STAT 509: STATISTICS FOR ENGINEERS

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Lecture Notes
Section 001

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Contents

1 Introduction

Definition: Statistics is the science of data; how to interpret and visualize data, analyze data, and design studies to collect data.

- Statistics is used in all disciplines; not just in engineering.
- "Statisticians get to play in everyone else's back yard." (John Tukey)

Examples:

1. In a reliability (time to event) study, engineers are interested in describing the time until failure for a jet engine fan blade.
2. In a genetics study involving patients with Alzheimer's disease, researchers wish to identify genes that are differentially expressed (when compared to non-AD patients).
3. In an agricultural experiment, researchers want to know which of four fertilizers (which vary in their nitrogen levels) produces the highest corn yield.
4. In a clinical trial, physicians want to determine which of two drugs is more effective for managing weight loss in pre-diabetic patients.
5. In a public health study involving "at-risk" teenagers, epidemiologists want to know how smoking behavior differs across demographic classes.
6. A food scientist is interested in determining how different feeding schedules (for pigs) could affect the spread of salmonella during the slaughtering process.
7. A pharmacist wants to determine if administering caffeine to premature infants increases the risk of necrotizing enterocolitis.
8. A research dietician wants to determine if academic achievement is related to BMI among students in the fourth grade.

What we do: Statisticians (and data scientists) use their skills in mathematics and computing to formulate statistical models and analyze data for a specific problem at hand. These models are then used to estimate important quantities of interest, to test the validity of proposed conjectures, and to predict future behavior. Being able to identify and model sources of **variability** are critical parts of this process.

Definition: A **deterministic model** makes no attempt to explain variability.

- In chemistry, the ideal gas law states

$$PV = nRT,$$

where P = pressure of a gas, V = volume, n = amount of substance of gas (number of moles), R = Boltzmann's constant, and T = temperature.

- In circuit analysis, Ohm's law states

$$V = IR,$$

  where V = voltage, I = current, and R = resistance.

In both of these models, the relationship among the variables is completely determined without ambiguity. In real life, this is rarely true for the obvious reason: there is natural variation that arises in the measurement process.

- For example, a common electrical engineering experiment involves setting up a simple circuit with a known resistance R. For a given current I, different students (using a mulitmeter) will then measure the voltage V.
  - With a class of 20 students, conducting the experiment with the same current I, we might get 20 different voltage measurements $V_1, V_2, ..., V_{20}$.
  - A deterministic model is too simplistic; it does not acknowledge the inherent variability that arises in the measurement process.

Important: Statistical models are not deterministic. They incorporate **variability** with the hope of describing what is going on in a larger population of individuals. They can also be used to **predict** future outcomes for specific individuals, a common task in machine learning and artificial intelligence.

Example 1.1. An article by Liu et al. (1996) in *Journal of Air and Waste Management Association* described a research study motivated by the waste disposal problems in Kaohsiung City, Taiwan. The goal was to develop a statistical model to explain how the response variable

$$Y = \text{ energy content of solid waste specimen when incinerated (kcal/kg)}$$

was related to four independent variables measured on each waste specimen

$$\begin{aligned} x_1 &= \text{plastic by weight (measured as \% of total weight)} \\ x_2 &= \text{paper by weight (measured as \% of total weight)} \\ x_3 &= \text{garbage by weight (measured as \% of total weight)} \\ x_4 &= \text{moisture percentage.} \end{aligned}$$

One way to think about this modeling problem−from a purely mathematical point of view−is to assume there is a function f that links the response variable Y to the independent variables for all waste specimens that will ever be collected, say

$$Y = f(x_1, x_2, x_3, x_4).$$

This is how a mathematician might formulate the problem−by using a **deterministic model**. Of course, the overarching problem is that the function f is likely unknown in real life so hence the model is not all that helpful. This is where statistics comes in.

Table 1.1: Waste incineration data. Measurements of energy, plastic percentage, paper percentage, garbage percentage, and moisture for a sample of 30 waste specimens.

Specimen	Energy (Y)	Plastic (x_1)	Paper (x_2)	Garbage (x_3)	Moisture (x_4)
1	947	18.69	15.65	45.01	58.21
2	1407	19.43	23.51	39.69	46.31
3	1452	19.24	24.23	43.16	46.63
4	1553	22.64	22.20	35.76	45.85
5	989	16.54	23.56	41.20	55.14
6	1162	21.44	23.65	35.56	54.24
7	1466	19.53	24.45	40.18	47.20
8	1656	23.97	19.39	44.11	43.82
9	1254	21.45	23.84	35.41	51.01
10	1336	20.34	26.50	34.21	49.06
11	1097	17.03	23.46	32.45	53.23
12	1266	21.03	26.99	38.19	51.78
13	1401	20.49	19.87	41.35	46.69
14	1223	20.45	23.03	43.59	53.57
15	1216	18.81	22.62	42.20	52.98
16	1334	18.28	21.87	41.50	47.44
17	1155	21.41	20.47	41.20	54.68
18	1453	25.11	22.59	37.02	48.74
19	1278	21.04	26.27	38.66	53.22
20	1153	17.99	28.22	44.18	53.37
21	1225	18.73	29.39	34.77	51.06
22	1237	18.49	26.58	37.55	50.66
23	1327	22.08	24.88	37.07	50.72
24	1229	14.28	26.27	35.80	48.24
25	1205	17.74	23.61	37.36	49.92
26	1221	20.54	26.58	35.40	53.58
27	1138	18.25	13.77	51.32	51.38
28	1295	19.09	25.62	39.54	50.13
29	1391	21.25	20.63	40.72	48.67
30	1372	21.62	22.71	36.22	48.19

Discussion: A statistician will think of this problem as

$$Y = f(x_1, x_2, x_3, x_4) + \epsilon,$$

where the extra term ϵ incorporates all the sources of variability that make Y different than $f(x_1, x_2, x_3, x_4)$. This could include

- independent variables that are not accounted for in the research study
- measurement error (e.g., are all the percentages measured correctly? the energy content measurements?)

- natural sampling variability, that is, the variability that arises from looking at a sample of waste specimens taken from a larger population.
  - Different samples of waste specimens will produce different data sets!

All of these sources of variability make ϵ random. We call

$$Y = f(x_1, x_2, x_3, x_4) + \epsilon,$$

a **statistical (or probabilistic) model** to acknowledge this. Statistical models acknowledge the relationship between (or among) variables is not perfect. This is more realistic.

Q: So, how do we estimate f with the sample of waste specimens like those in Table 1.1?
A: We could estimate f nonparametrically. That is, make no assumption about the form of f and use the observed data to select the function f that most closely matches the data.

- This is a challenging problem statistically and would give rise to a "wiggly" highly nonlinear function of x_1, x_2, x_3, and x_4 as the solution.
- The function chosen might be hard to interpret on practical grounds.
- Predictions might give far too much weight to the data. This would be bad if new waste specimens did not align with the sample.

A: Another approach (which is more common) is to make simplifying assumptions about the form of f, say, that f is linear function of the independent variables, that is,

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon.$$

This is called a **multiple linear regression model**.

- The coefficients β_0, β_1, β_2, β_3, and β_4 are called **regression parameters**.
- They describe how Y is related to the independent variables in the population of all waste specimens.
- Therefore, under the simplifying assumption that the relationship between Y and the independent variables is linear, we have reduced the problem of "estimating f" to finding values of β_0, β_1, β_2, β_3, and β_4 which "best fit" the observed data in Table 1.1. This problem can be solved easily using linear algebra calculations and will be discussed in Chapter 11.

Remark: Statistical models incorporate randomness. Randomness arises in probability, which is known as "the mathematics of uncertainty." Therefore, probability and uncertainty form the basis for all statistical analyses.

- Chapters 2-5 deal with probability and probability models for single variables.
- Chapter 6 is a "bridge" chapter. Chapters 7-12 deal with statistical methods to analyze data.

2 Probability

Example 2.1. A local television station's meteorologist announces,

"There is a 30 percent chance of rain tomorrow."

How do you interpret this statement?

(a) It will rain tomorrow for 30 percent of the time. That is, for 7.2 hours tomorrow, it will be raining. For the remaining 16.8 hours, it will not be raining.

(b) It will rain tomorrow in 30 percent of the region covered by the local television station. It will not rain in the other 70 percent of the region.

(c) Among all local meteorologists, 30 percent of them think it will rain tomorrow. The remaining 70 percent of the meteorologists think it will not rain tomorrow.

(d) Thirty percent of all inhabitants of the region covered by this local television station will see rain at least once during their day tomorrow; the remaining 70 percent will not see rain during their day.

(e) It will rain on 30 percent of the days in which this same forecast is made.

Discussion: The statement incorporates uncertainty about a future event−the event that it will rain tomorrow. The phrase "30 percent" can be interpreted as a probability. None of us know for sure whether it will rain tomorrow, so we are dealing with a **random** event. We can write this as

$$P(A) = 0.30,$$

where the event

$$A = \{\text{it rains tomorrow}\}.$$

In this example, we are given five different interpretations of $P(A) = 0.30$. I think interpretation (e) makes the most sense, but all five interpretations are valid depending on how one conceptualizes the problem.

Example 2.2. I have a class with 50 students in it. Assuming there are no twins (or other multiple births), what is the probability there is at least one shared birthday among the students? Remember there are 365 days in a year.

(a) $P(A) = 0.14$
(b) $P(A) = 0.28$
(c) $P(A) = 0.45$
(d) $P(A) = 0.81$
(e) $P(A) = 0.97$

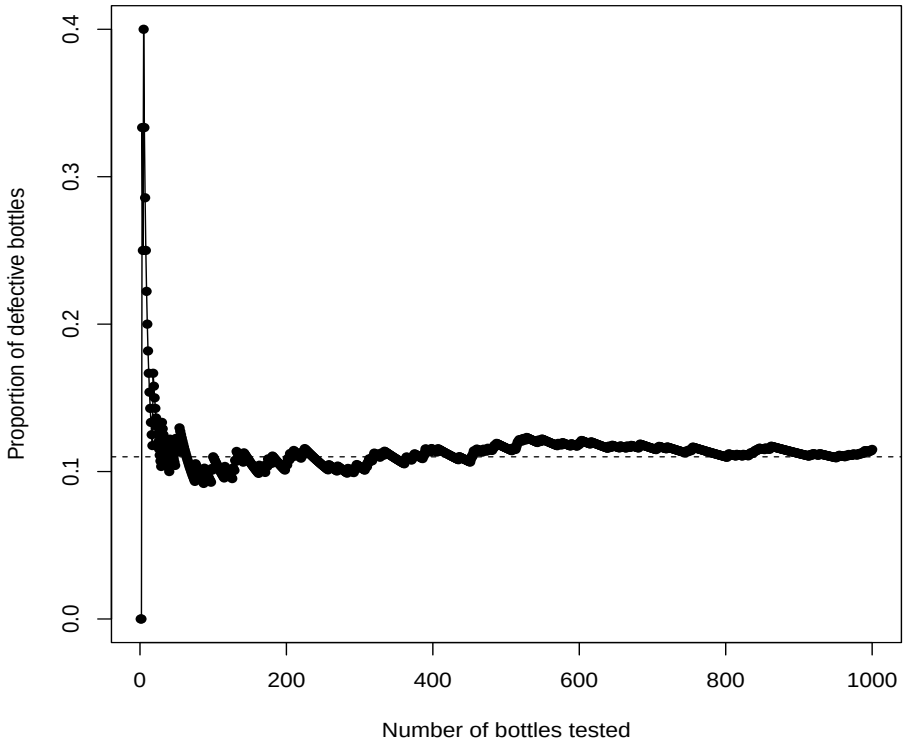


Figure 2.1: Relative frequency plot of the proportion of defective bottles (i.e., bottles that do not conform to specifications). A total of 1000 bottles are observed. A dotted horizontal line at 0.11 is added.

Q: For a future event A, how do we interpret what $P(A)$ means?
A: One way to think about $P(A)$ is that it represents the long-run proportion of times A would occur if we were to repeat the same phenomenon over and over again. The event A may occur on some repetitions and not on others; $P(A)$ is the proportion of times it will occur in the long-run. This is the **relative frequency** interpretation of probability.

Example 2.3. Plastic bottles for liquid laundry detergent are formed by blow molding, a manufacturing process used to create hollow plastic parts (often bottles and containers) by inflating a heated plastic tube inside a mold. Previous data from statistical process control monitoring suggests 11 percent of the bottles do not conform to specifications.

Imagine observing bottles one by one and define

$$A = \{\text{bottle does not conform to specifications}\}.$$

For each bottle observed, we note if A occurs or not. Figure 2.1 graphs what the relative frequency of the event A might look like over time when observing 1000 bottles.

2.1 Sample spaces and events

Remark: We use the phrase "random experiment" to mean an experiment which has many possible outcomes but we cannot predict with certainty which outcome will occur.

- Even if the experiment is performed the same way every time, we could still get different outcomes. "Cannot predict with certainty" means that each outcome (or collection of outcomes) has a probability associated with it.

Definition: The set of all possible outcomes for a random experiment is called the **sample space**, denoted by S. An **event** A is a subset of the sample space.

Result: If each outcome in S is equally likely (and $n_S < \infty$), then

$$P(A) = \frac{n_A}{n_S},$$

where

$$\begin{aligned} n_A &= \text{number of outcomes in } A \\ n_S &= \text{number of outcomes in } S. \end{aligned}$$

Example 2.4. Pick 3 is a three-digit number game from the South Carolina Education Lottery. We can think of playing this lottery as a random experiment with sample space

$$S = \{000, 001, 002, ..., 998, 999\}.$$

The number of outcomes in S is $n_S = 1000$. Suppose every week I purchase three tickets with the following numbers:

$$A = \{364, 446, 540\}.$$

The probability I win is

$$P(A) = \frac{n_A}{n_S} = \frac{3}{1000} = 0.003.$$

Q: Each ticket costs \$1. Why is the payout for a winning ticket only \$500? If the game was fair, shouldn't it be closer to \$1,000?

Example 2.5. Suppose we continue to observe plastic bottles in Example 2.3 until we find the first bottle that does not conform to specifications (i.e., is "defective"). The sample space is

$$S = \{\text{d}, \text{cd}, \text{ccd}, \text{cccd}, \text{ccccd}, \text{cccccd}, ...,\},$$

where "c" and "d" represent bottles that "conform" and are "defective," respectively.

Q: What is the probability we see the first defective bottle on the first or second bottle observed? This corresponds to the event

$$A = \{\text{d}, \text{cd}\}.$$

A: There are two problems. First of all, the sample space S does not contain a finite number of outcomes (i.e., it is countably infinite). Therefore, $n_S = +\infty$ and even writing

$$P(A) = \frac{n_A}{n_S}$$

would make no sense. Furthermore, the outcomes in S are not equally likely. It is reasonable to assign

$$P(\{\text{d}\}) = 0.11$$

for the first outcome in A because 11 percent of the bottles are thought to be defective. However, what is $P(\{\text{cd}\})$? We can't calculate this without making additional assumptions.

Definitions: The **union** of two events A and B is the event containing outcomes in A or B. The **intersection** of two events A and B is the event containing outcomes in A and B. We write

$$\begin{aligned} A \cup B &\longleftarrow \text{union (“or”)} \\ A \cap B &\longleftarrow \text{intersection (“and”).} \end{aligned}$$

Example 2.6. A medical professional observes adult male patients entering an emergency room. She classifies each patient according to his blood type (AB^+, AB^-, A^+, A^-, B^+, B^-, O^+, and O^-) and whether his systolic blood pressure (SBP) is low (L), normal (N), or high (H). Imagine observing the next male patient as a random experiment. The sample space is

$$\begin{aligned} S = \{&(\text{AB}^+,\text{L}),(\text{AB}^-,\text{L}),(\text{A}^+,\text{L}),(\text{A}^-,\text{L}),(\text{B}^+,\text{L}),(\text{B}^-,\text{L}),(\text{O}^+,\text{L}),(\text{O}^-,\text{L}), \\ &(\text{AB}^+,\text{N}),(\text{AB}^-,\text{N}),(\text{A}^+,\text{N}),(\text{A}^-,\text{N}),(\text{B}^+,\text{N}),(\text{B}^-,\text{N}),(\text{O}^+,\text{N}),(\text{O}^-,\text{N}), \\ &(\text{AB}^+,\text{H}),(\text{AB}^-,\text{H}),(\text{A}^+,\text{H}),(\text{A}^-,\text{H}),(\text{B}^+,\text{H}),(\text{B}^-,\text{H}),(\text{O}^+,\text{H}),(\text{O}^-,\text{H})\}. \end{aligned}$$

Remarks:

- There are 8 different blood types. There are 3 different categorizations of SBP. There are $8 \times 3 = 24$ possible outcomes in the sample space, which is formed by combining the two factors. This illustrates the **multiplication rule** of counting.
- Are these 24 outcomes equally likely? Probably not. O^+ is by far the most common blood type among American males (about 38 percent). On the other hand, AB^- is rare (only about 1 percent). Similarly, most American males have either normal or high SBP; fewer have low SBP.
- Even though we have listed all possible outcomes in S, we have not specified probabilities associated with the outcomes. We cannot assign probability to events like

  $$\begin{aligned} A &= \{\text{blood type with a } ^+ \text{ rhesus status}\} \\ B &= \{\text{high SBP}\} \end{aligned}$$

  without having this information.

List the outcomes in $A \cup B$ and $A \cap B$.

$$\begin{aligned} A \cup B &= \{\text{outcomes with a } ^+ \text{ rhesus status } \textbf{or} \text{ high SBP}\} \\ &= \{(\text{AB}^+, \text{L}), (\text{A}^+, \text{L}), (\text{B}^+, \text{L}), (\text{O}^+, \text{L}), (\text{AB}^+, \text{N}), (\text{A}^+, \text{N}), (\text{B}^+, \text{N}), (\text{O}^+, \text{N}), \\ &\quad (\text{AB}^+, \text{H}), (\text{AB}^-, \text{H}), (\text{A}^+, \text{H}), (\text{A}^-, \text{H}), (\text{B}^+, \text{H}), (\text{B}^-, \text{H}), (\text{O}^+, \text{H}), (\text{O}^-, \text{H})\} \end{aligned}$$

$$\begin{aligned} A \cap B &= \{\text{outcomes with a } ^+ \text{ rhesus status } \textbf{and} \text{ high SBP}\} \\ &= \{(\text{AB}^+, \text{H}), (\text{A}^+, \text{H}), (\text{B}^+, \text{H}), (\text{O}^+, \text{H})\} \end{aligned}$$

Discussion: The notions of union and intersection can be extended to more than two events. For example,

$$A \cup B \cup C$$

means either A, B, or C occurs. The event

$$A \cap B \cap C \cap D$$

means all four events A, B, C, and D occur. The event

$$(A \cap B) \cup (C \cap D \cap E)$$

means either $A \cap B$ or $C \cap D \cap E$ occurs. For any finite number of events $A_1, A_2, ..., A_n$, we write

$$\bigcup_{i=1}^{n} A_i = A_1 \cup A_2 \cup \cdots \cup A_n \quad \longleftarrow \quad \text{“at least one } A_i \text{ occurs”}$$

$$\bigcap_{i=1}^{n} A_i = A_1 \cap A_2 \cap \cdots \cap A_n \quad \longleftarrow \quad \text{“each } A_i \text{ occurs”}.$$

Definition: If the events A and B contain no common outcomes, we say the events are **mutually exclusive**. In this case,

$$P(A \cap B) = P(\emptyset) = 0.$$

It is not possible for A and B to both occur.

2.2 Counting techniques

Importance: When each outcome in S is equally likely, we learned

$$P(A) = \frac{n_A}{n_S},$$

where n_S and n_A count the (finite) number of outcomes in S and A, respectively. In some random experiments, counting techniques can help to determine n_S and n_A.

Multiplication rule (for counting): Suppose a random experiment involves k factors where

$$\begin{aligned} n_1 &= \text{number of outcomes for factor 1} \\ n_2 &= \text{number of outcomes for factor 2} \\ &\vdots \\ n_k &= \text{number of outcomes for factor } k. \end{aligned}$$

The total number of outcomes is

$$\prod_{i=1}^{k} n_i = n_1 \times n_2 \times \cdots \times n_k.$$

Example 2.7. A random experiment consists of selecting a standard South Carolina license plate which consists of 3 letters and 3 numbers. We can think of one outcome in the sample space S as having the following structure:

$$(\ \_\_\ \_\_\ \_\_\ \quad \_\_\ \_\_\ \_\_\ ).$$

Q: How many standard plates are possible; i.e., how many outcomes are in S?
A: There are

$$n_S = 26 \times 26 \times 26 \times 10 \times 10 \times 10 = 17,576,000$$

possible outcomes.

Q: Assume each outcome in S is equally likely (e.g., license plate letters/numbers are determined at random). What is the probability a randomly selected plate contains no repeat letters and no repeat numbers?
A: Define the event

$$A = \{\text{no repeat letters/numbers}\}.$$

The number of outcomes in A is

$$n_A = 26 \times 25 \times 24 \times 10 \times 9 \times 8 = 11,232,000.$$

Therefore,

$$P(A) = \frac{n_A}{n_S} = \frac{11232000}{17576000} \approx 0.639.$$

Permutations: Suppose a random experiment involves arranging distinct objects (e.g., people, parts, locations, etc.) in order.

- With n distinct objects, there are

  $$n! = n(n-1)(n-2) \times \cdots \times 2 \times 1$$

  ways to permute these objects (i.e., to arrange them in a particular order).

- With n distinct objects, there are

  $$P_r^n = \frac{n!}{(n-r)!}$$

  ways to select r objects and then permute these.

Example 2.8. A personnel director for a corporation has hired 12 new engineers.

Q: How many ways could the engineers be assigned to 12 different offices?
A: There are

$$12! = 12 \times 11 \times 10 \times \cdots \times 2 \times 1 = 479,001,600$$

ways an assignment could be made.

Q: Suppose the director needs to select 3 engineers to fill distinct positions: team leader, consultant, and support staff member. How many ways could this be done?
A: There are

$$P_3^{12} = \frac{12!}{(12-3)!} = 12 \times 11 \times 10 = 1320$$

ways this selection could be made.

Q: In the last part, suppose there are 6 engineers from USC and 6 from Clemson. What is the probability a USC graduate is selected as the team leader and the remaining 2 positions are filled by Clemson graduates?
A: Define the event

$$A = \{\text{USC team leader and Clemson graduates for other 2 positions}\}.$$

There are a total of

$$n_S = 1320$$

ways to select 3 engineers for the distinct positions (ignoring school; this was the last part). Assuming each of these outcomes is equally likely, then all we have to do is calculate the number of outcomes in A and use

$$P(A) = \frac{n_A}{n_S}.$$

We find n_A by using the multiplication rule:

$$\begin{aligned} n_1 &= \text{number of ways to select 1 USC graduate} = 6 \\ n_2 &= \text{number of ways to select 2 Clemson graduates} = P_2^6 \end{aligned}$$

The number of outcomes in A is

$$n_A = 6 \times P_2^6 = 6 \times 30 = 180.$$

Therefore,

$$P(A) = \frac{n_A}{n_S} = \frac{180}{1320} \approx 0.136.$$

Combinations: Combinations are like permutations except the ordering of the objects doesn't matter. With n distinct objects (e.g., people, parts, locations, etc.), there are

$$\binom{n}{r} = \frac{n!}{r!(n-r)!}$$

ways to select r objects.

Q: In Example 2.8, how many ways are there to select 3 engineers from 12?
A: Because the order of selection doesn't matter (i.e., there are no designations of team leader or anything like that), there are

$$\binom{12}{3} = \frac{12!}{3!\,9!} = \frac{12 \times 11 \times 10}{6} = 220$$

ways to select 3 engineers from 12.

Example 2.9. A bin of 50 manufactured parts contains 3 defective parts and 47 nondefective parts. A sample of 6 parts is selected at random and without replacement. That is, each part can be selected only once, and the sample is a subset of the 50 parts.

Q: What is the probability the sample contains exactly 2 defective parts?
A: Imagine the selection of 6 parts from the bin as a random experiment with outcomes in S having the form

$$(\ \_\_\ \_\_\ \_\_\ \_\_\ \_\_\ \_\_\ ).$$

One possible outcome is

$$(\ \underline{\text{ND}}\ \underline{\text{ND}}\ \underline{\text{ND}}\ \underline{\ \text{D}\ }\ \underline{\text{ND}}\ \underline{\text{ND}}\ )$$

meaning the fourth part selected was defective and the others were not.

How many outcomes are in the sample space? This is a combination question because we are simply selecting 6 parts from 50 and order doesn't matter. There are

$$n_S = \binom{50}{6} = 15,890,700$$

outcomes in S. How many outcomes are in

$$A = \{\text{sample contains 2 D and 4 ND parts}\}?$$

Use the multiplication rule with

$$\begin{aligned} n_1 &= \text{number of ways to select 2 D from 3} = \binom{3}{2} \\ n_2 &= \text{number of ways to select 4 ND from 47} = \binom{47}{4} \end{aligned}$$

The number of outcomes in A is

$$n_A = \binom{3}{2}\binom{47}{4} = 3 \times 178365 = 535,095.$$

Therefore, assuming each outcome in S is equally likely,

$$P(A) = \frac{n_A}{n_S} = \frac{535095}{15890700} \approx 0.034.$$

2.3 Axioms of probability and additive rules

Remark: Going forward, we need a formal set of rules (or axioms) which will govern how we determine probabilities in general. The following axioms are due to Kolmogorov.

Axioms: For any sample space S, assigning a probability P must satisfy

(1) $0 \leq P(A) \leq 1$, for any event A

(2) $P(S) = 1$

(3) If $A_1, A_2, ..., A_n$ are pairwise **mutually exclusive** events, then

$$P\left(\bigcup_{i=1}^{n} A_i\right) = \sum_{i=1}^{n} P(A_i).$$

- The term "pairwise mutually exclusive" means that $A_i \cap A_j = \emptyset$, for all $i \neq j$.
- Recall the event

$$\bigcup_{i=1}^{n} A_i = A_1 \cup A_2 \cup \cdots \cup A_n$$

means "at least one A_i occurs."

Discussion: The first axiom guarantees that probabilities must be between 0 and 1. Events with probability 0 can never occur. Events with probability 1 must occur. Both extremes are rare in real life. The third axiom provides the mathematical basis for intuitive calculations like in the following example.

Example 2.10. In the game of craps, two fair dice are rolled initially to start the game. Here is a probability model for the sum of the two faces.

Outcome	2	3	4	5	6	7	8	9	10	11	12
Probability	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{5}{36}$	$\frac{6}{36}$	$\frac{5}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{1}{36}$

Q: What is the probability of rolling a "7" or an "11?"
A: The third axiom assures we can add the probabilities, that is,

$$P(\text{rolling a 7 or 11}) = P(\text{rolling a 7}) + P(\text{rolling an 11}) = \frac{6}{36} + \frac{2}{36} = \frac{8}{36} \approx 0.222.$$

This is true because

$$\{\text{rolling a 7}\} \quad \text{and} \quad \{\text{rolling an 11}\}$$

are mutually exclusive events.

Complement Rule: The complement of the event A consists of all outcomes not in A. The complement is denoted by A'. The first two axioms can be used to show

$$P(A') = 1 - P(A).$$

That is, the probability A does not occur is one minus the probability it does.

Additive Rule: If A and B are two events, then

$$P(A \cup B) = P(A) + P(B) - P(A \cap B).$$

Of course, if A and B are mutually exclusive, then $P(A \cap B) = 0$ and

$$P(A \cup B) = P(A) + P(B).$$

This agrees with Axiom 3.

DeMorgan's Laws: If A and B are two events, then

$$\begin{aligned} (A \cup B)' &= A' \cap B' \\ (A \cap B)' &= A' \cup B'. \end{aligned}$$

Example 2.11. The probability that train 1 is on time is 0.95. The probability that train 2 is on time is 0.93. The probability that both are on time is 0.90. Define the events

$$\begin{aligned} A &= \{\text{train 1 is on time}\} \\ B &= \{\text{train 2 is on time}\}. \end{aligned}$$

We are given $P(A) = 0.95$, $P(B) = 0.93$, and $P(A \cap B) = 0.90$.

Q: What is the probability train 1 is not on time?

$$\begin{aligned} P(A') &= 1 - P(A) \\ &= 1 - 0.95 = 0.05. \end{aligned}$$

Q: What is the probability at least one train is on time?

$$\begin{aligned} P(A \cup B) &= P(A) + P(B) - P(A \cap B) \\ &= 0.95 + 0.93 - 0.90 = 0.98. \end{aligned}$$

Q: What is the probability neither train is on time?
A: Note that by DeMorgan's Law,

$$\{\text{neither train on time}\} = A' \cap B' = (A \cup B)'.$$

Therefore, by the complement rule,

$$\begin{aligned} P(A \cup B)' &= 1 - P(A \cup B) \\ &= 1 - 0.98 = 0.02. \end{aligned}$$

Remark: The additive rule also applies for more than two events. For example,

$$P(A \cup B \cup C) = P(A) + P(B) + P(C) - P(A \cap B) - P(A \cap C) - P(B \cap C) + P(A \cap B \cap C)$$

and

$$\begin{aligned} P(A \cup B \cup C \cup D) &= P(A) + P(B) + P(C) + P(D) \\ &\quad - P(A \cap B) - P(A \cap C) - P(A \cap D) - P(B \cap C) - P(B \cap D) - P(C \cap D) \\ &\quad + P(A \cap B \cap C) + P(A \cap B \cap D) + P(A \cap C \cap D) + P(B \cap C \cap D) \\ &\quad - P(A \cap B \cap C \cap D) \end{aligned}$$

for three and four events. The pattern continues, but the formula becomes increasingly impractical to work with (unless the events are mutually independent).

2.4 Conditional probability and independence

Remark: In many situations, we might want to calculate $P(A)$. However, this probability might be influenced by another event B. That is, the occurrence of B influences how we assign probability to A. This motivates conditional probability.

Definition: Let A and B be events in a sample space S with $P(B) > 0$. The **conditional probability** of A, given that B has occurred, is

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

Similarly,

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

provided $P(A) > 0$.

Example 2.12. In a manufacturing process, 10% of the parts contain surface flaws and 25% of the parts with surface flaws are (functionally) defective parts. However, only 5% of parts without surface flaws are defective parts.

There are two events of interest here:

$$\begin{aligned} D &= \{\text{part is defective}\} \\ F &= \{\text{part has surface flaws}\}. \end{aligned}$$

We are given $P(F) = 0.10$, $P(D|F) = 0.25$, and $P(D|F') = 0.05$. Therefore, how we assign probability to D depends on whether F occurs; i.e., it depends on whether the part has surface flaws (F) or not (F').

Exercise: What is $P(D)$? That is, what percentage of parts are defective overall regardless of surface flaw status?

Example 2.13. Brazilian scientists have identified a new strain of the H1N1 virus. The genetic sequence of the new strain consists of alterations in the hemagglutinin protein, making it significantly different than the usual H1N1 strain. Public health officials wish to study the population of residents in Rio de Janeiro. Suppose that in this population

- the probability of catching the usual strain is 0.10
- the probability of catching the new strain is 0.05
- the probability of catching both strains is 0.01.

Define the events

$$\begin{aligned} A &= \{\text{resident catches usual strain}\} \\ B &= \{\text{resident catches new strain}\}. \end{aligned}$$

From the information above, we have $P(A) = 0.10$, $P(B) = 0.05$, and $P(A \cap B) = 0.01$.

Q: Find the probability of catching the usual strain, given that the new strain is caught.
A: Using the definition of conditional probability,

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{0.01}{0.05} = 0.20.$$

This means among all residents who have caught the new strain, 20% of them will also catch the usual strain. Notice how $P(A)$ and $P(A|B)$ are different. That is, the occurrence of B has changed how we assign probability to A.

Q: Find the probability of catching the new strain, given that at least one strain is caught.
A: If "at least one strain is caught," this means $A \cup B$ has occurred. Therefore,

$$\begin{aligned} P(B|A \cup B) = \frac{P(B \cap (A \cup B))}{P(A \cup B)} &= \frac{P(B)}{P(A) + P(B) - P(A \cap B)} \\ &= \frac{0.05}{0.10 + 0.05 - 0.01} \approx 0.357. \end{aligned}$$

This means among all residents who have caught at least one strain, 35.7% of them have caught the new strain.

Multiplication Rule: If we take the conditional probability definitions

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \quad \text{and} \quad P(B|A) = \frac{P(A \cap B)}{P(A)},$$

we see that

$$\begin{aligned} P(A \cap B) &= P(A|B)P(B) \\ &= P(B|A)P(A). \end{aligned}$$

This is called the multiplication rule (although I'm not sure why). It gives us a way to calculate $P(A \cap B)$ when conditional probabilities are available.

- In general, we cannot determine $P(A \cap B)$ from $P(A)$ and $P(B)$ alone. We need more information or we have to make additional assumptions about A and B.

Curiosity: $P(A)$ and $P(A|B)$ are both probabilities for the event A. In the first, we look at A by itself. In the second, we incorporate knowledge that the event B has occurred. What does it mean when $P(A) = P(A|B)$? It means the knowledge gained from learning B occurred does not influence how we assign probability to the event A. This is the casual definition of **independence**.

Definition: When the occurrence or non-occurrence of B has no effect on whether or not A occurs, and vice-versa, we say the events A and B are **independent**. Mathematically, we define A and B to be independent if and only if

$$P(A \cap B) = P(A)P(B).$$

Note that if A and B are independent, then

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

and

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

Example 2.14. An electrical circuit consists of two components (e.g., resistors, capacitors, batteries, etc.). The probability the second component functions satisfactorily during its design life is 0.90. The probability at least one of the components does so is 0.96. The probability both components do so is 0.75.

Q: Do the two components function independently?
A: Define the events

$$\begin{aligned} A &= \{\text{component 1 functions}\} \\ B &= \{\text{component 2 functions}\}. \end{aligned}$$

We have $P(B) = 0.90$, $P(A \cup B) = 0.96$, and $P(A \cap B) = 0.75$. The additive rule gives

$$0.96 = P(A) + 0.90 - 0.75 \implies P(A) = 0.81.$$

However,

$$0.75 = P(A \cap B) \neq P(A)P(B) = 0.81(0.90) = 0.729.$$

Therefore, the events A and B are not independent. The two components do not function independently.

Example 2.15. In an engineering system, two components are placed in a **series**. This means the system is functional as long as both components are. Each component is functional with probability 0.95. Define the events

$$\begin{aligned} A_1 &= \{\text{component 1 is functional}\} \\ A_2 &= \{\text{component 2 is functional}\} \end{aligned}$$

so that $P(A_1) = P(A_2) = 0.95$. Because we need both components to be functional, the **system reliability** (i.e., the probability the system is functional) is $P(A_1 \cap A_2)$.

- If the components operate independently, then the system reliability is

$$P(A_1 \cap A_2) = P(A_1)P(A_2) = 0.95(0.95) = 0.9025.$$

- If the components do not operate independently; e.g., failure of one component affects the other, we can not determine the system reliability $P(A_1 \cap A_2)$ without additional knowledge or assumptions.

Remark: The notion of independence extends to more than two events. **Mutual independence** means the probability of all events in any sub-collection of $A_1, A_2, ..., A_n$ occurring equals the product of the probabilities of the events in the sub-collection. For example, if A_1, A_2, and A_3 are mutually independent, then

$$\begin{aligned} P(A_1 \cap A_2) &= P(A_1)P(A_2) \\ P(A_1 \cap A_3) &= P(A_1)P(A_3) \\ P(A_2 \cap A_3) &= P(A_2)P(A_3) \end{aligned}$$

considering all event sub-collections of size two. It must also be true that

$$P(A_1 \cap A_2 \cap A_3) = P(A_1)P(A_2)P(A_3).$$

Remark: Many random experiments can be envisioned as consisting of a sequence of n "trials" that are viewed as independent (e.g., flipping a coin 10 times). If A_i denotes the event associated with the ith trial, and the trials are mutually independent, then

$$P\left(\bigcap_{i=1}^{n} A_i\right) = \prod_{i=1}^{n} P(A_i).$$

Example 2.16. Samples of 30 parts from a metal punching process are selected every hour. Each part is tested. If a part does not conform to specifications, it is sent to another location where it is repaired (or "reworked").

Define the events

$$A_i = \{i\text{th part requires rework}\}, \quad i = 1, 2, ..., 30.$$

Assume the 30 events $A_1, A_2, ..., A_{30}$ are mutually independent and $P(A_i) = p$.

Q: Under these assumptions, what is the probability at least one part requires rework?
A: Define the event

$$A = \{\text{at least one part requires rework}\} = \bigcup_{i=1}^{30} A_i.$$

The complement of A is

$$A' = \{\text{no part requires rework}\} = \bigcap_{i=1}^{30} A_i'$$

by DeMorgan's Law. Because $A_1, A_2, ..., A_{30}$ are mutually independent, the complements $A_1', A_2', ..., A_{30}'$ are also mutually independent. Therefore,

$$P(A') = P\left(\bigcap_{i=1}^{30} A_i'\right) = \prod_{i=1}^{30} P(A_i') = (1-p)^{30}.$$

Finally,

$$P(A) = 1 - P(A') = 1 - (1-p)^{30}.$$

For example, if $p = 0.01$, that is, 1% of all parts require rework, then

$$1 - (0.99)^{30} \approx 0.260.$$

Therefore, rework will be required for at least one part 26% of the time when samples of size 30 are tested.

2.5 Law of Total Probability and Bayes' Rule

Law of Total Probability: Suppose A and B are events in a sample space S. We can express A as the union of two mutually exclusive events

$$A = (A \cap B) \cup (A \cap B').$$

Therefore,

$$\begin{aligned} P(A) &= P(A \cap B) + P(A \cap B') \\ &= P(A|B)P(B) + P(A|B')P(B'). \end{aligned}$$

Remark: The Law of Total Probability gives us a way to calculate $P(A)$ by relying instead on the conditional probabilities $P(A|B)$ and $P(A|B')$ and the probability of a related event B. Specifically, $P(A)$ is a linear combination of the conditional probabilities $P(A|B)$ and $P(A|B')$. Note that the "weights" in the linear combination, $P(B)$ and $P(B')$, add to 1.

Example 2.17. An insurance company classifies drivers as "accident-prone" and "non-accident-prone." The probability an accident-prone driver has an accident is 0.4. The probability a non-accident-prone driver has an accident is 0.2. The population is 30 percent accident-prone. Define the events

$$\begin{aligned} A &= \{\text{policy holder has an accident}\} \\ B &= \{\text{policy holder is accident-prone}\}. \end{aligned}$$

We are given $P(A|B) = 0.4$, $P(A|B') = 0.2$, and $P(B) = 0.3$.

Q: What is the probability a policy holder has an accident?
A: We want $P(A)$, which can be found by using the LOTP:

$$P(A) = P(A|B)P(B) + P(A|B')P(B') = 0.4(0.3) + 0.2(0.7) = 0.26.$$

Therefore, 26% of the company's policy holders will have an accident.

Q: If a policy holder has an accident, what is the probability s/he was "accident-prone?"
A: We want $P(B|A)$, which can be calculated as

$$P(B|A) = \frac{P(A \cap B)}{P(A)} = \frac{P(A|B)P(B)}{P(A)} = \frac{0.4(0.3)}{0.26} \approx 0.462.$$

Therefore, among all policy holders who had an accident, 46.2% of them are accident-prone.

Discussion: In the last part, note that if we write

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)} = \frac{P(A|B)P(B)}{P(A|B)P(B) + P(A|B')P(B')},$$

we obtain **Bayes' Rule** for two events.

Example 2.18. *Diagnostic testing.* A lab test is 95% effective at detecting a disease when it is present. It is 99% effective at declaring a subject negative when the subject is truly negative for the disease. Suppose 8% of the population has the disease.

Define the events

$$\begin{aligned} D &= \{\text{disease is present}\} \\ A &= \{\text{test is positive}\}. \end{aligned}$$

We are given the following information:

$$\begin{aligned} P(A|D) &= 0.95 \quad (\text{"sensitivity"}) \\ P(A'|D') &= 0.99 \quad (\text{"specificity"}) \\ P(D) &= 0.08 \quad (\text{"prevalence"}). \end{aligned}$$

Q: What is the probability a randomly selected subject will test positively?
A: We want $P(A)$. By the LOTP,

$$P(A) = P(A|D)P(D) + P(A|D')P(D') = 0.95(0.08) + 0.01(0.92) \approx 0.085.$$

Therefore, about 8.5% of the population will produce a positive test result.

Q: What is the probability a subject has the disease if his test is positive?
A: We want $P(D|A)$. By Bayes' Rule,

$$P(D|A) = \frac{P(A|D)P(D)}{P(A|D)P(D) + P(A|D')P(D')} = \frac{0.95(0.08)}{0.95(0.08) + 0.01(0.92)} \approx 0.892.$$

Therefore, among all subjects testing positively, about 89.2% of the subjects have the disease.

Remark: In general, Bayes' Rule allows us to update probabilities on the basis of observed information. In Example 2.18, the "observed information" we get to see is the test result.

Prior probability		Test result		**Posterior** probability
$P(D) = 0.08$	$\longrightarrow$	A	$\longrightarrow$	$P(D\|A) \approx 0.892$
$P(D) = 0.08$	$\longrightarrow$	A'	$\longrightarrow$	$P(D\|A') \approx 0.004$

2.6 Introduction to random variables

Terminology: A **random variable** is a variable whose value is determined by chance.

- By convention, we denote random variables by upper case letters towards the end of the alphabet; e.g., W, X, Y, Z, etc. The authors of the textbook for this course (Montgomery and Runger, 2018) favor the use of X.

Motivation: In Example 2.16, we considered samples of 30 parts from a metal punching process. Conceptualizing this as random experiment, the sample space can be written as

$$S = \{(0, 0, 0, ..., 0), (1, 0, 0, ..., 0), (0, 1, 0, ..., 0), ..., (1, 1, 1, ..., 1)\},$$

where "1" denotes a part that requires rework and "0" denotes a part that does not. There are

$$n_S = 2^{30} = 1,073,741,824$$

outcomes in this sample space! Examples like this illustrate why working with random variables is easier. After all, the line technician or quality control engineer is probably only interested in how many of the parts will require rework. If we let

$$X = \text{number of parts requiring rework (out of 30)},$$

then we no longer have to work with an unwieldy sample space with over a billion outcomes. We can instead work with events of the form

$$\{X = x\},$$

and designate probabilities for $P(X = x)$, for $x = 0, 1, 2, ..., 30$. This is much easier.

Terminology: Random variables generally break down into one of two types.

- If a random variable X can have only a finite (or countable) number of values, we say it is **discrete**.
  - For example, the random variable

    $$X = \text{number of parts requiring rework (out of 30)}$$

    is discrete because there are 31 possible values $x = 0, 1, 2, ..., 30$.

- If it makes more sense that X has values in an interval of numbers, we say X is **continuous**.
  - Measurements like part diameters (cm), temperature (deg C), energy expended (kcal), time (days, years, etc.), and distance (miles) are all best regarded as continuous random variables.

Terminology: The set of all values a random variable X can have is called its **support**.

Example 2.19. Classify the following random variables as discrete or continuous and specify the support of each:

$$\begin{aligned} V &= \text{number of unbroken eggs in a randomly selected carton (dozen)} \\ W &= \text{pH of an aqueous solution} \\ X &= \text{length of time between accidents at a factory} \\ Y &= \text{whether or not you pass this class} \\ Z &= \text{number of aircraft arriving tomorrow at CAE.} \end{aligned}$$

- The random variable V is **discrete**. It can have values in

$$\{0, 1, 2, ..., 12\}.$$

- The random variable W is **continuous**. It can have values in

$$\mathbb{R} = \{-\infty < w < \infty\}.$$

  With most solutions, it is more likely that W is not negative (although this is possible) and not larger than, say, 15 (a very reasonable upper bound).

- The random variable X is **continuous**. It can have values in

$$\mathbb{R}^+ = \{x > 0\}.$$

  The key point here is that a time cannot be negative. In theory, it is possible that X can be very large.

- The random variable Y is **discrete**. It can have values in

$$\{0, 1\},$$

  where I have arbitrarily labeled "1" for passing and "0" for failing. Random variables that can assume exactly two values (e.g., 0, 1) are **binary**.

- The random variable Z is **discrete**. It can have values in

$$\mathbb{N} = \{0, 1, 2, 3, ..., \}.$$

  I have allowed for the possibility of a very large number of aircraft arriving.

3 Discrete Distributions

3.1 Probability mass functions

Recall: A random variable X is **discrete** if it can have a finite or countable number of values.

Terminology: The **probability mass function** (pmf) of a discrete random variable X tells us two things:

1. the values X can have
2. a probability $p_X(x) = P(X = x)$ for each value of x.

The pmf of X,

$$p_X(x) = P(X = x),$$

describes the **distribution** of X. It tells us which values of x are possible (the support of X) and how to assign probabilities to these values.

Example 3.1. An automobile paint factory has 5 filling lines (lines where cans are filled with paint) which are in continuous operation. During a 24-hour time period, mechanics record

$$X = \text{the number of lines which require maintenance.}$$

Here is the distribution of X, described by its pmf:

x	0	1	2	3	4	5
$p_X(x)$	0.60	0.10	0.16	0.05	0.06	0.03

The support of X is

$$\{0, 1, 2, 3, 4, 5\}.$$

Also,

- the probabilities $p_X(x) = P(X = x)$ are all between 0 and 1
- the probabilities add to 1.

