \theta_p^{(0)}, \mathbf{y})$
3. Sample $\theta_2^{(0)} \sim \pi(\theta_2^{(0)} \mid, \theta_1^{(0)}, \theta_3^{(0)}, \dots, \theta_p^{(0)}, \mathbf{y})$
4. ...
5. Sample $\theta_p^{(0)} \sim \pi(\theta_p^{(0)} \mid \theta_1^{(0)}, \dots, \theta_{p-1}^{(0)}, \mathbf{y})$
6. Repeat many times, always sampling new observations conditional on your most recent guess (iteration) for each parameter!

It feels almost magical, but the end result is that we obtain many samples from the joint posterior distribution for all unknown parameters! MCMC methods such as Gibbs Samplers are what is known as "exact" methods for conducting Bayesian inference, because so long as sampling goes according to plan*, the posterior draws will be from the exactly correct, joint posterior distribution. This is opposed to Laplace approximation techniques which are, by definition, "approximate."

*Let's define "according to plan." Sometimes algorithms can go wrong. We saw an example of this with Newton-Raphson, where if we pick a terrible starting value, the algorithm can sometimes diverge. With Gibbs Samplers, we should be careful of checking convergence diagnostics. A visual tool for this is called a **Trace Plot**. Trace plots show the values of parameters that are being sampled across iterations. The values across iterations are referred to as **chains**.

Here are some examples of chains that have converged:



There are *many* other convergence diagnostics you will need to consider if you end up doing research involving MCMC algorithms. A recent research paper on convergence diagnostics that is generally accepted now as best practice among Bayesian statisticians can be found here.