

# Lecture 10: Bayesian Inference and Bayes' Rule

CS109A: Introduction to Data Science

Harvard University

- **Course:** CS109A: Introduction to Data Science
- **Lecture:** Lecture 10
- **Instructor:** Pavlos Protopapas, Kevin Rader, Chris Gumb
- **Objective:** Reviewing statistical inference, understanding the distinction between confidence and prediction intervals, learning Bayes' rule, and introducing Bayesian inference as an alternative paradigm to frequentist statistics

## Contents

# 1 Introduction and Motivation

## Lecture Overview

This lecture reviews statistical inference concepts and introduces a fundamentally different way of thinking about probability and parameters: **Bayesian inference**. The Bayesian approach treats parameters as random variables with probability distributions, rather than fixed unknown constants.

### Key Topics:

- **Review of Inference:** Standard errors, confidence intervals, hypothesis testing
- **Bootstrap vs. Permutation:** When to use which resampling method
- **Confidence Interval vs. Prediction Interval:** A crucial distinction
- **Likelihood Review:** The foundation for Bayesian methods
- **Bayes' Rule:** Flipping conditional probabilities
- **Bayesian Inference:** Updating beliefs based on evidence
- **Frequentist vs. Bayesian:** Two worldviews of statistics

## 1.1 Continuing the Housing Example

We continue with the Cambridge/Somerville housing data from last lecture:

- **Simple regression:** Price  $\sim$  Square footage
- **Estimated model:**  $\hat{y} = 247.4 + 0.5898x$
- **Interpretation:** Each additional square foot is associated with roughly \$600 higher selling price

### Correlation vs. Causation Reminder

“Be careful. Doesn’t mean it’s causal because there could be other confounders in that data set that we haven’t controlled for.”

The coefficient 0.5898 represents an *association*, not necessarily a causal effect. Other factors correlated with square footage (neighborhood quality, lot size, etc.) might be driving part of this relationship.

# 2 Review: Statistical Inference

## 2.1 Population vs. Sample

### Definition: Two Models

**Population Model** (what we want):

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

- $\beta_0, \beta_1$  are the *true* parameters for all homes in this geographic region

- $\sigma^2 = \text{Var}(\epsilon_i)$  is another unknown parameter

**Estimated Model** (what we have):

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$$

- $\hat{\beta}_0, \hat{\beta}_1$  are estimates from our sample of  $\sim 500$  homes
- These are one “realization” from the sampling distribution

## 2.2 Standard Errors: Understanding Uncertainty

The **standard error** (SE) quantifies how much our estimate would vary across different samples:

**Definition: Standard Error of the Slope**

$$\hat{SE}(\hat{\beta}_1) = \sqrt{\frac{\hat{\sigma}^2}{\sum_{i=1}^n (x_i - \bar{x})^2}}$$

where  $\hat{\sigma}^2$  is the estimated residual variance.

### 2.2.1 What Controls the Standard Error?

Looking at the formula, we can build intuition:

#### How to Reduce Standard Error

1. **Increase sample size ( $n$ ):**
  - More observations  $\rightarrow$  larger denominator
  - The sum  $\sum (x_i - \bar{x})^2$  increases with  $n$
  - **Most reliable way to reduce SE**
2. **Increase spread in  $X$ :**
  - Wider range of  $X$  values  $\rightarrow$  larger  $\sum (x_i - \bar{x})^2$
  - Hard to control in observational studies
  - In experiments, you can deliberately sample extreme  $X$  values
3. **Reduce residual variance ( $\hat{\sigma}^2$ ):**
  - Better model  $\rightarrow$  tighter fit around the line
  - Add relevant predictors, use transformations
  - Limited by irreducible error

### 2.2.2 What About Standardizing Predictors?

Professor Rader poses a “midterm type question”: What happens to the SE formula if you standardize the predictor?

**Example: The Standardization Trap**

At first glance, standardizing  $X$  (mean 0, variance 1) might seem to reduce SE since the denominator becomes smaller.