These two things must be true for any pmf (otherwise, we say the pmf is not valid).

Q: What is the probability no lines require maintenance during a 24-hour time period?

$$P(X = 0) = 0.60.$$

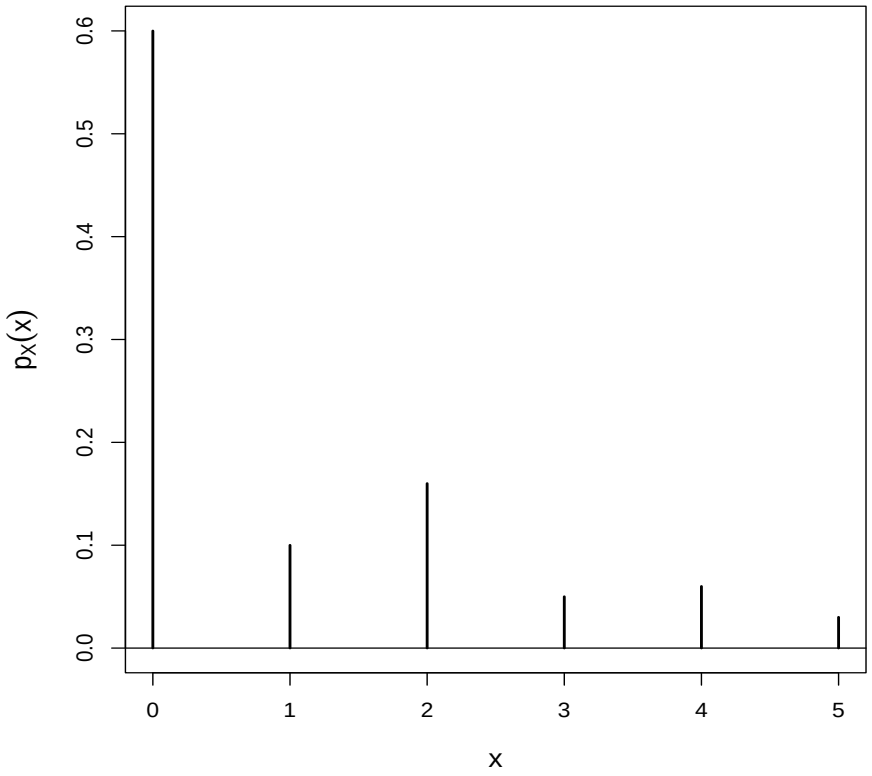


Figure 3.1: Probability mass function of X in Example 3.1.

Q: Upper management is contacted whenever 3 or more lines require maintenance during a 24-hour time period. What percentage of days will this occur?

$$\begin{aligned} P(X \geq 3) &= P(X = 3) + P(X = 4) + P(X = 5) \\ &= 0.05 + 0.06 + 0.03 = 0.14. \end{aligned}$$

Upper management will be contacted on 14% of the days.

Terminology: The **cumulative distribution function** (cdf) of a discrete random variable X gives probabilities of the form

$$F_X(x) = P(X \leq x)$$

for any real number x.

- When X is a discrete random variable, the cdf $F_X(x)$ is a step function.
- The range of $F_X(x)$ is

  $$0 \leq F_X(x) \leq 1.$$

  This makes sense because $F_X(x)$ is a probability.

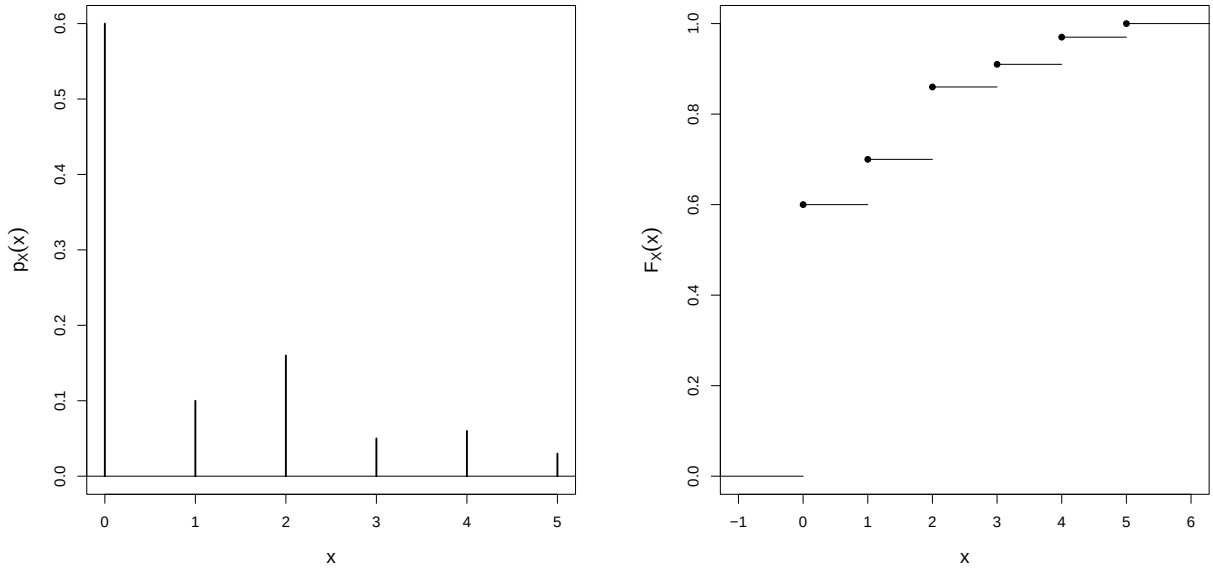


Figure 3.2: Left: Probability mass function (pmf) of X in Example 3.1. Right: Cumulative distribution function (cdf) of X.

Note: A discrete random variable's cdf cumulates (adds up) probability as we move from left to right on the pmf. The cdf of X in Example 3.1, shown above, can be written as

$$F_X(x) = \begin{cases} 0, & x < 0 \\ 0.60, & 0 \leq x < 1 \\ 0.70, & 1 \leq x < 2 \\ 0.86, & 2 \leq x < 3 \\ 0.91, & 3 \leq x < 4 \\ 0.97, & 4 \leq x < 5 \\ 1, & x \geq 5. \end{cases}$$

Example 3.1 (continued). Answer the following questions by using both the pmf and cdf in Figure 3.2.

Q: What is the probability there are at most 2 lines that require maintenance?
A: We want $P(X \leq 2)$.

PMF:

$$P(X \leq 2) = P(X = 0) + P(X = 1) + P(X = 2) = 0.60 + 0.10 + 0.16 = 0.86$$

CDF:

$$P(X \leq 2) = F_X(2) = 0.86.$$

Q: What is the probability there are at least 4 lines that require maintenance?
A: We want $P(X \geq 4)$.

PMF:

$$P(X \geq 4) = P(X = 4) + P(X = 5) = 0.06 + 0.03 = 0.09$$

CDF:

$$P(X \geq 4) = 1 - P(X \leq 3) = 1 - F_X(3) = 1 - 0.91 = 0.09.$$

Q: What is the probability there is exactly 1 line that requires maintenance?
A: We want $P(X = 1)$.

PMF:

$$P(X = 1) = 0.10$$

CDF:

$$P(X = 1) = P(X \leq 1) - P(X \leq 0) = F_X(1) - F_X(0) = 0.70 - 0.60 = 0.10.$$

3.2 Mean and variance

Terminology: Suppose X is a discrete random variable with pmf $p_X(x)$. The **expected value** of X is

$$\mu = E(X) = \sum_{\text{all } x} x p_X(x).$$

The expected value of a discrete random variable X is a weighted average of the possible values of X. Each value x is weighted by its probability $p_X(x)$. In statistical applications, $\mu = E(X)$ is called the **mean** or **population mean**.

Example 3.1 (continued). We examined the distribution of X, the number of filling lines which require maintenance during a 24-hour period. The probability mass function (pmf) of X is

x	0	1	2	3	4	5
$p_X(x)$	0.60	0.10	0.16	0.05	0.06	0.03

The expected value of X is

$$\begin{aligned} E(X) &= \sum_{\text{all } x} x p_X(x) \\ &= 0(0.60) + 1(0.10) + 2(0.16) + 3(0.05) + 4(0.06) + 5(0.03) = 0.96. \end{aligned}$$

Interpretations:

- $E(X)$ is the "center of gravity" of a discrete random variable's pmf. It's the location on the horizontal axis where $p_X(x)$ would balance if it were made of solid material.

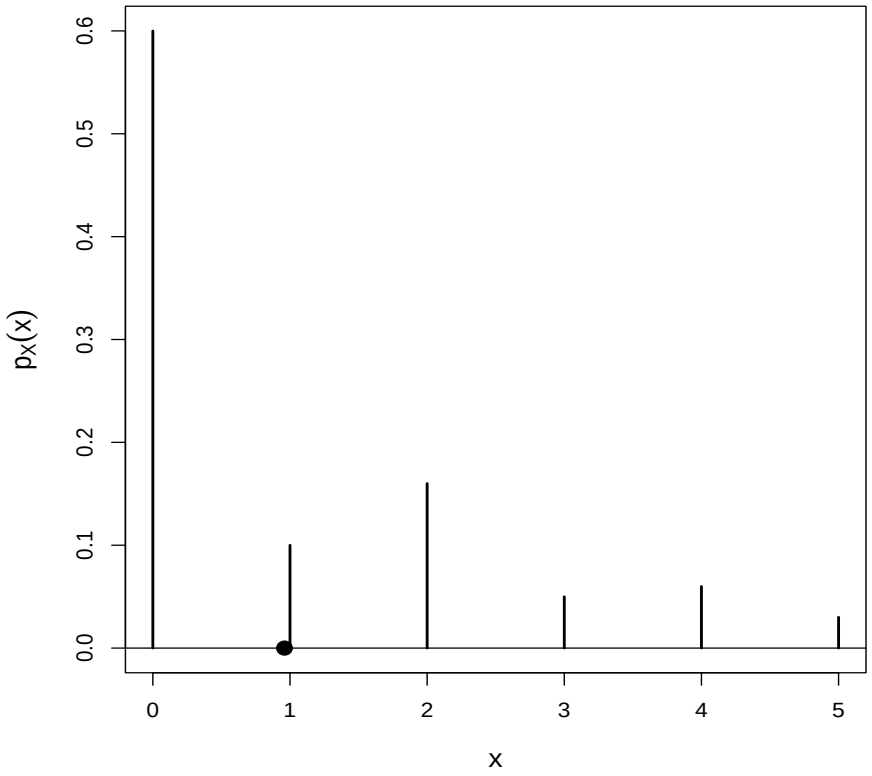


Figure 3.3: Probability mass function of X in Example 3.1. The expected value $E(X) = 0.96$ is shown by a solid circle.

- $E(X)$ is a "long-run average." That is, if we were to observe the value of X for many 24-hour periods in Example 3.1, the average of these observations should be "close" to $E(X)$. The more observations there are, the closer this average will be to $E(X)$. For example, the R code below simulates 365 measurements of X in Example 3.1 and averages them.

```
> options(digits=3) # control number of significant digits presented
> n = 365
> x = c(0,1,2,3,4,5)
> prob = c(0.60,0.10,0.16,0.05,0.06,0.03)
> lines = sample(x,n,replace=TRUE,prob=prob)
> mean(lines)
[1] 0.934
```

Result: Suppose X is a discrete random variable with pmf $p_X(x)$ and g is any function. Then $g(X)$ is also a random variable and its expectation (mean) is

$$E[g(X)] = \sum_{\text{all } x} g(x)p_X(x).$$

Linearity rules:

(a) $E(c) = c$, for any constant c

(b) $E[cg(X)] = cE[g(X)]$, for any constant c

(c) The expectation of the sum is the sum of the expectations; i.e.,

$$E[g_1(X) + g_2(X) + \cdots + g_k(X)] = E[g_1(X)] + E[g_2(X)] + \cdots + E[g_k(X)].$$

We say the expectation $E(\cdot)$ is a **linear operator**, that is, it preserves the operations of addition and scalar multiplication.

Example 3.2. In a one-hour period, the number of gallons of toxic waste produced at a local plant, say X, has the following pmf:

x	0	1	2	3
$p_X(x)$	0.2	0.3	0.3	0.2

This pmf is shown in Figure 3.4 (next page).

Q: What is $E(X)$?

$$E(X) = \sum_{\text{all } x} x p_X(x) = 0(0.2) + 1(0.3) + 2(0.3) + 3(0.2) = 1.5.$$

Therefore, we would expect 1.5 gallons of toxic waste to be produced per hour.

Q: Disposing toxic waste requires careful handling and adherence to regulations to protect human health and the environment. The cost C (in \$100s) to dispose X gallons of waste per hour is a quadratic function of X, specifically,

$$C = 3 - 1.4X + 4.6X^2.$$

What is the expected cost of disposal $E(C)$ in a one-hour period?
A: We can use the linearity rules stated above. Let's find $E(X^2)$ first:

$$E(X^2) = \sum_{\text{all } x} x^2 p_X(x) = 0^2(0.2) + 1^2(0.3) + 2^2(0.3) + 3^2(0.2) = 3.3.$$

Therefore,

$$\begin{aligned} E(C) = E(3 - 1.4X + 4.6X^2) &= 3 - 1.4E(X) + 4.6E(X^2) \\ &= 3 - 1.4(1.5) + 4.6(3.3) = 16.08. \end{aligned}$$

The expected hourly cost of toxic waste disposal is \$1,608.00.

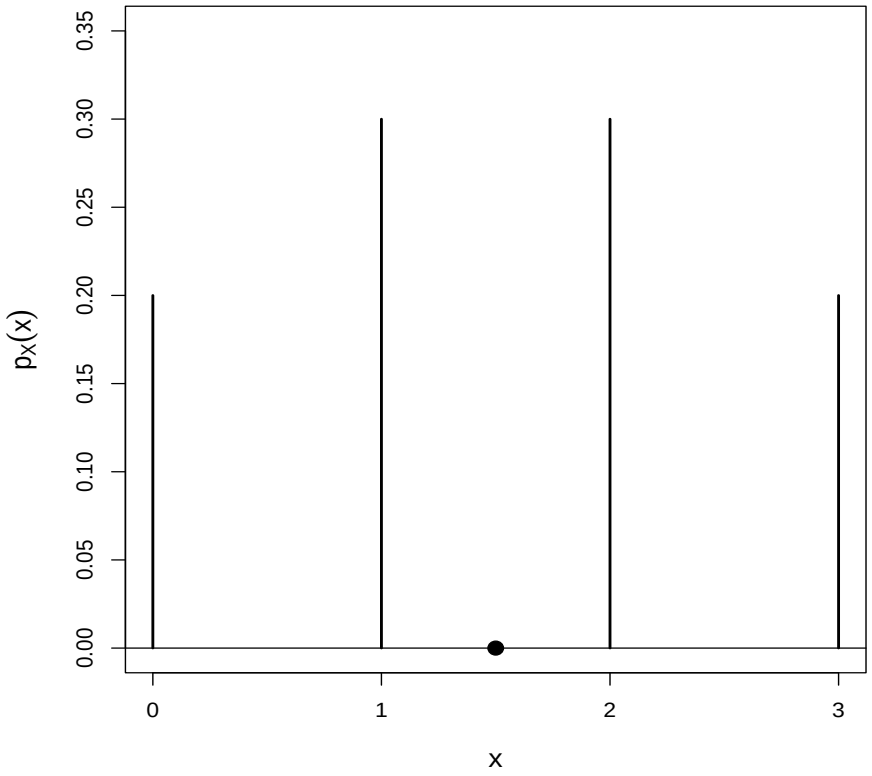


Figure 3.4: Probability mass function of X in Example 3.2. The expected value $E(X) = 1.5$ is shown by a solid circle.

Terminology: Suppose X is a discrete random variable with pmf $p_X(x)$ and mean $\mu = E(X)$. The **variance** of X is

$$\begin{aligned} \sigma^2 = V(X) &= E[(X-\mu)^2] \\ &= \sum_{\text{all } x} (x-\mu)^2 p_X(x). \end{aligned}$$

The **standard deviation** of X is the positive square root of the variance:

$$\sigma = \sqrt{\sigma^2} = \sqrt{V(X)}.$$

Example 3.2 (continued). Recall the pmf for the number of gallons of toxic waste produced (per hour) is

x	0	1	2	3
$p_X(x)$	0.2	0.3	0.3	0.2

Q: Find $V(X)$ and the standard deviation of X.

Using the definition of the variance, we have

$$\begin{aligned} V(X) &= \sum_{\text{all } x}(x-\mu)^2 p_X(x) \\ &= (0-1.5)^2(0.2) + (1-1.5)^2(0.3) + (2-1.5)^2(0.3) + (3-1.5)^2(0.2) = 1.05. \end{aligned}$$

The standard deviation of X is

$$\sigma = \sqrt{V(X)} = \sqrt{1.05} \approx 1.025.$$

Interpreting the variance and standard deviation:

1. Whereas $E(X)$ measures the "center" of a distribution, the variance $V(X)$ measures the "spread," that is, how spread out the values of X are about the mean.
2. The larger $V(X)$ is, the more spread (variability) in the distribution of X.
3. The variance $V(X) \geq 0$. The only time $V(X) = 0$ is when X has a **degenerate distribution**; i.e., all the probability mass is at one point.
4. $V(X)$ is measured in (units)^2 and σ is measured in original units.
5. From the definition,
$$V(X) = E[(X-\mu)^2]$$
is the expected squared distance between X and the mean. The standard deviation σ is (roughly) the expected distance between X and the mean.

Linear functions: Suppose X is a discrete random variable with pmf $p_X(x)$ and mean $\mu = E(X)$. Suppose a and b are constants. The mean and variance of the linear function $aX + b$ are

$$\begin{aligned} E(aX+b) &= aE(X) + b \\ V(aX+b) &= a^2 V(X). \end{aligned}$$

The expectation result follows from the linearity properties associated with $E(\cdot)$. The variance result is new.

- Taking $a = 0$, we see that $V(b) = 0$ for any constant b. This makes sense−the variance is a measure of variability for a random variable; a constant does not vary. This also means that additive shifts of b (to the left or right) do not affect the spread in the distribution of X.
- Taking $b = 0$, we see that $V(aX) = a^2 V(X)$. Multiplicative constants increase the variance when $|a| > 1$ and decrease the variance when $0 < |a| < 1$.

Example 3.3. Patient responses to a generic drug to control pain are scored on 5-point scale (1 = lowest pain level; 5 = highest pain level). In a certain population of patients, the pmf of the response X is given by

x	1	2	3	4	5
$p_X(x)$	0.38	0.27	0.18	0.11	0.06

This pmf is shown in Figure 3.5 (next page, left).

Q: Find the expected value and variance of X.
A: The expected value is

$$\begin{aligned} E(X) &= \sum_{\text{all } x} x p_X(x) \\ &= 1(0.38) + 2(0.27) + 3(0.18) + 4(0.11) + 5(0.06) = 2.2. \end{aligned}$$

In this application, it would be appropriate to call $E(X) = \mu = 2.2$ the **population mean**. It is the mean pain response for all patients in the population under study.

The variance is

$$\begin{aligned} V(X) &= \sum_{\text{all } x} (x-\mu)^2 p_X(x) \\ &= (1-2.2)^2(0.38) + (2-2.2)^2(0.27) + (3-2.2)^2(0.18) \\ &\qquad + (4-2.2)^2(0.11) + (5-2.2)^2(0.06) = 1.5. \end{aligned}$$

Similarly, it would be appropriate to call $V(X) = \sigma^2 = 1.5$ the **population variance**. It is the variance associated with the pain responses for all patients in the population.

Q: Find the mean and variance of $Y = 2X - 1$.
A: The mean of $Y = 2X - 1$ is

$$E(2X-1) = 2E(X) - 1 = 2(2.2) - 1 = 3.4.$$

The variance of $Y = 2X - 1$ is

$$V(2X-1) = 4V(X) = 4(1.5) = 6.$$

These are the mean and variance associated with the pmf of $Y = 2X - 1$:

y	1	3	5	7	9
$p_Y(y)$	0.38	0.27	0.18	0.11	0.06

This pmf is shown in Figure 3.5 (next page, right).

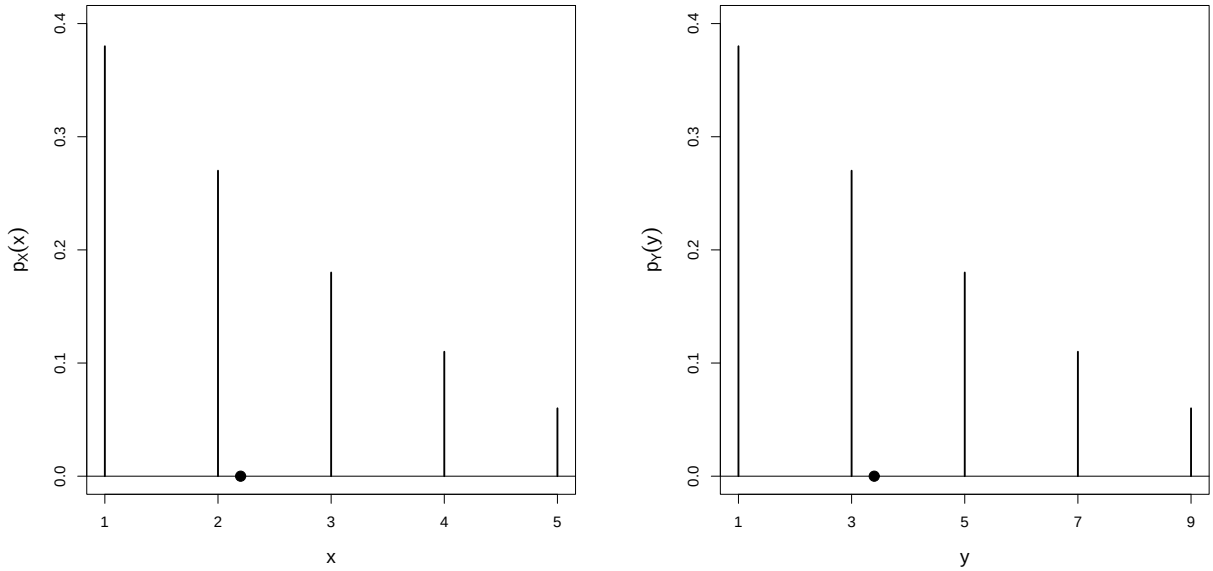


Figure 3.5: Left: Probability mass function of X in Example 3.3. Right: Probability mass function of $Y = 2X - 1$. The means $E(X) = 2.2$ and $E(Y) = 3.4$ are shown by solid circles.

Variance computing formula: Suppose X is a random variable (discrete or continuous) with mean $\mu = E(X)$. An alternative way to find $V(X)$ is by using

$$V(X) = E(X^2) - [E(X)]^2.$$

This formula is easy to remember and can make calculations easier. It also reminds us that

$$E(X^2) \neq [E(X)]^2.$$

Some students are tempted to write $E(X^2) = [E(X)]^2$, but this is not true! Provided X does not have a degenerate distribution (where all the probability is at one value), note that

$$V(X) > 0 \Longrightarrow E(X^2) > [E(X)]^2.$$

Example 3.3 (continued). For the pmf

x	1	2	3	4	5
$p_X(x)$	0.38	0.27	0.18	0.11	0.06

we have

$$\begin{aligned} E(X^2) &= \sum_{\text{all } x} x^2 p_X(x) \\ &= 1^2(0.38) + 2^2(0.27) + 3^2(0.18) + 4^2(0.11) + 5^2(0.06) = 6.34. \end{aligned}$$

Using the variance computing formula,

$$\begin{aligned} V(X) &= E(X^2) - [E(X)]^2 \\ &= 6.34 - (2.2)^2 = 1.5. \end{aligned}$$

This is the same answer we got for $V(X)$ when we used the definition of variance.

3.3 Binomial distribution

Bernoulli trials: Many random experiments can be envisioned as consisting of a sequence of "trials," where

1. each trial results in a "success" or a "failure" (only 2 outcomes are possible)
2. the trials are independent (the result on one trial is not affected by the results from other trials)
3. the probability of success p is the same on every trial.

Examples:

- When circuit boards used in the manufacture of laptops are tested, one percent of the boards are found to be defective.
  - circuit board = "trial"
  - defective board is observed = "success"
  - $p = 0.01$
- Ninety-eight percent of all air traffic radar signals are correctly interpreted the first time they are transmitted.
  - radar signal = "trial"
  - signal is correctly interpreted = "success"
  - $p = 0.98$
- Albino rats used to study the hormonal regulation of a metabolic pathway are injected with a drug that inhibits body synthesis of protein. Twenty percent of all rats will die before the study is complete.
  - rat = "trial"
  - dies before study is over = "success"
  - $p = 0.2$

- During her WNBA tenure, Caitlyn Clark's free throw percentage is 88.7%.
  - free throw = "trial"
  - made free throw = "success"
  - $p = 0.887$

Definition: A **binomial distribution** arises when we observe a fixed number of Bernoulli trials:

$$\begin{aligned} n &= \text{number of trials} \\ X &= \text{number of successes (out of } n\text{)}. \end{aligned}$$

If the Bernoulli trial assumptions hold, then the probability mass function (pmf) of X is given by the formula

$$p_X(x) = \begin{cases} \binom{n}{x} p^x (1-p)^{n-x}, & x = 0, 1, 2, ..., n \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim b(n, p)$, where p is the probability of success on any one trial.

Example 3.4. In an agricultural study, 40 percent of all plots respond to a certain treatment. In this context, we interpret

- plot = "trial"
- plot responds to treatment = "success"
- $p = 0.4$

Four plots are observed. If the Bernoulli trial assumptions hold (independent plots, same response probability for each plot), then

$$X = \text{number of plots responding to treatment} \sim b(n = 4, p = 0.4).$$

This pmf is shown in Figure 3.6 (next page). Here are all the pmf calculations:

$$\begin{aligned} P(X = 0) &= \binom{4}{0}(0.4)^0(0.6)^4 = 0.1296 \\ P(X = 1) &= \binom{4}{1}(0.4)^1(0.6)^3 = 0.3456 \\ P(X = 2) &= \binom{4}{2}(0.4)^2(0.6)^2 = 0.3456 \\ P(X = 3) &= \binom{4}{3}(0.4)^3(0.6)^1 = 0.1536 \\ P(X = 4) &= \binom{4}{4}(0.4)^4(0.6)^0 = 0.0256. \end{aligned}$$

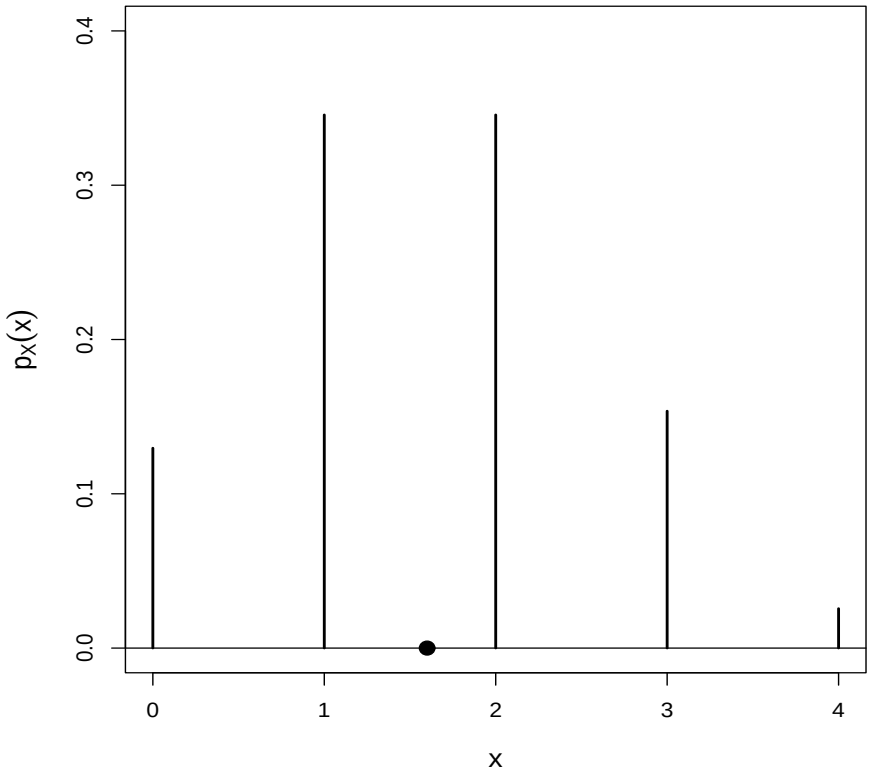


Figure 3.6: Probability mass function of $X \sim b(4, 0.4)$ in Example 3.4. The expected value $E(X) = 1.6$ is shown by a solid circle.

Putting these in tabular form (like before), we have

x	0	1	2	3	4
$p_X(x)$	0.1296	0.3456	0.3456	0.1536	0.0256

MEAN/VARIANCE: If $X \sim b(n, p)$, then

$$\begin{aligned} E(X) &= np \\ V(X) &= np(1-p). \end{aligned}$$

Example 3.4 (continued). The expected number of plots which respond to treatment is

$$E(X) = 4(0.4) = 1.6 \text{ plots.}$$

The variance is

$$V(X) = 4(0.4)(0.6) = 0.96 \text{ (plots)}^2.$$

The standard deviation is

$$\sigma = \sqrt{0.96} \approx 0.98 \text{ plots.}$$

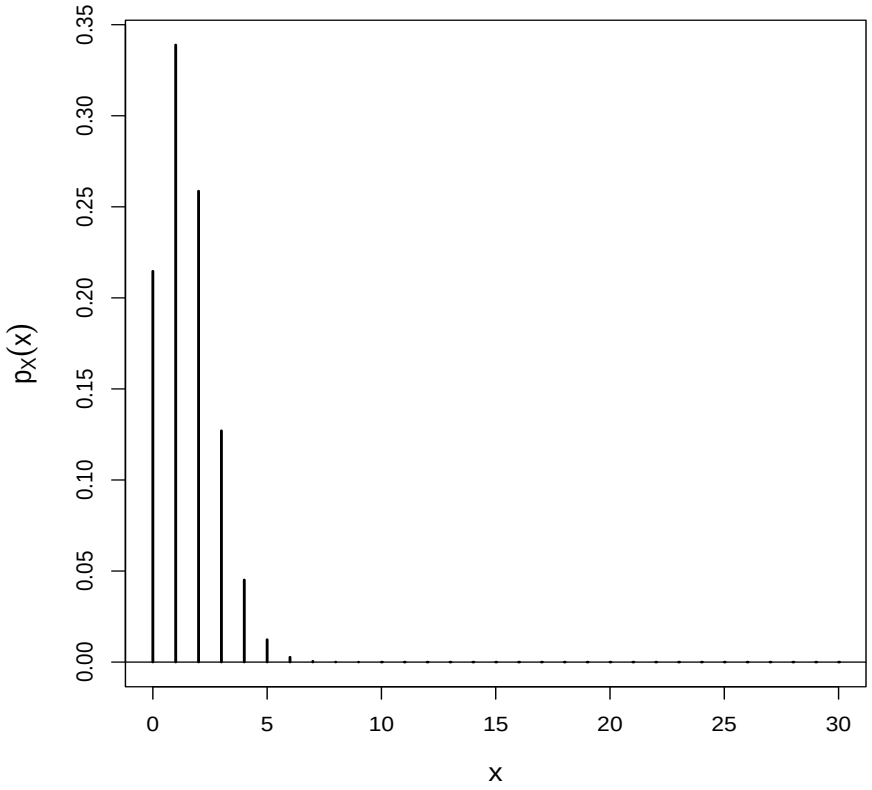


Figure 3.7: Probability mass function of $X \sim b(30, 0.05)$ in Example 3.5.

Example 3.5. A computer's power supply unit (PSU) is hardware that converts high-voltage alternating current (from a wall outlet) into lower-voltage direct current power which is needed by a computer's components (e.g., CPU, etc.). A manufacturer claims "no more than 5 percent" of its power supply units need servicing during their warranty period. We can interpret

- PSU = "trial"
- PSU needs service during warranty period = "success"
- $p = 0.05$ (in fact, the manufacturer claims p is no larger than 0.05).

Technicians access a sample of 30 units and simulate their usage during the warranty period. If the Bernoulli trial assumptions hold (independent units, same probability of needing service for each unit), then

$$X = \text{number of PSUs needing service during warranty period} \sim b(n = 30, p = 0.05).$$

This pmf is shown in Figure 3.7 (above).

Q: Among the 30 units tested, what is the probability the technicians find 5 or more PSUs requiring service during the warranty period?
A: We want $P(X \geq 5)$. We could calculate

$$P(X = 5) + P(X = 6) + P(X = 7) + \cdots + P(X = 29) + P(X = 30),$$

but this would require using the binomial pmf formula 26 times and adding up the results. It is easier to write

$$\begin{aligned} P(X \geq 5) &= 1 - P(X \leq 4) \\ &= 1 - P(X = 0) - P(X = 1) - P(X = 2) - P(X = 3) - P(X = 4) \end{aligned}$$

which requires using the binomial pmf formula only 5 times. Note that

$$\begin{aligned} P(X = 0) &= \binom{30}{0}(0.05)^0(0.95)^{30} \approx 0.2146 \\ P(X = 1) &= \binom{30}{1}(0.05)^1(0.95)^{29} \approx 0.3389 \\ P(X = 2) &= \binom{30}{2}(0.05)^2(0.95)^{28} \approx 0.2586 \\ P(X = 3) &= \binom{30}{3}(0.05)^3(0.95)^{27} \approx 0.1270 \\ P(X = 4) &= \binom{30}{4}(0.05)^4(0.95)^{26} \approx 0.0451. \end{aligned}$$

Therefore,

$$P(X \geq 5) \approx 1 - 0.2146 - 0.3389 - 0.2586 - 0.1270 - 0.0451 = 0.0158.$$

Under the $b(30, 0.05)$ model, it is unlikely the technicians would find 5 or more PSUs requiring service during the warranty period. This would occur only in 1.58% of the samples of size 30 tested.

Discussion: What if the technicians *did* observe 5 PSUs which required service during the warranty period? What might be true?

BINOMIAL R CODE: Suppose $X \sim b(n, p)$.

$p_X(x) = P(X = x)$	$F_X(x) = P(X \leq x)$
`dbinom(x,n,p)`	`pbinom(x,n,p)`

```
> options(digits=4)
> dbinom(2,30,0.05) # P(X=2)
[1] 0.2586
> 1-pbinom(4,30,0.05) # 1-P(X<=4)
[1] 0.01564
```

Note: Another way in R to calculate $P(X \geq 5)$ in this example would be to use the code

```
> sum(dbinom(5:30,30,0.05))
[1] 0.01564
```

The `dbinom(5:30,30,0.05)` command creates a vector containing the binomial pmf probabilities $p_X(5), p_X(6), ..., p_X(30)$. The `sum` command adds them.

3.4 Geometric and negative binomial distributions

Note: Both the geometric and negative binomial distributions arise from observing Bernoulli trials.

Definition: A **geometric distribution** arises when we continue to observe Bernoulli trials until the first success occurs. Specifically, define

$$X = \text{number of trials to observe the 1st success.}$$

If the Bernoulli trial assumptions hold, then the probability mass function (pmf) of X is given by the formula

$$p_X(x) = \begin{cases} (1-p)^{x-1}p, & x = 1, 2, 3, ..., \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim \text{geom}(p)$, where p is the probability of success on any one trial.

Example 3.6. An EPA engineer is tasked with testing water specimens from lakes in northeast Georgia. In this region, each specimen has a 20 percent chance of containing a particular organic pollutant. We interpret

- specimen = "trial"
- specimen contains the pollutant = "success"
- $p = 0.2$

Define

$$X = \text{number of specimens tested to find the first one containing the pollutant.}$$

If the Bernoulli trial assumptions hold (independent specimens, each specimen has the same probability of containing the pollutant), then $X \sim \text{geom}(p = 0.2)$. This pmf is shown in Figure 3.8 (next page).

Q: What is the probability the engineer finds the first polluted specimen on the 5th specimen tested?
A: We want

$$P(X = 5) = (0.8)^4(0.2) \approx 0.082.$$

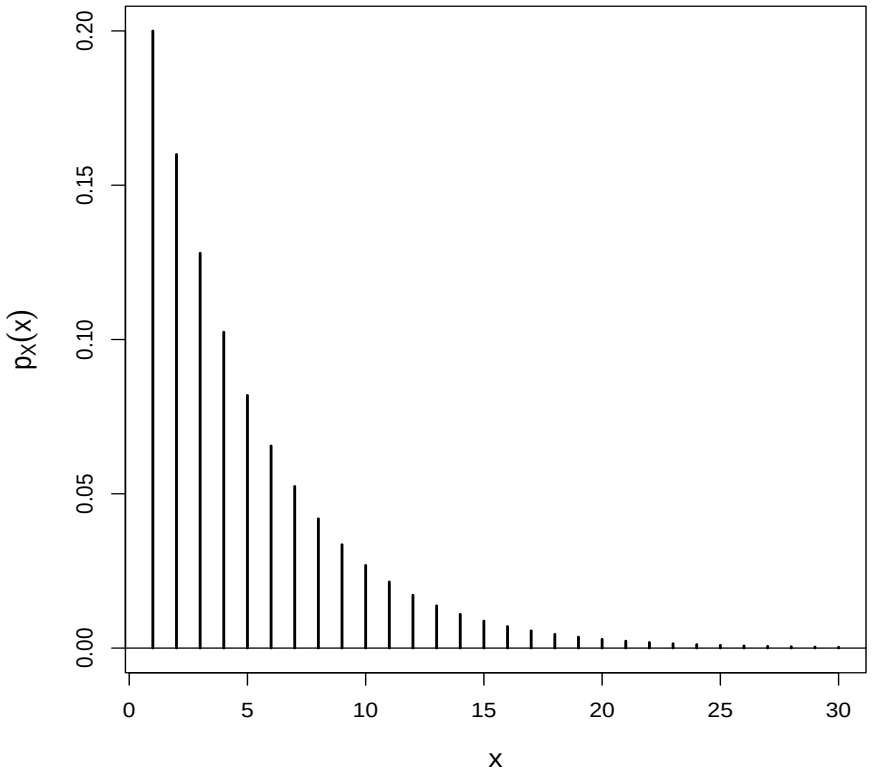


Figure 3.8: Probability mass function of $X \sim \text{geom}(p = 0.2)$ in Example 3.6.

Q: What is the probability the first polluted specimen is found before the 4th specimen is tested?
A: We want

$$\begin{aligned} P(X \leq 3) &= P(X = 1) + P(X = 2) + P(X = 3) \\ &= (0.8)^0(0.2) + (0.8)^1(0.2) + (0.8)^2(0.2) = 0.488. \end{aligned}$$

GEOMETRIC R CODE: Suppose $X \sim \text{geom}(p)$.

$p_X(x) = P(X = x)$	$F_X(x) = P(X \leq x)$
`dgeom(x-1,p)`	`pgeom(x-1,p)`

```
> options(digits=3)
> dgeom(5-1,0.2) # P(X=5)
[1] 0.0819
> pgeom(3-1,0.2) # P(X<=3)
[1] 0.488
```

Definition: A **negative binomial distribution** arises when we continue to observe Bernoulli trials until the rth success occurs. Specifically, define

$$X = \text{number of trials to observe the } r\text{th success.}$$

If the Bernoulli trial assumptions hold, then the probability mass function (pmf) of X is given by the formula

$$p_X(x) = \begin{cases} \binom{x-1}{r-1}(1-p)^{x-r}p^r, & x = r, r+1, r+2, ..., \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim \text{nib}(r, p)$, where p is the probability of success on any one trial.

Note: Some authors call r the **waiting parameter** in the distribution, because we are "waiting" to observe the rth success. Of course, if $r = 1$, then the negative binomial pmf reduces to the geometric pmf.

Example 3.7. At an automotive paint factory, 25 percent of all batches sent to the lab for chemical analysis do not conform to specifications. This might occur for batches that were not prepared properly in the mixing and/or grinding stages. In this situation, we interpret

- batch = "trial"
- batch does not conform = "success"
- $p = 0.25$

Q: What is the probability the 2nd nonconforming batch is found on the 6th batch tested?
A: We are "waiting" until we find the 2nd nonconforming batch ($r = 2$). If the Bernoulli trial assumptions hold (independent batches, same probability of nonconforming for each batch), then

$$\begin{aligned} X &= \text{the number of batches tested to find the second nonconforming} \\ &\sim \text{nib}(r = 2, p = 0.25). \end{aligned}$$

This pmf is shown in Figure 3.9 (next page).

We want

$$P(X = 6) = \binom{5}{1}(0.75)^4(0.25)^2 \approx 0.099.$$

Q: What is the probability we need to observe 20 or more batches to find the 2nd nonconforming batch?
A: We want

$$\begin{aligned} P(X \geq 20) &= 1 - P(X \leq 19) \\ &= 1 - P(X = 2) - P(X = 3) - \cdots - P(X = 19) \\ &= \underbrace{1 - \binom{1}{1}(0.75)^0(0.25)^2 - \binom{2}{1}(0.75)^1(0.25)^2 - \cdots - \binom{18}{1}(0.75)^{17}(0.25)^2}_{\text{there are 18 terms here}} \approx 0.031. \end{aligned}$$

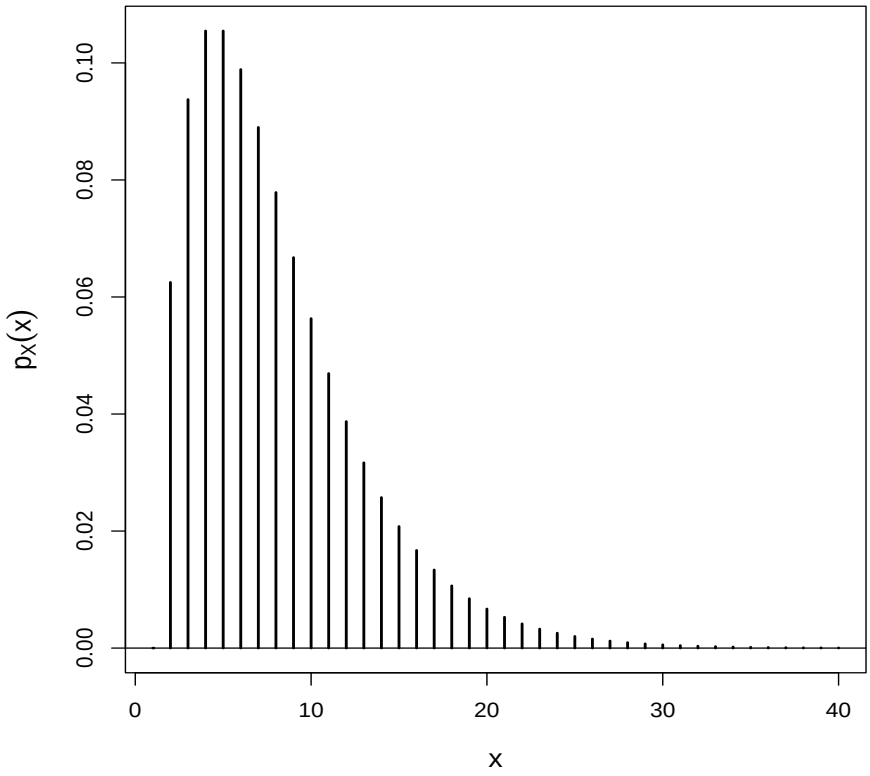


Figure 3.9: Probability mass function of $X \sim \text{nib}(2, 0.25)$ in Example 3.7.

NEGATIVE BINOMIAL R CODE: Suppose $X \sim \text{nib}(r, p)$.

$p_X(x) = P(X = x)$	$F_X(x) = P(X \leq x)$
`dnbinom(x-r,r,p)`	`pnbinom(x-r,r,p)`

```
> dnbinom(6-2,2,0.25) # P(X=6)
[1] 0.0989
> 1-pnbinom(19-2,2,0.25) # 1-P(X<=19)
[1] 0.031
```

MEAN/VARIANCE: If $X \sim \text{nib}(r, p)$, then

$$\begin{aligned} E(X) &= \frac{r}{p} \\ V(X) &= \frac{r(1-p)}{p^2}. \end{aligned}$$

Letting $r = 1$ in the formulas above gives $E(X)$ and $V(X)$ for $X \sim \text{geom}(p)$.

3.5 Hypergeometric distribution

Setting: Consider a population of N objects and suppose each object belongs to one of two classes: Class 1 or Class 2. For example, the objects might be people (infected/not), parts (defective/not), plots of land (respond to treatment/not), etc. We have

$$\begin{aligned} N &= \text{total number of objects} \\ K &= \text{number of objects in Class 1} \\ N-K &= \text{number of objects in Class 2.} \end{aligned}$$

A sample of n objects is taken from the population at random and without replacement (after an object is selected, it is not replaced).

Definition: In the setting above, a **hypergeometric distribution** arises when we observe

$$X = \text{number of Class 1 objects in the sample (out of } n\text{).}$$

The probability mass function (pmf) of X is given by the formula

$$p_X(x) = \begin{cases} \dfrac{\binom{K}{x}\binom{N-K}{n-x}}{\binom{N}{n}}, & x \leq K \text{ and } n-x \leq N-K \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim \text{hyper}(N, n, K)$, where N is the population size, n is the sample size, and K is the number of Class 1 objects in the population.

Discussion: The motivation for the hypergeometric distribution should remind us of the underlying framework for the binomial; i.e., we record the number of Class 1 objects ("successes") out of n ("trials"). The difference here is that

- the population size N is finite
- sampling is done without replacement.

To understand further, suppose

$$p = \frac{K}{N} = \text{proportion of Class 1 objects in the population.}$$

Because sampling from the population is done **without replacement**, the value of p changes from trial to trial. This violates the Bernoulli trial assumptions, so technically the binomial model does not apply. However, if the population size N is "large," the hyper(N, n, K) distribution and the $b(n, p = K/N)$ distribution should be very close to each other even when one samples without replacement. Of course, if one samples from the population **with replacement**, then $p = K/N$ remains fixed and hence the binomial model applies regardless of how large N is.

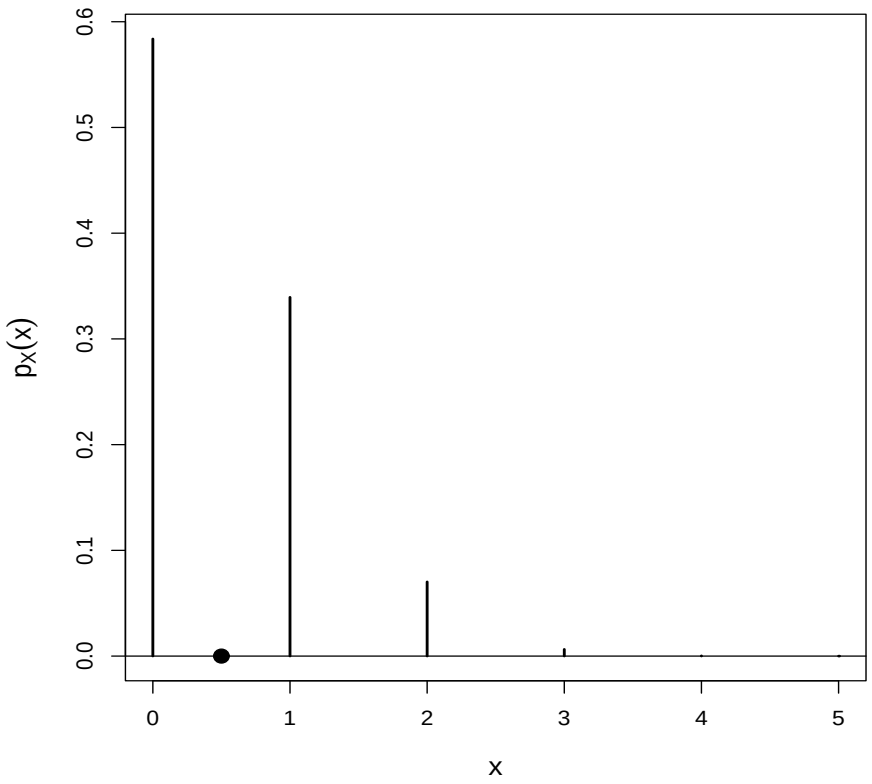


Figure 3.10: Probability mass function of $X \sim \text{hyper}(100, 5, 10)$ in Example 3.8. The expected value $E(X) = 0.5$ is shown by a solid circle.

Example 3.8. A supplier ships parts to a company in lots of 100 parts. The company has an acceptance sampling plan which adopts the following rule:

> "....sample 5 parts at random and without replacement. If there are no defectives in the sample, accept the entire lot; otherwise, reject the entire lot."

Suppose a lot contains 10 defective parts and 90 non-defective parts (this information would usually not be known to the company). Define

$$X = \text{number of defective parts in the sample (out of 5)}$$

so that $X \sim \text{hyper}(N = 100, n = 5, K = 10)$. This pmf is shown in Figure 3.10 (above).

Q: Following the rule above, what is the probability the company accepts the lot?
A: We want $P(X = 0)$. The lot will be accepted only when there are no defectives in the sample.

$$P(X = 0) = \frac{\binom{10}{0}\binom{90}{5}}{\binom{100}{5}} \approx 0.584.$$

Q: What is the probability there are at most 2 defectives in the sample?

$$\begin{aligned} P(X \leq 2) &= P(X=0) + P(X=1) + P(X=2) \\ &= \frac{\binom{10}{0}\binom{90}{5}}{\binom{100}{5}} + \frac{\binom{10}{1}\binom{90}{4}}{\binom{100}{5}} + \frac{\binom{10}{2}\binom{90}{3}}{\binom{100}{5}} \approx 0.993. \end{aligned}$$

HYPERGEOMETRIC R CODE: Suppose $X \sim \text{hyper}(N, n, K)$.

$p_X(x) = P(X = x)$	$F_X(x) = P(X \leq x)$
`dhyper(x,K,N-K,n)`	`phyper(x,K,N-K,n)`

```
> options(digits=3)
> dhyper(0,10,100-10,5) # P(X=0)
[1] 0.584
> phyper(2,10,100-10,5) # P(X<=2)
[1] 0.993
```

MEAN/VARIANCE: If $X \sim \text{hyper}(N, n, K)$, then

$$\begin{aligned} E(X) &= n\left(\frac{K}{N}\right) \\ V(X) &= n\left(\frac{K}{N}\right)\left(1 - \frac{K}{N}\right)\left(\frac{N-n}{N-1}\right). \end{aligned}$$

Note that these formulas are similar to $E(X) = np$ and $V(X) = np(1-p)$ when $X \sim b(n, p)$ and $p = K/N$ is the proportion of Class 1 objects in the population. The extra term in the variance formula is called the **finite population correction factor** (it adjusts for the fact one is sampling from a finite population−not one which is regarded to be infinite in size).

Example 3.8 (continued). The expected number of defective parts sampled is

$$E(X) = 5\left(\frac{10}{100}\right) = 0.5 \text{ parts.}$$

The variance is

$$V(X) = 5\left(\frac{10}{100}\right)\left(1 - \frac{10}{100}\right)\left(\frac{95}{99}\right) = 0.432 \text{ (parts)}^2.$$

The standard deviation is

$$\sigma = \sqrt{0.432} \approx 0.657 \text{ parts.}$$

3.6 Poisson distribution

Relevance: The Poisson distribution is the most common probability distribution when modeling **counts** such as

- the number of customers entering a post office per hour
- the number of insurance claims received per day
- the number of machine breakdowns per month
- the number of severe weather events per year
- the number of raw material defects per square foot
- the number of airborne aerosol particles per cubic inch.

Definition: A **Poisson distribution** arises when we are counting the number of "occurrences" over a unit interval of time (e.g., hour, day, month, year etc.) or a unit region of space (e.g., square foot, cubic inch, etc.). These occurrences must obey the following postulates:

P1. The number of occurrences in non-overlapping intervals of time (or regions of space) are independent.

P2. The probability of an occurrence is proportional to the length of the interval of time (or area/volume of the region of space).

P3. The probability of 2 or more occurrences in a sufficiently small interval of time (or region of space) is zero.

Define

$$X = \text{number of occurrences in a unit interval of time (or region of space).}$$

If the Poisson postulate assumptions hold, then the probability mass function (pmf) of X is given by the formula

$$p_X(x) = \begin{cases} \dfrac{\lambda^x e^{-\lambda}}{x!}, & x = 0, 1, 2, ... \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim \text{Poisson}(\lambda)$, where λ is the mean number of occurrences per unit interval of time or region of space.

MEAN/VARIANCE: If $X \sim \text{Poisson}(\lambda)$, then

$$\begin{aligned} E(X) &= \lambda \\ V(X) &= \lambda. \end{aligned}$$

This is a unique feature of the Poisson distribution−its mean and variance are equal.

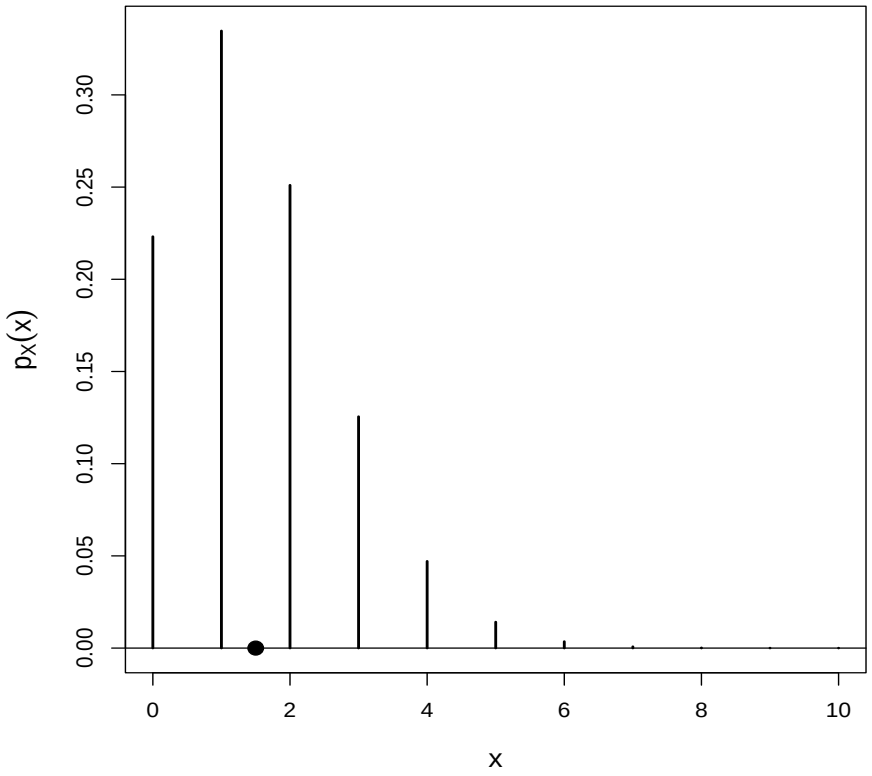


Figure 3.11: Probability mass function of $X \sim$ Poisson(1.5) in Example 3.9. The expected value $E(X) = 1.5$ is shown by a solid circle.

Example 3.9. In a certain region in the northeast US, the number of severe weather events per year X is assumed to have a Poisson distribution with mean $\lambda = 1.5$. The pmf of X is shown in Figure 3.11 (above).

Q: What is the probability there are exactly 2 severe weather events in a given year?

$$P(X = 2) = \frac{(1.5)^2 e^{-1.5}}{2!} \approx 0.251.$$

Q: What is the probability there are more than 3 severe weather events in a given year?
A: We want $P(X \geq 4)$.

$$\begin{aligned} P(X \geq 4) &= 1 - P(X \leq 3) \\ &= 1 - P(X = 0) - P(X = 1) - P(X = 2) - P(X = 3) \\ &= 1 - \frac{(1.5)^0 e^{-1.5}}{0!} - \frac{(1.5)^1 e^{-1.5}}{1!} - \frac{(1.5)^2 e^{-1.5}}{2!} - \frac{(1.5)^3 e^{-1.5}}{3!} \approx 0.066. \end{aligned}$$

POISSON R CODE: Suppose $X \sim$ Poisson(λ).

$p_X(x) = P(X = x)$	$F_X(x) = P(X \leq x)$
`dpois(x,`λ`)`	`ppois(x,`λ`)`

```
> options(digits=3)
> dpois(2,1.5) # P(X=2)
[1] 0.251
> 1-ppois(3,1.5) # 1-P(X<=3)
[1] 0.0656
```

Example 3.9 (continued). A local company in this region buys an insurance policy in the event severe weather shuts down business. The policy pays nothing for the first severe weather event of the year but pays \$25,000 for each one thereafter, until the end of the year.

Q: Calculate the expected amount paid to the company under this policy during a one-year period.
A: First note that if $X = 0$ or $X = 1$, then the company receives nothing according to the policy. It is only when there are 2 or more severe weather events does a payout occur, and this payout is \$25,000 for each severe weather event. Therefore, the payout when viewed as a function of X is

$$g(X) = \begin{cases} 0, & X = 0, 1 \\ 25000(X-1), & X = 2, 3, 4, ... \end{cases}$$

and we want to calculate $E[g(X)]$. From the definition of expectation, we have

$$\begin{aligned} E[g(X)] &= \sum_{x=0}^{\infty} g(x) \frac{(1.5)^x e^{-1.5}}{x!} \\ &= 0 \times \frac{(1.5)^0 e^{-1.5}}{0!} + 0 \times \frac{(1.5)^1 e^{-1.5}}{1!} + \sum_{x=2}^{\infty} 25000(x-1) \frac{(1.5)^x e^{-1.5}}{x!} \\ &= 25000 \sum_{x=2}^{\infty} (x-1) \frac{(1.5)^x e^{-1.5}}{x!} \\ &= 25000 \left[\sum_{x=0}^{\infty} (x-1) \frac{(1.5)^x e^{-1.5}}{x!} - (1-1) \times \frac{(1.5)^1 e^{-1.5}}{1!} - (0-1) \times \frac{(1.5)^0 e^{-1.5}}{0!} \right]. \end{aligned}$$

Note that

$$\sum_{x=0}^{\infty} (x-1) \frac{(1.5)^x e^{-1.5}}{x!} = E(X-1) = E(X) - 1 = 1.5 - 1 = 0.5.$$

Therefore,

$$E[g(X)] = 25000(0.5 - 0 + e^{-1.5}) \approx 18078.25.$$

The expected payout to the company during a one-year period is \$18078.25.

4 Continuous Distributions

4.1 Probability density functions

Recall: A random variable X is **continuous** if, at least in theory, it can have any value in an interval of numbers. For example,

- X = pH of an aqueous solution $\longrightarrow \mathbb{R} = \{-\infty < x < \infty\}$
- X = length of time (days) between accidents at a factory $\longrightarrow \mathbb{R}^+ = \{x > 0\}$
- X = proportion of parts which require rework $\longrightarrow [0, 1] = \{0 \leq x \leq 1\}$
- X = current (mA) measured in a thin copper wire $\longrightarrow [4.9, 5.1] = \{4.9 \leq x \leq 5.1\}$
- X = diameter (mm) of a hole drilled in sheet metal $\longrightarrow (12.5, \infty) = \{x > 12.5\}$.

Important: Assigning probabilities to events with continuous random variables is different than in the discrete case. We do not assign probability to specific values like $x = 2$ as we might in discrete models. Instead, we assign probabilities to events which are **intervals** like $1 < x < 3$, acknowledging that X can have any value between 1 and 3.

Terminology: The **probability density function** (pdf) of a continuous random variable X is a function $f_X(x)$ which has the following characteristics:

1. $f_X(x) \geq 0 \longrightarrow f_X(x)$ is nonnegative.
2. the area under any pdf is equal to 1, that is,

$$\int_{-\infty}^{\infty} f_X(x)dx = 1.$$

Result: If X is a continuous random variable with pdf $f_X(x)$, then

$$P(a < X < b) = \int_a^b f_X(x)dx.$$

Probabilities with continuous random variables are found by integrating the pdf.

Example 4.1. The amount of loss/damage (in millions of dollars) due to catastrophic weather is a continuous random variable X with pdf

$$f_X(x) = \begin{cases} \dfrac{3000}{(10+x)^4}, & x \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

This pdf is shown in Figure 4.1 (next page).

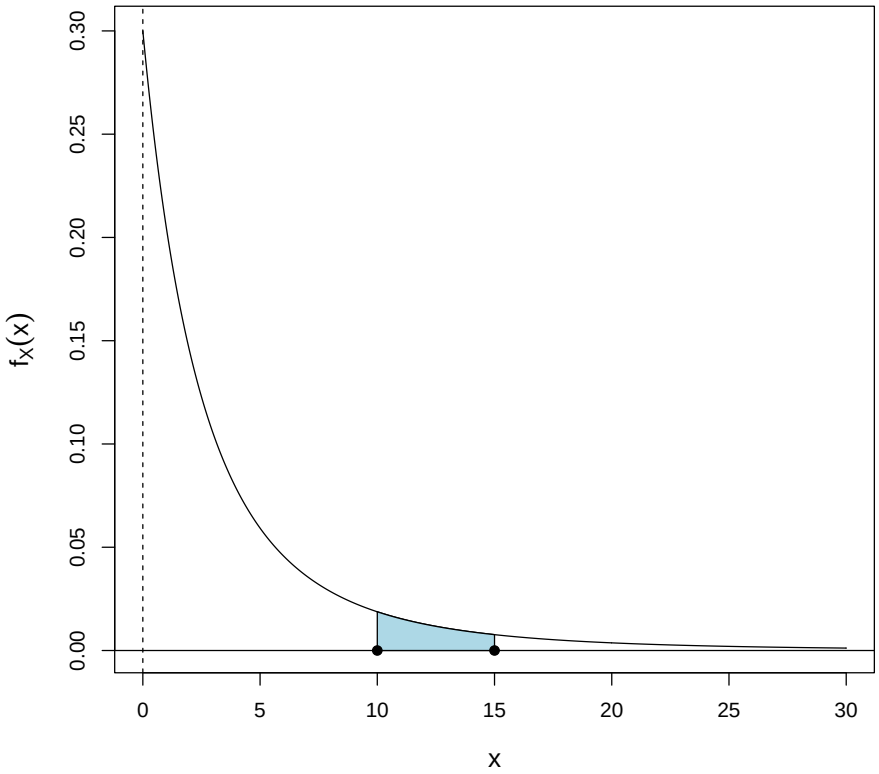


Figure 4.1: Probability density function of X in Example 4.1. The shaded area under the curve is $P(10 < X < 15)$.

Q: What is the probability the amount of loss/damage is between 10 and 15 million dollars?
A: We want

$$P(10 < X < 15) = \int_{10}^{15} f_X(x)dx = \int_{10}^{15} \frac{3000}{(10+x)^4}dx.$$

To do this integral, let

$$u = 10 + x \implies du = dx.$$

With this u-substitution (noting the change in limits), the last integral equals

$$\int_{20}^{25} \frac{3000}{u^4}du = 3000\int_{20}^{25} \frac{1}{u^4}du = 3000\left(-\frac{1}{3}\frac{1}{u^3}\right)\Bigg|_{20}^{25} = 1000\left(\frac{1}{20^3} - \frac{1}{25^3}\right) = 0.061.$$

Therefore,

$$P(10 < X < 15) = 0.061.$$

That is, 6.1% of all loss/damage amounts from catastrophic weather will be between 10 and 15 million dollars.

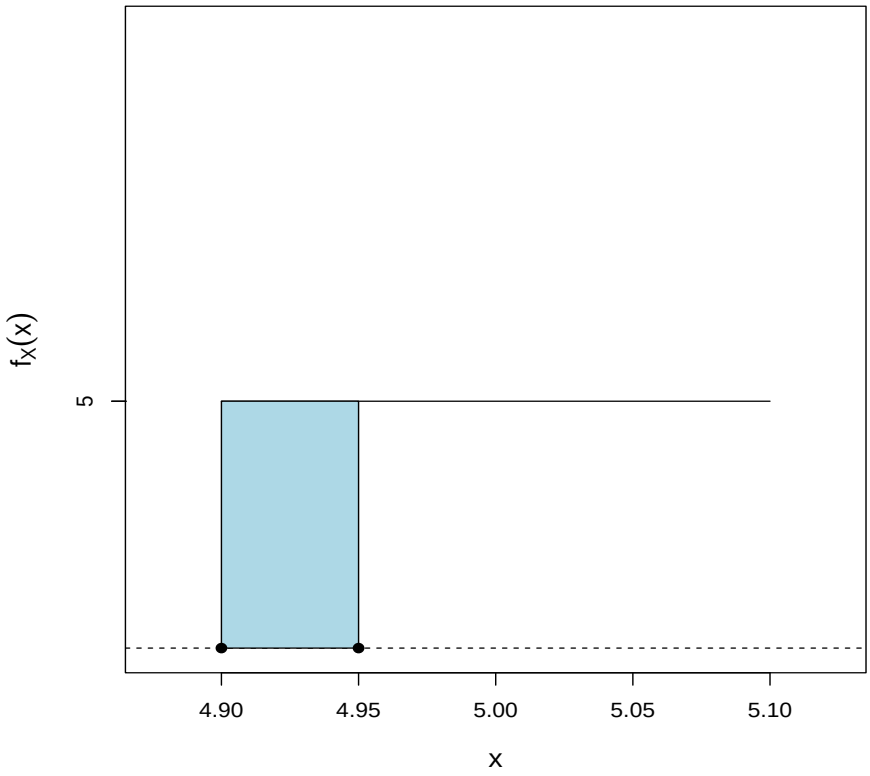


Figure 4.2: Probability density function of X in Example 4.2. The shaded area under the curve is $P(X < 4.95)$.

Integration in R: One-dimensional integrals can be found numerically using the `integrate` function in R. In Example 4.1,

```
> pdf <- function(x){3000/(10+x)^4}
> integrate(pdf,lower=10,upper=15) # P(10<X<15)
0.061 with absolute error < 6.8e-16
```

The absolute error arises from the adaptive quadrature method used to perform numerical integration (it is generally very small for "well behaved" functions we are integrating).

Example 4.2. Let the continuous random variable X denote the current measured in a thin copper wire (in milliamperes, mA). Assume the range (support) of X is $[4.9, 5.1]$ mA and the pdf of X is

$$f_X(x) = \begin{cases} 5, & 4.9 \leq x \leq 5.1 \\ 0, & \text{otherwise.} \end{cases}$$

This pdf is shown in Figure 4.2 (above).

Q: What is the probability the current measurement is less than 4.95 mA?
A: We want

$$P(X < 4.95) = \int_{4.9}^{4.95} f_X(x)dx = \int_{4.9}^{4.95} 5\ dx = 5\left(x\Big|_{4.9}^{4.95}\right) = 5(4.95 - 4.9) = 0.25.$$

That is, 25% of all current measurements will be less than 4.95 mA.

Remark: In Example 4.2, the pdf is constant across the range (support) of X. We call this a **uniform distribution**. Probability is assigned equally to intervals of the same size across the support of X.

Example 4.3. UPS ships millions of packages every month in a specific 1-ft^3 packing container. Define

$$X = \text{amount of space occupied in this container (in ft}^3\text{)}.$$

The pdf of X is given by

$$f_X(x) = \begin{cases} 90x^8(1-x), & 0 < x < 1 \\ 0, & \text{otherwise.} \end{cases}$$

This pdf is shown in Figure 4.3 (next page).

Q: What is the probability a package will be filled at 0.9 ft^3 or more?
A: We want

$$\begin{aligned} P(X \geq 0.9) = \int_{0.9}^{1} f_X(x)dx &= \int_{0.9}^{1} 90x^8(1-x)dx \\ &= 90\int_{0.9}^{1}(x^8 - x^9)dx \\ &= 90\left(\frac{x^9}{9} - \frac{x^{10}}{10}\right)\Big|_{0.9}^{1} = 90\left(\frac{1}{9} - \frac{1}{10} - \frac{0.9^9}{9} + \frac{0.9^{10}}{10}\right) \approx 0.264. \end{aligned}$$

That is, approximately 26.4% of all containers will be filled at 0.9 ft^3 or more.

R: Here is how to calculate this probability in R:

```
> options(digits=3)
> pdf <- function(x){90*x^8*(1-x)}
> integrate(pdf,lower=0.9,upper=1) # P(X>=0.9)
0.264 with absolute error < 2.9e-15
```

Discussion: Discrete distributions (last chapter) assign positive probability to specific points. Calculating probabilities with continuous distributions is done by integration. We integrate a continuous random variable's pdf $f_X(x)$ over the range defined by the event of interest. In continuous distributions, all single points are assigned zero probability.

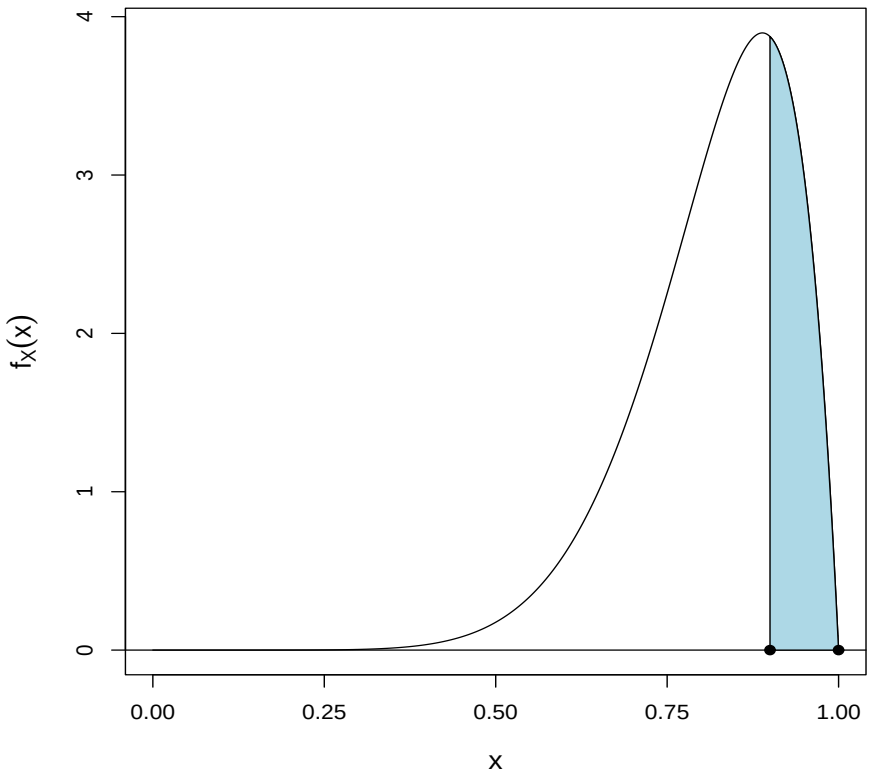


Figure 4.3: Probability density function of X in Example 4.3. The shaded area under the curve is $P(X \geq 0.9)$.

Why? This makes sense if you think about it using calculus. Suppose a is a number in the support of X. The probability

$$P(X = a) = \int_a^a f_X(x)dx = 0.$$

The area under $f_X(x)$ above a single point is always zero. This highlights the salient difference between discrete and continuous random variables. In discrete models, specific points have positive probability. In continuous models, they don't. It follows that

$$P(a < X < b) = P(a \leq X < b) = P(a < X \leq b) = P(a \leq X \leq b)$$

and each one equals

$$\int_a^b f_X(x)dx.$$

The endpoints simply don't matter when X is continuous. Of course, this is not true in discrete distributions.

Terminology: The **cumulative distribution function** (cdf) of a continuous random variable X gives probabilities of the form

$$F_X(x) = P(X \leq x) = \int_{-\infty}^{x} f_X(t)dt$$

for any real number x.

- When X is a continuous random variable, the cdf $F_X(x)$ is a continuous function.
- Applying the Fundamental Theorem of Calculus (part 1), it follows that

$$\frac{d}{dx}F_X(x) = \frac{d}{dx}\int_{-\infty}^{x} f_X(t)dt = f_X(x).$$

That is, differentiating a continuous random variable's cdf produces the pdf.

Example 4.1 (continued). The amount of loss/damage (in millions of dollars) due to catastrophic weather is a continuous random variable X with pdf

$$f_X(x) = \begin{cases} \dfrac{3000}{(10+x)^4}, & x \geq 0 \\ 0, & \text{otherwise.} \end{cases}$$

The cdf of X is

$$F_X(x) = \begin{cases} 0, & x < 0 \\ 1 - \left(\dfrac{10}{10+x}\right)^3, & x \geq 0. \end{cases}$$

The pdf and cdf are shown side by side in Figure 4.4 (next page). We previously calculated

$$P(10 < X < 15) = \int_{10}^{15} f_X(x)dx = \int_{10}^{15} \frac{3000}{(10+x)^4}dx = 0.061$$

by integrating the pdf over $(10, 15)$. We can also get this from the cdf:

$$\begin{aligned} P(10 < X < 15) &= P(X < 15) - P(X < 10) \\ &= F_X(15) - F_X(10) = \left[1 - \left(\frac{10}{10+15}\right)^3\right] - \left[1 - \left(\frac{10}{10+10}\right)^3\right] = 0.061. \end{aligned}$$

This example illustrates the following general result for **continuous** random variables:

$$P(a < X < b) = \int_a^b f_X(x)dx = F_X(b) - F_X(a),$$

which, in essence, applies the Fundamental Theorem of Calculus (part 2).

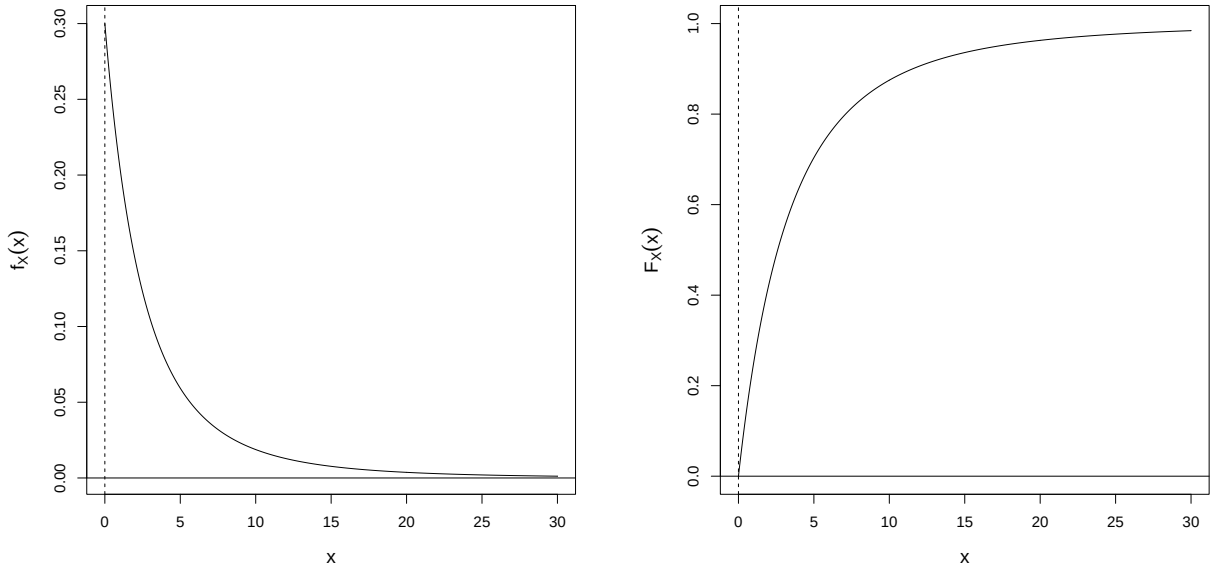


Figure 4.4: Left: Probability density function (pdf) of X in Example 4.1. Right: Cumulative distribution function (cdf) of X.

Examples 4.2 and 4.3 (continued). The pdfs and cdfs are

$$\textbf{4.2.} \quad f_X(x) = \begin{cases} 5, & 4.9 \leq x \leq 5.1 \\ 0, & \text{otherwise} \end{cases} \implies F_X(x) = \begin{cases} 0, & x < 4.9 \\ 5x - 24.5, & 4.9 \leq x \leq 5.1 \\ 1, & x > 5.1 \end{cases}$$

$$\textbf{4.3.} \quad f_X(x) = \begin{cases} 90x^8(1-x), & 0 < x < 1 \\ 0, & \text{otherwise} \end{cases} \implies F_X(x) = \begin{cases} 0, & x \leq 0 \\ 10x^9 - 9x^{10}, & 0 < x < 1 \\ 1, & x \geq 1 \end{cases}.$$

These functions are shown in Figures 4.5 and 4.6 (next page).

- In Example 4.2, using the cdf gives

$$P(X < 4.95) = F_X(4.95) = 5(4.95) - 24.5 = 0.25.$$

- In Example 4.3, using the cdf gives

$$P(X \geq 0.9) = 1 - P(X \leq 0.9) = 1 - F_X(0.9) = 1 - \left[10(0.9)^9 - 9(0.9)^{10}\right] \approx 0.264.$$

Note: These are the same answers we got by using the pdfs (and integrating). The lesson here is that knowing a random variable's cdf can greatly simplify our work. For upcoming "named" continuous distributions, like the exponential, gamma, normal, and others, the corresponding cdfs are available in R.

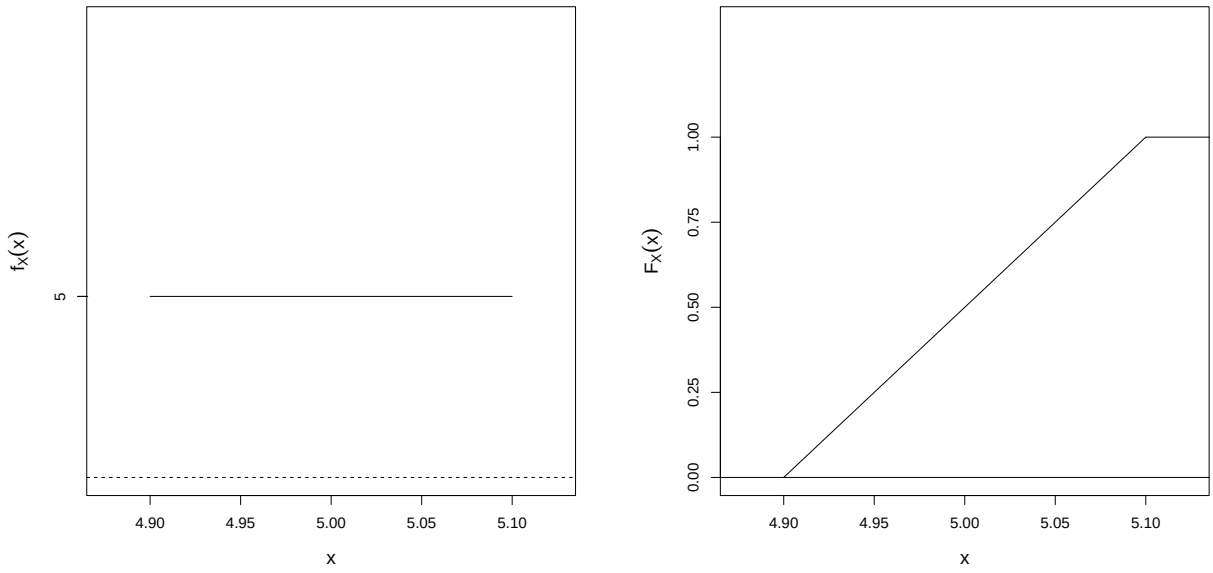


Figure 4.5: Left: Probability density function (pdf) of X in Example 4.2. Right: Cumulative distribution function (cdf) of X.

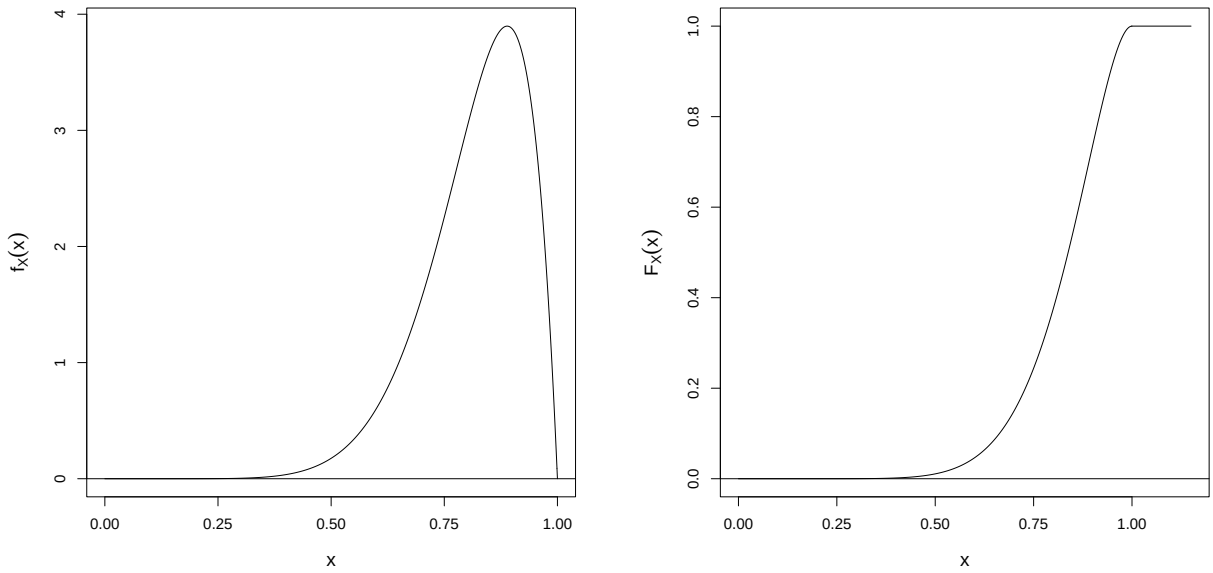


Figure 4.6: Left: Probability density function (pdf) of X in Example 4.3. Right: Cumulative distribution function (cdf) of X.

4.2 Mean, variance, and percentiles

Terminology: Suppose X is a continuous random variable with pdf $f_X(x)$. The **expected value** of X is

$$\mu = E(X) = \int_{-\infty}^{\infty} x f_X(x) dx.$$

We interpret $E(X)$ the same way as we did in the discrete case:

- a center of gravity or "balance point" on the pdf
- a "long-run average."

In statistical applications, $\mu = E(X)$ is called the **mean** or **population mean**.

Remark: The limits of the integral in the definition $E(X)$ above, while technically correct, will always be the lower and upper limits corresponding to the nonzero part of the pdf.

Example 4.4. Let the continuous random variable X denote the diameter of a hole drilled in a sheet metal component. The target diameter is 12.5 millimeters. However, random disturbances to the drilling process result in larger diameters. Historical data show the distribution of X can be modeled by the pdf

$$f_X(x) = \begin{cases} 20e^{-20(x-12.5)}, & x > 12.5 \\ 0, & \text{otherwise.} \end{cases}$$

This pdf is shown in Figure 4.7 (next page).

Q: Find the mean diameter $E(X)$.
A: We calculate

$$E(X) = \int_{12.5}^{\infty} x f_X(x) dx = \int_{12.5}^{\infty} 20x e^{-20(x-12.5)} dx = 20e^{20(12.5)} \int_{12.5}^{\infty} x e^{-20x} dx.$$

To do the last integral, use integration by parts with

$$\begin{aligned} u &= x & du &= dx \\ dv &= e^{-20x} dx & v &= -\frac{1}{20} e^{-20x} \end{aligned}$$

so that

$$\begin{aligned} \int_{12.5}^{\infty} x e^{-20x} dx &= \left(-\frac{x}{20} e^{-20x} \Big|_{12.5}^{\infty} \right) - \int_{12.5}^{\infty} -\frac{1}{20} e^{-20x} dx \\ &= \frac{12.5}{20} e^{-20(12.5)} - 0 + \frac{1}{20} \left(-\frac{1}{20} e^{-20x} \Big|_{12.5}^{\infty} \right) = \frac{12.5}{20} e^{-20(12.5)} + \frac{1}{400} e^{-20(12.5)}. \end{aligned}$$

Therefore,

$$E(X) = 20e^{20(12.5)} \left[\frac{12.5}{20} e^{-20(12.5)} + \frac{1}{400} e^{-20(12.5)} \right] = 12.5 + \frac{1}{20} = 12.55 \text{ mm}.$$

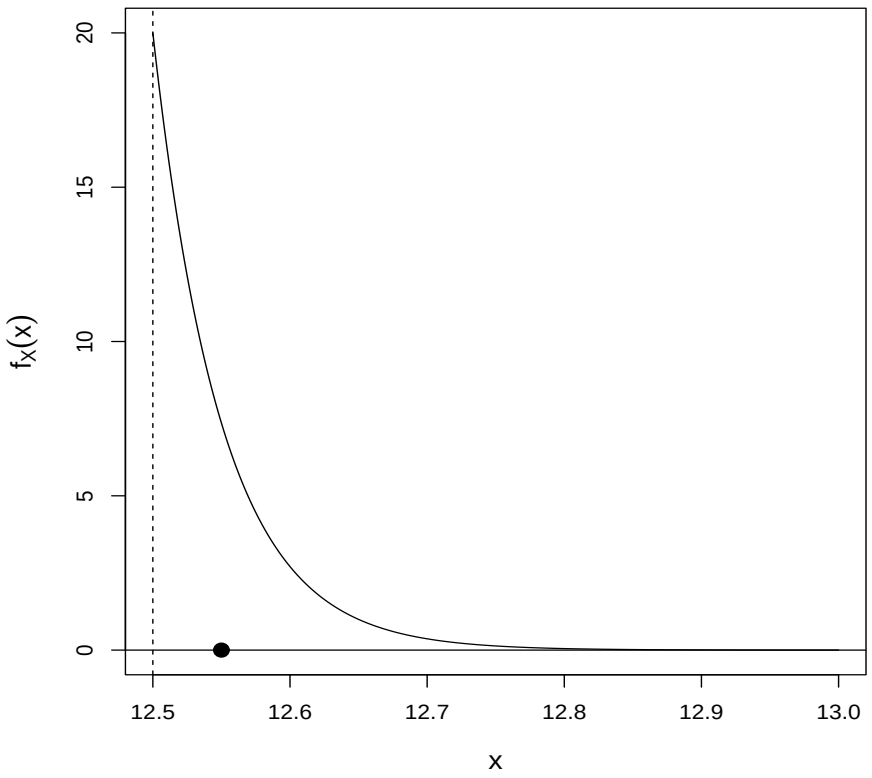


Figure 4.7: Probability density function of X in Example 4.4. The expected value $E(X) = 12.55$ is shown by a solid circle.

R: Here is how to calculate $E(X)$ in R:

```
> x.times.pdf = function(x){x*20*exp(-20*(x-12.5))}
> integrate(x.times.pdf,lower=12.5,upper=Inf) # E(X)
12.55 with absolute error < 1.3e-07
```

Result: Suppose X is a continuous random variable with pdf $f_X(x)$ and g is any function. Then $g(X)$ is also a random variable and its expectation (mean) is

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

Linearity rules: These rules are the same as they were in the discrete case:

(a) $E(c) = c$, for any constant c

(b) $E[cg(X)] = cE[g(X)]$, for any constant c

(c) The expectation of the sum is the sum of the expectations; i.e.,

$$E[g_1(X) + g_2(X) + \cdots + g_k(X)] = E[g_1(X)] + E[g_2(X)] + \cdots + E[g_k(X)].$$

Terminology: Suppose X is a continuous random variable with pdf $f_X(x)$ and mean $\mu = E(X)$. The **variance** of X is

$$\begin{aligned}\sigma^2 = V(X) &= E[(X-\mu)^2] \\ &= \int_{-\infty}^{\infty}(x-\mu)^2 f_X(x)dx.\end{aligned}$$

The **standard deviation** of X is the positive square root of the variance:

$$\sigma = \sqrt{\sigma^2} = \sqrt{V(X)}.$$

Variance computing formula: Suppose X is a random variable (discrete or continuous) with mean $\mu = E(X)$. An alternative way to find $V(X)$ is by using

$$V(X) = E(X^2) - [E(X)]^2.$$

Linear functions: Suppose X is a continuous random variable with pdf $f_X(x)$ and mean $\mu = E(X)$. Suppose a and b are constants. The mean and variance of the linear function $aX + b$ are

$$\begin{aligned}E(aX+b) &= aE(X)+b \\ V(aX+b) &= a^2V(X).\end{aligned}$$

These rules are the same as they were in the discrete case.

Example 4.5. Conductive coatings are applied to a wide variety of materials to make them electrically conductive or to shield them from electromagnetic interference. The thickness of a coating applied to a medical device (measured in micrometers) is a continuous random variable X with pdf

$$f_X(x) = \begin{cases} \dfrac{1200}{x^2}, & 400 < x < 600 \\ 0, & \text{otherwise.} \end{cases}$$

This pdf is shown in Figure 4.8 (next page).

Q: Find $E(X)$ and $V(X)$.
A: The mean is

$$\begin{aligned}E(X) = \int_{400}^{600} x f_X(x)dx &= \int_{400}^{600}\frac{1200x}{x^2}dx \\ &= 1200\int_{400}^{600}\frac{1}{x}\,dx \\ &= 1200\left(\ln x\Big|_{400}^{600}\right) = 1200(\ln 600 - \ln 400) \approx 486.6\ \mu\text{m}.\end{aligned}$$

To find the variance, let's use the variance computing formula. First, we find

$$E(X^2) = \int_{400}^{600} x^2 f_X(x)dx = \int_{400}^{600}\frac{1200x^2}{x^2}dx = 1200\int_{400}^{600}1dx = 1200(600-400) = 240000.$$

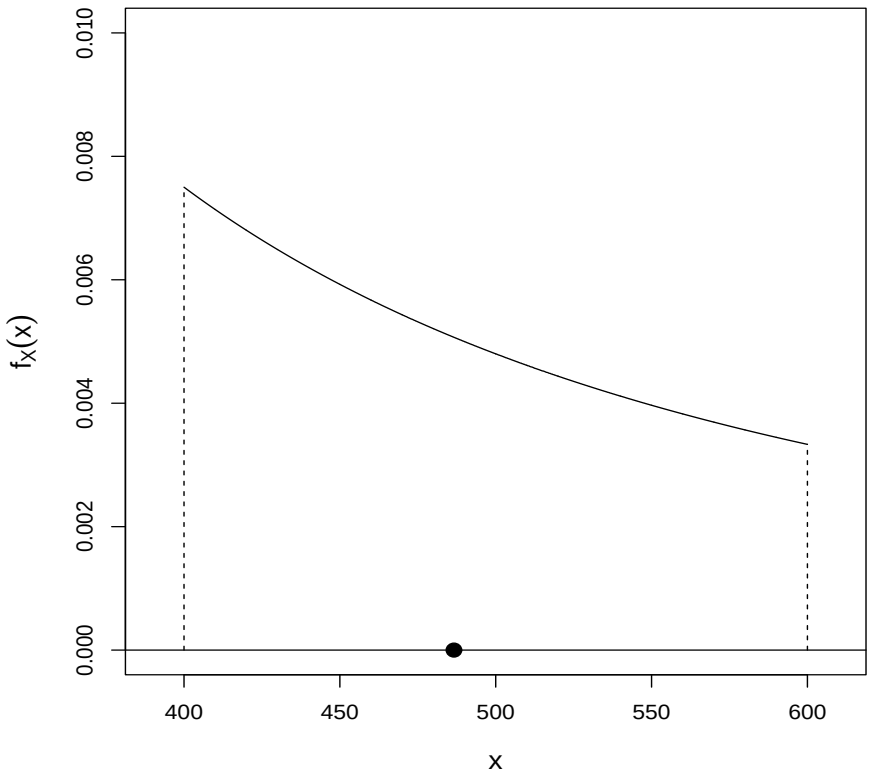


Figure 4.8: Probability density function of X in Example 4.5. The expected value $E(X) \approx 486.6$ is shown by a solid circle.