**But wait!**

When you standardize  $X$ :

- The denominator  $\sum(x_i - \bar{x})^2$  decreases
- BUT  $\hat{\beta}_1$  itself changes (different units!)
- Interpretation changes from “per unit  $X$ ” to “per standard deviation of  $X$ ”

**Net effect:** The t-statistic remains the same!

$$t = \frac{\hat{\beta}_1}{\hat{SE}(\hat{\beta}_1)}$$

Standardizing doesn’t magically make your predictor more “significant.” The narrower CI is offset by a smaller  $\hat{\beta}_1$ .

## 2.3 Confidence Intervals: Formula-Based

**Definition: Confidence Interval Formula**

$$\text{CI for } \beta_1 : \hat{\beta}_1 \pm t^* \cdot \hat{SE}(\hat{\beta}_1)$$

where  $t^*$  is the critical value from the t-distribution (roughly 2 for 95% CI with large samples).

### 2.3.1 Why t-distribution Instead of Normal?

**t-Distribution vs. Normal Distribution**

**Normal (Z) distribution:** Used when  $\sigma$  is *known* (rare in practice).

**t-distribution:** Used when  $\sigma$  must be *estimated* from data.

- Estimating  $\sigma$  adds extra uncertainty
- t-distribution has “fatter tails” to account for this
- As sample size  $\rightarrow \infty$ , t-distribution  $\rightarrow$  normal distribution
- With  $n \geq 50$ , the difference is minimal

## 2.4 Hypothesis Testing Review

**Hypothesis Testing for  $\beta_1$** 

**Hypotheses:**

- $H_0 : \beta_1 = 0$  (no association between  $X$  and  $Y$ )
- $H_A : \beta_1 \neq 0$  (there is an association)

**Test Statistic:**

$$t = \frac{\hat{\beta}_1 - 0}{\hat{SE}(\hat{\beta}_1)} = \frac{\hat{\beta}_1}{\hat{SE}(\hat{\beta}_1)}$$

This measures: “How many standard errors is our estimate from zero?”

**p-value:** Probability of observing a  $|t|$  this extreme or more extreme, assuming  $H_0$  is true.

**Decision:** If p-value  $< 0.05$ , reject  $H_0$ .

## 2.5 Two-Sided Tests and Absolute Values

**Example: Why Absolute Values in p-value Calculation?**

The p-value formula often looks like:

$$\text{p-value} = P(|T| \geq |t_{\text{observed}}|)$$

**Why absolute values?**

Because our alternative hypothesis is  $\beta_1 \neq 0$  (two-sided). We consider evidence against  $H_0$  whether the association is positive or negative.

If we observed  $t = -4$ :

- Area to the left of  $-4$  (extreme negative)
- Plus area to the right of  $+4$  (equally extreme positive)

## 3 Bootstrap vs. Permutation Tests

### 3.1 When to Use Each

**Very Important: Bootstrap vs. Permutation: Critical Distinction**

**Bootstrap:** For **confidence intervals**

- Resample *with replacement* from your data
- Preserves the relationships in your data
- Estimates the sampling distribution of your statistic

**Permutation Test:** For **hypothesis testing (p-values)**

- Shuffle the response variable  $Y$ , keep  $X$  fixed
- **Enforces the null hypothesis** (no relationship between  $X$  and  $Y$ )
- Builds a reference distribution *under*  $H_0$

**Why not bootstrap for hypothesis testing?**

Bootstrap doesn't enforce  $H_0$ . Under certain conditions (violated assumptions, multicollinearity), it can lead to **inflated Type I error**—rejecting  $H_0$  too often when it's actually true.

**Example: Permutation Testing Procedure**

To test  $H_0 : \beta_1 = 0$ :

1. **Shuffle**: Randomly permute the  $Y$  values (break the  $X$ - $Y$  relationship)
  2. **Refit**: Calculate  $\hat{\beta}_1^*$  on the shuffled data
  3. **Repeat**: Do this many times (e.g., 1000 permutations)
  4. **Result**: A distribution of  $\hat{\beta}_1^*$  values, centered at 0 (since  $H_0$  is enforced)
- The p-value is the proportion of permuted  $|\hat{\beta}_1^*|$  values that exceed your observed  $|\hat{\beta}_1|$ .

**3.2 Comparing Bootstrap and Formula-Based CIs**

From the housing data:

Method	95% CI for $\beta_1$	Width
statsmodels (formula)	(0.544, 0.636)	0.092
Bootstrap	(0.487, 0.705)	0.218

**Table 1:** Comparison of confidence intervals

**Why the Difference?**

The bootstrap CI is **wider** because:

- The formula-based CI assumes constant variance (homoscedasticity)
- Our data shows clear heteroscedasticity (variance fanning out with larger homes)
- When assumptions are violated, formulas give **incorrectly narrow** CIs
- Bootstrap makes fewer assumptions and captures the true variability

**Lesson:** When in doubt, bootstrap is safer!

**3.3 Linear Regression Assumptions (LINE)****The LINE Assumptions**

1. **Linearity**: The relationship is linear
2. **Independence**: Observations are independent (most important!)
3. **Normality**: Residuals are normally distributed (least important if  $n > 50$ )
4. **Equal variance**: Constant variance (homoscedasticity)

**Bootstrap**: Relaxes N and E, still requires L and I

**Formula-based**: Requires all four

**4 Confidence Interval vs. Prediction Interval**

This is one of the most commonly confused distinctions in regression!

## 4.1 Two Different Questions

### Definition: CI vs. PI

**Confidence Interval (CI):** Uncertainty about the *mean* response

- Question: “What is the **average** selling price of *all* homes with 2860 sqft?”
- Only includes uncertainty in the regression line ( $\hat{\beta}$ 's)

**Prediction Interval (PI):** Uncertainty about a *single* new observation

- Question: “What will *this specific new home* with 2860 sqft sell for?”
- Includes uncertainty in the line **AND** the individual noise ( $\sigma^2$ )

## 4.2 Why PI is Always Wider

### Two Sources of Uncertainty for Predictions

**Source 1:** Uncertainty in the regression line

- We estimated  $\hat{\beta}_0$  and  $\hat{\beta}_1$  from a sample
- Different samples would give different estimates
- This is what the CI captures

**Source 2:** Individual observation variability (irreducible error)

- Even if we knew the exact population line, individual homes vary around it
- This is  $\sigma^2$  (the variance of  $\epsilon$ )
- No matter how much data you collect, this never goes away!

**Prediction Interval:**

$$\text{PI} = \hat{y} \pm t^* \cdot \sqrt{(\text{SE of fit})^2 + \hat{\sigma}^2}$$

The extra  $\hat{\sigma}^2$  term is why PI is always wider than CI.

### Example: Game Time Question

Use this output to predict with 95% uncertainty the selling price of a home that is 2860 sqft:

Intercept: 247.4, sqft coef: 0.5898, SE(sqft): 0.023

Options:

- $0.5898 \pm 2 \times 0.023$  (CI for slope)
- $247.4 + 0.5898 \times 2860$  (point prediction only)
- $247.4 + 0.5898(2860) \pm 2 \times 0.023$  (CI for mean response)
- $247.4 + 0.5898(2860) \pm 2\sqrt{0.023^2 + \hat{\sigma}^2}$  (PI for new observation)

**Answer: D!**

Since we're predicting “a home”—a single new observation—we need the **Prediction Interval**, which includes both the model uncertainty and the residual variance  $\hat{\sigma}^2$ .

## 5 Likelihood Review

Before diving into Bayesian inference, let's solidify our understanding of likelihood.