Therefore,

$$V(X) = E(X^2) - [E(X)]^2 \approx 240000 - (486.6)^2 \approx 3220.4 \ (\mu\text{m})^2.$$

Q: The coating costs $C = 40 + 0.15X$ dollars to apply to each device. That is, there is a fixed cost of 40 dollars plus an additional cost of 0.15 dollars for each micrometer of coating applied. Find $E(C)$ and $V(C)$.
A: The cost C is a linear function of X. We have

$$E(C) = E(40 + 0.15X) = 40 + 0.15E(X) \approx 40 + 0.15(486.6) \approx 112.99 \text{ dollars.}$$

The variance is

$$V(C) = V(40 + 0.15X) = (0.15)^2 V(X) \approx (0.15)^2(3220.4) \approx 72.46 \ (\text{dollars})^2.$$

The standard deviation of C is

$$\sigma_C = \sqrt{V(C)} \approx \sqrt{72.46} \approx 8.51 \text{ dollars.}$$

Terminology: Suppose X is a **continuous** random variable with cdf $F_X(x)$ and pdf $f_X(x)$. The p**th quantile** $(0 < p < 1)$ of X, denoted by ϕ_p, satisfies

$$P(X \leq \phi_p) = \int_{-\infty}^{\phi_p} f_X(x)dx = F_X(\phi_p) = p.$$

In other words, ϕ_p is the value for which $100p\%$ of the possible values of X are below ϕ_p. Some authors call ϕ_p the $100p$**th percentile** of the distribution of X. For example,

- $\phi_{0.10} = 10$th percentile. This means 10 percent of the values of X are below $\phi_{0.10}$, and 90 percent of the values are above $\phi_{0.10}$.
- $\phi_{0.50} = 50$th percentile. This means 50 percent of the values of X are below $\phi_{0.50}$, and 50 percent of the values are above $\phi_{0.50}$. This is also called the **median** of X.
- $\phi_{0.99} = 99$th percentile. This means 99 percent of the values of X are below $\phi_{0.99}$, and 1 percent of the values are above $\phi_{0.99}$.

Example 4.4 (continued). The diameter X (in millimeters) of a hole drilled in a sheet metal component has pdf

$$f_X(x) = \begin{cases} 20e^{-20(x-12.5)}, & x > 12.5 \\ 0, & \text{otherwise.} \end{cases}$$

The cdf of X is

$$F_X(x) = \begin{cases} 0, & x < 0 \\ 1 - e^{-20(x-12.5)}, & x > 12.5. \end{cases}$$

The pdf and cdf are shown side by side in Figure 4.9.

Q: Five percent of the diameters will be larger than what value?
A: We want $\phi_{0.95}$, the 95th percentile of the distribution of X. We solve

$$P(X \leq \phi_{0.95}) = \int_{12.5}^{\phi_{0.95}} 20e^{-20(x-12.5)}dx = 1 - e^{-20(\phi_{0.95}-12.5)} = 0.95$$

for $\phi_{0.95}$. This is done as follows:

$$\begin{aligned} 1 - e^{-20(\phi_{0.95}-12.5)} = 0.95 &\implies e^{-20(\phi_{0.95}-12.5)} = 0.05 \\ &\implies -20(\phi_{0.95} - 12.5) = \ln(0.05) \\ &\implies \phi_{0.95} - 12.5 = -\frac{\ln(0.05)}{20} \\ &\implies \phi_{0.95} = 12.5 - \frac{\ln(0.05)}{20} \approx 12.65. \end{aligned}$$

Therefore, approximately 5 percent of the hole diameters will be larger than 12.65 mm.

Exercise: Find $\phi_{0.50}$, the median coating thickness in Example 4.5. How does $\phi_{0.50}$ compare to $E(X)$?

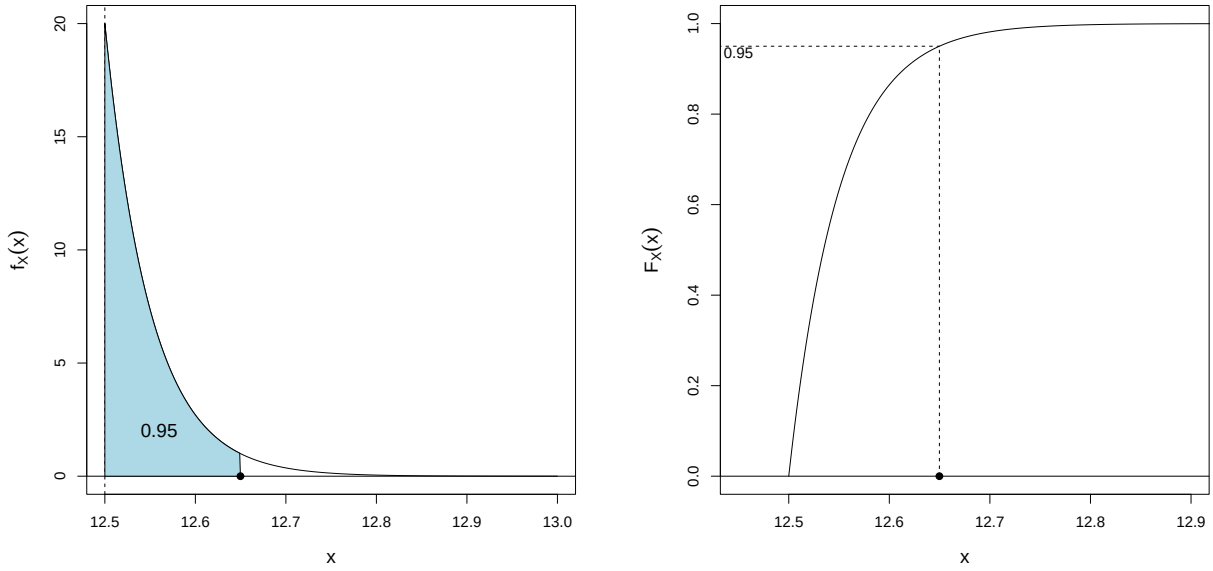


Figure 4.9: Left: Probability density function (pdf) of X in Example 4.4. Right: Cumulative distribution function (cdf) of X. The 95th percentile $\phi_{0.95} \approx 12.65$ is shown in each figure.

4.3 Exponential distribution

Definition: A continuous random variable X has an **exponential distribution** with parameter $\lambda > 0$ if its pdf is given by

$$f_X(x) = \begin{cases} \lambda e^{-\lambda x}, & x > 0 \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim$ exponential(λ). Different values of λ give different pdfs. All pdfs have the same exponential decay shape; the value of λ controls the scale; see Figure 4.10 (next page).

Remarks:

- The first thing we note is the exponential distribution is for positive quantities ($x > 0$). This include things like part dimensions, weights, biomarkers, and times.
- The exponential distribution is used in **reliability analysis** and other areas which focus on "time-to-event" random variables, for example,
  - the time until part failure
  - the time until disease onset
  - the time until an insurance claim is filed
  - the time until a catastrophic weather event.

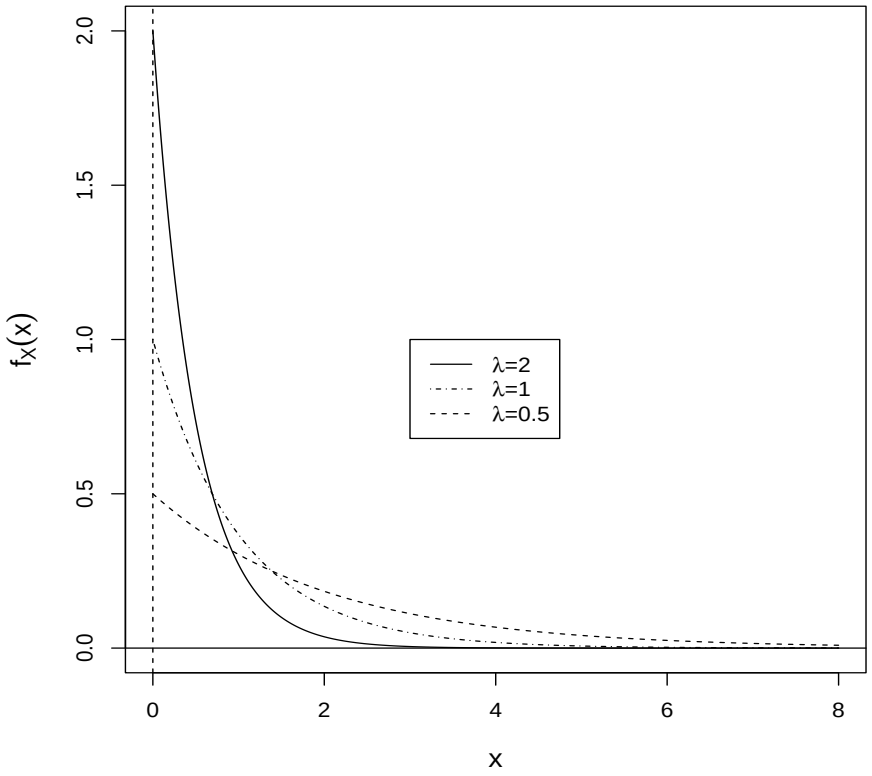


Figure 4.10: Exponential pdfs for different values of λ.

MEAN/VARIANCE: If $X \sim$ exponential(λ), then

$$\begin{aligned} E(X) &= \frac{1}{\lambda} \\ V(X) &= \frac{1}{\lambda^2}. \end{aligned}$$

CDF: If $X \sim$ exponential(λ), then the cdf of X is

$$F_X(x) = \begin{cases} 0, & x \leq 0 \\ 1 - e^{-\lambda x}, & x > 0. \end{cases}$$

Example 4.6. The monthly precipitation in Columbia, SC, is a continuous random variable X which is assumed to follow an exponential distribution with mean 4 inches.

Q: What is the probability a given month will have more than 10 inches of precipitation?
A: First note that

$$E(X) = 4 \implies \lambda = 0.25.$$

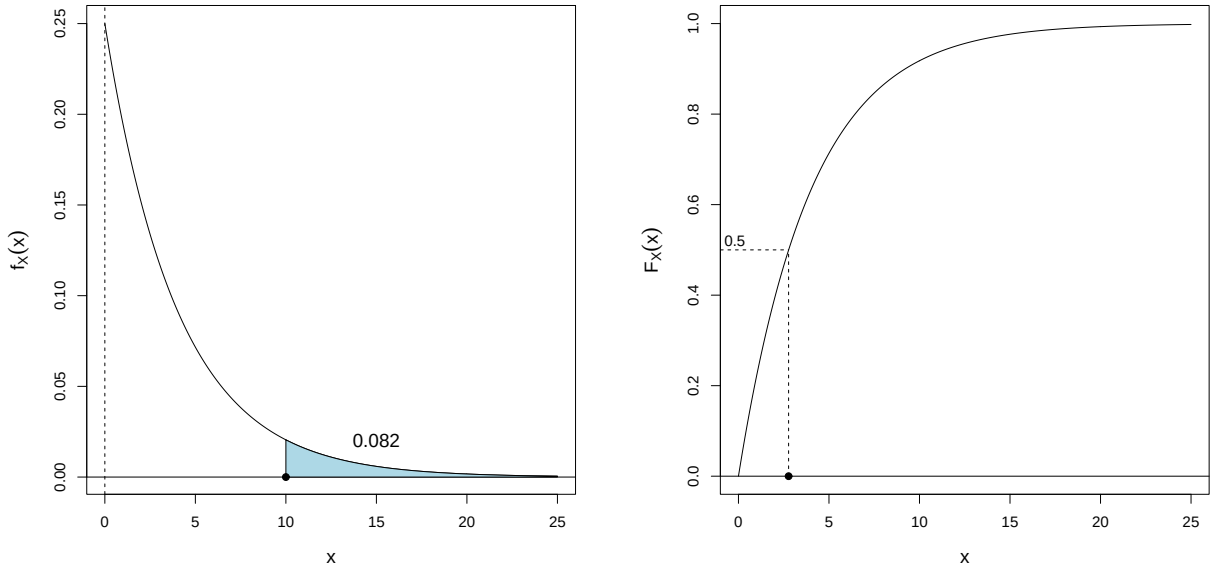


Figure 4.11: Left: Probability density function (pdf) of X in Example 4.6. The probability $P(X > 10) \approx 0.082$ is shown shaded. Right: Cumulative distribution function (cdf) of X. The median $\phi_{0.50} \approx 2.77$ is shown by a solid circle.

The pdf and cdf of X are

$$f_X(x) = \begin{cases} 0.25e^{-0.25x}, & x > 0 \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad F_X(x) = \begin{cases} 0, & x \leq 0 \\ 1 - e^{-0.25x}, & x > 0 \end{cases},$$

shown in Figure 4.11 (above). We want

$$\begin{aligned} P(X > 10) &= 1 - P(X \leq 10) \\ &= 1 - F_X(10) \\ &= 1 - [1 - e^{-0.25(10)}] = e^{-2.5} \approx 0.082. \end{aligned}$$

Therefore, approximately 8.2% of the months will have precipitation amounts larger than 10 inches.

Q: What is the median monthly precipitation?
A: We want to solve

$$\begin{aligned} F_X(\phi_{0.50}) = 0.5 &\implies 1 - e^{-0.25\phi_{0.50}} = 0.5 \\ &\implies e^{-0.25\phi_{0.50}} = 0.5 \\ &\implies -0.25\phi_{0.50} = \ln(0.5) \implies \phi_{0.50} = -\frac{\ln(0.5)}{0.25} \approx 2.77 \text{ inches.} \end{aligned}$$

This means 50 percent of the months will have precipitation amounts less than 2.77 inches (and 50 percent of the months will be greater).

EXPONENTIAL R CODE: Suppose $X \sim$ exponential(λ).

$F_X(x) = P(X \leq x)$	ϕ_p
`pexp(x,`λ`)`	`qexp(p,`λ`)`

```
> options(digits=3)
> 1-pexp(10,0.25) # 1-P(X<=10)
[1] 0.0821
> qexp(0.5,0.25) # median
[1] 2.77
```

POISSON-EXPONENTIAL RELATIONSHIP: Recall a Poisson distribution arises when we are counting the number of "occurrences" over a unit interval of time (see Section 3.6, notes). Define

$$X = \text{ the } \textbf{time} \text{ until the first occurrence.}$$

This is a continuous random variable and it follows an exponential distribution with parameter λ, where λ is the mean number of occurrences per unit interval of time in the Poisson counting process. That is, $X \sim$ exponential(λ).

Example 4.7. In a corporate computer network, user log-ons to the system are modeled as a Poisson process with a mean of $\lambda = 25$ log-ons per hour.

Q: What is the probability it takes longer than 10 minutes for the first user log-on to occur? Note that 10 minutes = 1/6 of one hour.
A: The time until the first user log-on X follows an exponential distribution with $\lambda = 25$. The pdf and cdf of X are

$$f_X(x) = \begin{cases} 25e^{-25x}, & x > 0 \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad F_X(x) = \begin{cases} 0, & x \leq 0 \\ 1 - e^{-25x}, & x > 0 \end{cases}.$$

We want

$$\begin{aligned} P(X > 1/6) &= 1 - P(X \leq 1/6) \\ &= 1 - F_X(1/6) \\ &= 1 - [1 - e^{-25(1/6)}] = e^{-25/6} \approx 0.016. \end{aligned}$$

```
> 1-pexp(1/6,25) # 1-P(X<=1/6)
[1] 0.016
```

Remark: Another interesting fact is the time between any two successive occurrences in a Poisson process follows the same exponential(λ) distribution. Times between successive occurrences are called **interarrival times**. In Example 4.7,

- the time until the first user log-on is exponential($\lambda = 25$),
- the time between the first user log-on and the second is exponential($\lambda = 25$),
- the time between the second user log-on and the third is exponential($\lambda = 25$),

and so on.

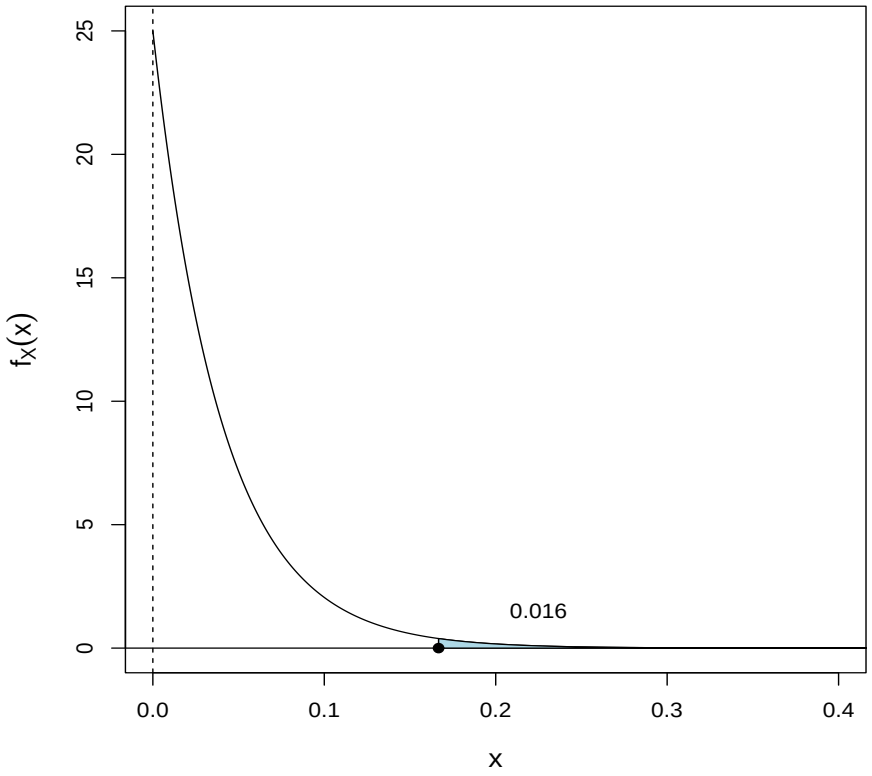


Figure 4.12: Probability density function of X in Example 4.7. The shaded area under the curve is $P(X > 1/6) \approx 0.016$.

MEMORYLESS PROPERTY: A unique property of the exponential distribution is its "lack of memory." Suppose a continuous random variable X measures the time until some event occurs (e.g., part failure, disease onset, claim is filed, catastrophic weather, etc.). If $X \sim$ exponential(λ), then

$$P(X > t_1 + t_2 | X > t_1) = P(X > t_2).$$

In the context of a part failing, here is how this can be intepreted:

- We have one part in the field whose failure time X is known to be larger than t_1, that is, the part has been in operation and has not failed before time t_1.
- We have a second part that has just been put in operation (at "time zero").
- The memoryless property says the probability the first part does not fail before an additional time of t_2 is the same as the second part not failing before time t_2. In other words, the fact the first part has been in operation for time t_1 has been "forgotten."

Remark: The memoryless property is mandated whenever one makes an exponential distribution assumption about the time to event. It is a restrictive condition and may not be realistic. For example, in the part failure context, an exponential distribution assumption for X requires that parts in the field do not "wear out" or "get stronger" over time.

Example 4.8. At a hospital's intensive care unit (ICU), the time until patient discharge (in days) is a continuous random variable X which is assumed to have an exponential distribution with $\lambda = 1/7$. The pdf and cdf of X are

$$f_X(x) = \begin{cases} \frac{1}{7}e^{-x/7}, & x > 0 \\ 0, & \text{otherwise} \end{cases} \quad \text{and} \quad F_X(x) = \begin{cases} 0, & x \leq 0 \\ 1 - e^{-x/7}, & x > 0 \end{cases}.$$

Q: One patient has been in the ICU for 5 days. What is the probability the patient is still in the ICU after 8 days?
A: From the memoryless property, we know

$$P(X > 8|X > 5) = P(X > 3).$$

This equals

$$1 - P(X \leq 3) = 1 - F_X(3) = e^{-3/7} \approx 0.65.$$

4.4 Gamma distribution

Definition: A continuous random variable X has a **gamma distribution** with parameters $r > 0$ and $\lambda > 0$ if its pdf is given by

$$f_X(x) = \begin{cases} \frac{\lambda^r}{\Gamma(r)}x^{r-1}e^{-\lambda x}, & x > 0 \\ 0, & \text{otherwise.} \end{cases}$$

We write $X \sim \text{gamma}(r, \lambda)$. We call

- $r =$ shape parameter
- $\lambda =$ scale parameter.

Different values of r and λ give different pdfs; see Figure 4.13 (next page). The gamma distribution is more flexible than the exponential distribution. Introducing the extra parameter r allows for different shapes, whereas the exponential distribution imposes the same exponential decay shape regardless of what λ is.

Q: What is $\Gamma(r)$?
A: It is a constant defined as the following integral

$$\Gamma(r) = \int_0^\infty u^{r-1}e^{-u}du,$$

provided that $r > 0$. In mathematical analysis, this is called the **gamma function**.

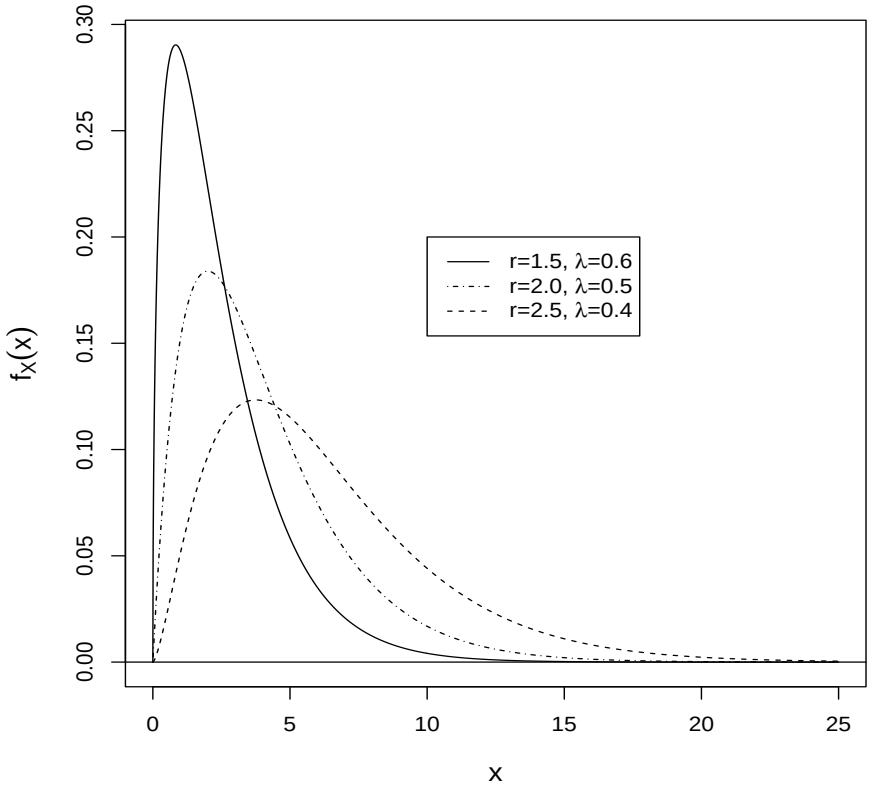


Figure 4.13: Gamma pdfs for different values of r and λ.

Important: When $r = 1$, the gamma(r, λ) distribution reduces to the exponential(λ) distribution. This is true because

$$\Gamma(1) = \int_0^\infty e^{-u} du = 1$$

and therefore the gamma(r, λ) pdf

$$\frac{\lambda^r}{\Gamma(r)} x^{r-1} e^{-\lambda x} = \lambda e^{-\lambda x}, \quad \text{provided that } r = 1.$$

GAMMA R CODE: Suppose $X \sim$ gamma(r, λ).

$F_X(x) = P(X \leq x)$	ϕ_p
`pgamma(x,r,λ)`	`qgamma(p,r,λ)`

Note: Probability and quantile calculations for the gamma distribution can be carried out using R. The cdf of $X \sim$ gamma(r, λ) does not exist in closed form for all values of $r > 0$, so numerical evaluation is required.

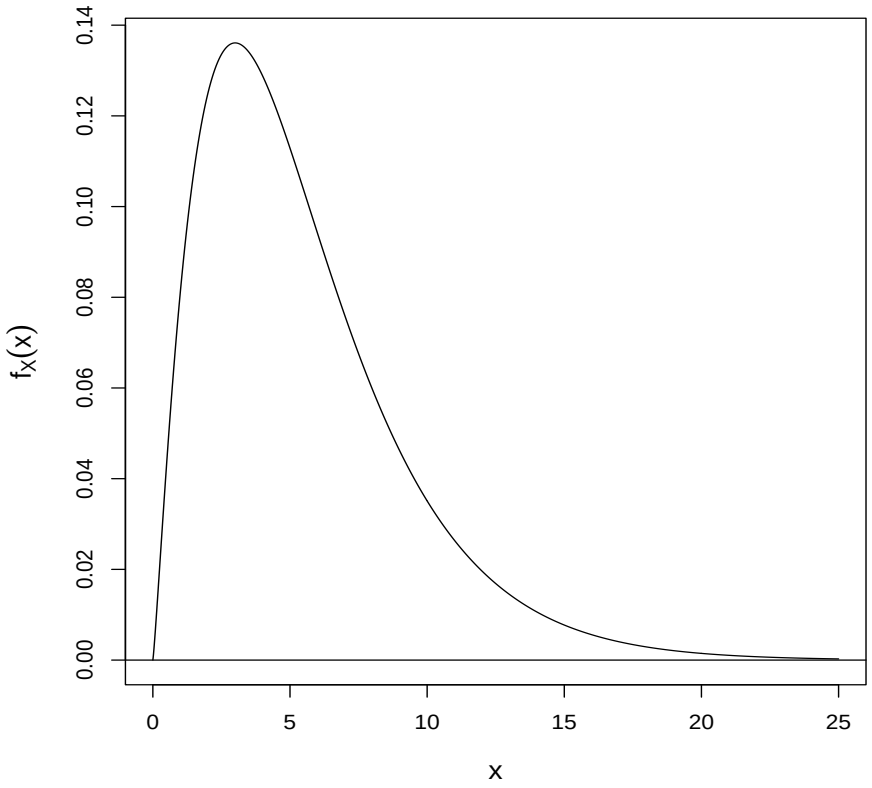


Figure 4.14: Probability density function of X in Example 4.9.

Example 4.9. The lifetime of a diesel engine fan blade X (in 1000s of hours) is modeled using a gamma distribution with $r = 2.2$ and $\lambda = 0.4$. This pdf is shown in Figure 4.14.

Q: What is the probability a fan blade fails before 5000 hours of operation?
A: We want

$$P(X < 5) = \int_0^5 \frac{(0.4)^{2.2}}{\Gamma(2.2)}\, x^{1.2} e^{-0.4x} dx \approx 0.536.$$

This probability is calculated numerically using the R code:

```
> options(digits=3)
> pgamma(5,2.2,0.4)
[1] 0.536
```

Q: Find the 90th percentile of this distribution and interpret what it means.

```
> options(digits=5)
> qgamma(0.9,2.2,0.4)
[1] 10.461
```

Ninety percent of all fan blades will fail before 10,461 hours of operation.

MEAN/VARIANCE: If $X \sim \text{gamma}(r, \lambda)$, then

$$\begin{aligned} E(X) &= \frac{r}{\lambda} \\ V(X) &= \frac{r}{\lambda^2}. \end{aligned}$$

Letting $r = 1$ in the formulas above gives $E(X)$ and $V(X)$ for $X \sim \text{exponential}(\lambda)$.

POISSON-GAMMA RELATIONSHIP: Recall a Poisson distribution arises when we are counting the number of "occurrences" over a unit interval of time (see Section 3.6, notes). Define

$$X = \text{ the } \textbf{time} \text{ until the } r\text{th occurrence.}$$

This is a continuous random variable and it follows a gamma(r, λ) distribution, where λ is the mean number of occurrences per unit interval of time in the Poisson counting process. That is, $X \sim \text{gamma}(r, \lambda)$.

- Of course, if $r = 1$, then X is the time until the **first** occurrence, which we know is exponential(λ).

Example 4.7 (continued). In a corporate computer network, user log-ons to the system are modeled as a Poisson process with a mean of $\lambda = 25$ log-ons per hour.

- the time until the first user log-on is exponential$(\lambda = 25)$,
- the time until the second user log-on is gamma$(r = 2, \lambda = 25)$,
- the time until the third user log-on is gamma$(r = 3, \lambda = 25)$,

and so on.

4.5 Normal distribution

Definition: A continuous random variable X has a **normal distribution** with mean μ and variance σ^2 if its pdf is given by

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} \, e^{-(x-\mu)^2/2\sigma^2}, \quad \text{for } -\infty < x < \infty.$$

We write $X \sim \mathcal{N}(\mu, \sigma^2)$. This is also called the **Gaussian distribution**. The parameters μ and σ^2 are the mean and variance of X, respectively, that is,

$$\begin{aligned} E(X) &= \mu \\ V(X) &= \sigma^2. \end{aligned}$$

The mean μ identifies where the "center" of the distribution is. The variance σ^2 measures the "spread" of the distribution.

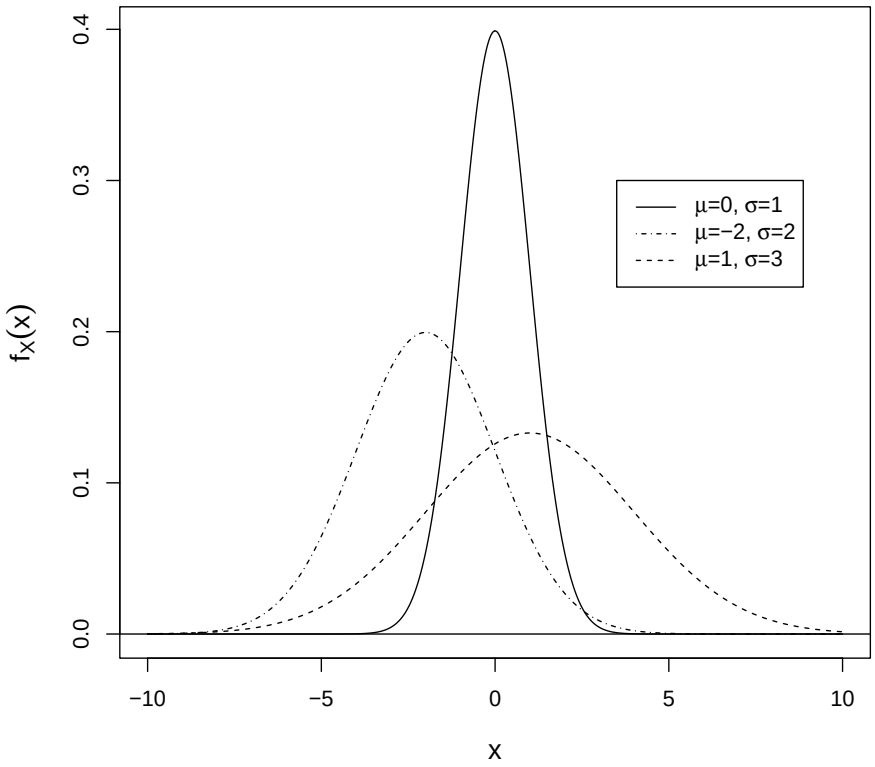


Figure 4.15: Normal pdfs for different values of μ and σ^2. Note the standard deviation σ is used instead of the variance σ^2.

Facts:

- The $\mathcal{N}(\mu, \sigma^2)$ pdf is **symmetric** about the mean μ.
- The $\mathcal{N}(\mu, \sigma^2)$ pdf has points of inflection at $\mu - \sigma$ and $\mu + \sigma$.
- The $\mathcal{N}(\mu, \sigma^2)$ pdf follows the **68-95-99.7% Rule**:

$$\begin{aligned} P(\mu - \sigma < X < \mu + \sigma) &\approx 0.68 \\ P(\mu - 2\sigma < X < \mu + 2\sigma) &\approx 0.95 \\ P(\mu - 3\sigma < X < \mu + 3\sigma) &\approx 0.997. \end{aligned}$$

  That is, approximately 68% of the observations x will be within 1 standard deviation of the mean, approximately 95% of the observations will be within 2 standard deviations of the mean, and approximately 99.7% of the observations will be within 3 standard deviations of the mean.

  - It is unlikely for a $\mathcal{N}(\mu, \sigma^2)$ random variable to have a value x further than 3 standard deviations away from its mean in either direction; this probability is approximately 0.003 or 0.3%.

NORMAL R CODE: Suppose $X \sim \mathcal{N}(\mu, \sigma^2)$.

$F_X(x) = P(X \leq x)$	ϕ_p
`pnorm(x,`μ`,`σ`)`	`qnorm(p,`μ`,`σ`)`

Note: Probability and quantile calculations for the normal distribution can be carried out using R. The cdf of $X \sim \mathcal{N}(\mu, \sigma^2)$ does not exist in closed form, so numerical evaluation is required. Note that R parameterizes the normal distribution by the standard deviation σ (not the variance σ^2).

Example 4.10. The daily demand for water use in Atlanta, GA, is a continuous random variable X, measured in millions of gallons. Suppose the distribution of X is normal (Gaussian) with mean $\mu = 447$ and standard deviation $\sigma = 32$. This pdf is shown in Figure 4.16 (next page).

Q: What is the probability the daily water demand will be less than 400 million gallons?
A: We want

$$P(X < 400) = \int_{-\infty}^{400} \frac{1}{\sqrt{2\pi}(32)} \, e^{-(x-447)^2/2(32)^2} dx \approx 0.071.$$

This probability is calculated numerically using the R code:

```
> options(digits=3)
> pnorm(400,447,32)
[1] 0.071
```

Q: City reservoirs are filled daily to a designated capacity. What capacity is needed so that the probability the daily demand exceeds the capacity is only 0.01?
A: We want $\phi_{0.99}$, the 99th percentile of this distribution. From R,

```
> options(digits=9)
> qnorm(0.99,447,32)
[1] 521.443132
```

Therefore, the capacity should be set at 521,443,132 gallons.

Terminology: A normal random variable with mean 0 and variance 1 is called a **standard normal** random variable. The pdf of $Z \sim \mathcal{N}(0, 1)$ is

$$f_Z(z) = \frac{1}{\sqrt{2\pi}} \, e^{-z^2/2}, \quad \text{for } -\infty < z < \infty.$$

The cdf of Z can be written as

$$F_Z(z) = P(Z \leq z) = \int_{-\infty}^{z} \frac{1}{\sqrt{2\pi}} \, e^{-t^2/2} dt.$$

The term $e^{-t^2/2}$ in the integrand does not have an antiderivative in closed form, so probabilities and quantiles associated with the standard normal distribution (and, in fact, any normal distribution) must be calculated numerically.

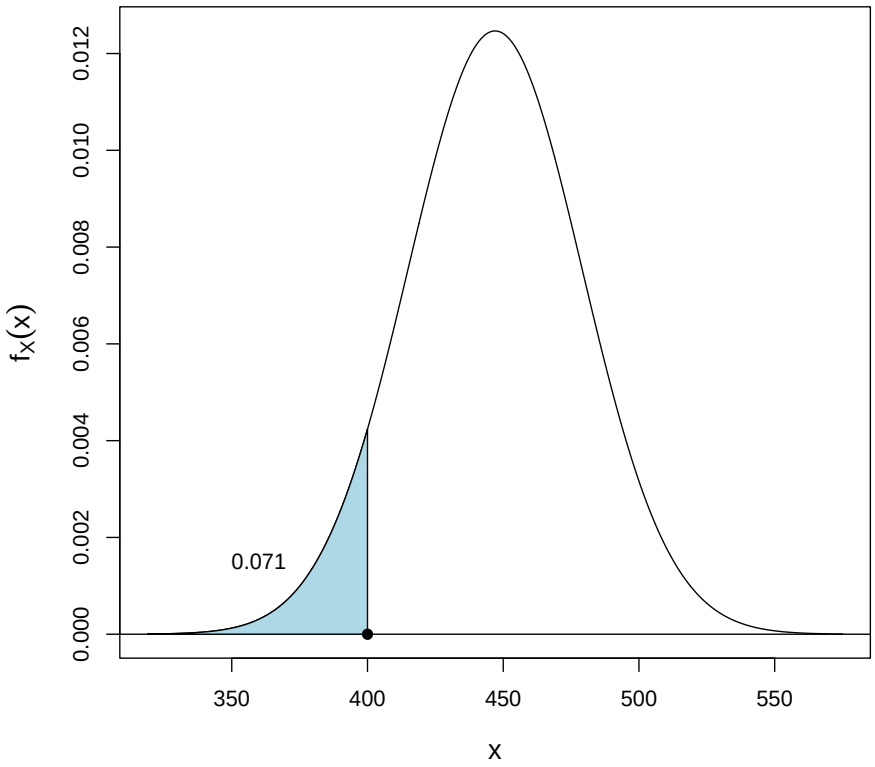


Figure 4.16: Probability density function of X in Example 4.10. The shaded area under the curve is $P(X < 400) \approx 0.071$.

Important: If $X \sim \mathcal{N}(\mu, \sigma^2)$, then

$$Z = \frac{X - \mu}{\sigma} \sim \mathcal{N}(0, 1).$$

This result says any normal random variable X can be "converted" to a standard normal random variable Z by applying this linear transformation. This conversion is known as **standardization**. For example, suppose exam scores for a population of students have mean $\mu = 70$ and standard deviation $\sigma = 10$. A student's score of 85 has standardized value

$$z = \frac{85 - 70}{10} = 1.5.$$

This means the student's score is 1.5 standard deviations above the mean. Similarly, a student's score of 55 produces

$$z = \frac{55 - 70}{10} = -1.5,$$

meaning the score is 1.5 standard deviations below the mean. From the 68-95-99.7% Rule, we know almost all standardized values z will be between -3 and 3.

5 Reliability Analysis and Lifetime Distributions

Terminology: Reliability analysis deals with the analysis of "time-to-event data." This means we are interested in a continuous random variable T which measures the time until something occurs. For example,

$$\begin{aligned} T &= \text{time until part failure} \\ T &= \text{time until maintenance is required} \\ T &= \text{time until a warranty claim is filed} \\ T &= \text{lifespan of a biological organism.} \end{aligned}$$

It is understood we are measuring something for which there is an unambiguous start and end, with the time in between corresponding to T. We call T a **lifetime random variable** because $P(T \geq 0) = 1$, that is, T assumes positive values only.

Terminology: A **lifetime distribution** describes the distribution of a lifetime random variable T. It has positive support. Some common choices are

- Weibull $\longleftarrow$ by far the most common in engineering applications
- lognormal
- gamma
- exponential (arises as a special gamma and as a special Weibull).

Although the normal distribution is the most widely used distribution in all of statistics, it is rarely used for reliability analyses. Typical time-to-event data are positive and skewed to the right. These characteristics are incongruous with normal distributions.

5.1 Weibull distribution

Definition: A continuous random variable T has a **Weibull distribution** with parameters $\beta > 0$ and $\eta > 0$ if its pdf is given by

$$f_T(t) = \begin{cases} \dfrac{\beta}{\eta}\left(\dfrac{t}{\eta}\right)^{\beta-1} \exp\left[-\left(\dfrac{t}{\eta}\right)^{\beta}\right], & t > 0 \\ 0, & \text{otherwise.} \end{cases}$$

We write $T \sim \text{Weibull}(\beta, \eta)$. We call

- β = shape parameter
- η = scale parameter.

Different values of β and η give different pdfs; see Figure 5.1 (next page). Weibull distributions have positive support and are generally skewed to the right.

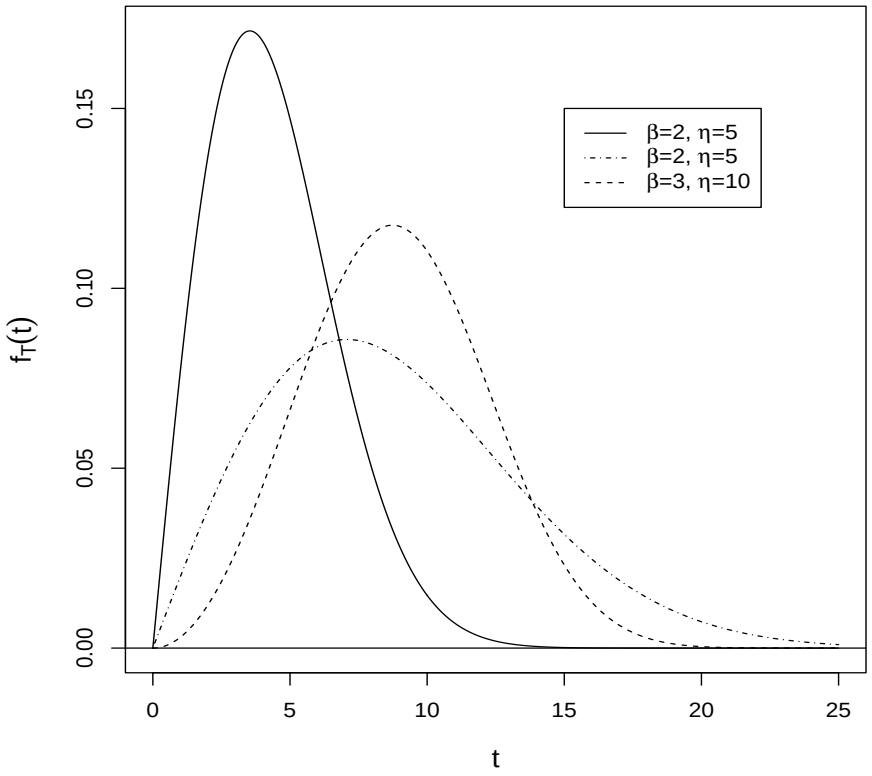


Figure 5.1: Weibull pdfs for different values of β and η.

Important: When $\beta = 1$, the Weibull(β, η) distribution reduces to the exponential(λ) distribution, where $\lambda = 1/\eta$. This is true because the Weibull(β, η) pdf

$$\frac{\beta}{\eta}\left(\frac{t}{\eta}\right)^{\beta-1}\exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right] = \frac{1}{\eta}e^{-t/\eta}, \quad \text{provided that } \beta = 1.$$

MEAN/VARIANCE: If $T \sim$ Weibull(β, η), then

$$\begin{aligned} E(T) &= \eta\Gamma\left(1+\frac{1}{\beta}\right) \\ V(T) &= \eta^2\left\{\Gamma\left(1+\frac{2}{\beta}\right) - \left[\Gamma\left(1+\frac{1}{\beta}\right)\right]^2\right\}, \end{aligned}$$

where recall $\Gamma(\cdot)$ is the gamma function defined in Section 4.4 (notes). The R code `gamma(r)` will calculate

$$\Gamma(r) = \int_0^\infty u^{r-1}e^{-u}du,$$

for any $r > 0$.

CDF: If $T \sim \text{Weibull}(\beta, \eta)$, then the cdf of T is

$$F_T(t) = \begin{cases} 0, & t \leq 0 \\ 1 - \exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right], & t > 0. \end{cases}$$

Therefore, Weibull probabilities of the form $F_T(b) = P(T \leq b)$ and

$$P(a < T < b) = F_T(b) - F_T(a)$$

can be calculated without using numerical methods. Quantiles ϕ_p can be found by solving

$$F_T(\phi_p) = 1 - \exp\left[-\left(\frac{\phi_p}{\eta}\right)^{\beta}\right] = p.$$

WEIBULL R CODE: Suppose $T \sim \text{Weibull}(\beta, \eta)$.

$F_T(t) = P(T \leq t)$	ϕ_p
`pweibull(t,`β`,`η`)`	`qweibull(p,`β`,`η`)`

Example 5.1. In a mechanical assembly, a bearing allows a shaft to rotate smoothly with minimal friction. The time until the bearing fails (in hours) is modeled as a Weibull random variable T with $\beta = 1.5$ and $\eta = 3000$. The pdf and cdf of T are shown side by side in Figure 5.2 (next page).

Q: What is the probability the bearing fails before 5000 hours of operation?
A: We want

$$P(T < 5000) = F_T(5000) = 1 - \exp\left[-\left(\frac{5000}{3000}\right)^{1.5}\right] = 1 - e^{-(5/3)^{1.5}} \approx 0.884.$$

That is, 88.4% of all bearings will fail before 5000 hours of operation.

```
> options(digits=3)
> pweibull(5000,1.5,3000)
[1] 0.884
```

Remark: When T measures the time to failure, we can think of the cdf $F_T(t)$ as the proportion of all units (here, shaft bearings) in the population which have "failed" before time t. Of course, if a unit has not failed before time t, then it is still operational and hence has "survived" up until time t. We call

$$S_T(t) = 1 - F_T(t)$$

the **survivor function** for this reason. It represents the proportion of all units in the population still "alive" at time t.

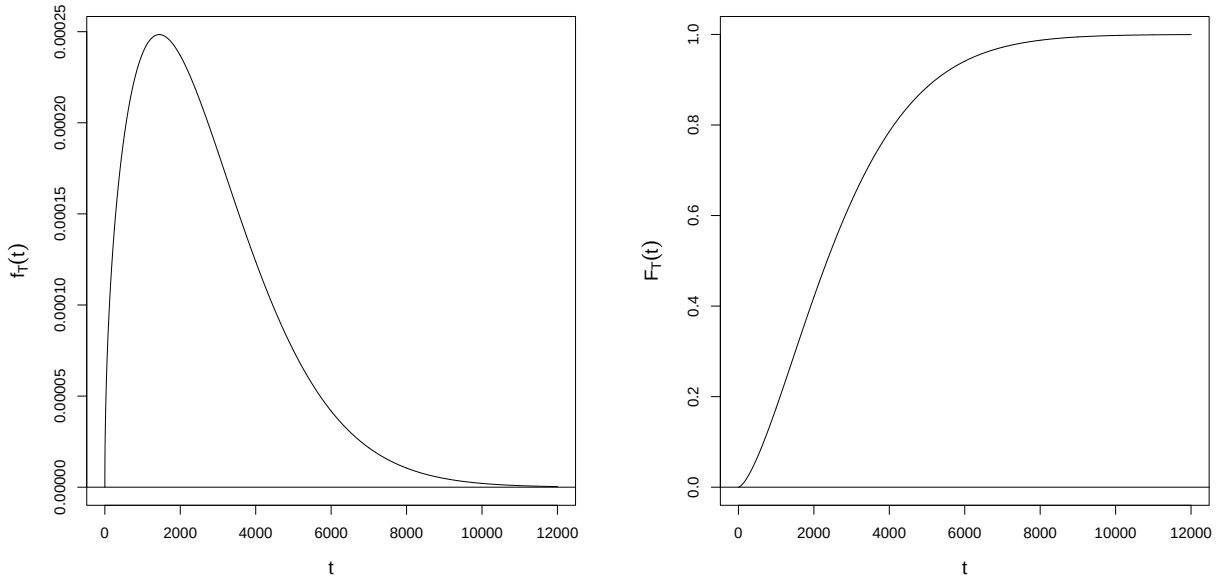


Figure 5.2: Left: Probability density function (pdf) of T in Example 5.1. Right: Cumulative distribution function (cdf) of T.

Q: Find the mean and median time to bearing failure.
A: The mean time to failure is

$$E(T) = 3000\ \Gamma\left(1 + \frac{1}{1.5}\right) = 3000\ \Gamma\left(\frac{5}{3}\right) \approx 2708.2 \text{ hours.}$$

The median time to failure $\phi_{0.5}$ solves

$$\begin{aligned} F_T(\phi_{0.5}) = 1 - \exp\left[-\left(\frac{\phi_{0.5}}{3000}\right)^{1.5}\right] = 0.5 &\implies \exp\left[-\left(\frac{\phi_{0.5}}{3000}\right)^{1.5}\right] = 0.5 \\ &\implies -\left(\frac{\phi_{0.5}}{3000}\right)^{1.5} = \ln(0.5) \\ &\implies \left(\frac{\phi_{0.5}}{3000}\right)^{1.5} = -\ln(0.5) \\ &\implies \frac{\phi_{0.5}}{3000} = [-\ln(0.5)]^{1/1.5} \\ &\implies \phi_{0.5} = 3000[-\ln(0.5)]^{1/1.5} \approx 2349.7 \text{ hours.} \end{aligned}$$

```
> options(digits=5)
> 3000*gamma(5/3) # E(T)
[1] 2708.2
> qweibull(0.5,1.5,3000) # median
[1] 2349.7
```

5.2 Reliability functions

Goal: We now summarize some different, but equivalent, ways of defining the distribution of a continuous lifetime random variable T. We also introduce a new function which is used in reliability studies.

- The **cumulative distribution function** (cdf)

$$F_T(t) = P(T \leq t).$$

  This can be interpreted as the proportion of units (individuals) in the population that have failed at or before time t.

- The **survivor function**

$$S_T(t) = P(T > t) = 1 - F_T(t).$$

  This can be interpreted as the proportion of units (individuals) in the population that have not failed by time t; e.g., unit is still operational, warranty claim has not been made, organism is still alive, etc.

- The **probability density function** (pdf)

$$f_T(t) = \frac{d}{dt}F_T(t) = -\frac{d}{dt}S_T(t).$$

  Also, recall

$$F_T(t) = \int_0^t f_T(u)du \longleftarrow \text{ area under the pdf over } (0, t)$$

  and

$$S_T(t) = \int_t^\infty f_T(u)du \longleftarrow \text{ area under the pdf over } (t, \infty).$$

Terminology: The **hazard function** of a lifetime random variable T is defined as

$$h_T(t) = \lim_{\epsilon \to 0} \frac{P(t \leq T < t + \epsilon | T \geq t)}{\epsilon},$$

for $\epsilon > 0$. The hazard function is not a probability; rather, it is a **probability rate**. It characterizes the instantaneous potential for failure to occur, given that a unit (individual) has already survived up to a certain point in time t.

Interpretation: The hazard function offers a useful interpretation. *It indicates how the rate of failure varies with time.*

- Distributions with increasing hazard functions are seen in units (individuals) where some kind of aging or "wear out" takes place. The population gets weaker over time.

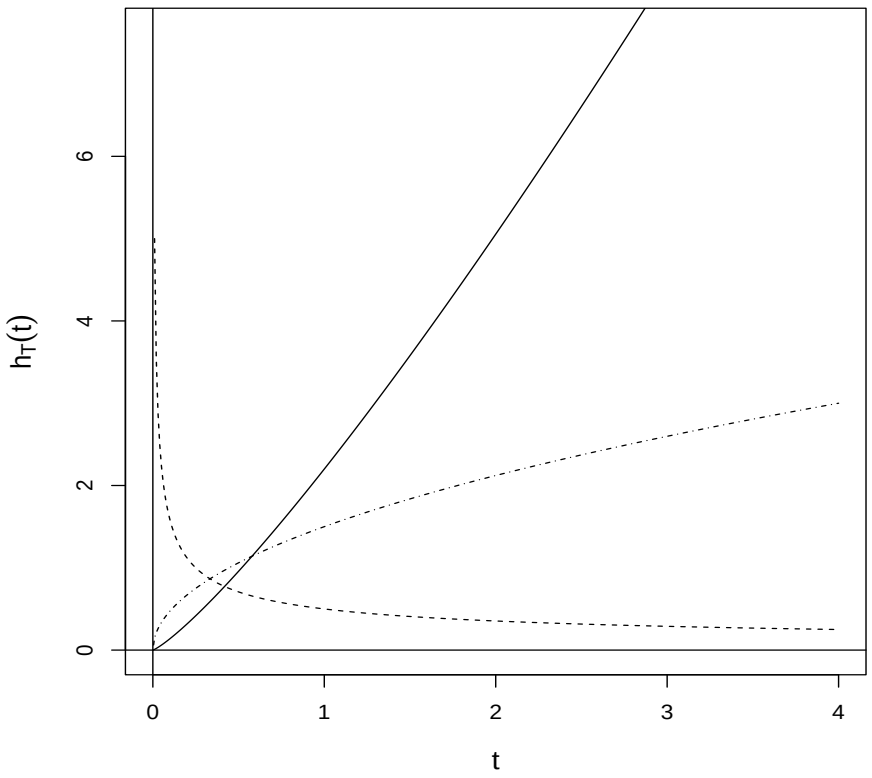


Figure 5.3: Examples of hazard functions. Increasing hazards correspond to the population getting weaker over time.

- Distributions with decreasing hazard functions correspond to a population getting stronger over time. This is observed in scenarios like the "infant mortality" phase in manufacturing, where initial defects are weeded out, or in situations where components become more robust with use.
- In some populations, the hazard function decreases initially, stays constant for a period of time, and then increases. This corresponds to a population whose units get stronger initially (defective units "die out" early), exhibit random failures for a period of time (constant hazard), and then eventually the population starts to weaken (e.g., due to wear/old age, etc.). These hazard functions are **bathtub-shaped**.

Result: Suppose T is a lifetime random variable with pdf $f_T(t)$ and survivor function $S_T(t)$. The hazard function

$$h_T(t) = \frac{f_T(t)}{S_T(t)}.$$

We can therefore describe the distribution of T by using either $f_T(t)$, $F_T(t)$, $S_T(t)$, or $h_T(t)$. If we know one of these functions, we can always retrieve the other three.

Note: The previous result can be shown by using the definitions of conditional probability (Chapter 2) and of the derivative from calculus. Note that

$$\begin{aligned} h_T(t) &= \lim_{\epsilon \to 0} \frac{P(t \leq T < t+\epsilon | T \geq t)}{\epsilon} \\ &= \lim_{\epsilon \to 0} \frac{P(t \leq T < t+\epsilon \text{ and } T \geq t)}{\epsilon \; P(T \geq t)} \\ &= \lim_{\epsilon \to 0} \frac{P(t \leq T < t+\epsilon)}{\epsilon \; S_T(t)} \\ &= \frac{1}{S_T(t)} \underbrace{\lim_{\epsilon \to 0} \frac{F_T(t+\epsilon) - F_T(t)}{\epsilon}}_{=\frac{d}{dt}F_T(t)} = \frac{f_T(t)}{S_T(t)}. \end{aligned}$$

WEIBULL HAZARD: If $T \sim \text{Weibull}(\beta, \eta)$, then the hazard function of T is

$$h_T(t) = \frac{f_T(t)}{S_T(t)} = \frac{f_T(t)}{1 - F_T(t)} = \frac{\frac{\beta}{\eta}\left(\frac{t}{\eta}\right)^{\beta-1} \exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right]}{1 - \left\{1 - \exp\left[-\left(\frac{t}{\eta}\right)^{\beta}\right]\right\}} = \frac{\beta}{\eta}\left(\frac{t}{\eta}\right)^{\beta-1}.$$

Interpretation: For a Weibull distribution,

- $h_T(t)$ is **increasing** if $\beta > 1$ (wear out; population gets weaker)
- $h_T(t)$ is **constant** if $\beta = 1$ (random failures; exponential distribution)
- $h_T(t)$ is **decreasing** if $\beta < 1$ (infant mortality; population gets stronger).

In other words, the value of the shape parameter β completely summarizes the relevant feature of the hazard function. This is one reason the Weibull distribution is popular. Engineers can characterize the rate of failure over time by knowing this single number. Other lifetime distributions (e.g., gamma, lognormal, etc.) have hazard functions which are more complex. They are not amenable to this easy interpretation.

Example 5.1 (continued). In a mechanical assembly, a bearing allows a shaft to rotate smoothly with minimal friction. The time until the bearing fails (in hours) is modeled as a Weibull random variable T with $\beta = 1.5$ and $\eta = 3000$. The hazard function

$$h_T(t) = \frac{1.5}{3000}\left(\frac{t}{3000}\right)^{1.5-1} = \frac{1.5}{(3000)^{3/2}}\, t^{1/2}$$

is an increasing function of t; see Figure 5.4 (next page). This means that (under the Weibull model assumption) the rate of bearing failure increases over time. This corresponds to "aging" or "wear out" in the population of bearings over time.

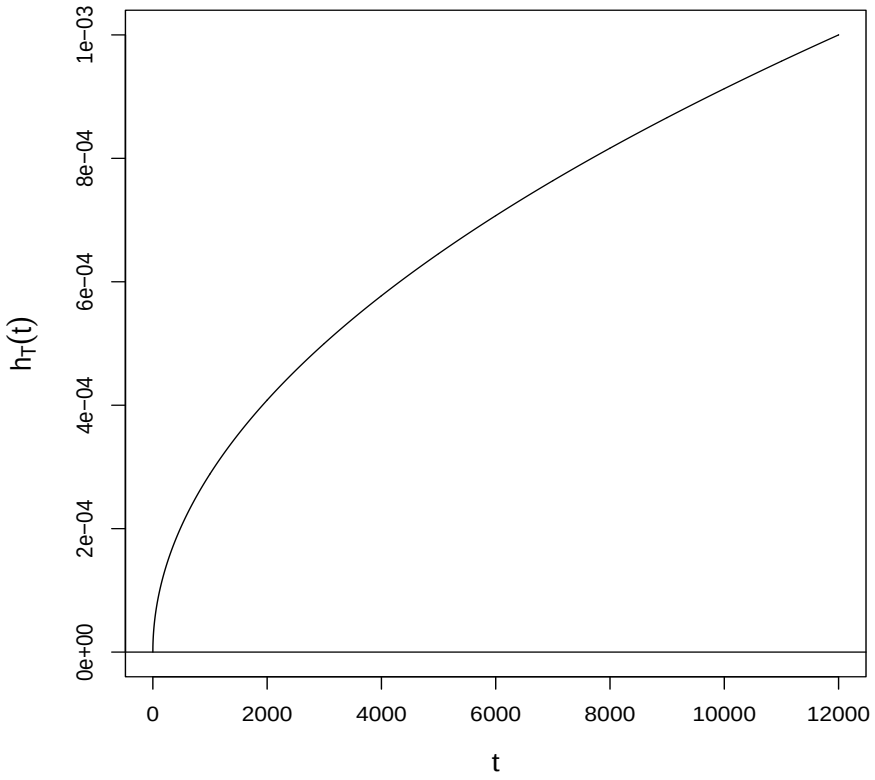


Figure 5.4: Hazard function of T in Example 5.1.

5.3 Fitting a Weibull distribution to data

Curiosity: In Example 5.1, we used a Weibull distribution with $\beta = 1.5$ and $\eta = 3000$ to model T, the time until shaft bearing failure. A natural question to ask is, "Where do the values of β and η come from?" or "How do we know these values are correct?"

- Formulating a good answer to the first question is easy, sort of. The reason for the ambiguity is that β and η are **population parameters**. They represent the shape and scale of the Weibull distribution that is selected to model the time to failure for all shaft bearings in the population.
- Therefore, the only way we could determine β and η without ambiguity is to observe the failure time T for all shaft bearings in the population! This is not possible. For this reason, population parameters like β and η will be unknown in real life (and, thus, no one can answer the second question above).
- What can we do? We do the next best thing. If we observe a **sample** of shaft bearings from the population, we can find **estimates** of β and η by using the failure times in

the sample. If the sample is representative of the population, then the estimates of β and η we calculate should be reasonable "guesses" of what the true β and η are.

- Of course, a deeper foundational question is "How do we know if the Weibull distribution is the correct lifetime distribution for the population of all shaft bearings?" Again, this question cannot be answered, because "correct" is too strong a word (it would require us to observe the failure time of all shaft bearings in the population). We *can* assess empirically whether the Weibull model is "reasonable" by using a representative sample. This is done in the next section.

Example 5.2. A shock absorber is a suspension component that controls the up-and-down motion of a vehicle's wheels. The following data are $n = 38$ distances (in km) driven to failure for a specific brand of shock absorber under extreme driving conditions.

6700	6950	7820	9120	9660	9820	11310	11690	11850	11880
12140	12200	12870	13150	13330	13470	14040	14300	17520	17540
17890	18450	18960	18980	19410	20100	20100	20150	20320	20900
22700	23490	26510	27410	27490	27890	28100	30050		

We will assume a Weibull(β, η) distribution for

$$T = \text{ distance until failure (in km).}$$

Because the population parameters β and η are not given to us, our first task is to estimate them. We do this by finding the values of β and η that "most closely agree" with the data above. Form the **likelihood function**

$$\begin{aligned} L(\beta,\eta) = \prod_{i=1}^{38} f_T(t_i) &= \prod_{i=1}^{38} \frac{\beta}{\eta}\left(\frac{t_i}{\eta}\right)^{\beta-1} \exp\left[-\left(\frac{t_i}{\eta}\right)^{\beta}\right] \\ &= \left(\frac{\beta}{\eta^{\beta}}\right)^{38}\left(\prod_{i=1}^{38} t_i\right)^{\beta-1} \exp\left[-\sum_{i=1}^{38}\left(\frac{t_i}{\eta}\right)^{\beta}\right], \end{aligned}$$

where $t_1, t_2, ..., t_{38}$ are the 38 distances. Informally, the likelihood function describes the probability of the observed data. Therefore, the values of β and η that "most closely agree" with the data are the values that maximize $L(\beta, \eta)$.

- Let $\widehat{\beta}$ and $\widehat{\eta}$ denote the values of β and η, respectively, that maximize $L(\beta, \eta)$. We call $\widehat{\beta}$ and $\widehat{\eta}$ **maximum likelihood estimates**.
- Finding $\widehat{\beta}$ and $\widehat{\eta}$ is a multivariable calculus problem we will solve numerically using R.
- In statistics speak, we say that $\widehat{\beta}$ and $\widehat{\eta}$ are **estimates** of the population parameters β and η, respectively. The population here is the universe of all shock absorbers of this specific brand.

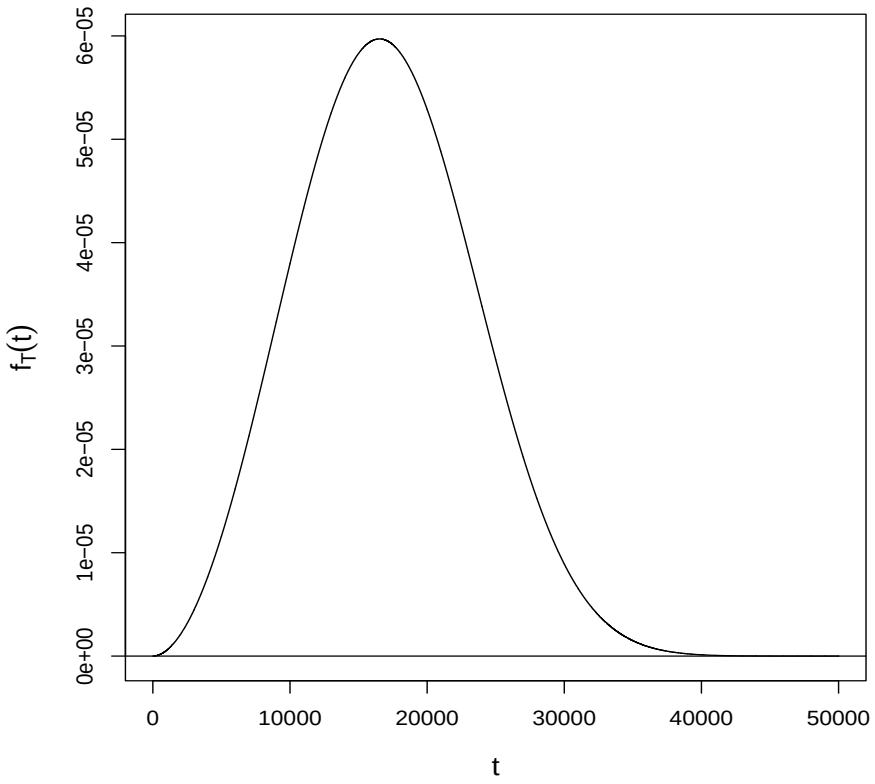


Figure 5.5: (Estimated) probability density function of T in Example 5.2.

Implementation in R: We can use the `fitdistrplus` package:

```
> library(fitdistrplus)
> distance.to.failure = c(6700,6950,7820, ..., 30050) # Enter the data
> options(digits=3)
> fitdist(distance.to.failure,distr="weibull",method="mle")

Fitting of the distribution ' weibull ' by maximum likelihood
Parameters:
      estimate Std. Error
shape      2.9      0.367
scale  19125.6   1140.512
```

This output produces

$$\begin{aligned} \widehat{\beta} &\approx 2.9 \\ \widehat{\eta} &\approx 19125.6. \end{aligned}$$

These are the **estimates** of β and η based on the data from the previous page.

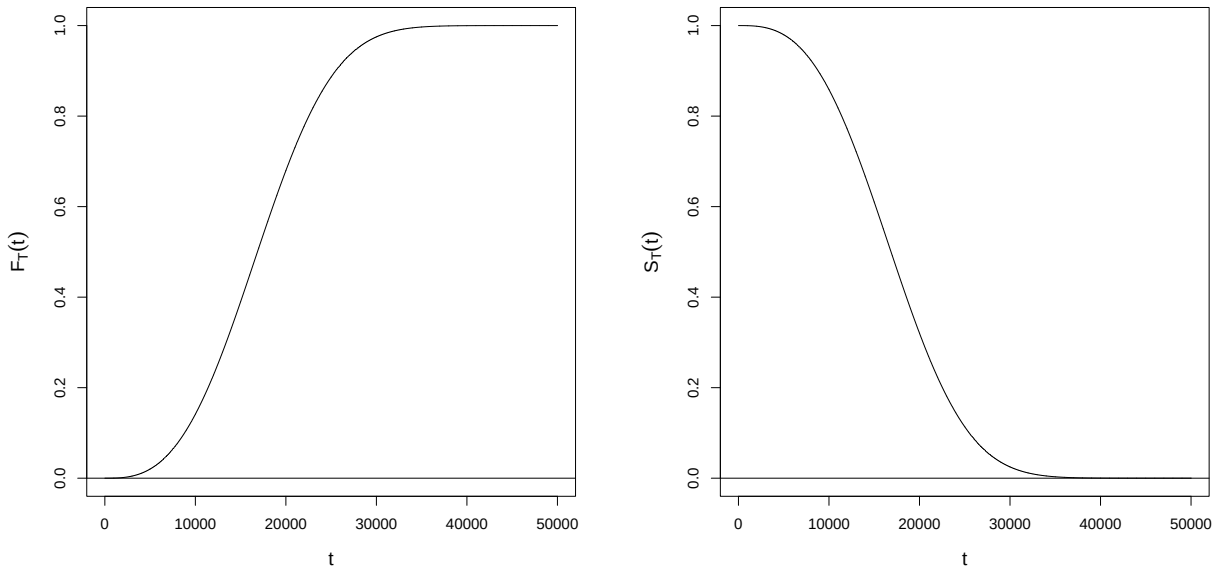


Figure 5.6: Left: (Estimated) cumulative distribution function T in Example 5.2. Right: (Estimated) survivor function of T.

Here are the estimated functions for the shock absorber data in Example 5.2:

PDF:

$$f_T(t) = \begin{cases} \dfrac{2.9}{19125.6}\left(\dfrac{t}{19125.6}\right)^{1.9} \exp\left[-\left(\dfrac{t}{19125.6}\right)^{2.9}\right], & t > 0 \\ 0, & \text{otherwise.} \end{cases}$$

CDF/Survivor:

$$F_T(t) = \begin{cases} 0, & t \leq 0 \\ 1 - \exp\left[-\left(\dfrac{t}{19125.6}\right)^{2.9}\right], & t > 0 \end{cases} \quad S_T(t) = \begin{cases} 1, & t \leq 0 \\ \exp\left[-\left(\dfrac{t}{19125.6}\right)^{2.9}\right], & t > 0 \end{cases}.$$

Q: Estimate the proportion of shock absorbers in this population that will still be operational at 30,000 km.
A: We want

$$P(T \geq 30000) = S_T(30000) = \exp\left[-\left(\frac{30000}{19125.6}\right)^{2.9}\right] \approx 0.025.$$

About 2.5% of all shock absorbers in the population will still be operational at 30,000 km.

```
> 1-pweibull(30000,2.9,19125.6) # P(T>=30000)
[1] 0.025
```

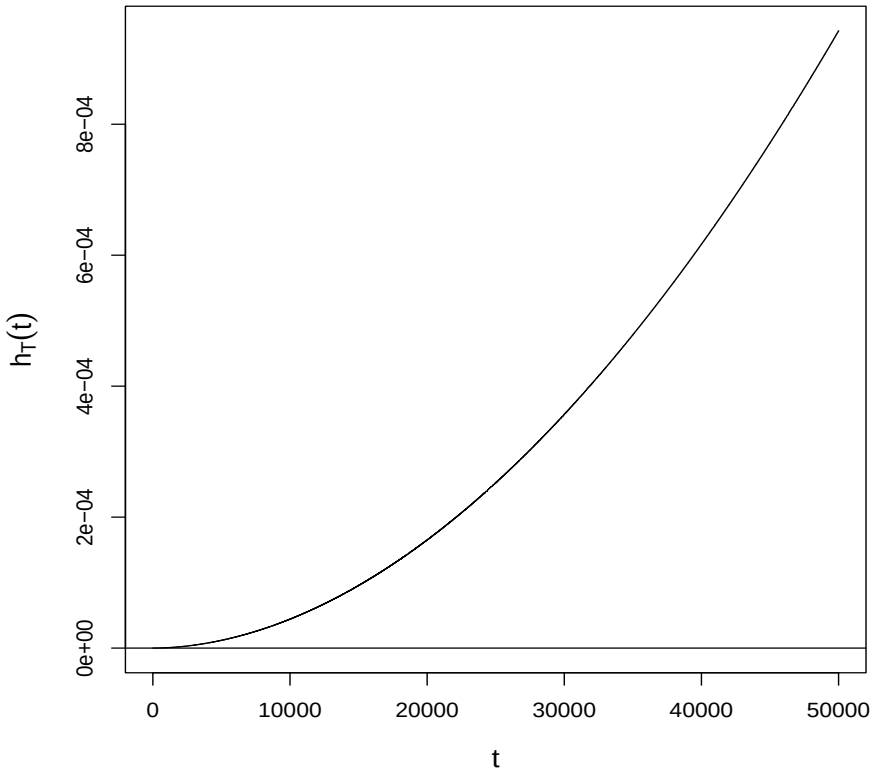


Figure 5.7: (Estimated) hazard function of T in Example 5.2.

Hazard:

$$h_T(t) = \frac{2.9}{19125.6}\left(\frac{t}{19125.6}\right)^{1.9}.$$

This function is shown in Figure 5.7 (above). Because the hazard function is increasing, this means the population of shock absorbers gets weaker over time.

5.4 Quantile-quantile plots

Importance: In a reliability analysis, we will typically assume a lifetime random variable T has a specific distribution, like the Weibull distribution. How do we know if this assumption is reasonable?

- Because we are making an assumption about the distribution of all units (individuals) in the population, we never get to know for sure if the distribution we have chosen is correct.
- We *can* assess if the distribution we have chosen is "reasonable" based on the observed data in the sample.

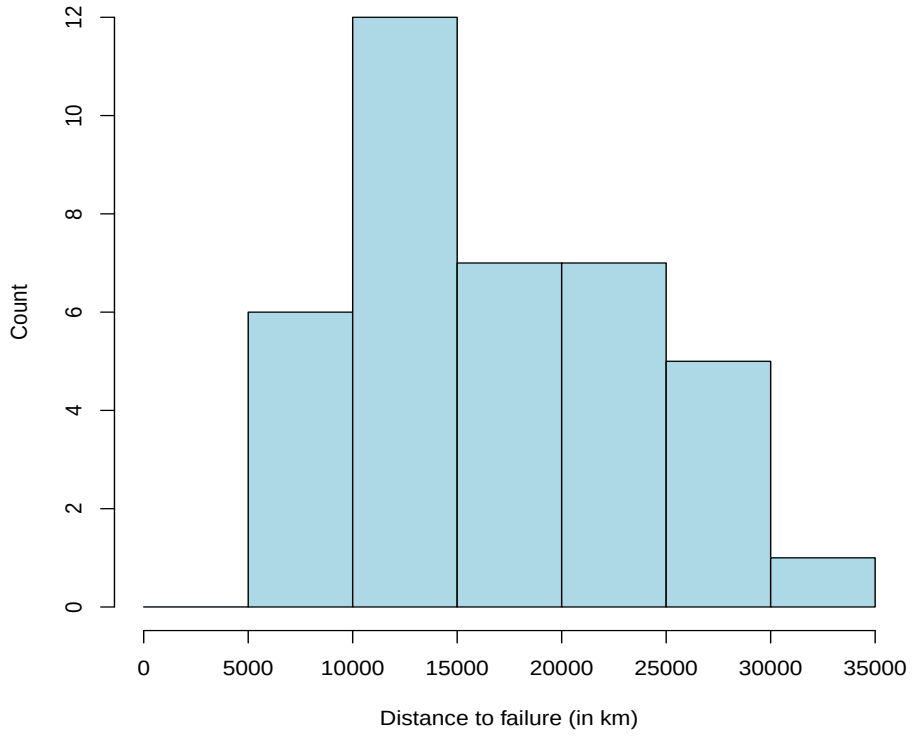


Figure 5.8: Histogram of the shock absorber data in Example 5.2.

- This is part of the "model diagnostics" phase of any data analysis. This means we are assessing (or diagnosing) the plausibility of the assumptions made as part of the analysis.

Remark: The first thing I do in any data analysis is look at the data graphically. A histogram of the $n = 38$ shock absorber distances is shown in Figure 5.8 (above). With such a small sample, it's hard to make good prognostications about "what's going on" in the population of all shock absorbers. However, the shape we see in the histogram does align with the right-skewed shape we know is characteristic of a Weibull pdf. This is reassuring but by no means determinative. There are many types of skewed right distributions.

Terminology: A **quantile-quantile plot** (**qq plot**) is a graphical display that can help assess how well a distribution fits a data set. Here is how the plot is constructed:

- On the vertical axis, we plot the observed data ordered from low to high.
- On the horizontal axis, we plot the same number of (ordered) quantiles from the distribution assumed for the observed data.

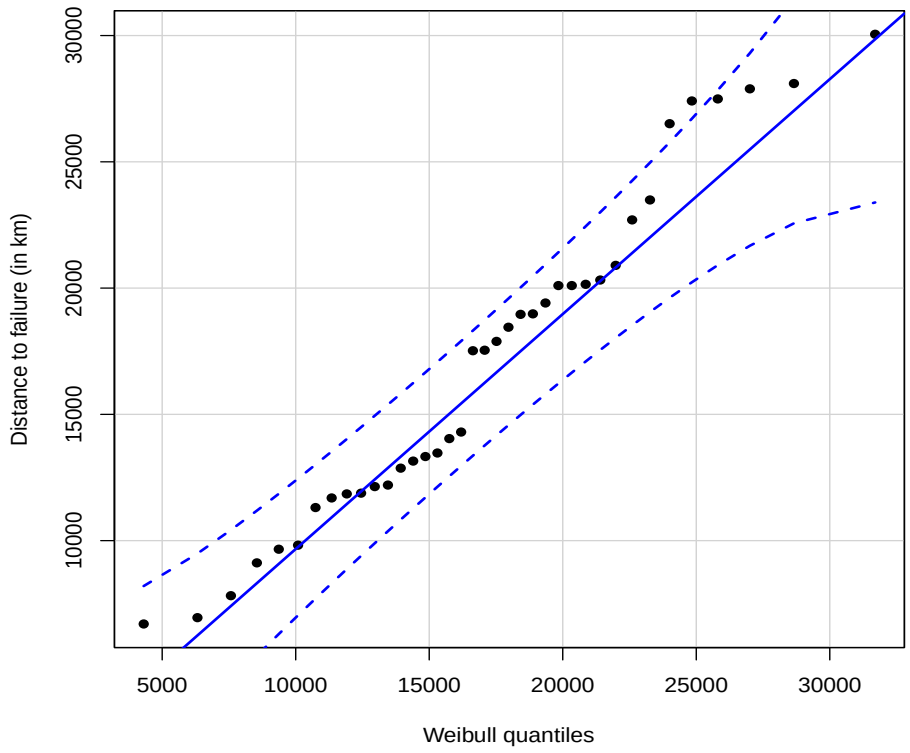


Figure 5.9: Quantile-quantile plot of the shock absorber data in Example 5.2. This is a plot of the observed data (vertical axis) versus quantiles of a Weibull distribution with shape $\widehat{\beta} = 2.9$ and scale $\widehat{\eta} = 19125.6$ (horizontal axis).

Our intuition should suggest the following:

- If the observed data align with the distribution's quantiles, then the qq plot should look like a **straight line**. This suggests the distribution fits the data well and is therefore a reasonable choice for the population.
- If the observed data do not align with the distribution's quantiles, then the qq plot should have **curvature** in it. This suggests the distribution may not be a good choice for the population.

Assessment: The qq plot in Figure 5.9 (above) looks linear for the most part. Even though the agreement isn't perfect, the Weibull distribution appears to be reasonable for the shock absorber data in Example 5.2.

Important: When you interpret qq plots, you are looking for **general agreement**. The observed data will never line up perfectly with the distribution's quantiles due to natural variability−even when the distribution is correct! In other words, don't be "too picky" when interpreting these plots, especially with small sample sizes (like $n = 38$).

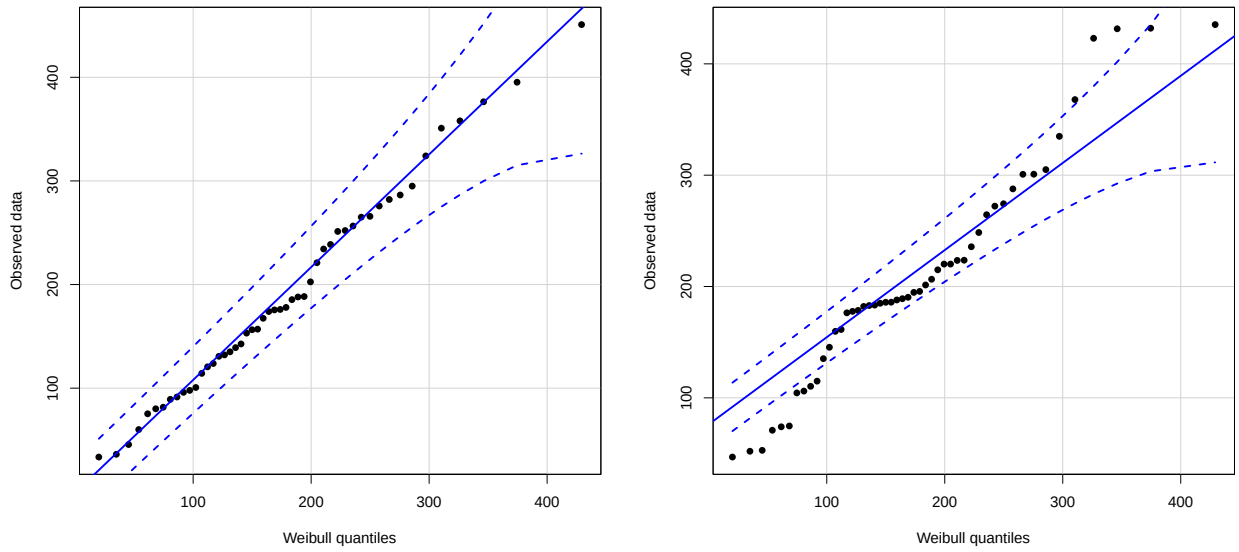


Figure 5.10: Two qq plots with sample size $n = 50$. The Weibull$(2, 200)$ distribution is assumed for the population.

- If there is disagreement, it will usually happen in the tails of the distribution (left or right). With time-to-event data, disagreement in the right tail is more common.
- The bands in Figure 5.9 are shown to give the viewer a reference for how much variability about the line "is allowed." However, even if a couple of points fall outside the bands, especially if these points are in the tail, this should not cause dramatic concern.

Exercise: Figure 5.10 (above) shows two qq plots, each with sample size $n = 50$. The population distribution is assumed to be Weibull with $\beta = 2$ and $\eta = 200$.

Q: I simulated two data sets. I then constructed qq plots (above) for each data set under the assumption the Weibull$(2, 200)$ population distribution is correct. Which plot do you think used data simulated from the correct distribution?
A: This was a trick question! Both qq plots show data sets simulated from the correct distribution.

- In reality, I simulated about 20 data sets from the correct Weibull$(2, 200)$ distribution and constructed qq plots for each one.
- I then selected the qq plot that looked "the best" (left) and the one that looked "the worst" (right).
- The lesson here is that qq plots, while helpful in model assessment, should not be meticulously overanalyzed. This is especially true with small sample sizes.

6 Bridge to Statistical Inference

6.1 Populations and samples (Parameters and statistics)

Goal: We now shift our focus to **statistical inference**. This deals with making statements about a population of individuals based on information that is available in a sample taken from the population.

- In most situations, it is not possible to observe all individuals in a population (e.g., all power supply units, all shaft bearings, all shock absorbers, etc.). The population is too large, and it would be too time consuming to measure every individual in it.
- If the observed sample is representative of the population, then what we see in the sample should approximate "what's going on" in the population.
- In this class, we will assume the sample of individuals is a **random sample**. Mathematically, this means all observations are independent and follow the same probability distribution.
- Selecting a random sample is our best hope of obtaining individuals that are representative of the entire population.

Notation: We will denote a random sample of observations by using random variable notation:

$$X_1, X_2, ..., X_n.$$

That is, X_1 is the value of X for the first individual in the sample, X_2 is the value of X for the second individual in the sample, and so on. The **sample size** tells us how many individuals are in the sample and is denoted by n. Lower case notation $x_1, x_2, ..., x_n$ is used when citing numerical values. We will typically call these **data**.

Example 6.1. Aluminum-lithium alloys are primarily used in the aerospace industry due to their high strength-to-weight ratio and stiffness. The data below are the compressive strengths (in psi) of $n = 80$ specimens of a new alloy undergoing evaluation as a possible material for aircraft structural elements.

105	221	183	186	121	181	180	143	97	154	153	174	120	168	167	141
245	228	174	199	181	158	176	110	163	131	154	115	160	208	158	133
207	180	190	193	194	133	156	123	134	178	76	167	184	135	229	146
218	157	101	171	165	172	158	169	199	151	142	163	145	171	148	158
160	175	149	87	160	237	150	135	196	201	200	176	150	170	118	149

Population: all alloy specimens (of this type) produced using the current process
Sample: the 80 specimens

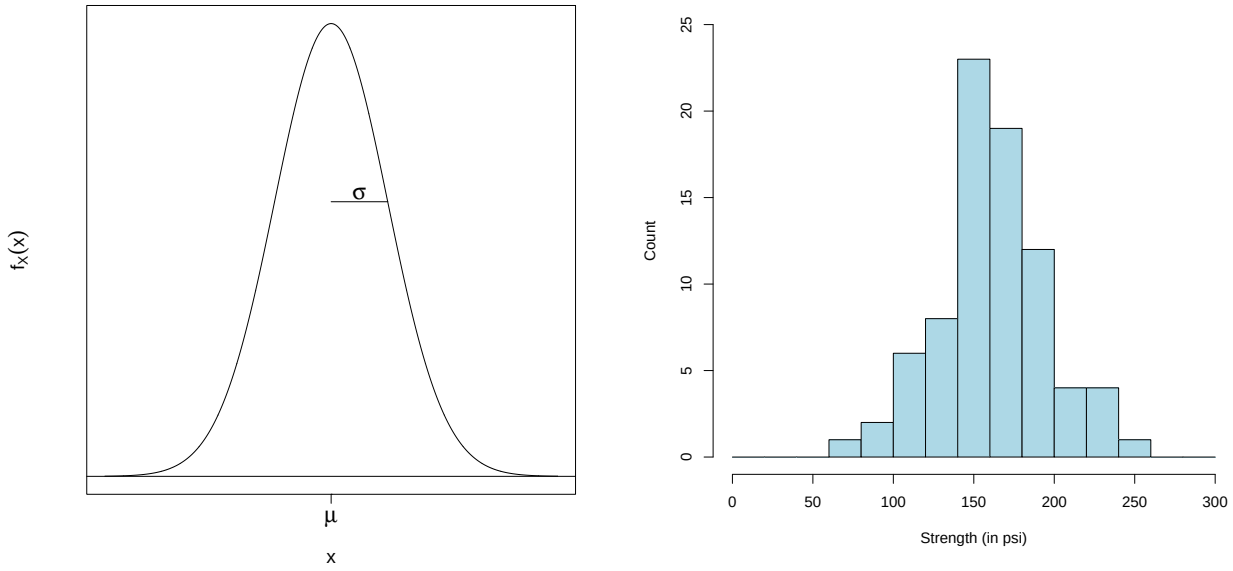


Figure 6.1: Left: $\mathcal{N}(\mu, \sigma^2)$ pdf for X in Example 6.1. This serves as a model for the population of all alloy specimens. Right: Histogram of the sample of $n = 80$ alloy specimens.

Engineers assume the random variable

$$X = \text{strength of alloy specimen (in psi)}$$

is normally distributed with mean μ and variance σ^2. That is, $X \sim \mathcal{N}(\mu, \sigma^2)$. This is called the **population distribution**. We use the term "population distribution" to mean the distribution of X for all individuals (alloy specimens) in the population. The data, shown above in Figure 6.1 (right), can be conceptualized as 80 independent observations from this population distribution.

Remark: This example illustrates a common situation encountered in practice. The engineers are willing to assume the population distribution is $\mathcal{N}(\mu, \sigma^2)$, but the **population parameters** associated with this distribution

$$\begin{aligned} \mu &= \text{population mean} \\ \sigma^2 &= \text{population variance} \end{aligned}$$

are unknown. The statistical inference question then becomes, "How do we **estimate** these parameters with the observed data?"

Remark: This is analogous to our discussion in the last chapter where we assumed a Weibull(β, η) population distribution for a lifetime random variable T; see Example 5.2. We assumed a Weibull(β, η) distribution for the population of all shock absorbers. We then estimated the population parameters β and η with the $n = 38$ shock absorbers in the sample and used qq plots to assess the Weibull assumption.

Terminology: A **parameter** is a numerical quantity that describes a population (more specifically, all individuals in the population). In most situations, population parameters are unknown. Some common examples are:

$$\begin{aligned} \mu &= \text{population mean} \\ \sigma^2 &= \text{population variance} \\ \sigma &= \text{population standard deviation} \\ p &= \text{population proportion.} \end{aligned}$$

Terminology: Suppose $X_1, X_2, ..., X_n$ is a random sample from a population with mean μ and variance σ^2.

- The **sample mean** is
$$\overline{X} = \frac{1}{n}\sum_{i=1}^{n} X_i.$$
- The **sample variance** is
$$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X})^2.$$
- The **sample standard deviation** is the positive square root of the sample variance; i.e.,
$$S = \sqrt{S^2} = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(X_i - \overline{X})^2}.$$

Terminology: A **statistic** is a numerical quantity that is calculated from a sample of observations. In statistical inference, (sample) statistics are used to estimate (population) parameters. We say

- the sample mean $\overline{X}$ is an estimate of the population mean μ
- the sample variance S^2 is an estimate of the population variance σ^2
- the sample standard deviation S is an estimate of the population standard deviation σ.

Example 6.1 (continued). We use R to calculate statistics for the alloy strength data:

```
> options(digits=4)
> mean(strength) # sample mean
[1] 162.7
> var(strength) # sample variance
[1] 1141
> sd(strength) # sample standard deviation
[1] 33.77
```

Therefore, we would conclude:

- the population mean μ can be estimated using $\overline{x} = 162.7$ psi
- the population variance σ^2 can be estimated using $s^2 = 1141$ (psi)^2
- the population standard deviation σ can be estimated using $s = 33.77$ psi.

Discussion: It is important to understand that when we calculate an estimate of a population parameter, that's all we are doing−we are taking a "guess" at what it is. There is no guarantee we are correct or even close for that matter.

- Different samples will give different statistic values. For example, if engineers in Example 6.1 sampled another $n = 80$ alloy specimens the following day, they would get different strength measurements and, thus, all statistics' values would change.
- Statistics' values will change from sample to sample. On the other hand, population parameters do not change. They continue to describe the entire population regardless of how many times we sample from it.
- One desirable characteristic of a statistic, in general, is that it estimates the population parameter "correctly on average." This does not mean one sample will estimate the parameter correctly (some samples will underestimate; some samples will overestimate). This means that over the long run, if one took many samples, the statistic would estimate the parameter correctly on average. This is the definition of **unbiasedness**.
- It also makes sense to think about how variable a statistic's value might be from sample to sample. Doing this will help us understand how much variability is associated with the statistics we calculate. In turn, this will help us form **confidence intervals** for parameters we wish to estimate (next chapter).

6.2 Point estimation and sampling distributions

Note: The ideas in this section can be applied to a variety of situations. Therefore, to keep our discussion general, we let θ denote an arbitrary population parameter.

- For example, θ could denote a population mean, a population variance, a population proportion, a Weibull population distribution parameter, etc.
- It could also denote a parameter in a linear regression model (Chapters 10-11) or other statistical model.
- Whatever the quantity θ represents, the salient point is that it is unknown because it describes the entire population. We want to estimate it using a random sample.