### 5.1 Flipping the Perspective

#### Definition: Likelihood Function

**PDF/PMF:**  $f(x|\theta)$  — Given parameters, what's the probability of the data?

**Likelihood:**  $L(\theta|x)$  — Given data, how plausible is each parameter value?

**Mathematically:** They're the same function! The difference is conceptual:

- PDF:  $\theta$  is fixed,  $x$  varies
- Likelihood:  $x$  is fixed (observed),  $\theta$  varies

### 5.2 Why Products Become Sums

#### Log-Likelihood

For independent observations  $x_1, \dots, x_n$ :

$$L(\theta) = \prod_{i=1}^n f(x_i|\theta)$$

Taking the log:

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^n \log f(x_i|\theta)$$

**Why use log?**

1. Products  $\rightarrow$  sums (much easier calculus!)
2. Numerical stability (avoids underflow from multiplying many small numbers)
3. Same maximum:  $\arg \max L(\theta) = \arg \max \ell(\theta)$

### 5.3 The OLS-MLE Connection (Review)

#### OLS

If we assume  $\epsilon_i \sim N(0, \sigma^2)$ , then maximizing the likelihood is equivalent to minimizing the sum of squared errors.

**Why?** The negative log-likelihood becomes:

$$-\ell(\beta_0, \beta_1) = \text{constant} + \frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \beta_0 - \beta_1 x_i)^2$$

Minimizing this with respect to  $\beta_0, \beta_1$  is the same as minimizing SSE!



## 6 Bayes' Rule: Flipping Conditional Probabilities

### 6.1 The Basic Formula

#### Definition: Bayes' Rule

For events  $A$  and  $B$ :

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

**Extended version** (using Law of Total Probability for denominator):

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B|A) \cdot P(A) + P(B|A^c) \cdot P(A^c)}$$

### 6.2 Example: CS and STAT Concentrators

#### Example: Conditional Probability Practice

In a hypothetical CS109A class (among undergrads):

- 40% are STAT concentrators:  $P(\text{STAT}) = 0.40$
- 60% are CS concentrators:  $P(\text{CS}) = 0.60$
- 20% are both (joint/double):  $P(\text{STAT} \cap \text{CS}) = 0.20$

**Question 1:** Among STAT concentrators, what fraction are also CS?

$$P(\text{CS}|\text{STAT}) = \frac{P(\text{STAT} \cap \text{CS})}{P(\text{STAT})} = \frac{0.20}{0.40} = 0.50$$

**Question 2:** Among CS concentrators, what fraction are also STAT?

$$P(\text{STAT}|\text{CS}) = \frac{P(\text{STAT} \cap \text{CS})}{P(\text{CS})} = \frac{0.20}{0.60} = 0.333$$

**Key Insight:**  $P(\text{CS}|\text{STAT}) \neq P(\text{STAT}|\text{CS})$ !

These are fundamentally different questions—don't confuse them.

### 6.3 Independence and Dependence

#### Are STAT and CS Independent?

Events are **independent** if  $P(A \cap B) = P(A) \cdot P(B)$ .

Check:  $P(\text{STAT}) \cdot P(\text{CS}) = 0.40 \times 0.60 = 0.24$

But  $P(\text{STAT} \cap \text{CS}) = 0.20 \neq 0.24$

**Conclusion:** They are **dependent**!

**Meaning:** Knowing someone's CS status gives you information about whether they're also STAT. The probability changes once you have additional information.

## 7 Bayes' Rule in Diagnostic Testing

This is a classic application that will connect directly to classification later.

### Example: Pregnancy Test Example

A pregnancy test has:

- **Sensitivity:**  $P(\text{Test} + | \text{Pregnant}) = 0.97$  (true positive rate)
- **Specificity:**  $P(\text{Test} - | \text{Not Pregnant}) = 0.99$  (true negative rate)

Among people taking this test, about 30% are actually pregnant:  $P(\text{Pregnant}) = 0.30$

**Question:** If someone tests positive, what's the probability they're actually pregnant?

**We want:**  $P(\text{Pregnant} | \text{Test} +)$

**We have:**  $P(\text{Test} + | \text{Pregnant})$

We need to **flip the conditional**—use Bayes' Rule!