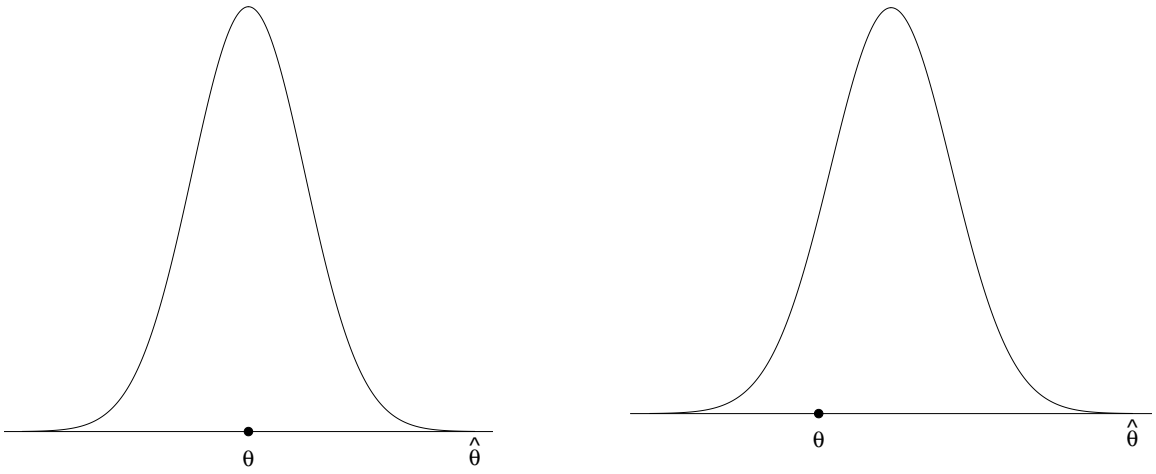


Figure 6.2: Sampling distribution of the point estimator $\widehat{\theta}$. Left: $\widehat{\theta}$ is an unbiased estimator. Right: $\widehat{\theta}$ is a biased estimator.

Terminology: A **point estimator** $\widehat{\theta}$ is a statistic that estimates a population parameter θ. Common examples are:

$$\begin{aligned} \overline{X} &\longrightarrow \text{ a point estimator for the population mean } \mu \\ S^2 &\longrightarrow \text{ a point estimator for the population variance } \sigma^2 \\ S &\longrightarrow \text{ a point estimator for the population standard deviation } \sigma. \end{aligned}$$

Important: Because a point estimator $\widehat{\theta}$ is a statistic, its value depends on the sample that is observed, and, as we just discussed, its value will be different for different samples. Therefore, it makes sense to think about the distribution of all possible values of $\widehat{\theta}$ that could arise from sampling.

Terminology: The distribution of a point estimator $\widehat{\theta}$ is called its **sampling distribution**. This distribution describes how $\widehat{\theta}$ would vary in repeated sampling from the same population. We say that $\widehat{\theta}$ is an **unbiased estimator** of θ if

$$E(\widehat{\theta}) = \theta.$$

In other words, the mean of the sampling distribution of $\widehat{\theta}$ is equal to θ. This means that $\widehat{\theta}$ will estimate θ "correctly on average."

Result: Suppose $X_1, X_2, ..., X_n$ is a random sample from a population with mean μ and variance σ^2. Mathematics can show

$$\begin{aligned} E(\overline{X}) &= \mu \\ E(S^2) &= \sigma^2. \end{aligned}$$

That is, the sample mean $\overline{X}$ is an unbiased estimator of the population mean μ. The sample variance S^2 is an unbiased estimator of the population variance σ^2.

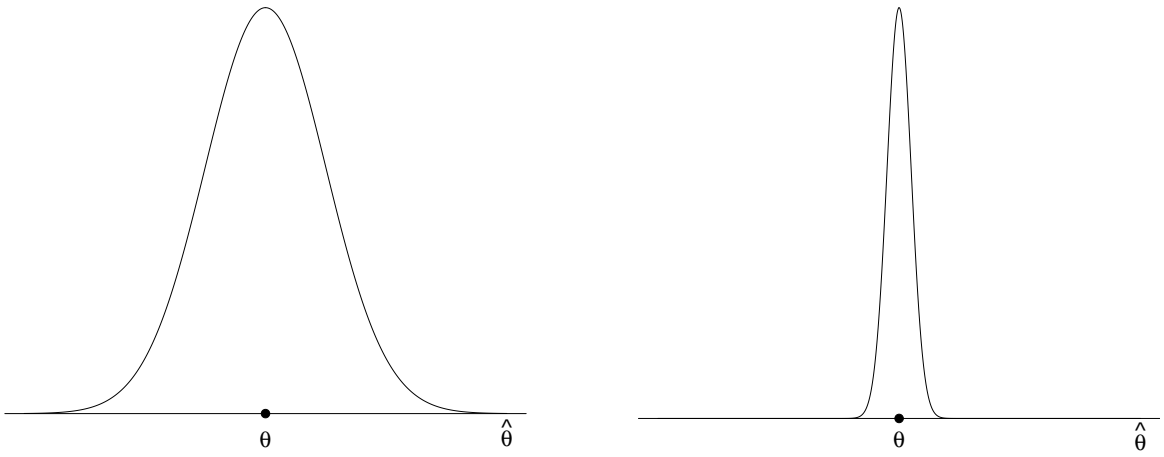


Figure 6.3: Sampling distribution of the point estimator $\widehat{\theta}$. The variability associated with $\widehat{\theta}$ is smaller for the sampling distribution on the right.

Discussion: Unbiasedness is a desirable property for a point estimator $\widehat{\theta}$ to possess. This deals with **accuracy**.

- Unbiased estimators are perfectly accurate. This does not mean $\widehat{\theta}$ will estimate θ perfectly for a given sample. Over the long run, $\widehat{\theta}$ will estimate θ correctly on average.
- In the light of the last remark, it is important to understand that $\widehat{\theta}$ will probably miss θ for a given sample−even when $\widehat{\theta}$ is unbiased. By how much will it miss? This is a question about **precision**.
- Figure 6.3 (above) shows two sampling distributions, and $\widehat{\theta}$ is an unbiased estimator in both. However, the variability in the sampling distribution on the right is smaller. That is, when $\widehat{\theta}$ "misses" θ, it doesn't miss by as much. The point estimator $\widehat{\theta}$ whose sampling distribution is depicted on the right is more precise.
- **Best of both worlds:** We would prefer point estimators $\widehat{\theta}$ to be unbiased (perfectly accurate) and have small variance (highly precise). In practice, improving the precision of a point estimator $\widehat{\theta}$ can usually be accomplished by increasing the sample size.

Terminology: The **standard error** of a point estimator $\widehat{\theta}$ quantifies how variable it is. Specifically, it equals

$$\text{se}(\widehat{\theta}) = \sqrt{V(\widehat{\theta})}.$$

In other words, the standard error of $\widehat{\theta}$ is the standard deviation of its sampling distribution. Therefore,

$$\text{smaller se}(\widehat{\theta}) \iff \widehat{\theta} \text{ more precise.}$$

Recall: We have seen standard errors before. In Example 5.2, we estimated a Weibull(β, η) distribution for the distance until failure (in km) for a population of shock absorbers. Here was the R output:

```
> options(digits=3)
> fitdist(distance.to.failure,distr="weibull",method="mle")

Fitting of the distribution ' weibull ' by maximum likelihood
Parameters:
      estimate Std. Error
shape      2.9      0.367
scale  19125.6   1140.512
```

In our new estimation language, we would say

- $\widehat{\beta} = 2.9$ is a point estimate for β, the population shape parameter
- $\widehat{\eta} = 19125.6$ is a point estimate for η, the population scale parameter
- The R output above also displays the standard errors of both point estimates. These describe how variable the point estimates are.
- Point estimates and standard errors will play an important role in writing confidence intervals. We start this discussion in the next chapter.

6.3 Sampling distribution of $\overline{X}$

Importance: Averages (sample means) are the most widely used statistics, so it is important to understand how they vary in repeated sampling. For example,

- average yield of a chemical production process
- average time to part failure
- average precipitation level
- average number of defects per piece of raw material.

Result 1: Suppose $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution. The sample mean $\overline{X}$ has the following sampling distribution:

$$\overline{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right).$$

- Our first observation here is

$$\text{normal population distribution} \implies \text{sampling distribution of } \overline{X} \text{ is also normal.}$$

- This result also reminds us that
$$E(\overline{X}) = \mu,$$
that is, the sample mean $\overline{X}$ is an unbiased estimator of the population mean μ.

- This result shows the standard error of $\overline{X}$ is
$$\text{se}(\overline{X}) = \sqrt{V(\overline{X})} = \sqrt{\frac{\sigma^2}{n}} = \frac{\sigma}{\sqrt{n}}.$$
This reveals the variability in the possible values of $\overline{X}$ depends on
  - the population standard deviation σ (for individuals in the population)
  - the sample size n.

Implication: Larger samples will reduce the variability associated with $\overline{X}$ as a point estimator of μ. This will lead to more precise estimates. This is also true when the population distribution is non-normal (Result 2; coming up).

Example 6.2. In cardiology, an ejection fraction (EF) measures your heart's ability to pump oxygen-rich blood out to your body. This is measured as a percentage and quantifies the amount of blood pumped out of the left ventricle when your heart contracts. Suppose for a population of healthy male subjects, the ejection fraction X is normally distributed with mean $\mu = 56$ and standard deviation $\sigma = 8$.

Q: What is the population distribution?
A: $X \sim \mathcal{N}(56, 64)$. This is the distribution of EF for all male subjects in the population.

Q: A random sample of $n = 16$ males is selected from the population and the EF is measured on each subject producing $X_1, X_2, ..., X_{16}$. What is the sampling distribution of $\overline{X}$, the sample mean EF?
A: Use Result 1:
$$\overline{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right) \implies \overline{X} \sim \mathcal{N}\left(56, \frac{64}{16}\right) \implies \overline{X} \sim \mathcal{N}(56, 4).$$
The sample mean $\overline{X}$ is normally distributed with mean 56 and variance 4.

Q: In the last part, what is the standard error of $\overline{X}$?
A: The standard error of $\overline{X}$ is the standard deviation of its sampling distribution, here,
$$\text{se}(\overline{X}) = \sqrt{4} = 2.$$
Note that this is also
$$\text{se}(\overline{X}) = \frac{\sigma}{\sqrt{n}} = \frac{8}{\sqrt{16}} = 2$$
using the formula above.

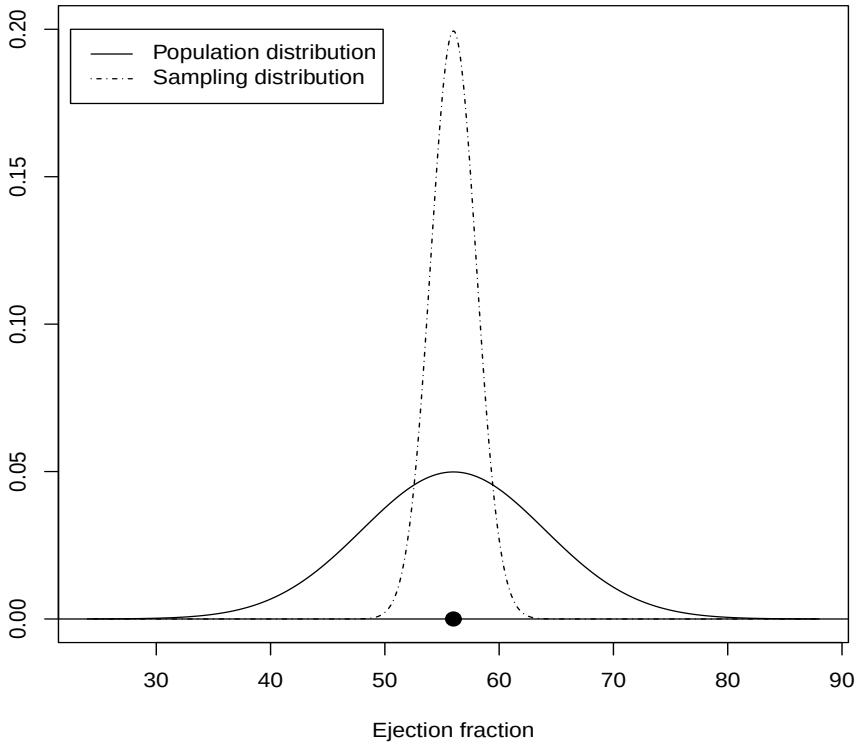


Figure 6.4: $\mathcal{N}(56, 64)$ pdf for X in Example 6.2. This serves as a model for the population of all healthy male subjects. The sampling distribution of $\overline{X}$ with $n = 16$ is also shown.

Q: Calculate $P(X > 60)$ and $P(\overline{X} > 60)$ and explain what these mean.
A: We want

$$P(X > 60) = P\left(\frac{X - 56}{8} > \frac{60 - 56}{8}\right) = P(Z > 0.5) \approx 0.309.$$

This means about 30.9% of the population of all male subjects will have an EF larger than 60. Also,

$$P(\overline{X} > 60) = P\left(\frac{\overline{X} - 56}{8/\sqrt{16}} > \frac{60 - 56}{8/\sqrt{16}}\right) = P(Z > 2) \approx 0.0228.$$

If we observed a random sample of $n = 16$ male subjects from this population, the probability the sample mean ejection fraction $\overline{X}$ would be larger than 60 is about 0.0228.

```
> options(digits=3)
> 1-pnorm(0.5,0,1)
[1] 0.309
> 1-pnorm(2,0,1)
[1] 0.0228
```

Recall: Result 1 informed us that when $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, the sample mean

$$\overline{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right).$$

Q: What if the population distribution is something else other than a normal distribution? What is the sampling distribution of $\overline{X}$ in this case?
A: We answer this question now, stating one of the most fascinating results in statistics.

Result 2: Suppose $X_1, X_2, ..., X_n$ is a random sample from a population distribution with mean μ and variance σ^2. When the sample size n is large, the sample mean

$$\overline{X} \sim \mathcal{AN}\left(\mu, \frac{\sigma^2}{n}\right).$$

The symbol $\mathcal{AN}$ is read "approximately normal." This result is called the **Central Limit Theorem (CLT)**.

Remark: The CLT implies the sample mean $\overline{X}$ will behave like a normal random variable (approximately) regardless of what the population distribution looks like. The population distribution could be skewed, bimodal, discrete, binary, or whatever. The only mathematical requirement is that the population variance $\sigma^2 < \infty$, which holds for nearly all probability distributions.

Example 6.3. In a textile production process, the number of defects (per square meter) in a certain fabric is assumed to follow a Poisson distribution with mean $\lambda = 1.5$. A quality control plan involves sampling 50 square meter pieces per day and inspecting them for defects.

Q: What is the population distribution?
A: Define

$$X = \text{number of defects per square meter of fabric.}$$

The population distribution is Poisson($\lambda = 1.5$). This is the distribution of the number of defects X for each square meter piece of fabric in the population.

Q: What is the sampling distribution of $\overline{X}$, the average number of defects for the 50 pieces observed on a given day?
A: The population mean is $\mu = 1.5$ and the population variance is $\sigma^2 = 1.5$. Recall that in the Poisson distribution, the mean and variance are equal. Now, use Result 2 (CLT):

$$\overline{X} \sim \mathcal{AN}\left(\mu, \frac{\sigma^2}{n}\right) \implies \overline{X} \sim \mathcal{AN}\left(1.5, \frac{1.5}{50}\right) \implies \overline{X} \sim \mathcal{AN}(1.5, 0.03).$$

Q: Assuming the population distribution is correct, how likely would it be to observe a sample mean $\overline{X}$ larger than 2 as part of the daily quality control plan?

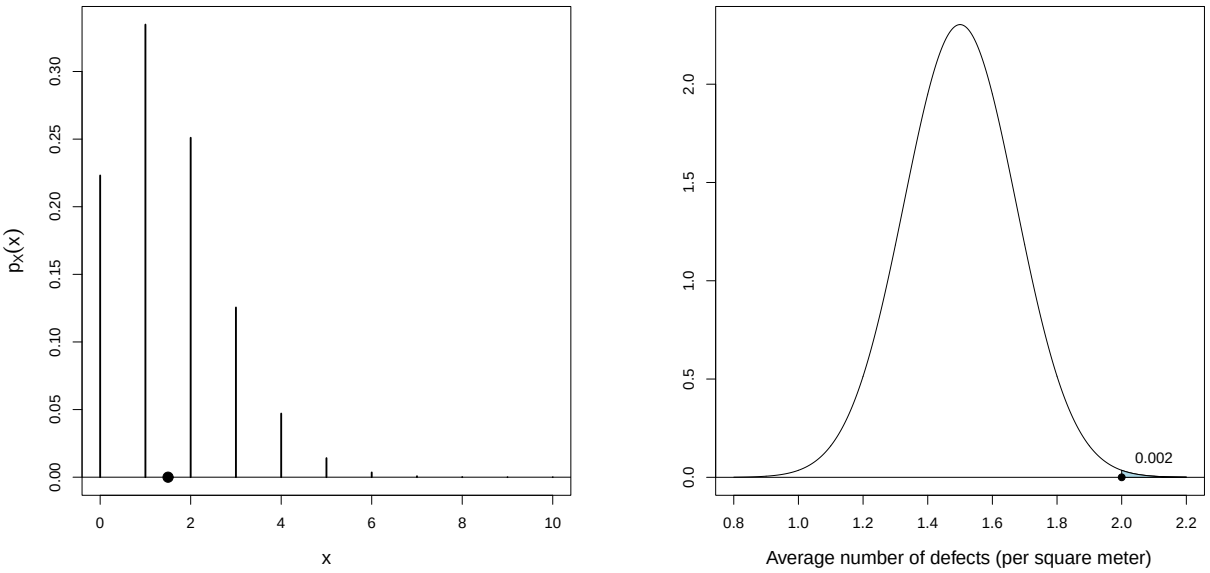


Figure 6.5: Left: Population distribution of $X \sim \text{Poisson}(\lambda = 1.5)$. The population mean $\mu = 1.5$ is shown using a solid circle. Right: Approximate sampling distribution of $\overline{X}$, the sample mean of $n = 50$ observations from the population. The probability $P(\overline{X} > 2) \approx 0.002$ is shown shaded.

A: We can calculate

$$P(\overline{X} > 2) = P\left(\frac{\overline{X} - 1.5}{\sqrt{1.5/50}} > \frac{2 - 1.5}{\sqrt{1.5/50}}\right) \approx P(Z > 2.89) \approx 0.002.$$

```
> options(digits=1)
> 1-pnorm(2.89,0,1)
[1] 0.002
```

Question for thought: Because $P(\overline{X} > 2) \approx 0.002$ is so small, what might be true if we actually observed a sample mean $\overline{X}$ larger than 2 on any given day? This would certainly not be expected if the population distribution was correct.

Back to the CLT: Because the CLT only approximates the sampling distribution of $\overline{X}$, that is,

$$\overline{X} \sim \mathcal{AN}\left(\mu, \frac{\sigma^2}{n}\right),$$

it is natural to wonder how good the approximation actually is. This depends primarily on two factors:

1. the sample size n. The larger the sample size, the better the approximation.
2. the amount of skewness in the population distribution. The closer the population distribution is to being **symmetric**, the better the approximation.

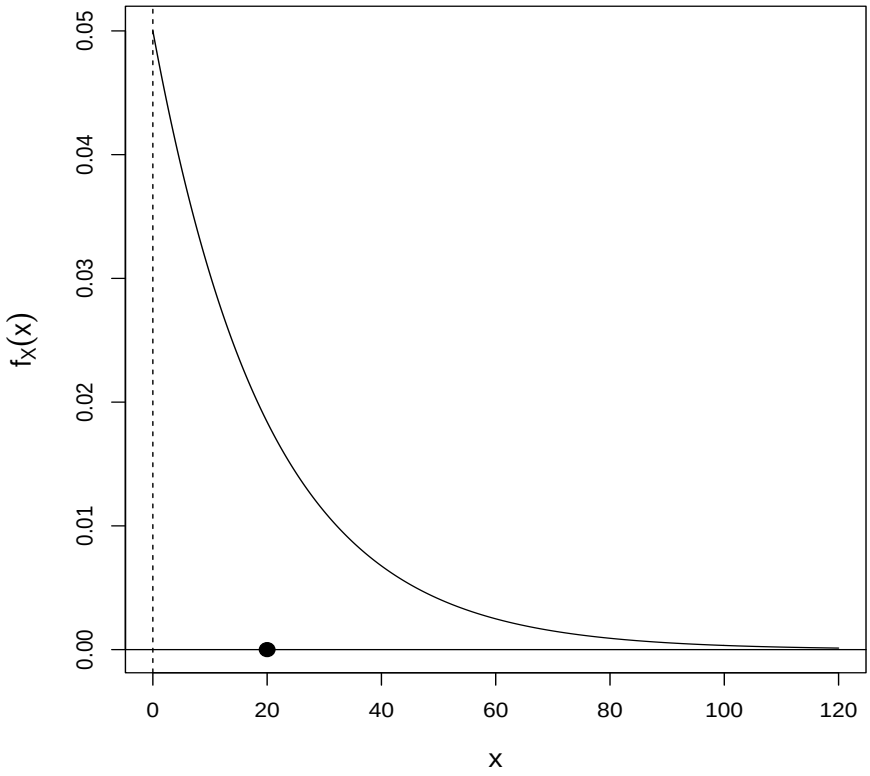


Figure 6.6: Population distribution of $X \sim$ exponential($\lambda = 0.05$) in Example 6.4. The population mean $\mu = 20$ is shown using a solid circle.

Remark: There is no "one sample size n that fits all" to ensure the CLT will offer a good approximation (although some textbooks claim $n \geq 30$ is the magic threshold). For population distributions which are symmetric or approximately symmetric, the sample size n doesn't have to be that large. For severely skewed distributions or distributions with other nonstandard shapes, the sample size might have to be larger.

Misinterpretation: Some students (and not-so-smart researchers) will interpret the CLT as "with a large enough sample, the data should look approximately normal." This is not correct. When you are sampling from a population, the population distribution remains fixed−it doesn't change. The fact that you have a larger sample simply means that you have more observations from the population. The CLT is a statement about the sampling distribution of the sample mean $\overline{X}$; not the shape of the population from which you are sampling. The population doesn't "become more normal" when you have larger samples.

Example 6.4. A clinical trial is being planned to test the effectiveness of semaglutide for weight loss in pre-diabetic patients. The time X (in days) to enroll a patient from this population into the trial follows an exponential distribution with $\lambda = 0.05$ so that the

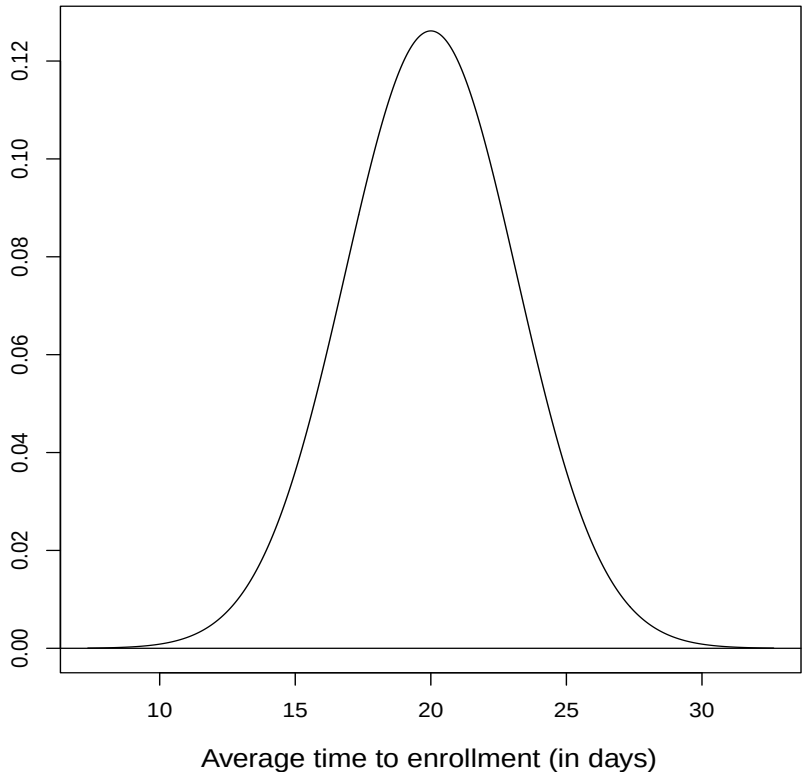


Figure 6.7: Approximate sampling distribution of $\overline{X}$ in Example 6.4.

population mean is

$$\mu = \frac{1}{\lambda} = \frac{1}{0.05} = 20 \text{ days.}$$

The population variance is

$$\sigma^2 = \frac{1}{\lambda^2} = \frac{1}{(0.05)^2} = 400 \text{ (days)}^2.$$

The goal is recruit 40 patients.

Q: What is the population distribution?
A: $X \sim$ exponential($\lambda = 0.05$). This is the distribution of the time to enrollment for individual patients in this population.

Q: What is the sampling distribution of $\overline{X}$, the sample mean time to enrollment for the 40 patients?
A: Use Result 2 (CLT):

$$\overline{X} \sim \mathcal{AN}\left(\mu, \frac{\sigma^2}{n}\right) \implies \overline{X} \sim \mathcal{AN}\left(20, \frac{400}{40}\right) \implies \overline{X} \sim \mathcal{AN}(20, 10).$$

This sampling distribution is shown in Figure 6.7 (above).

6.4 The t distribution

Recall: Suppose $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution. Result 1 informed us that

$$\overline{X} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right).$$

Therefore, if we standardize $\overline{X}$, that is, subtract its mean and divide through by its standard deviation (standard error), we obtain

$$Z = \frac{\overline{X} - \mu}{\sigma/\sqrt{n}} \sim \mathcal{N}(0, 1).$$

The random variable Z follows a **standard normal distribution**.

New result: If we replace the population standard deviation σ with the sample standard deviation S in the quantity above, we get a new distribution:

$$T = \frac{\overline{X} - \mu}{S/\sqrt{n}} \sim t(n-1),$$

a t **distribution** with $n-1$ degrees of freedom. This result will be used in the next chapter when we discuss confidence intervals for a population mean μ. More generally, the t distribution is widely used in statistical inference.

Facts: The t distribution has the following characteristics:

- Its pdf is continuous and symmetric about 0 (just like the standard normal pdf); see Figure 6.8 (next page).
- It is indexed by a value ν called the **degrees of freedom**. In practice, ν is usually an integer that depends on the sample size.
- When compared to the standard normal pdf, the t pdf is less peaked and has more probability (area) in the tails.
- As $\nu \to \infty$, the t pdf approaches the standard normal pdf. For $\nu \geq 30$ or so, it is very hard to distinguish the t pdf from the standard normal pdf with the naked eye.

MEAN/VARIANCE: If $T \sim t(\nu)$, then

$$\begin{aligned} E(T) &= 0 \\ V(T) &= \frac{\nu}{\nu - 2}. \end{aligned}$$

The mean is $E(T) = 0$, provided that $\nu > 1$. The variance formula above is only applicable when $\nu > 2$.

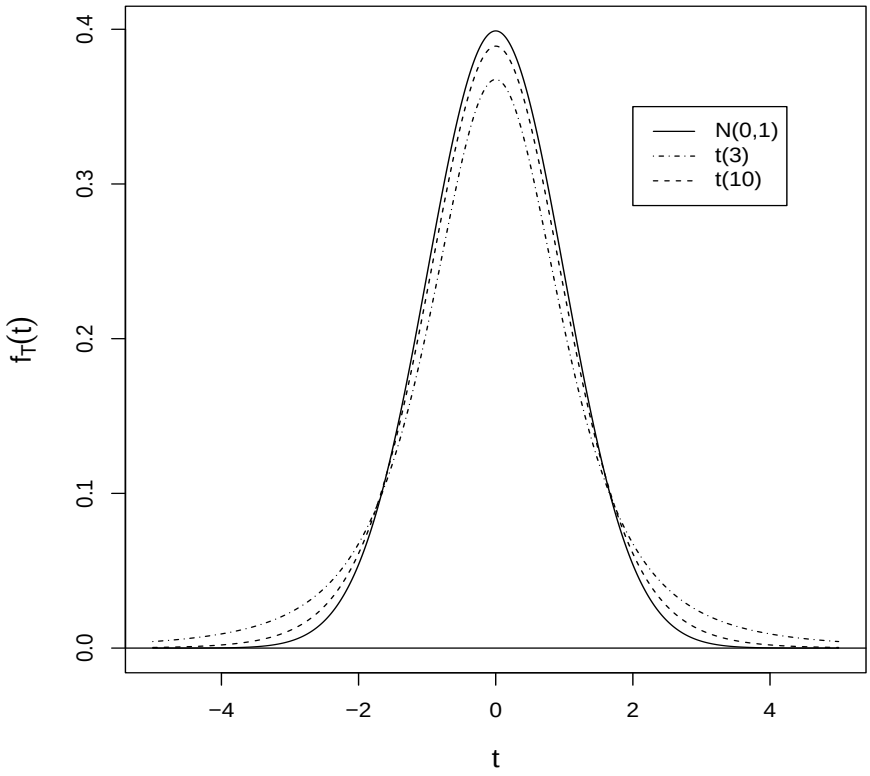


Figure 6.8: t pdfs with $\nu = 3$ and $\nu = 10$ degrees of freedom. The $\mathcal{N}(0, 1)$ pdf is shown as a reference.

Remark: There is a t pdf formula, but it is complicated and unnecessary for our purposes. R will compute probabilities and quantiles from any t distribution.

t **R CODE:** Suppose $T \sim t(\nu)$.

$F_T(t) = P(T \leq t)$	ϕ_p
`pt(t,`ν`)`	`qt(p,`ν`)`

For example, here are the 95th percentiles of each distribution in Figure 6.8 above:

```
> options(digits=3)
> qt(0.95,3) # 95th percentile of t(3)
[1] 2.35
> qt(0.95,10) # 95th percentile of t(10)
[1] 1.81
> qnorm(0.95,0,1) # 95th percentile of N(0,1)
[1] 1.64
```

6.5 Normal quantile-quantile plots

Recall: In the last chapter, we used **quantile-quantile (qq) plots** to assess whether the Weibull(β, η) population distribution was appropriate for a lifetime data set. We can make similar plots to assess whether a normal population distribution is appropriate.

Importance: We have just learned that when $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, the quantity

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

In other words, for the t distribution to result, we are assuming the population distribution (from which the data arise) is normal. Normality is a common assumption with many statistical inference techniques we will learn going forward. We need to have a way to assess whether this assumption is reasonable.

Recall: We can use qq plots to assess the normality assumption for the observed data in a sample. Recall how this plot is constructed:

- On the vertical axis, we plot the observed data ordered from low to high.
- On the horizontal axis, we plot the same number of (ordered) quantiles from the population distribution assumed for the observed data (here, a normal distribution).

Linearity in the qq plot supports the normal population assumption. A strong departure from linearity (e.g., extreme curvature) refutes it. Remember, we are looking for **general agreement** when we examine these plots.

Example 6.1 (continued). We observed a sample of 80 alloy specimens and measured the compressive strength (in psi) of each specimen:

105	221	183	186	121	181	180	143	97	154	153	174	120	168	167	141
245	228	174	199	181	158	176	110	163	131	154	115	160	208	158	133
207	180	190	193	194	133	156	123	134	178	76	167	184	135	229	146
218	157	101	171	165	172	158	169	199	151	142	163	145	171	148	158
160	175	149	87	160	237	150	135	196	201	200	176	150	170	118	149

Q: Is it reasonable to assume these data arise from a normal population distribution?
A: We can construct a qq plot for the data to answer this question; see Figure 6.9 (next page).

- The plot reveals some minor departures in both tails (lower and upper), but nothing that is too extreme.
- The plot is mostly supportive of the normality assumption for the population of alloy specimens; at least, there isn't strong evidence to refute normality here.

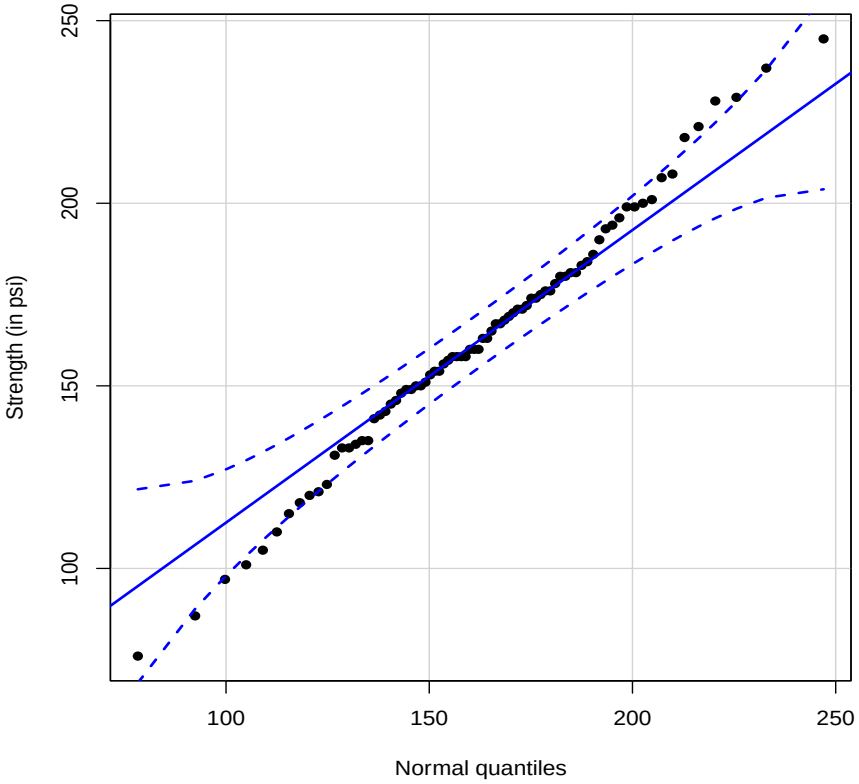


Figure 6.9: Normal quantile-quantile plot of the alloy strength data in Example 6.1.

Example 6.5. Arsenic (As) is a chemical element found naturally in ground water. Excessive levels may result from contamination caused by hazardous waste or by industries that make or use arsenic. Environmental engineers sampled $n = 102$ water wells in Texas and measured the arsenic concentration X (in parts per billion, ppb) for each well. The observed data are shown below:

17.6	10.4	13.5	4.0	19.9	16.0	12.0	12.2	11.4	12.7	3.0	10.3	21.4	19.4	9.0
6.5	10.1	8.7	9.7	6.4	9.7	63.0	15.5	10.7	18.2	7.5	6.1	6.7	6.9	0.8
73.5	12.0	28.0	12.6	9.4	6.2	15.3	7.3	10.7	15.9	5.8	1.0	8.6	1.3	13.7
2.8	2.4	1.4	2.9	13.1	15.3	9.2	11.7	4.5	1.0	1.2	0.8	1.0	2.4	4.4
2.2	2.9	3.6	2.5	1.8	5.9	2.8	1.7	4.6	5.4	3.0	3.1	1.3	2.6	1.4
2.3	1.5	4.0	1.8	2.6	3.4	1.4	10.7	18.2	7.7	6.5	12.2	10.1	6.4	10.7
6.1	0.8	12.0	28.1	9.4	6.2	7.3	9.7	62.1	15.5	6.4	9.5			

Q: Is it reasonable to assume these data arise from a normal population distribution?
A: Figure 6.10 (next page) shows the histogram and the normal qq plot for these data.

- The histogram shows a strong skewed right shape with multiple outliers, which we know doesn't align with the normal distribution.

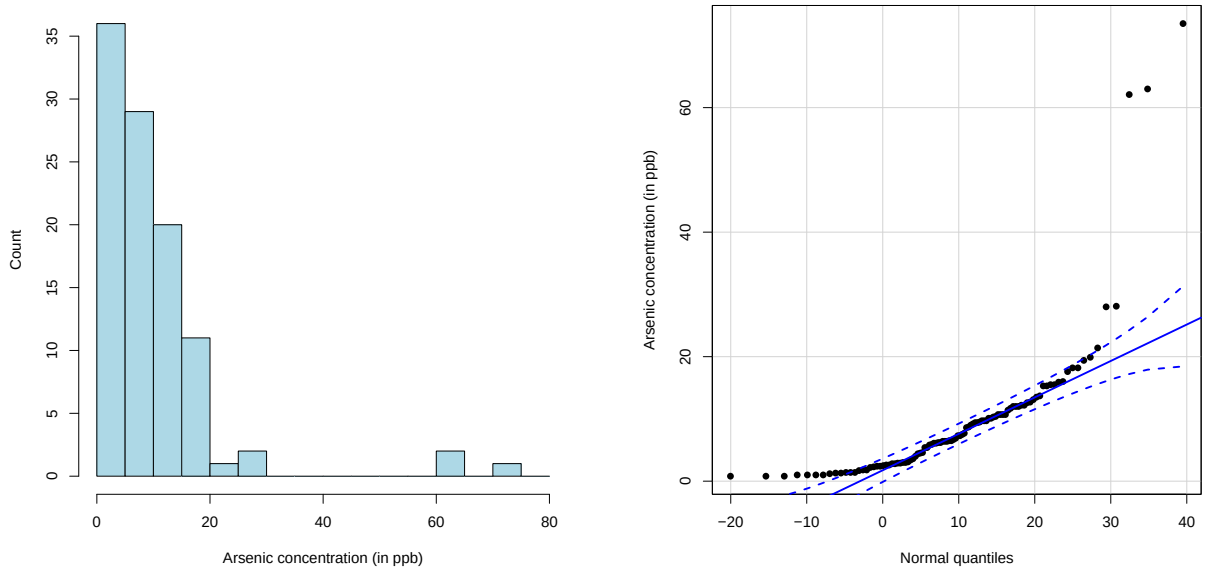


Figure 6.10: Left: Histogram of the $n = 102$ arsenic concentrations in Example 6.5. Right: Normal quantile-quantile plot.

- The appearance of the histogram appears to align more with an exponential or gamma population distribution.
- Not surprisingly, we see **strong disagreement** in the observed data and the normal quantiles in the qq plot. Normality is not a good assumption for these data.

Robustness: We know when $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, the quantity

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

Q: What if $X_1, X_2, ..., X_n$ is a random sample from some other population distribution (e.g., Poisson, exponential, etc.)? Does the sampling distribution for T above still hold?
A: No, it doesn't, but it may be approximately correct even when the population distribution is not normal. The approximation is best when

- the sample size n is larger
- the population distribution is more symmetric.

Terminology: In statistical inference, we say that a result or method is **robust** when the accuracy of the result (or success of the method) does not depend critically on the underlying assumptions. The t sampling distribution result above is robust to the normality assumption for the population distribution. This means the normality assumption isn't that critical, especially when the two conditions above are met.

7 One-Sample Inference

Preview: In this chapter, we will discuss one-sample inference for three population parameters:

- a population **mean** μ (Section 7.1)
- a population **variance** σ^2 (Section 7.2)
- a population **proportion** p (Section 7.3).

Remember these quantities describe an entire population, so they are unknown. Our goal is to use sample information to estimate them. This is what statistical inference is all about. To "infer" means to "draw a conclusion about something based on evidence."

Example 7.1. A general contractor buys standard-sized bricks from a local brick supplier. The manufactured specifications call for each brick to weigh 4.5 lbs, but there has been recent concern on the contractor's part the supplier is selling bricks that do not conform to this specified weight on average. The contractor asks for a sample of bricks to be selected and each brick weighed, producing the data below.

4.54	4.64	4.58	4.78	4.58	4.62	4.55	4.63	4.51	4.49	4.50	4.51
4.63	4.47	4.36	4.61	4.53	4.45	4.26	4.40	4.48	4.63	4.47	4.46
4.57	4.41	4.50	4.62	4.50	4.61	4.49	4.79	4.39	4.70	4.39	4.45

There are $n = 36$ bricks in the sample, but this is a small collection when compared to the tens of thousands of bricks produced each day by the supplier. We can think of the population here as all bricks manufactured by the supplier using the current production process.

- One statistical inference question is, "What are the plausible values of the population mean brick weight μ that are consistent with the data in the sample?" Is 4.5 lbs included within this range of plausible values? If not, then it would appear there is something wrong with the brick supply in terms of the average weight.
- Another equally important question deals with variability. The target specification is 4.5 lbs, but we notice from the data above there is variation in the sample observations (some weights are below 4.5 lbs; some are above). Is there "too much" weight variation in the population of all bricks? A range of plausible values of σ^2, the population variance, would be helpful in assessing whether there is excessive weight variability in the brick supply.

Statistical formulation: How do we answer these questions? That is what we will do in this chapter. We begin by assuming a random sample of observations $X_1, X_2, ..., X_n$ is available from a population described by a normal distribution with mean μ and variance σ^2. Our goal is to use the evidence in the sample to formulate (or "to infer") a range of plausible values for these population parameters.

7.1 Confidence interval for a population mean μ

Recall: From the last chapter, we learned that if $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, then

$$T = \frac{\overline{X} - \mu}{S/\sqrt{n}} \sim t(n-1),$$

a t distribution with $n-1$ degrees of freedom. This describes the sampling distribution of T, that is, how T will vary probabilistically when sampling from a $\mathcal{N}(\mu, \sigma^2)$ population.

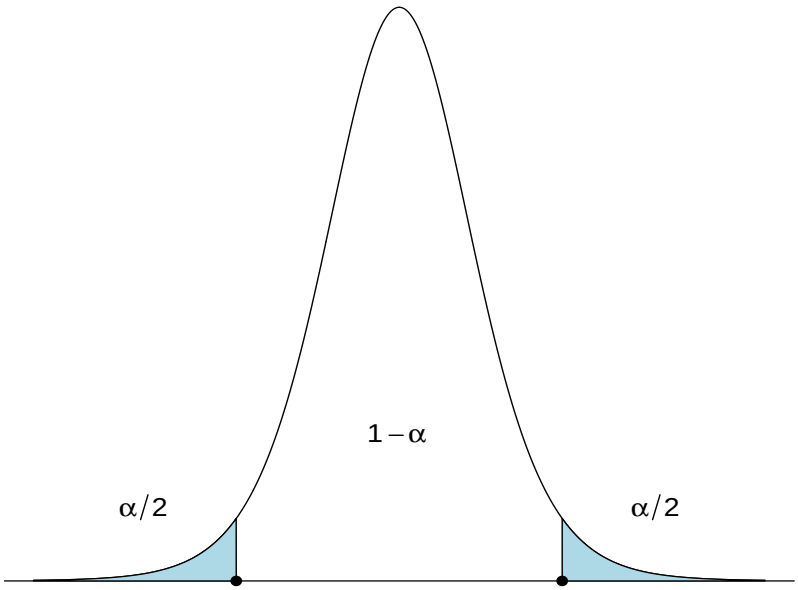


Figure 7.1: t pdf with $n-1$ degrees of freedom. The lower $\alpha/2$ quantile $-t_{n-1,\alpha/2}$ and the upper $\alpha/2$ quantile $t_{n-1,\alpha/2}$ are shown using solid circles.

Notation: We introduce notation that identifies quantiles from a $t(n-1)$ distribution. Define

$$\begin{aligned} t_{n-1,\alpha/2} &= \textbf{upper } \alpha/2 \text{ quantile from } t(n-1) \text{ pdf} \\ -t_{n-1,\alpha/2} &= \textbf{lower } \alpha/2 \text{ quantile from } t(n-1) \text{ pdf.} \end{aligned}$$

Because the $t(n-1)$ pdf is symmetric about zero, these two quantiles are equal in absolute value (the upper quantile is positive; the lower quantile is negative); see Figure 7.1. For example, if $n = 10$ and $\alpha = 0.05$, then

$$\begin{aligned} t_{9,0.025} &\approx 2.26 \\ -t_{9,0.025} &\approx -2.26. \end{aligned}$$

We can obtain quantiles like these using the `qt` function in R:

```
> options(digits=3)
> qt(0.975,9) # upper 0.025 quantile
[1] 2.26
> qt(0.025,9) # lower 0.025 quantile
[1] -2.26
```

Derivation: For any value of α, $0 < \alpha < 1$, we can write

$$\begin{aligned}
1-\alpha &= P\left(-t_{n-1,\alpha/2} < T < t_{n-1,\alpha/2}\right) \quad \longleftarrow \text{ this comes from Figure 7.1.} \\
&= P\left(-t_{n-1,\alpha/2} < \frac{\overline{X}-\mu}{S/\sqrt{n}} < t_{n-1,\alpha/2}\right) \\
&= P\left(-t_{n-1,\alpha/2}\frac{S}{\sqrt{n}} < \overline{X}-\mu < t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}\right) \\
&= P\left(t_{n-1,\alpha/2}\frac{S}{\sqrt{n}} > \mu-\overline{X} > -t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}\right) \\
&= P\left(\overline{X}+t_{n-1,\alpha/2}\frac{S}{\sqrt{n}} > \mu > \overline{X}-t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}\right) \\
&= P\left(\overline{X}-t_{n-1,\alpha/2}\frac{S}{\sqrt{n}} < \mu < \overline{X}+t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}\right).
\end{aligned}$$

We call

$$\left(\overline{X}-t_{n-1,\alpha/2}\frac{S}{\sqrt{n}},\ \overline{X}+t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}\right)$$

a $100(1-\alpha)\%$ **confidence interval** for the population mean μ. This is written more succinctly as

$$\overline{X} \pm t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}.$$

Example 7.1 (continued). Calculate a 95% confidence interval for the population mean brick weight μ using the sample data in Example 7.1:

4.54	4.64	4.58	4.78	4.58	4.62	4.55	4.63	4.51	4.49	4.50	4.51
4.63	4.47	4.36	4.61	4.53	4.45	4.26	4.40	4.48	4.63	4.47	4.46
4.57	4.41	4.50	4.62	4.50	4.61	4.49	4.79	4.39	4.70	4.39	4.45

Sample statistics: We use R to first find the sample mean $\overline{x}$ and the sample standard deviation s for these data:

```
> options(digits=3)
> mean(bricks) # sample mean
[1] 4.53
> sd(bricks) # sample standard deviation
[1] 0.113
```

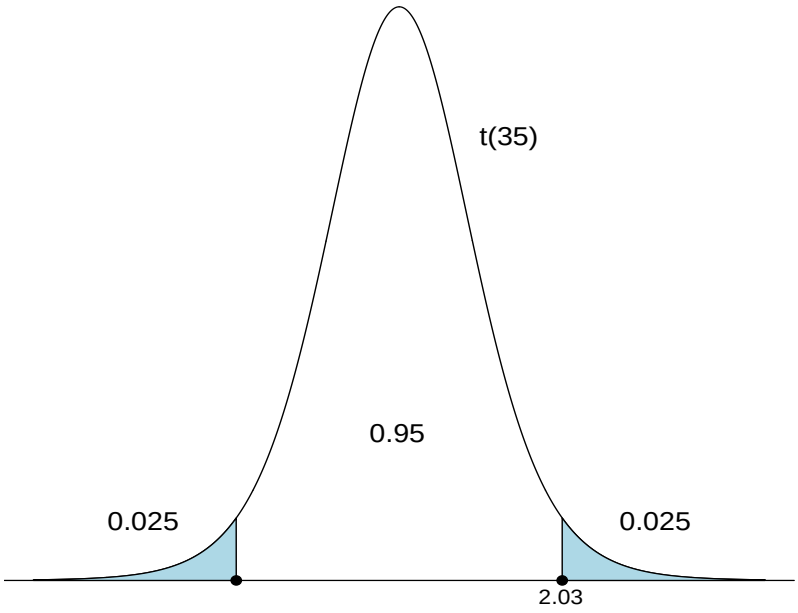
Therefore, we have

$$\begin{aligned} \overline{x} &\approx 4.53 \text{ lbs} \\ s &\approx 0.113 \text{ lbs.} \end{aligned}$$

Quantiles: With a sample of size $n = 36$, we use the $t(35)$ distribution. Note that

$$95\% \text{ confidence} \implies \alpha = 0.05 \implies \alpha/2 = 0.025 \implies t_{35,0.025} \approx 2.03.$$

```
> qt(0.975,35)
[1] 2.03
```



A 95% confidence interval for the population mean μ is

$$\overline{x} \pm t_{n-1,\alpha/2}\frac{s}{\sqrt{n}} \implies 4.53 \pm 2.03\left(\frac{0.113}{\sqrt{36}}\right) \implies (4.49, 4.57).$$

Interpretation: We are 95% confident the population mean brick weight μ is between 4.49 and 4.57 lbs.

Implementation in R: We can calculate confidence intervals for a population mean μ using the `t.test` function in R:

```
> options(digits=3)
> t.test(bricks,conf.level=0.95)$conf.int
[1] 4.49 4.57
```

Using this function avoids the piecemeal approach outlined above, although it is helpful to see all the parts that go into the calculation of the interval.

Discussion: We now make several remarks about the confidence interval

$$\overline{X} \pm t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}$$

for a population mean μ. Many of these remarks apply to other types of confidence intervals we will learn later.

- First, note the form of the interval:

$$\underbrace{\text{point estimate}}_{\overline{X}} \pm \underbrace{\text{quantile}}_{t_{n-1,\alpha/2}} \times \underbrace{\text{standard error}}_{S/\sqrt{n}}.$$

  Other confidence intervals we will learn have this same form.

- Here is how we interpret the interval:

  "We are $100(1-\alpha)\%$ confident the population mean μ is in this interval."

- Unfortunately, the word "confident" does not mean "probability."

  - The word "confidence" means if we sampled from the population over and over again, each time calculating a $100(1-\alpha)\%$ confidence interval for the population mean μ, then $100(1-\alpha)\%$ of the intervals we calculated would contain μ.

- In other words, "confidence" refers to "long term behavior" of many intervals; not probability for the interval we calculated. For example, in Example 7.1, it would **not** be correct to write

$$P(4.49 < \mu < 4.57) = 0.95$$

  or say "the population mean brick weight μ is between 4.49 and 4.57 lbs with probability 0.95." Remember, the population mean μ is a fixed number−it isn't random. It does not make sense to assign probabilities to events that are not random.

- Unfortunately, there is no way to tell if the confidence interval we calculated contains μ or not. Remember, μ is a population-level parameter so it is unknown. The only way we could determine if the interval contains μ would be to observe every individual in the population. Of course, in this unrealistic scenario, we could determine μ exactly so there would be no need to estimate it with a confidence interval.

- Standard confidence levels are

  - 90% ($\alpha = 0.10$)
  - 95% ($\alpha = 0.05$) $\longleftarrow$ the most common
  - 99% ($\alpha = 0.01$)

  The larger the confidence level, the larger the "long term percentage" of intervals that will contain the population mean μ. Larger confidence levels will produce wider intervals to guarantee this.

- We have all heard the aphorism, "There is no free lunch."
  - If you use a larger confidence level, then what you get is a larger percentage of confidence intervals that will contain μ. The price you pay is that your interval will be wider and, therefore, less precise.
  - Smaller confidence levels will produce a narrower interval which is more precise. The price you pay is that a smaller percentage of confidence intervals will actually contain μ.
  - Therefore, when writing confidence intervals, there is always a tradeoff between "confidence" and "precision."

Assumptions: Statistical inference procedures (like confidence intervals) are derived from certain assumptions. It is important to know what these assumptions are, how critical they are, and how to check them. The confidence interval

$$\overline{X} \pm t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}$$

for a population mean μ is created under the following assumptions:

1. $X_1, X_2, ..., X_n$ is a random sample from the population
2. The population distribution is $\mathcal{N}(\mu, \sigma^2)$.

It is under these assumptions that

$$T = \frac{\overline{X} - \mu}{S/\sqrt{n}} \sim t(n-1),$$

and this was the starting point to derive the interval above.

- The random sampling assumption is critical. We must assume all observations are coming from the same population distribution and that the observations are mutually independent. This ensures our sample will be representative of the population.
- The normality assumption for the population is not so critical. Remember, we learned in the last chapter the sampling distribution result for T above is **robust** to the normality assumption for the population.
  - This means we can still use the confidence interval formula above even when the normal population assumption does not hold exactly.
  - We can check the normality assumption by using qq plots with the observed sample. As long as there are no **serious departures** from normality detected in the plot, the confidence interval above will likely operate close to the nominal confidence level.
  - Even if there are serious departures from normality, the effect of this is usually small when the sample size n is large. This is a consequence of the CLT.

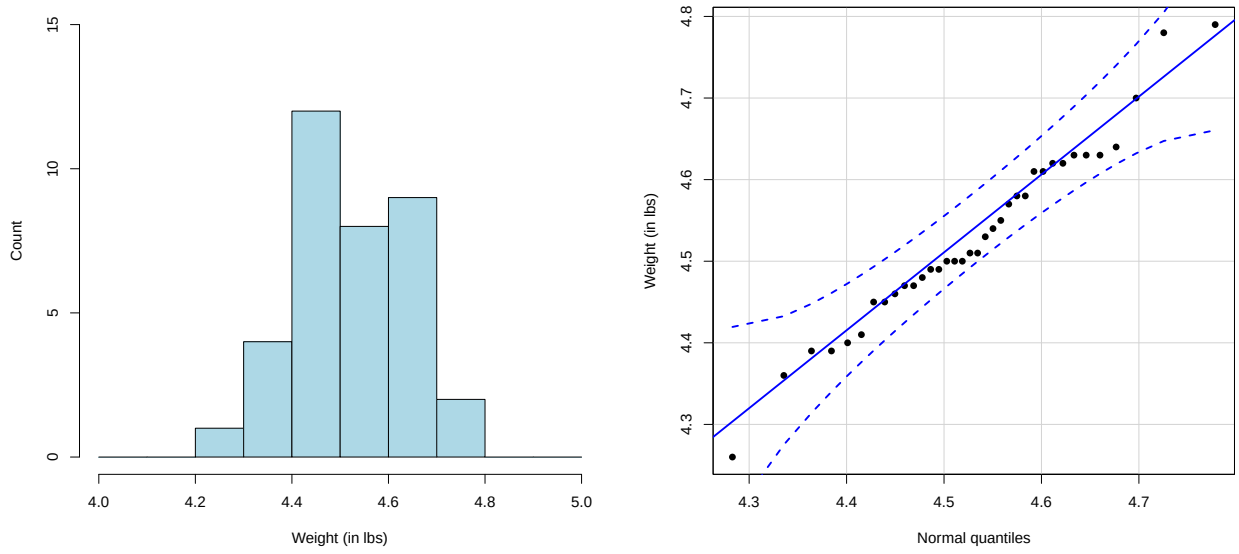


Figure 7.2: Left: Histogram of the $n = 36$ brick weights in Example 7.1. Right: Normal quantile-quantile plot.

Brick weight data: The qq plot for the brick weight data in Figure 7.2 (above, right) does not reveal any serious departures from normality. We can feel comfortable reporting $(4.49, 4.57)$ as a 95% confidence interval for μ, the population mean brick weight.

7.2 Confidence interval for a population variance σ^2

Remark: In some situations, we aren't concerned with the mean of the population but the variance instead. This is especially true in manufacturing settings. Too much variation can lead to inconsistent product quality and reduced customer satisfaction. On the other hand, small levels of variation are associated with predictability. Ensuring predictable results in production and construction is essential for meeting specifications and maintaining a positive reputation with customers.

New result: If $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, then

$$Q = \frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1),$$

a χ^2 **distribution** with $n-1$ degrees of freedom. This describes the sampling distribution of Q, that is, how Q will vary probabilistically when sampling from a $\mathcal{N}(\mu, \sigma^2)$ population.

Importance: The χ^2 distribution (and this sampling distribution result above) will be used to develop a confidence interval for the population variance σ^2.

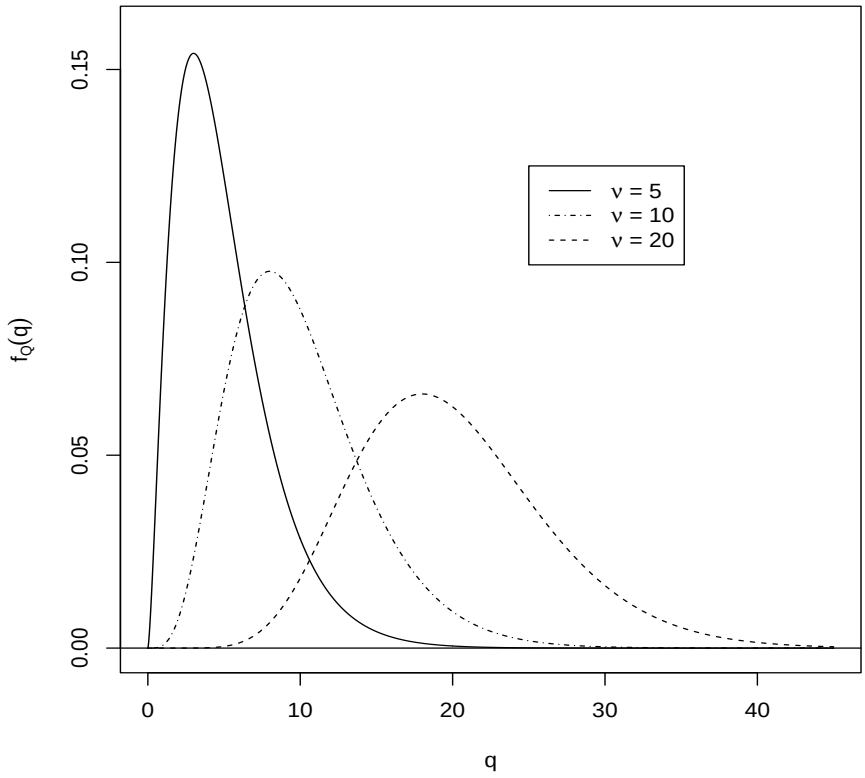


Figure 7.3: χ^2 pdfs with different degrees of freedom.

Facts: The χ^2 distribution has the following characteristics:

- Its pdf is continuous, skewed right, and its support is positive values only (no negative values); see Figure 7.3 above.
- It is indexed by a value ν called the **degrees of freedom**. In practice, ν is usually an integer that depends on the sample size.
- The χ^2 pdf formula is unnecessary for our purposes. R will compute probabilities and quantiles from any χ^2 distribution.

χ^2 **R CODE:** Suppose $Q \sim \chi^2(\nu)$.

$F_Q(q) = P(Q \leq q)$	ϕ_p
`pchisq(q,`ν`)`	`qchisq(p,`ν`)`

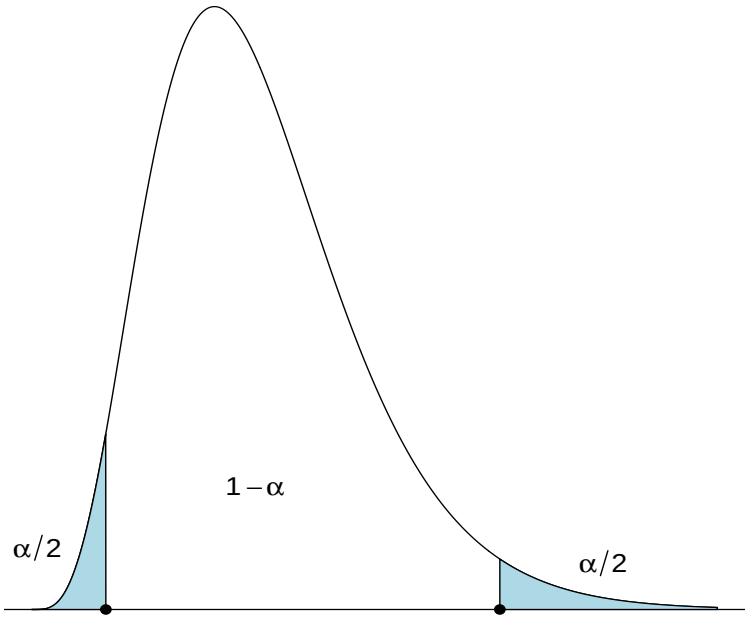


Figure 7.4: χ^2 pdf with $n-1$ degrees of freedom. The lower $\alpha/2$ quantile $\chi^2_{n-1,\alpha/2}$ and the upper $\alpha/2$ quantile $\chi^2_{n-1,1-\alpha/2}$ are shown using solid circles.

Notation: We introduce notation that identifies quantiles from a $\chi^2(n-1)$ distribution. Define

$$\begin{aligned} \chi^2_{n-1,1-\alpha/2} &= \textbf{upper } \alpha/2 \text{ quantile from } \chi^2(n-1) \text{ pdf} \\ \chi^2_{n-1,\alpha/2} &= \textbf{lower } \alpha/2 \text{ quantile from } \chi^2(n-1) \text{ pdf.} \end{aligned}$$

For example, if $n = 10$ and $\alpha = 0.05$, then

$$\begin{aligned} \chi^2_{9,0.975} &\approx 19.02 \\ \chi^2_{9,0.025} &\approx 2.7. \end{aligned}$$

We can obtain quantiles like these using the `qchisq` function in R:

```
> options(digits=4)
> qchisq(0.975,9) # upper 0.025 quantile
[1] 19.02
> qchisq(0.025,9) # lower 0.025 quantile
[1] 2.7
```

Derivation: For any value of α, $0 < \alpha < 1$, we can write

$$\begin{aligned}
1-\alpha &= P\left(\chi^2_{n-1,\alpha/2} < Q < \chi^2_{n-1,1-\alpha/2}\right) \quad \longleftarrow \text{ this comes from Figure 7.4.} \\
&= P\left(\chi^2_{n-1,\alpha/2} < \frac{(n-1)S^2}{\sigma^2} < \chi^2_{n-1,1-\alpha/2}\right) \\
&= P\left(\frac{1}{\chi^2_{n-1,\alpha/2}} > \frac{\sigma^2}{(n-1)S^2} > \frac{1}{\chi^2_{n-1,1-\alpha/2}}\right) \\
&= P\left(\frac{(n-1)S^2}{\chi^2_{n-1,\alpha/2}} > \sigma^2 > \frac{(n-1)S^2}{\chi^2_{n-1,1-\alpha/2}}\right) \\
&= P\left(\frac{(n-1)S^2}{\chi^2_{n-1,1-\alpha/2}} < \sigma^2 < \frac{(n-1)S^2}{\chi^2_{n-1,\alpha/2}}\right).
\end{aligned}$$

This shows

$$\left(\frac{(n-1)S^2}{\chi^2_{n-1,1-\alpha/2}}, \frac{(n-1)S^2}{\chi^2_{n-1,\alpha/2}}\right)$$

is a $100(1-\alpha)\%$ **confidence interval** for the population variance σ^2. We interpret the interval in the same way:

> "We are $100(1-\alpha)\%$ confident the population variance σ^2 is in this interval."

Note: A $100(1-\alpha)\%$ confidence interval for the **population standard deviation** σ arises from simply taking the square root of the endpoints of the σ^2 interval.

- That is,
$$\left(\sqrt{\frac{(n-1)S^2}{\chi^2_{n-1,1-\alpha/2}}}, \sqrt{\frac{(n-1)S^2}{\chi^2_{n-1,\alpha/2}}}\right)$$
is a $100(1-\alpha)\%$ confidence interval for the population standard deviation σ.
- This is usually preferred over the σ^2 interval, because standard deviation measures variability in terms of the original units (e.g., dollars, inches, days, etc.).
- Recall the variance σ^2 is measured in squared units (e.g., dollars^2, in^2, days^2, etc.) and is harder to interpret.

Example 7.2. A furniture company sells items designed for the customer to assemble him or herself. One item uses screws which are supposed to have a mean diameter of 1.200 cm. Periodically, quality control is performed to assess whether there is excessive variation in various screw dimensions. Specifications mandate the population standard deviation σ of the diameters should not exceed 0.005 cm. Otherwise, there is excessive variation in the production of this critical part which could lead to difficulty in construction and customer dissatisfaction.

Below are diameter measurements for a random sample $n = 40$ screws:

1.194	1.177	1.204	1.195	1.209	1.208	1.210	1.206	1.187	1.187
1.219	1.198	1.196	1.194	1.194	1.208	1.207	1.201	1.214	1.203
1.198	1.195	1.207	1.185	1.189	1.191	1.204	1.199	1.196	1.212
1.198	1.188	1.203	1.199	1.211	1.215	1.202	1.206	1.212	1.189

Q: Find a 99% confidence interval for the population standard deviation σ.
A: We will first find a 99% confidence interval for the population variance σ^2 and then take the square root of each interval endpoint.

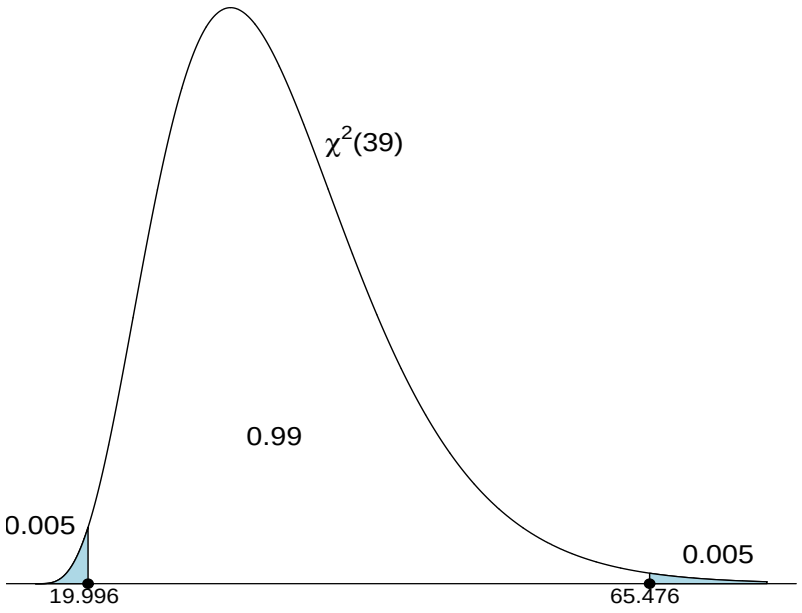
Sample statistics: We use R to first find the sample variance s^2 for these data:

```
> options(digits=5)
> var(screws) # sample variance
[1] 8.9372e-05
```

Therefore, we have

$$s^2 \approx 8.9372 \times 10^{-5} \text{ or } 0.000089372 \text{ cm}^2.$$

I'm retaining many digits due to the small numbers here (this will mitigate the impact of rounding error later).



Quantiles: With a sample of size $n = 40$, we use the $\chi^2(39)$ distribution. Note that

$$99\% \text{ confidence} \implies \alpha = 0.01 \implies \alpha/2 = 0.005 \implies \begin{cases} \chi^2_{39,0.005} \approx 19.996 \\ \chi^2_{39,0.995} \approx 65.476 \end{cases}$$

```
> qchisq(0.005,39)
[1] 19.996
> qchisq(0.995,39)
[1] 65.476
```

Therefore, a 99% confidence interval for the population variance σ^2 is

$$\left(\frac{(n-1)s^2}{\chi^2_{n-1,1-\alpha/2}}, \frac{(n-1)s^2}{\chi^2_{n-1,\alpha/2}}\right) \implies \left(\frac{39(0.000089372)}{65.476}, \frac{39(0.000089372)}{19.996}\right)$$
$$\implies (0.00005323, 0.00017431).$$

Interpretation: We are 99% confident the population variance σ^2 of the screw diameters is between 0.00005323 and 0.00017431 cm^2.

A 99% confidence interval for the population standard deviation σ is

$$(\sqrt{0.00005323}, \sqrt{0.00017431}) \implies (0.007, 0.013).$$

Interpretation: We are 99% confident the population standard deviation σ of the screw diameters is between 0.007 and 0.013 cm.

Discussion: This analysis suggests there is too much variation in the process producing the screws. The confidence interval consists entirely of values which are larger than 0.005 cm. It would be advised to revisit the production process and see if we can find assignable causes of variability−those causes which are inflating the variation in the diameters beyond the acceptable upper limit of 0.005 cm.

Implementation in R: There is no handy internal function in R that calculates a confidence interval for a population variance σ^2, so I wrote one. The function `var.ci` below asks the user to input the data set (`data`) and specify the confidence level.

```
var.ci = function(data,conf.level=0.99){
    df = length(data)-1
    chi.lower = qchisq((1-conf.level)/2,df)
    chi.upper = qchisq((1+conf.level)/2,df)
    s2 = var(data)
    c(df*s2/chi.upper,df*s2/chi.lower)
    }
```

Applying this function to the screw diameter data, we get the output

```
> options(digits=5)
> var.ci(screws,conf.level=0.99) # CI for population variance
[1] 5.3234e-05 1.7431e-04
> options(digits=1)
> sqrt(var.ci(screws,conf.level=0.99)) # CI for population standard deviation
[1] 0.007 0.013
```

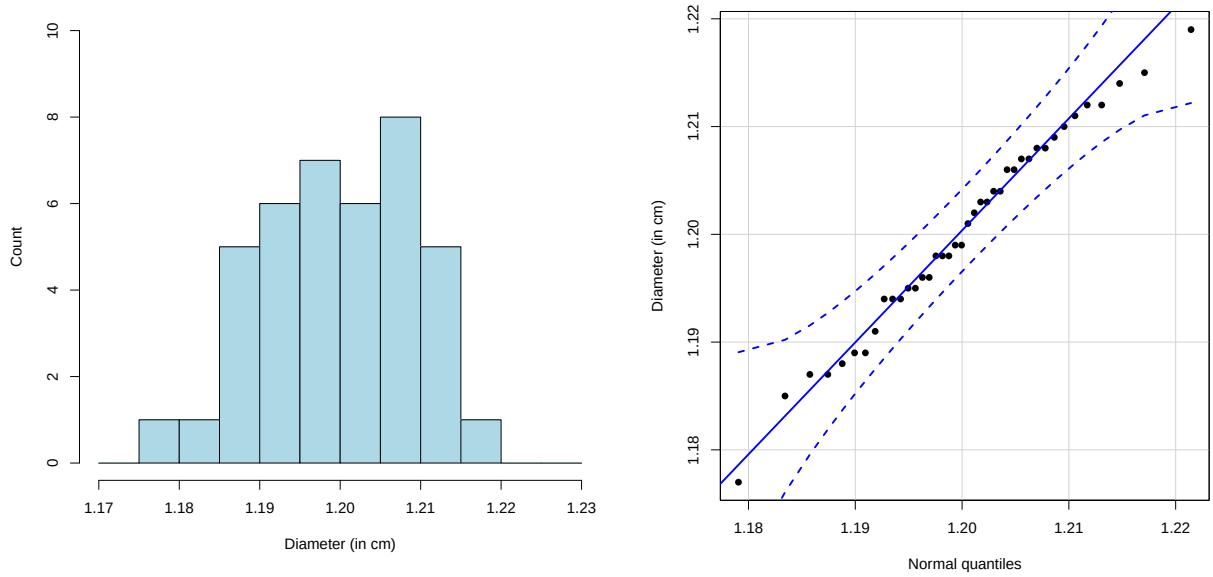


Figure 7.5: Left: Histogram of the $n = 40$ screw diameters in Example 7.2. Right: Normal quantile-quantile plot.

Assumptions: The confidence interval

$$\left(\frac{(n-1)S^2}{\chi^2_{n-1,1-\alpha/2}}, \frac{(n-1)S^2}{\chi^2_{n-1,\alpha/2}} \right)$$

for a population variance σ^2 is created under the following assumptions:

1. $X_1, X_2, ..., X_n$ is a random sample from the population
2. The population distribution is $\mathcal{N}(\mu, \sigma^2)$.

It is under these assumptions that

$$Q = \frac{(n-1)S^2}{\sigma^2} \sim \chi^2(n-1),$$

and this was the starting point to derive the interval above.

- The random sampling assumption is critical. We must assume all observations are coming from the same population distribution and that the observations are mutually independent. This ensures our sample will be representative of the population.
- The normality assumption for the population is also critical. The sampling distribution result for Q above is **not** robust to departures from the normality assumption for the population.

- This means the confidence interval for σ^2 (and therefore the one for σ too) is only meaningful when the population is $\mathcal{N}(\mu, \sigma^2)$. Departures from normality could cause the confidence intervals for σ^2 and σ to be misleading.
- This is different than what we learned with a confidence interval for a population mean μ using the t distribution. This interval is robust to the normality assumption.

Screw diameter data: The qq plot for the screw diameter data in Figure 7.5 (last page, right) does not reveal any serious departures from normality. We can feel comfortable reporting $(0.007, 0.013)$ as a 99% confidence interval for σ, the population standard deviation σ of the diameters.

7.3 Confidence interval for a population proportion p

Scenario: We now switch gears and focus on estimating a population proportion p. This parameter is relevant when we measure a binary characteristic on each individual. Here are some examples:

p = proportion of defective circuit boards
p = proportion of power supply units requiring service during a warranty period
p = proportion of customers who are satisfied
p = proportion of payments received on time
p = proportion of patients who respond to treatment.

To start our discussion, we need to recall the **Bernoulli trial** assumptions for each individual in the population:

1. each individual is categorized as a "success" or "failure"
2. the individuals are independent
3. the probability of "success" p is the same for every individual in the population.

In our examples above,

"success" $\longrightarrow$ circuit board defective
"success" $\longrightarrow$ PSU requires service during a warranty period
"success" $\longrightarrow$ customer satisfied
"success" $\longrightarrow$ payment received on time
"success" $\longrightarrow$ patient responds to treatment.

The parameter p is the proportion of "successes" in the population. Our goal is to estimate p with a confidence interval.

Recall: A **binomial distribution** arises when we observe a fixed number of Bernoulli trials and record

$$X = \text{number of successes (out of } n).$$

- In a statistical inference context, we envision each individual (e.g., circuit board, PSU, customer, payment, patient, etc.) in a random sample as a "trial," and we record a "success" or "failure" on each individual in the sample.
- If p is the proportion of "successes" in the population, then $X \sim b(n, p)$.

Point estimation: If X is the number of "successes" in a random sample of size n, then

$$\widehat{p} = \frac{X}{n}$$

is the **sample proportion**. This is simply the proportion of successes in the sample. We will use $\widehat{p}$ as a point estimator for the population proportion p. Mathematics can show these two results:

$$\begin{aligned} E(\widehat{p}) &= p \\ V(\widehat{p}) &= \frac{p(1-p)}{n}. \end{aligned}$$

The first result says the sample proportion $\widehat{p}$ is an **unbiased estimator** of the population proportion p. From the second result, we can find the standard error

$$\text{se}(\widehat{p}) = \sqrt{V(\widehat{p})} = \sqrt{\frac{p(1-p)}{n}}.$$

Recall the standard error of a point estimator (like $\widehat{p}$) measures how much variation is attached to it.

Important: Knowing the sampling distribution of $\widehat{p}$ is critical if we are going to develop a confidence interval for p. We appeal to an approximation (conferred by the CLT) which says

$$\widehat{p} \sim \mathcal{AN}\left(p, \frac{p(1-p)}{n}\right),$$

when the sample size n is large. Standardizing $\widehat{p}$, that is, subtracting the mean and dividing through by the standard deviation (standard error), we get

$$Z = \frac{\widehat{p} - p}{\sqrt{\frac{p(1-p)}{n}}} \sim \mathcal{AN}(0, 1),$$

an approximate **standard normal distribution**. We will use this result to write a confidence interval for p.

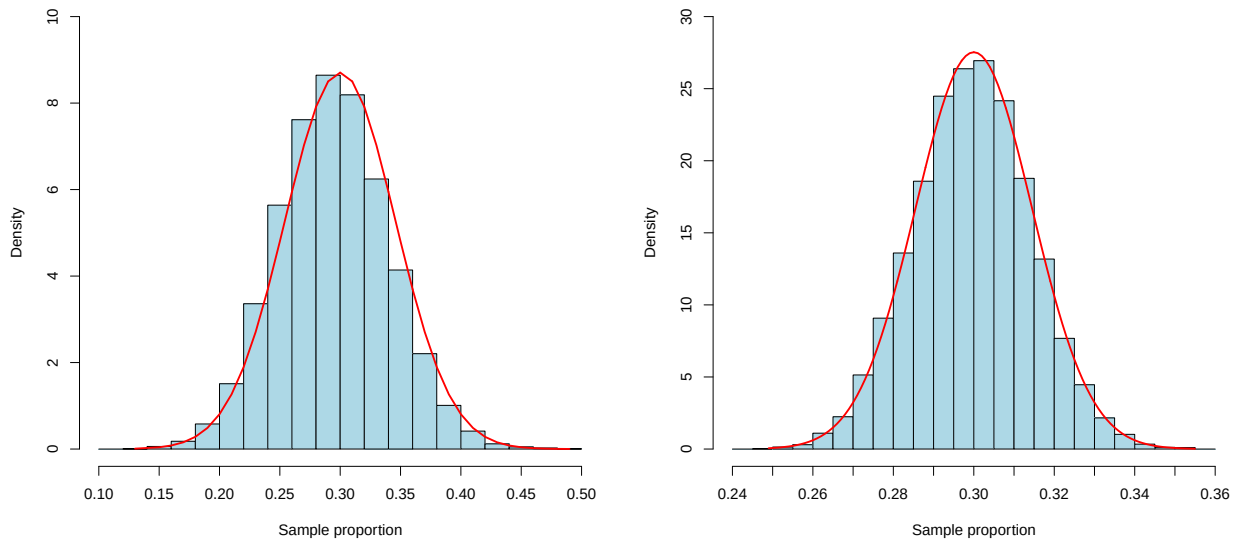


Figure 7.6: Left: Histogram of the 10,000 sample proportions $\widehat{p}$ when $n = 100$ and $p = 0.30$. Right: $n = 1000$ and $p = 0.30$. A normal pdf has been superimposed over each histogram. Density histograms have been used so that total histogram areas equal one.

Monte Carlo simulation: Before we develop the confidence interval for p, you should be reasonably convinced the sampling distribution result for $\widehat{p}$ on the previous page is correct (at least the approximate normality part).

- The histograms in Figure 7.6 (above) each show 10,000 simulated values of $\widehat{p}$ when the population proportion is $p = 0.30$; i.e., 30% of individuals in the population are "successes."
- The normal approximation to the histogram when $n = 100$ (left) is pretty good. The approximation is outstanding when $n = 1000$ (right). This illustrates how the normal approximation for the sampling distribution of $\widehat{p}$ is better for larger sample sizes.
- Notice how the histograms of $\widehat{p}$ are centered at $p = 0.30$. This is because $\widehat{p}$ is an unbiased estimator.
- Also notice how the variation in the sampling distribution is much smaller when the sample size $n = 1000$ (right). This can be seen also through standard error calculations:

$$\text{Left: } \text{se}(\widehat{p}) = \sqrt{\frac{0.30(0.70)}{100}} \approx 0.046$$

$$\text{Right: } \text{se}(\widehat{p}) = \sqrt{\frac{0.30(0.70)}{1000}} \approx 0.014.$$

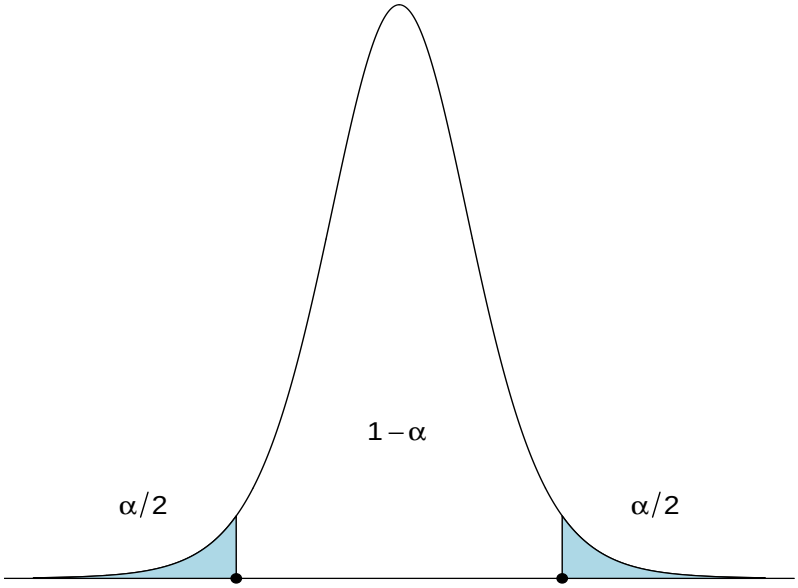


Figure 7.7: $\mathcal{N}(0,1)$ pdf. The lower $\alpha/2$ quantile $-z_{\alpha/2}$ and the upper $\alpha/2$ quantile $z_{\alpha/2}$ are shown using solid circles.

Notation: We introduce notation that identifies quantiles from a $\mathcal{N}(0,1)$ distribution. Define

$$\begin{aligned} z_{\alpha/2} &= \textbf{upper } \alpha/2 \text{ quantile from } \mathcal{N}(0,1) \text{ pdf} \\ -z_{\alpha/2} &= \textbf{lower } \alpha/2 \text{ quantile from } \mathcal{N}(0,1) \text{ pdf.} \end{aligned}$$

Because the $\mathcal{N}(0,1)$ pdf is symmetric about zero, these two quantiles are equal in absolute value (the upper quantile is positive; the lower quantile is negative); see Figure 7.7. For example, if $\alpha = 0.05$, then

$$\begin{aligned} z_{0.025} &\approx 1.96 \\ -z_{0.025} &\approx -1.96. \end{aligned}$$

We can obtain quantiles like these using the `qnorm` function in R:

```
> options(digits=3)
> qnorm(0.975,0,1)
[1] 1.96
> qnorm(0.025,0,1)
[1] -1.96
```

Derivation: For any value of α, $0 < \alpha < 1$, we can write

$$\begin{aligned}
1-\alpha &\approx P(-z_{\alpha/2} < Z < z_{\alpha/2}) \quad \longleftarrow \text{ this comes from Figure 7.7.} \\
&\approx P\left(-z_{\alpha/2} < \frac{\widehat{p}-p}{\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}} < z_{\alpha/2}\right) \quad \longleftarrow \text{ using an estimate of the standard error.} \\
&= P\left(-z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} < \widehat{p}-p < z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right) \\
&= P\left(z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} > p-\widehat{p} > -z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right) \\
&= P\left(\widehat{p}+z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} > p > \widehat{p}-z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right) \\
&= P\left(\widehat{p}-z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} < p < \widehat{p}+z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right).
\end{aligned}$$

We call

$$\left(\widehat{p}-z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}},\ \widehat{p}+z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}\right)$$

a $100(1-\alpha)\%$ **confidence interval** for the population proportion p. This is written more succinctly as

$$\widehat{p} \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}.$$

We interpret the interval in the same way:

> "We are $100(1-\alpha)\%$ confident the population proportion p is in this interval."

Discussion: Note the familiar form of the interval:

$$\underbrace{\text{point estimate}}_{\widehat{p}} \ \pm \ \underbrace{\text{quantile}}_{z_{\alpha/2}} \ \times \ \underbrace{\text{standard error}}_{\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}}.$$

This interval should be used only when the sample size n is "large." A common **rule of thumb** is to require

$$\begin{aligned}
n\widehat{p} &\geq 5 \\
n(1-\widehat{p}) &\geq 5.
\end{aligned}$$

Under these conditions, the CLT should adequately describe the sampling distribution of $\widehat{p}$, thereby making the confidence interval formula above approximately valid.

Example 7.3. One source of water pollution is gasoline leakage from underground storage tanks. In Pennsylvania, a random sample of $n = 74$ gasoline stations is selected from the state and the tanks are inspected; 10 stations are found to have at least one leaking tank.

Q: Calculate a 95% confidence interval for p, the population proportion of gasoline stations in Pennsylvania with at least one leaking tank.
A: In this example, we interpret

- gasoline station = "trial"
- at least one leaking tank at station = "success."

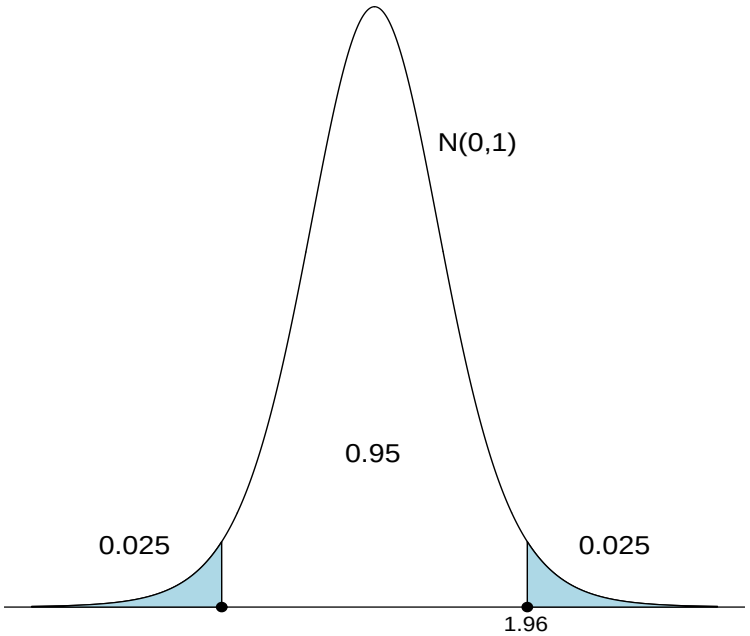
Note: There are about 10,000 gas stations in Pennsylvania. Therefore, p represents the proportion of stations with at least one leaking tank for this entire population. We have a random sample of 74 stations from this population.

Sample statistics: The sample proportion of stations with at least one leaking tank is

$$\widehat{p} = \frac{10}{74} \approx 0.135.$$

Quantiles: We use the $\mathcal{N}(0,1)$ distribution. Note that

$$95\% \text{ confidence} \implies \alpha = 0.05 \implies \alpha/2 = 0.025 \implies z_{0.025} \approx 1.96.$$




```
> options(digits=3)
> qnorm(0.975,0,1)
[1] 1.96
```

A 95% confidence interval for the population proportion p is

$$0.135 \pm 1.96\sqrt{\frac{0.135(1-0.135)}{74}} \implies (0.057, 0.213).$$

Interpretation: We are 95% confident the population proportion p of stations in Pennsylvania with at least one leaking tank is between 0.057 and 0.213.

CLT approximation check: We have

$$\begin{aligned} n\widehat{p} &= 74\left(\frac{10}{74}\right) = 10 \\ n(1-\widehat{p}) &= 74\left(1-\frac{10}{74}\right) = 64. \end{aligned}$$

Both of these are larger than 5, so we can feel comfortable using this confidence interval formula.

Implementation in R: There are various R functions and packages which produce confidence intervals for proportions, but they are far more elaborate than what we need. I wrote a simple function `p.ci` that automates the calculations. It requires the user to input the number of successes (`x`), the number of trials (`n`), and the confidence level:

```
p.ci = function(x,n,conf.level=0.95){
    est = x/n
    se = sqrt(est*(1-est)/n)
    z.upper = qnorm((1+conf.level)/2,0,1)
    c(est-z.upper*se,est+z.upper*se)
    }
```

Using this function with $x = 10$ and $n = 74$ in Example 7.3, we get

```
> options(digits=2)
> p.ci(10,74,conf.level=0.95)
[1] 0.057 0.213
```

7.4 Sample size determination

Importance: In the planning stages of an experiment or observational study, we need to first determine how many individuals should be sampled from a population. For example,

- We want to write a 90% confidence interval for the population mean time to part failure. How many parts should be sampled?
- We want to write a 95% confidence interval for the population proportion of patients who respond to a treatment. How many patients should we recruit?

The sample size n determines how precise confidence intervals will be. Larger sample sizes will give narrower (more precise) confidence intervals. Of course, sampling from a population always costs money, and larger samples will usually cost more too (think of the Pennsylvania gas station example). We will discuss statistical issues associated with sample size determination. There is a complementary set of practical issues like cost, time spent in sampling, personnel training, and other factors, which are also important.

Sample size for a population mean: Recall that if $X_1, X_2, ..., X_n$ is a random sample from a $\mathcal{N}(\mu, \sigma^2)$ population distribution, then

$$\overline{X} \pm t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}$$

is a $100(1-\alpha)\%$ confidence interval for the population mean μ. This interval is formed by taking a point estimate $\overline{X}$ and then adding/subtracting

$$t_{n-1,\alpha/2}\frac{S}{\sqrt{n}}.$$

We call this quantity the **margin of error** associated with the confidence interval. It consists of two parts:

- the quantile $t_{n-1,\alpha/2}$, which depends on the confidence level $100(1-\alpha)\%$
- $S/\sqrt{n}$, which is a point estimate of the population standard error $\sigma/\sqrt{n}$. Note the population standard error depends on the population standard deviation σ and the sample size n.

Recall the t distribution is similar to the standard normal distribution $\mathcal{N}(0,1)$, especially when the degrees of freedom $(n-1)$ is larger. Therefore, the margin of error above should be approximately equal to

$$B = z_{\alpha/2}\frac{\sigma}{\sqrt{n}}.$$

Solving this equation for n, we get

$$n = \left(\frac{z_{\alpha/2}\sigma}{B}\right)^2.$$

This is the sample size which will guarantee a prescribed confidence level $100(1-\alpha)\%$ and a margin of error B.

Note: To use the formula, we have to specify three things:

1. the confidence level $100(1-\alpha)\%$; this determines the $\mathcal{N}(0,1)$ quantile $z_{\alpha/2}$.
2. the margin of error B; note the interval length is twice the margin of error. Therefore, when you specify B, you are specifying how narrow (how precise) you want the interval to be.

3. the population standard deviation σ. This is the hardest part, because σ is a population-level parameter (so it is unknown). Generally, an "estimate" or "guess" is provided here. An upper bound for σ is used if you want to be **conservative**. This will provide a sample size larger than what is actually needed.

Example 7.4. In a biomedical experiment, we would like to estimate the population mean time to death μ for healthy rats (in days) when given a toxic substance. The research protocol requires a 95% confidence interval for μ with a margin of error equal to $B = 2$ days. From past studies, the time to death after administration of the toxin has been modeled by a normal distribution with standard deviation $\sigma = 8$ days.

Q: How many rats should we use for the experiment?
A: With $z_{0.05/2} = z_{0.025} \approx 1.96$, $B = 2$, and $\sigma = 8$, the minimum sample size is

$$n = \left(\frac{z_{\alpha/2}\sigma}{B}\right)^2 = \left(\frac{1.96 \times 8}{2}\right)^2 \approx 61.5.$$

We would need a random sample of $n = 62$ rats to achieve these goals. This will produce a 95% confidence interval for μ with a margin of error no larger than $B = 2$ days (total interval length no larger than 4 days).

Remark: We could weaken our requirements to (a) a lower 90% confidence level and (b) a margin of error of $B = 3$ days, which is less precise. The minimum sample size is now

$$n = \left(\frac{z_{\alpha/2}\sigma}{B}\right)^2 = \left(\frac{1.65 \times 8}{3}\right)^2 \approx 19.4.$$

We would need to sample only $n = 20$ rats to meet these weaker requirements.