### 7.1 Applying Bayes' Rule

$$\begin{aligned}
 P(\text{Preg} | T+) &= \frac{P(T+ | \text{Preg}) \cdot P(\text{Preg})}{P(T+)} \\
 &= \frac{P(T+ | \text{Preg}) \cdot P(\text{Preg})}{P(T+ | \text{Preg}) \cdot P(\text{Preg}) + P(T+ | \text{Not Preg}) \cdot P(\text{Not Preg})} \\
 &= \frac{0.97 \times 0.30}{0.97 \times 0.30 + 0.01 \times 0.70} \\
 &= \frac{0.291}{0.291 + 0.007} = \frac{0.291}{0.298} \approx 0.977
 \end{aligned}$$

### Belief Update: Prior to Posterior

- **Prior probability** of being pregnant: 30%
- **Evidence:** Positive test result
- **Posterior probability** of being pregnant: 97.7%

The positive test dramatically updated our belief from 30% to 97.7%!

**This is the essence of Bayesian inference:** Using evidence to update our beliefs.

## 8 Bayesian Inference: A New Paradigm

### 8.1 From Events to Parameters

Now we apply this same logic to statistical parameters:

**Definition: Bayesian Inference Formula**

$$f(\theta|X) = \frac{f(X|\theta) \cdot f(\theta)}{f(X)}$$

**Components:**

- $f(\theta|X)$  — **Posterior Distribution**: Our updated belief about  $\theta$  after seeing data
- $f(X|\theta)$  — **Likelihood**: How probable is our data given  $\theta$ ?
- $f(\theta)$  — **Prior Distribution**: Our initial belief about  $\theta$  before seeing data
- $f(X)$  — **Evidence/Marginal Likelihood**: A normalizing constant

**Simplified:**

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

**8.2 The Bayesian Philosophy****Very Important: Frequentist vs. Bayesian Worldviews****8.3 Example: Three Coins****Example: Discrete Bayesian Inference**

You have three coins in your pocket:

- Coin A:  $P(\text{Heads}) = 0.1$  (biased toward tails)
- Coin B:  $P(\text{Heads}) = 0.5$  (fair)
- Coin C:  $P(\text{Heads}) = 0.9$  (biased toward heads)

You randomly select one coin (equal probability) and flip it 4 times.

**Data observed:** 3 Heads, 1 Tail

**Question:** Which coin did you probably pick?

**Step 1: Prior**

Before seeing any flips, each coin is equally likely:

$$P(p = 0.1) = P(p = 0.5) = P(p = 0.9) = \frac{1}{3}$$

**Step 2: Likelihood**

Calculate probability of “3H, 1T” for each coin using binomial distribution:

$$L(p = 0.1) = \binom{4}{3} (0.1)^3 (0.9)^1 = 4 \times 0.001 \times 0.9 = 0.0036$$

$$L(p = 0.5) = \binom{4}{3} (0.5)^3 (0.5)^1 = 4 \times 0.125 \times 0.5 = 0.2500$$

$$L(p = 0.9) = \binom{4}{3} (0.9)^3 (0.1)^1 = 4 \times 0.729 \times 0.1 = 0.2916$$

**Step 3: Posterior (unnormalized)**

$$P(p = 0.1|\text{data}) \propto 0.0036 \times \frac{1}{3} = 0.0012$$

$$P(p = 0.5|\text{data}) \propto 0.2500 \times \frac{1}{3} = 0.0833$$

$$P(p = 0.9|\text{data}) \propto 0.2916 \times \frac{1}{3} = 0.0972$$

**Step 4: Normalize** (sum = 0.0012 + 0.0833 + 0.0972 = 0.1817)

$$P(p = 0.1|\text{data}) = \frac{0.0012}{0.1817} \approx 0.007 \quad (0.7\%)$$

$$P(p = 0.5|\text{data}) = \frac{0.0833}{0.1817} \approx 0.458 \quad (45.8\%)$$

$$P(p = 0.9|\text{data}) = \frac{0.0972}{0.1817} \approx 0.535 \quad (53.5\%)$$

**Conclusion:** Our belief shifted from (33.3%, 33.3%, 33.3%) to (0.7%, 45.8%, 53.5%). We now believe we most likely picked the biased-toward-heads coin!

## 9 Game Time: Bootstrap Sample Size

**Example: Class Question**

What happens to the bootstrap distribution when  $B$  (number of bootstrap samples) increases?

Options:

- A. The distribution becomes more normal
- B. The variance decreases
- C. The confidence intervals become narrower
- D. The distribution gets smoother

**Correct Answer: D** (and arguably A)

**What increasing  $B$  does:**

- Gets a more *precise estimate* of the true sampling distribution
- Makes the histogram smoother (less jagged)
- Does NOT change the underlying variability of your estimate!

**What increasing  $B$  does NOT do:**

- Narrow confidence intervals
- Reduce the variance of  $\hat{\beta}$

**To actually narrow CIs**, you need to increase  $n$  (original sample size), not  $B$ !

## 10 Quick Reference Summary

### Lecture 10 Quick Reference Card

#### 1. CI vs. PI

- **CI:** Uncertainty in mean response (where is the line?)
- **PI:** Uncertainty in single observation (includes  $\hat{\sigma}^2$ )
- PI is **always wider!**

#### 2. Bootstrap vs. Permutation

- **Bootstrap:** Confidence intervals (resample with replacement)
- **Permutation:** Hypothesis tests (shuffle  $Y$ , enforces  $H_0$ )

#### 3. Bayes' Rule

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

Allows “flipping” conditional probabilities!

#### 4. Bayesian Inference

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

$$f(\theta|X) \propto f(X|\theta) \cdot f(\theta)$$

#### 5. Frequentist vs. Bayesian

- **Frequentist:**  $\theta$  is fixed constant, probability = long-run frequency
- **Bayesian:**  $\theta$  has a distribution, probability = belief

## 11 Common Questions and Answers

**Q: The prior seems subjective. Isn't that a problem?**

A: It can be, but:

1. Use “informative priors” based on previous research or domain knowledge
2. Use “uninformative/flat priors” when you have no prior knowledge
3. Most importantly: **With enough data, the prior gets overwhelmed.** The posterior converges to the same answer regardless of (reasonable) prior choices.

**Q: When should I use Bayesian vs. Frequentist methods?**

A: Both have their place:

- **Frequentist:** Simpler, faster computation, standard in clinical trials

- **Bayesian:** Can incorporate prior knowledge, gives full posterior distribution, better for small samples

Modern data science often uses both and compares results.

**Q: Why does increasing bootstrap samples  $B$  not narrow the CI?**

A:  $B$  controls how accurately you *estimate* the sampling distribution. But the *width* of the sampling distribution depends on your original sample size  $n$ . More bootstrap samples give you a smoother histogram of the same width.

## 12 The Monty Hall Problem (Bonus)

Professor Rader mentions this classic probability puzzle:

### Example: The Monty Hall Problem

#### Setup:

- 3 doors: 1 car (prize), 2 goats (losers)
- You pick a door (say, Door 1)
- Host (who knows where the car is) opens another door revealing a goat
- You're offered: "Do you want to switch to the remaining door?"

#### Counterintuitive Result:

- Stay: Win probability =  $1/3$
- Switch: Win probability =  $2/3$

#### Intuition (100 doors version):

- Pick 1 door out of 100. Probability you picked the car =  $1/100$ .
- Host reveals 98 goats, leaving 2 doors.
- If you switch, you win unless you initially picked the car (probability  $99/100$ )!

This demonstrates how conditional probability can be counterintuitive!

## 13 Looking Ahead

In the next lecture, we'll:

- Work through the three-coins example in more detail
- Explore continuous priors and posteriors
- See how Bayesian inference connects to regression
- Start applying these ideas in Python

The Bayesian framework will also be crucial when we move to classification, where we'll care about  $P(\text{Class}|\text{Features})$ —a natural application of Bayes' Rule!