Sample size for a population proportion: A $100(1-\alpha)\%$ confidence interval for a population proportion p is

$$\widehat{p} \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}}.$$

The margin of error associated with the interval

$$z_{\alpha/2}\sqrt{\frac{\widehat{p}(1-\widehat{p})}{n}} \quad \text{is an estimate of} \quad z_{\alpha/2}\sqrt{\frac{p(1-p)}{n}}.$$

A small problem arises, namely, the (population-level) margin of error

$$z_{\alpha/2}\sqrt{\frac{p(1-p)}{n}}$$

depends on p, which is what we are trying to estimate with a confidence interval. The "workaround" is to elicit a "guess" of what p is, say p_0, and use

$$B = z_{\alpha/2}\sqrt{\frac{p_0(1-p_0)}{n}}$$

instead. Solving this equation for n, we get

$$n = \left(\frac{z_{\alpha/2}}{B}\right)^2 p_0(1-p_0).$$

This is the sample size which will guarantee a prescribed confidence level $100(1-\alpha)\%$ and a margin of error B.

Remark: If there is no sensible guess for p available, use $p_0 = 0.5$. The resulting sample size n will be as large as possible. Put another way, using $p_0 = 0.5$ gives the most **conservative** solution. This is true because

$$n = n(p_0) = \left(\frac{z_{\alpha/2}}{B}\right)^2 p_0(1-p_0),$$

when viewed as a function of p_0, is maximized when $p_0 = 0.5$. However, the resulting sample size could be very large, perhaps much larger than is practical to use.

Example 7.5. You have been asked to estimate the proportion of parts in a certain manufacturing process that need to be "scrapped;" e.g., the part is so defective that it can not be used or reworked. If this proportion is larger than 10 percent, it will be deemed by management to be an unacceptable continued operating cost and a substantial process overhaul will be performed. Past experience suggests the scrap rate is about 5 percent, but recent information suggests this rate may be increasing.

You would like to write a 95% confidence interval for p, the population proportion of parts that will be scrapped, with a margin of error equal to $B = 0.02$.

Q: How many parts should you ask to be sampled?
A: For 95% confidence, we use $z_{0.05/2} = z_{0.025} \approx 1.96$. In providing an initial guess p_0, we have different options; we could use

$$\begin{aligned} p_0 &= 0.05 \text{ (historical scrap rate)} \\ p_0 &= 0.10 \text{ ("critical mass" value)} \\ p_0 &= 0.50 \text{ (most conservative choice).} \end{aligned}$$

For these choices, we have

$$\begin{aligned} n &= \left(\frac{1.96}{0.02}\right)^2 0.05(1-0.05) \approx 457 \\ n &= \left(\frac{1.96}{0.02}\right)^2 0.10(1-0.10) \approx 865 \\ n &= \left(\frac{1.96}{0.02}\right)^2 0.50(1-0.50) \approx 2401. \end{aligned}$$

This shows how the "guess" p_0 can have a substantial impact on the final sample size calculation. Furthermore, it may not be practical to sample 2,401 parts, as would be required by the most conservative approach.

8 Two-Sample Inference

Preview: We now move to situations where there are two populations of interest. We have a random sample from each population and the goal is to infer how the populations compare with each other. For example,

- We would like to compare the mean arsenic concentration of ground water wells in urban areas to the mean concentration of wells in rural areas. How do the population means μ_1 and μ_2 compare?
- We would like to compare the variation in brick weights from two different suppliers who manufacture the same standard-size brick. How do the population variances σ_1^2 and σ_2^2 compare?
- We would like to compare the proportion of patients who respond to a new treatment to the proportion who respond to a conventional treatment. How do the population proportions p_1 and p_2 compare?

Comparing two groups (populations) is one of the most common goals in the practice of statistics. In this chapter, we will examine statistical inference methods which allow us to make these types of comparisons above. The outline has the same structure as the last chapter, namely, we will

- compare two population **means** μ_1 and μ_2 (Sections 8.1 and 8.2)
- compare two population **variances** σ_1^2 and σ_2^2 (Section 8.3)
- compare two population **proportions** p_1 and p_2 (Section 8.4).

In each setting, we will form specific confidence intervals which allow us to compare one population parameter to the other.

8.1 Comparing two population means with independent samples

Setting: Suppose we have two **independent** random samples:

Sample 1 : $X_{11}, X_{12}, ..., X_{1n_1}$ is a random sample from a $\mathcal{N}(\mu_1, \sigma_1^2)$ population
Sample 2 : $X_{21}, X_{22}, ..., X_{2n_2}$ is a random sample from a $\mathcal{N}(\mu_2, \sigma_2^2)$ population.

Our goal is to compare the population means μ_1 and μ_2. This will be done by forming a confidence interval for the **population mean difference**

$$\Delta = \mu_1 - \mu_2.$$

Importantly, note that if the two population means are equal (i.e., $\mu_1 = \mu_2$), then the population mean difference is $\Delta = \mu_1 - \mu_2 = 0$.

Note: Here are some clarifying remarks about the two-sample setting:

- When we say the two samples are **independent**, informally, we mean observations on individuals in one sample are not influenced by the observations on individuals in the other sample.
- The double subscript notation in X_{ij} is needed to identify which sample the observation is in ($i = 1$ means first sample; $i = 2$ means second sample) and which observation we are talking about in that sample. In general,

  $$X_{ij} = j\text{th observation in the } i\text{th sample},$$

  for $i = 1, 2$, and $j = 1, 2, ..., n_i$. For example,
  - X_{11} is the first observation in Sample 1
  - X_{23} is the third observation in Sample 2.
- The sample size of the first random sample is n_1. The sample size of the second random sample is n_2. The sample sizes don't have to be equal. For example, we might sample $n_1 = 25$ wells in urban areas and $n_2 = 20$ wells in rural areas.
- There are four population-level parameters: the two population means μ_1 and μ_2 and the two population variances σ_1^2 and σ_2^2. All of these are unknown.
- We assume each population distribution is normal. As in the last chapter, it will be important to think about how critical this assumption is (robustness).

Sample statistics: We define the sample means and sample variances for both samples:

$$\overline{X}_{1+} = \frac{1}{n_1}\sum_{j=1}^{n_1} X_{1j} = \text{sample mean for sample 1}$$

$$\overline{X}_{2+} = \frac{1}{n_2}\sum_{j=1}^{n_2} X_{2j} = \text{sample mean for sample 2}$$

$$S_1^2 = \frac{1}{n_1 - 1}\sum_{j=1}^{n_1}(X_{1j} - \overline{X}_{1+})^2 = \text{sample variance for sample 1}$$

$$S_2^2 = \frac{1}{n_2 - 1}\sum_{j=1}^{n_2}(X_{2j} - \overline{X}_{2+})^2 = \text{sample variance for sample 2.}$$

A natural **point estimator** for the population mean difference $\Delta = \mu_1 - \mu_2$ is

$$\widehat{\Delta} = \overline{X}_{1+} - \overline{X}_{2+}.$$

We will form a confidence interval for Δ using $\widehat{\Delta}$ as a point estimator. This requires us to learn about the sampling distribution of $\widehat{\Delta}$ so that we can identify correct quantiles and estimate its standard error.

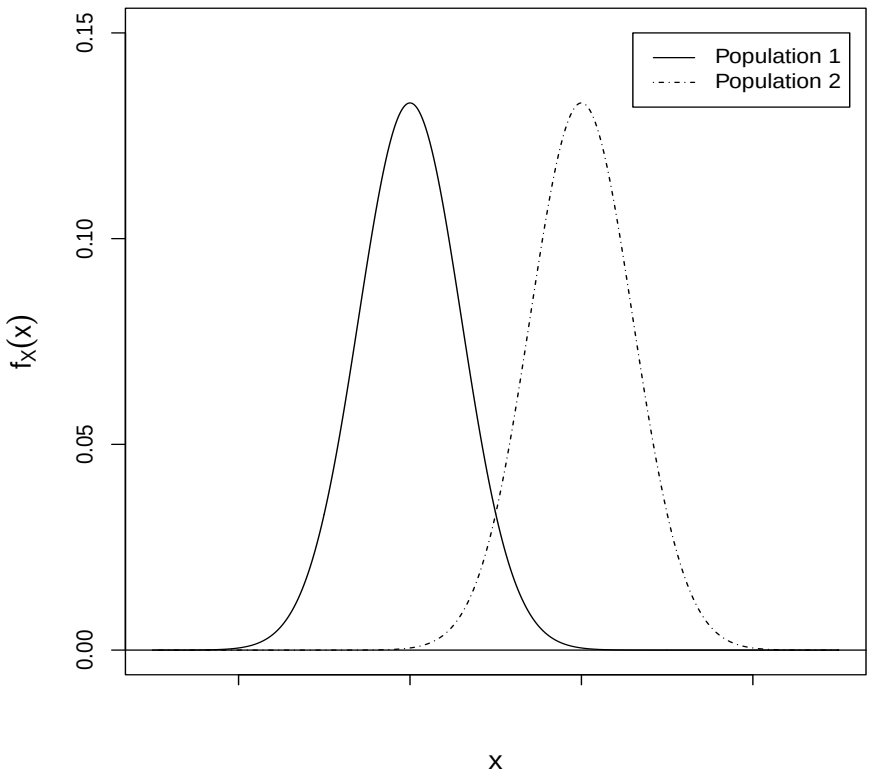


Figure 8.1: Two normal pdfs with equal variances ($\sigma_1^2 = \sigma_2^2$). Note the population mean difference $\Delta = \mu_1 - \mu_2 < 0$.

Interesting: Precisely how we form a confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ depends on which assumption we make regarding the population variances σ_1^2 and σ_2^2. There are two cases:

- $\sigma_1^2 = \sigma_2^2 \longrightarrow$ the two population variances are equal (Section 8.1.1)
- $\sigma_1^2 \neq \sigma_2^2 \longrightarrow$ the two population variances are not equal (Section 8.1.2).

8.1.1 Confidence interval for $\Delta = \mu_1 - \mu_2$ when $\sigma_1^2 = \sigma_2^2$

Result: Under the assumptions outlined at the beginning of this section (i.e., independent random samples, normal populations) and when $\sigma_1^2 = \sigma_2^2$, the quantity

$$T = \frac{(\overline{X}_{1+} - \overline{X}_{2+}) - (\mu_1 - \mu_2)}{\sqrt{S_p^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} \sim t(n_1 + n_2 - 2),$$

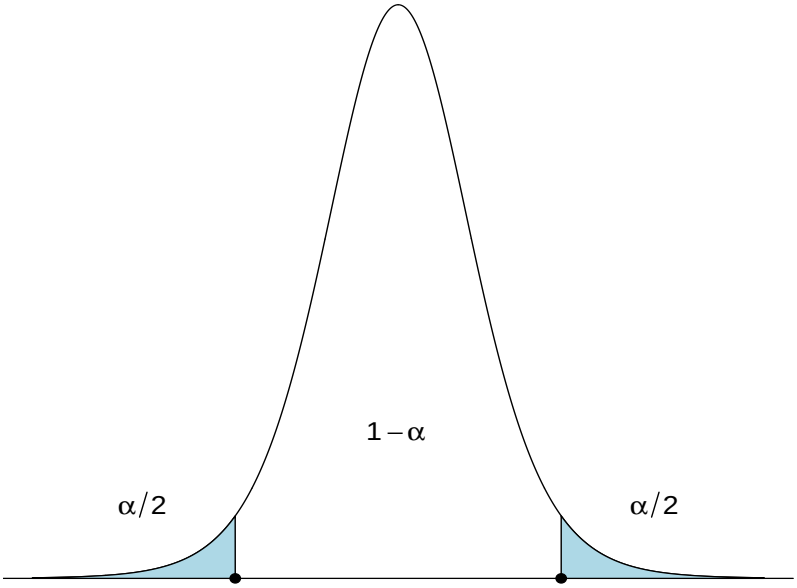


Figure 8.2: t pdf with $n_1 + n_2 - 2$ degrees of freedom. The lower $\alpha/2$ quantile $-t_{n_1+n_2-2,\alpha/2}$ and the upper $\alpha/2$ quantile $t_{n_1+n_2-2,\alpha/2}$ are shown using solid circles.

a t distribution with $n_1 + n_2 - 2$ degrees of freedom; see Figure 8.2 above. This describes the sampling distribution of T, that is, how T will vary probabilistically when sampling from two (independent) normal populations with equal variances.

Remarks:

- The **pooled variance estimator**

$$S_p^2 = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2}{n_1 + n_2 - 2}$$

  is an unbiased estimator of the common population variance $\sigma_1^2 = \sigma_2^2 = \sigma^2$. It is a weighted average of the sample variances S_1^2 and S_2^2 from the two samples. This is an unbiased estimator only when the population variances are equal.

- The sampling distribution $T \sim t(n_1 + n_2 - 2)$, shown above, depends on the sample sizes n_1 and n_2.

- Define

$$\begin{aligned} t_{n_1+n_2-2,\alpha/2} &= \textbf{upper } \alpha/2 \text{ quantile from } t(n_1 + n_2 - 2) \text{ pdf} \\ -t_{n_1+n_2-2,\alpha/2} &= \textbf{lower } \alpha/2 \text{ quantile from } t(n_1 + n_2 - 2) \text{ pdf.} \end{aligned}$$

  Because the $t(n_1 + n_2 - 2)$ pdf is symmetric about zero, these two quantiles are equal in absolute value (the upper quantile is positive; the lower quantile is negative).

From Figure 8.2 (previous page), we have

$$\begin{aligned} 1-\alpha &= P(-t_{n_1+n_2-2,\alpha/2} < T < t_{n_1+n_2-2,\alpha/2}) \\ &= P\left(-t_{n_1+n_2-2,\alpha/2} < \frac{(\overline{X}_{1+} - \overline{X}_{2+}) - (\mu_1 - \mu_2)}{\sqrt{S_p^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}} < t_{n_1+n_2-2,\alpha/2} \right). \end{aligned}$$

After performing algebraic rearrangements similar to those in the last chapter, we obtain

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{n_1+n_2-2,\alpha/2}\sqrt{S_p^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}$$

as a $100(1-\alpha)\%$ **confidence interval** for the population mean difference $\Delta = \mu_1 - \mu_2$.

- We see this interval has the familiar form:

$$\underbrace{\text{point estimate}}_{\overline{X}_{1+}-\overline{X}_{2+}} \pm \underbrace{\text{quantile}}_{t_{n_1+n_2-2,\alpha/2}} \times \underbrace{\text{standard error}}_{\sqrt{S_p^2\left(\frac{1}{n_1}+\frac{1}{n_2}\right)}}.$$

- We interpret the interval in the same way:

> "We are $100(1-\alpha)\%$ confident the population mean difference $\Delta = \mu_1 - \mu_2$ is in this interval."

Important: Here is how we use the confidence interval to compare the population means μ_1 and μ_2 when a $100(1-\alpha)\%$ confidence level is used:

- If the confidence interval for Δ consists entirely of positive values; e.g., (5.5, 12.3), we would infer
$$\Delta = \mu_1 - \mu_2 > 0 \implies \mu_1 > \mu_2.$$

- If the confidence interval for Δ consists entirely of negative values; e.g., $(-12.3, -5.5)$, we would infer
$$\Delta = \mu_1 - \mu_2 < 0 \implies \mu_1 < \mu_2.$$

- If the confidence interval for Δ contains "0;" e.g., $(-5.5, 12.3)$, we cannot infer an ordering between μ_1 and μ_2. What this would suggest is that
$$\Delta = \mu_1 - \mu_2 = 0$$
is a plausible value for the population mean difference. In other words, we don't have sufficient evidence that one population mean is larger than the other.

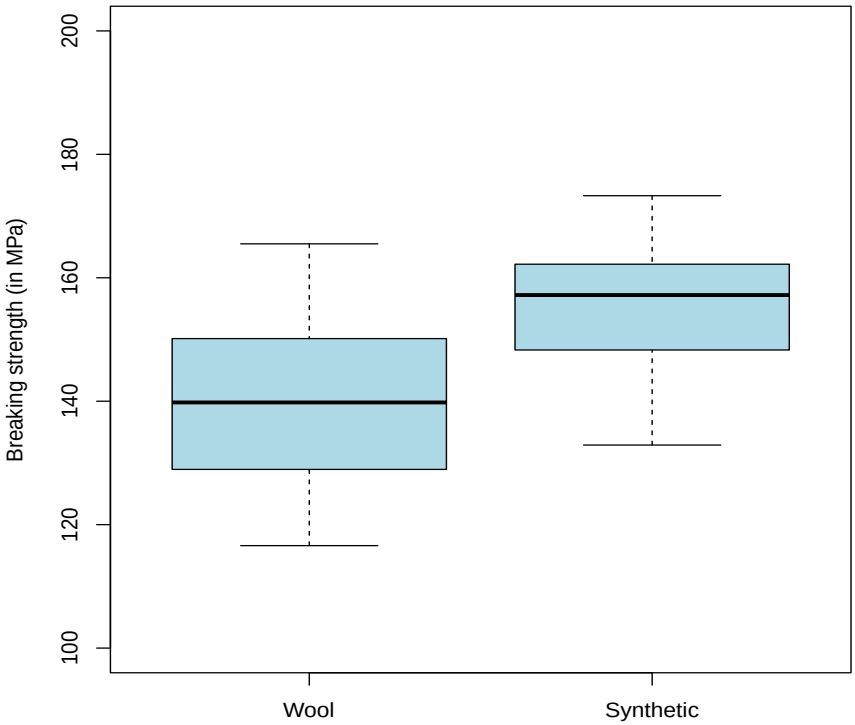


Figure 8.3: Fabric strength data. Boxplots of breaking strengths (in MPa) for independent samples of wool and synthetic fabric.

Example 8.1. Textile engineers would like to compare the mean breaking strength (in megapascals, MPa) of two types of fabric: wool and synthetic. Independent random samples of fabric material are taken from each group and the strength of each piece is measured using a tensile testing machine which stretches the fabric until it breaks. The data are shown below:

Wool	116.6	123.8	148.8	127.7	141.3	129.1	139.9	149.4	148.8	130.1
($n_1 = 20$)	135.9	125.5	128.8	154.7	155.1	155.9	132.9	165.5	150.9	139.7
Synthetic	157.2	144.5	157.9	161.3	144.4	165.8	169.3	163.4	151.3	140.2
($n_2 = 25$)	157.1	162.6	158.7	161.9	173.3	148.3	149.0	158.8	149.0	162.2
	132.9	170.3	134.1	151.4	138.6					

Boxplots of the two samples are shown in Figure 8.3 above; these plots use the five-number summary statistics from each sample:

```
> options(digits=4)
> quantile(wool,type=2) # 5-number summary
   0%   25%   50%   75%  100%
116.6 128.9 139.8 150.2 165.5
```

```
> quantile(synthetic,type=2)
   0%   25%   50%   75%  100%
132.9 148.3 157.2 162.2 173.3
```

Q: Find a 95% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$.
A: We can use the `t.test` function in R to calculate the confidence interval directly:

```
> options(digits=2)
> t.test(wool,synthetic,conf.level=0.95,var.equal=TRUE)$conf.int
[1] -21.8  -7.2
```

A 95% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ is

$$(-21.8, -7.2) \text{ MPa.}$$

Interpretation: We are 95% confident the population mean difference $\Delta = \mu_1 - \mu_2$ is between -21.8 and -7.3 MPa. Because this interval consists entirely of negative values, we can infer the population mean breaking strength of the wool fabric (μ_1) is less than the population mean breaking strength of the synthetic fabric (μ_2).

Assumptions: The confidence interval

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{n_1+n_2-2,\alpha/2}\sqrt{S_p^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}$$

for the population mean difference $\Delta = \mu_1 - \mu_2$ is created using four assumptions:

1. We have random samples from each population.
2. The two samples are independent.
3. The population variances σ_1^2 and σ_2^2 are equal.
4. The population distributions are normal.

Discussion: The confidence interval above is **not robust** to departures of the first three assumptions.

- The random sampling assumption ensures that each sample is representative of its population. The independence assumption (between samples) is also important.
- It is **critical** the equal population variance assumption $\sigma_1^2 = \sigma_2^2$ holds; otherwise, the pooled sample variance S_p^2 is not estimating anything meaningful, and the standard error of the point estimator $\widehat{\Delta} = \overline{X}_{1+} - \overline{X}_{2+}$ could be way off−especially if the sample sizes n_1 and n_2 are vastly different. This would produce a confidence interval that is too short or too long for the confidence level we are using.

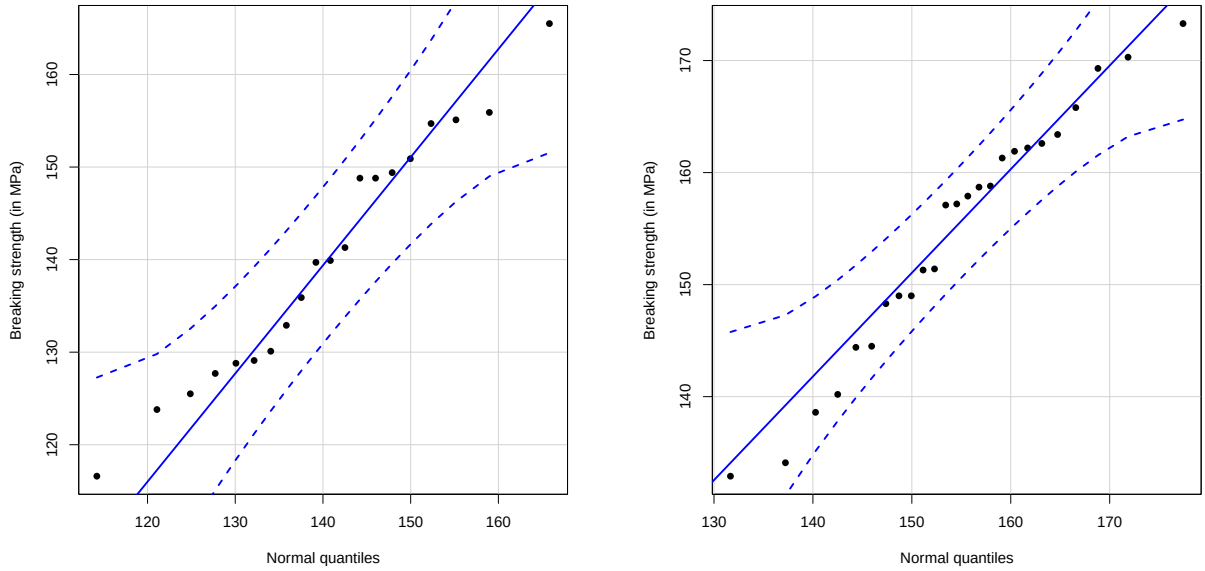


Figure 8.4: Fabric strength data. Normal qq plots for wool (left) and synthetic (right) breaking strengths.

Robustness: The normality assumption for the two populations is not so critical especially when the sample sizes are larger (a consequence of the CLT). In other words, slight or even modest departures from normality should not affect the confidence interval's performance that much. We can check this assumption using qq plots for each sample separately.

Fabric strength data: The qq plots for the fabric breaking strength data in Figure 8.4 (above) do not reveal any departures from normality. We can feel comfortable reporting $(-21.8, -7.2)$ as a 95% confidence interval for $\Delta = \mu_1 - \mu_2$, the population mean difference in breaking strength for the two fabric types.

8.1.2 Confidence interval for $\Delta = \mu_1 - \mu_2$ when $\sigma_1^2 \neq \sigma_2^2$

Note: When the population variances are not equal ($\sigma_1^2 \neq \sigma_2^2$), we should not use

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{n_1+n_2-2,\alpha/2}\sqrt{S_p^2\left(\frac{1}{n_1} + \frac{1}{n_2}\right)}$$

as a $100(1-\alpha)\%$ confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$. This interval is only valid when the population variances are equal ($\sigma_1^2 = \sigma_2^2$).

- Why? The pooled sample variance estimator S_p^2 estimates the common population variance $\sigma_1^2 = \sigma_2^2 = \sigma^2$ correctly on average (unbiasedly) only when the population variances are equal.

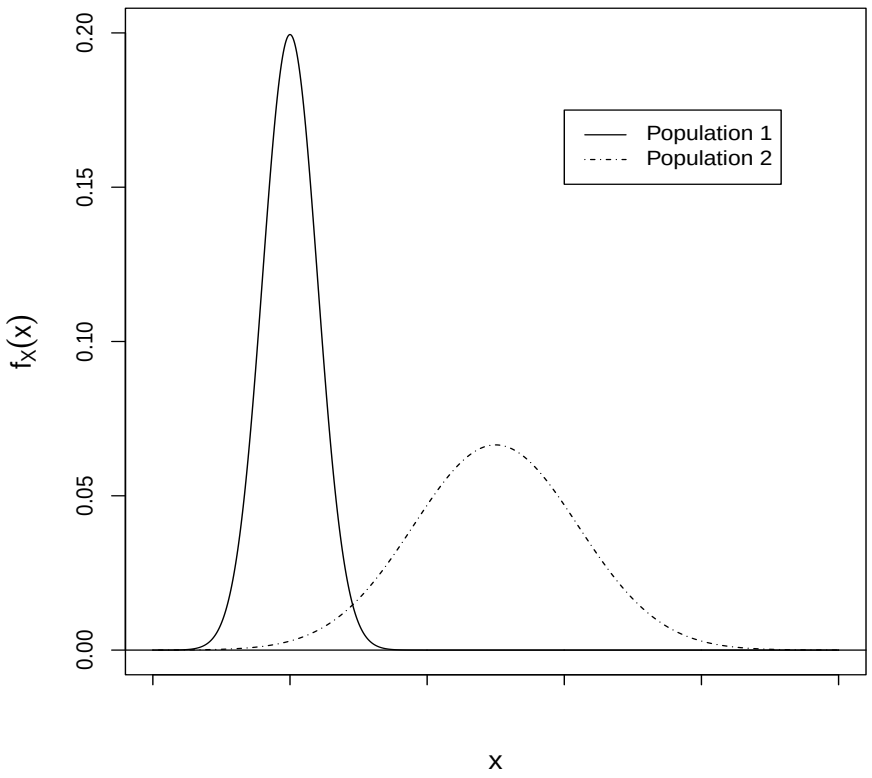


Figure 8.5: Two normal pdfs with unequal variances ($\sigma_1^2 \neq \sigma_2^2$). Note the population mean difference $\Delta = \mu_1 - \mu_2 < 0$.

Q: How should we compare the population means μ_1 and μ_2 if we are unwilling to make an equal population variance assumption?

Result: Mathematics shows that regardless of how the population variances σ_1^2 and σ_2^2 compare to each other (i.e., equal or not equal), the interval

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{\nu,\alpha/2}\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}$$

always serves as an **approximate** $100(1-\alpha)\%$ confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$. The degrees of freedom ν is calculated using

$$\nu = \frac{\left(\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}\right)^2}{\frac{(S_1^2/n_1)^2}{n_1 - 1} + \frac{(S_2^2/n_2)^2}{n_2 - 1}}.$$

This is the value of ν that identifies the best t distribution to approximate the sampling

distribution of

$$T = \frac{(\overline{X}_{1+} - \overline{X}_{2+}) - (\mu_1 - \mu_2)}{\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}} \sim t(\nu).$$

The approximate confidence interval

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{\nu,\alpha/2}\sqrt{\frac{S_1^2}{n_1} + \frac{S_2^2}{n_2}}$$

is derived from this approximate sampling distribution. Note that this interval does not use a "pooled" sample variance estimator; instead, we are using the sample variances S_1^2 and S_2^2 to estimate the population variances σ_1^2 and σ_2^2 separately.

Assumptions: This new confidence interval no longer requires the equal population variance assumption ($\sigma_1^2 = \sigma_2^2$), but it still requires the following:

1. We have random samples from each population. $\longleftarrow$ critical
2. The two samples are independent. $\longleftarrow$ critical
3. The population distributions are normal. $\longleftarrow$ not critical; robust to departures like before.

Example 8.2. Infection of chickens with the avian flu is a threat to both poultry production and human health. A research team created transgenic (genetically altered) chickens resistant to avian flu infection, but there was a concern this modification could affect the hatching weight. The researchers took independent samples of transgenic and commercial (unaltered) chickens of the same breed and weighed them at birth. The hatching weights (in grams, g) are displayed below:

Transgenic ($n_1 = 45$)	38.8	39.0	39.7	40.0	40.8	40.9	41.0	41.0	41.0	42.5
	42.6	43.0	43.0	43.4	43.5	43.5	43.8	44.4	44.7	44.7
	44.7	45.3	45.7	45.8	46.4	46.5	46.6	46.7	46.7	46.8
	46.9	47.1	47.1	47.1	47.3	47.6	47.7	48.1	48.3	49.3
	49.3	49.8	50.3	50.9	52.1					
Commercial ($n_2 = 54$)	36.7	37.1	38.9	39.5	39.5	39.8	40.0	40.2	40.3	40.5
	40.5	40.7	41.1	41.2	41.5	41.5	41.6	41.6	41.7	42.4
	43.1	43.3	43.3	43.4	43.7	44.1	44.2	45.2	45.3	45.4
	46.0	46.1	46.4	46.6	46.6	46.9	47.3	47.5	48.1	48.2
	48.4	48.6	49.0	49.1	49.3	49.6	50.1	50.2	50.4	50.6
	52.2	53.0	55.5	56.4						

Boxplots of the two samples are shown in Figure 8.6 (next page).

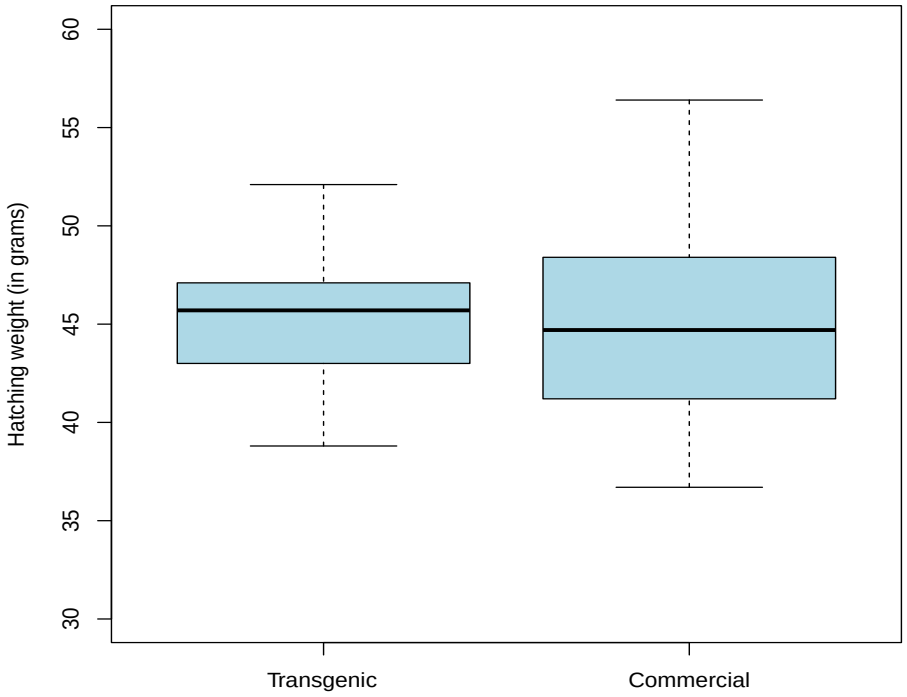


Figure 8.6: Hatching weight data. Boxplots of hatching weights (in grams) for independent samples of transgenic and commercial chickens.

Q: Find a 99% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$.
A: We can use the `t.test` function in R to calculate the confidence interval directly:

```
> options(digits=2)
> t.test(transgenic,commercial,conf.level=0.99,var.equal=FALSE)$conf.int
[1] -1.9  2.2
```

A 99% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ is

$$(-1.9, 2.2) \text{ grams.}$$

Interpretation: We are 99% confident the population mean difference $\Delta = \mu_1 - \mu_2$ is between -1.9 and 2.2 grams. Because this interval contains "0," we cannot conclude the population mean hatching weight for transgenic chickens (μ_1) is different than the population mean hatching weight for commerical chickens (μ_2).

Hatching weight data: The qq plots for the hatching weight data in Figure 8.7 (next page) do not reveal any serious departures from normality. We can feel comfortable reporting $(-1.9, 2.2)$ as a 99% confidence interval for $\Delta = \mu_1 - \mu_2$, the population mean difference in hatching weight for the two types of chickens.

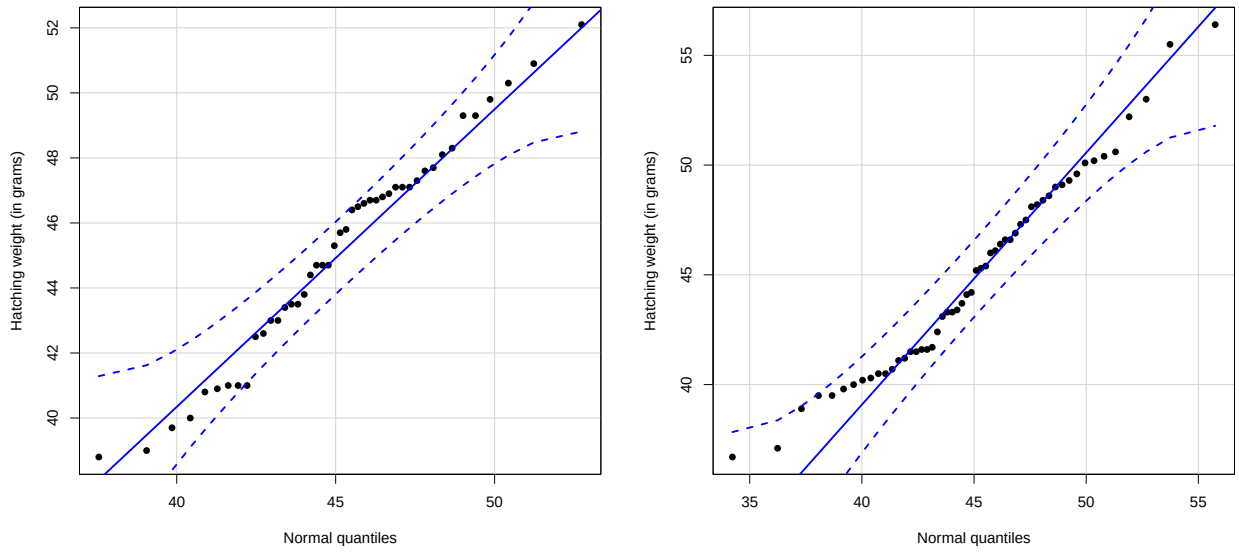


Figure 8.7: Hatching weight data. Normal qq plots for transgenic (left) and commercial (right) hatching weights.

Discussion: We have presented two approaches to construct a $100(1-\alpha)\%$ confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ with independent random samples−one which assumes equal population variances

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{n_1+n_2-2,\alpha/2}\sqrt{S_p^2\left(\frac{1}{n_1}+\frac{1}{n_2}\right)}$$

and one which does not

$$(\overline{X}_{1+} - \overline{X}_{2+}) \pm t_{\nu,\alpha/2}\sqrt{\frac{S_1^2}{n_1}+\frac{S_2^2}{n_2}}.$$

Advice: Only use the equal variance interval if there is strong evidence the population variances σ_1^2 and σ_2^2 are equal.

- Examining graphical displays like those in Figures 8.3 and 8.6 can be helpful, but these displays only show the samples. The equal population variance assumption is an assumption about the population variances. These may be different than the variation we see in the samples.
- In Section 8.3, we will describe a statistical inference procedure which allows you to compare σ_1^2 and σ_2^2 formally.

Some authors (not yours) advocate to always use the second interval−the one that makes no assumptions about the population variances. These authors argue that the second interval is always "adequate," despite the fact that it is created from an approximate t sampling

distribution. Make no mistake−the equal variance interval is a better confidence interval for $\Delta = \mu_1 - \mu_2$ when all of its assumptions hold, most importantly, when σ_1^2 and σ_2^2 are equal. The concern these authors have is this assumption is simply too prohibitive and ultimately is unnecessary. Personally, when I do two group comparisons like this, I just look at both intervals and see if they are giving me wildly different assessments. This is easy to do because R automates everything.

8.2 Matched pairs comparisons

Example 8.3. Tetrachlorodibenzodioxin (TCDD) is a toxic contaminant in Agent Orange, a herbicide used by the US military to clear foliage during the Vietnam War. Exposure to TCDD at high levels has been linked to serious health issues in Vietnam veterans, including various cancers, neurological disorders, heart conditions, diabetes, and birth defects in their children. A study reported the levels of TCDD in 20 Vietnam veterans who may have been exposed to Agent Orange during the war. The levels (in parts per trillion, ppt) in plasma and fat tissue were measured in each veteran. These data are below:

Veteran	Plasma	Fat	Veteran	Plasma	Fat
1	2.5	4.9	11	6.9	7.0
2	3.1	5.9	12	3.9	2.9
3	2.1	4.4	13	4.2	4.6
4	3.5	6.9	14	1.6	1.4
5	3.1	9.0	15	7.2	7.7
6	1.8	4.2	16	1.8	1.1
7	6.0	10.0	17	20.0	11.0
8	3.0	5.5	18	2.0	2.5
9	36.0	41.0	19	2.5	2.3
10	4.7	4.4	20	4.1	1.5

The goal of the study was to learn how the population mean TCDD level in plasma (μ_1) compared to the population mean TCDD level in fat tissue (μ_2).

Terminology: A **matched pairs design** arises when one obtains two measurements on each individual: one measurement under one condition and one measurement under a different condition.

- The goal is still to compare the population means μ_1 and μ_2. We can do this by forming a confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ like before.
- The difference in a matched pairs design is that the two sets of measurements (e.g., plasma, fat tissue) are no longer independent. Each individual contributes one measurement to both samples. Therefore, the confidence intervals in Section 8.1 are not applicable. These require independent samples.

Advantage: When compared to using two independent samples (Section 8.1), matched pairs study designs allow one to compare the population means μ_1 and μ_2 under more homogeneous conditions. This allows one to make more precise inference for $\Delta = \mu_1 - \mu_2$, the population mean difference.

- To see why, suppose researchers had performed the Vietnam veteran study with two independent samples:
  - Sample 1 with 20 veterans: measure TCDD level in plasma
  - Sample 2 with 20 different veterans: measure TCDD level in fat tissue.
- Think about the sources of variation that are present for a pair of measurements in different samples:

Design	Sources of variation
Two independent samples	difference between the two group means variation between the two veterans
Matched pairs	difference between the two group means

- In a matched pairs design, the extra source of variation that makes two different veterans different is removed (or blocked out). This is because you are making both measurements on the **same** veteran−not one measurement on one veteran and one measurement on another.
- In general, when you remove extra variation by pairing, this enables you to compare the two population means more precisely. This gives you a better chance of identifying a population mean difference if one really exists.
- On the other hand, in a design with two independent samples, the extra variation among individuals in different groups could prevent us from being able to identify this difference. Confidence intervals for $\Delta = \mu_1 - \mu_2$ may include "0" when, in fact, the population means are really different.

Implementation: Data from matched pairs studies are analyzed by writing a one-sample confidence interval using the **data differences**. Specifically, find

$$D_j = X_{1j} - X_{2j},$$

for each individual. After doing this, we have essentially created a "one-sample problem" like in Section 7.1 where our data are

$$D_1, D_2, ..., D_n.$$

A $100(1-\alpha)\%$ confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ is

$$\overline{D} \pm t_{n-1,\alpha/2}\frac{S_D}{\sqrt{n}},$$

where $\overline{D}$ and S_D are the sample mean and sample standard deviation of the data differences, respectively. We interpret this interval the same as before.

Example 8.3 (continued). Here are the TCDD veteran data with the data differences:

Veteran	Plasma	Fat	Difference	Veteran	Plasma	Fat	Difference
1	2.5	4.9	−2.4	11	6.9	7.0	−0.1
2	3.1	5.9	−2.8	12	3.9	2.9	1.0
3	2.1	4.4	−2.3	13	4.2	4.6	−0.4
4	3.5	6.9	−3.4	14	1.6	1.4	0.2
5	3.1	9.0	−5.9	15	7.2	7.7	−0.5
6	1.8	4.2	−2.4	16	1.8	1.1	0.7
7	6.0	10.0	−4.0	17	20.0	11.0	9.0
8	3.0	5.5	−2.5	18	2.0	2.5	−0.5
9	36.0	41.0	−5.0	19	2.5	2.3	0.2
10	4.7	4.4	0.3	20	4.1	1.5	2.6

Q: Find a 95% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$.
A: We can use the `t.test` function in R like before. We form a one-sample confidence interval using the data differences (`diff`):

```
> options(digits=1)
> t.test(diff,conf.level=0.95)$conf.int
[1] -2.4  0.6
```

A 95% confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ is

$$(-2.4, 0.6) \text{ ppt.}$$

Interpretation: We are 95% confident the population mean difference $\Delta = \mu_1 - \mu_2$ is between −2.4 and 0.6 ppt. Because this interval contains "0," we cannot conclude the population mean TCDD level in plasma (μ_1) is different than the population mean TCDD level in fat tissue (μ_2).

Curiosity: Suppose we had analyzed the data **incorrectly** as data from two independent random samples. Here is the corresponding confidence interval:

```
> options(digits=2)
> t.test(plasma,fat,conf.level=0.95,var.equal=FALSE)$conf.int
[1] -6.2  4.4
```

See how much longer this interval is? This shows how a matched pairs analysis is more precise than a two independent sample analysis. When you use pairing to remove the variation among individuals in different groups, confidence intervals for the population mean difference $\Delta = \mu_1 - \mu_2$ are much shorter.

Assumptions: A matched pairs analysis makes two assumptions:

1. We have a random sample of individuals from the population of interest (critical).
2. The population distribution of the data differences $D_1, D_2, ..., D_n$ is normal. This is preferred but not critical; confidence intervals using the t distribution are robust to departures like before.

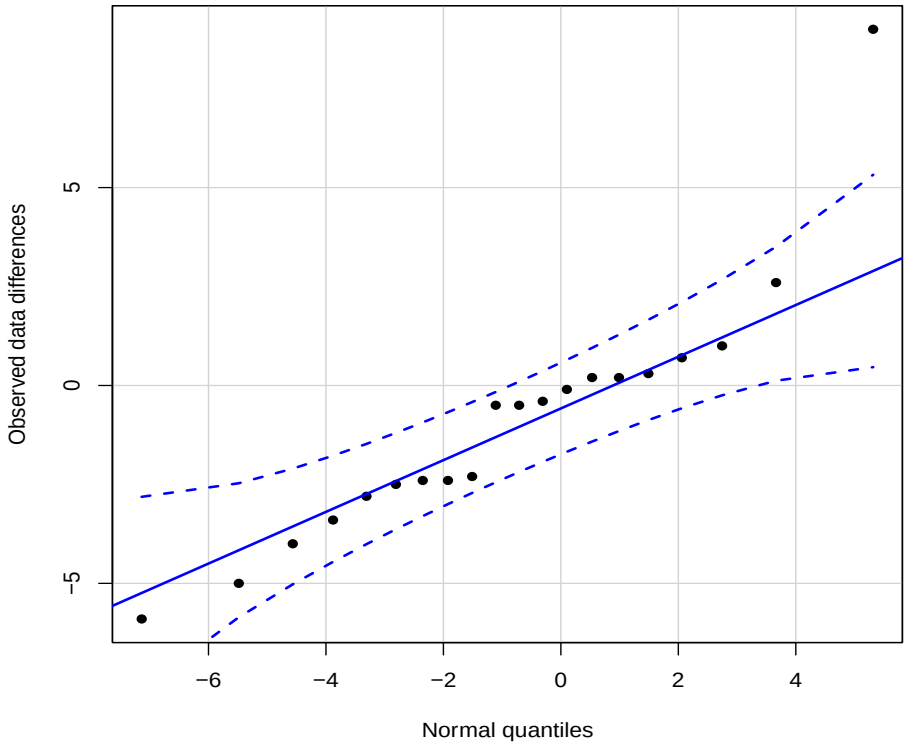


Figure 8.8: TCDD veteran data. Normal qq plot for the data differences.

TCDD veteran data: The qq plot for the data differences in Figure 8.8 (above) does not reveal a departure from normality overall, but it does identify a clear **outlier** for Veteran 17 whose difference is $d_{17} = 9.0$ ppt.

Curiosity: What effect does this one outlier have? The following shows what would happen if we removed Veteran 17 and redid the analysis:

```
> options(digits=1)
> t.test(diff[diff<5],conf.level=0.95)$conf.int
[1] -2.5 -0.4
```

Therefore, removing Veteran 17 would produce a 95% confidence interval

$$(-2.5, -0.4) \text{ ppt}$$

for the population mean difference $\Delta = \mu_1 - \mu_2$, which does not include "0." In other words, we would now conclude the population mean TCDD level in plasma (μ_1) is less than the population mean TCDD level in fat tissue (μ_2). The one observation (Veteran 17) changed our population level assessment entirely!

8.3 Comparing two population variances with independent samples

Setting: Suppose we have two **independent** random samples:

Sample 1 : $X_{11}, X_{12}, ..., X_{1n_1}$ is a random sample from a $\mathcal{N}(\mu_1, \sigma_1^2)$ population
Sample 2 : $X_{21}, X_{22}, ..., X_{2n_2}$ is a random sample from a $\mathcal{N}(\mu_2, \sigma_2^2)$ population.

Our goal is to compare the population variances σ_1^2 and σ_2^2. This will be done by forming a confidence interval for the **population variance ratio**

$$\Lambda = \frac{\sigma_2^2}{\sigma_1^2}.$$

Importantly, note that if the two population variances are equal (i.e., $\sigma_1^2 = \sigma_2^2$), then the population variance ratio is $\Lambda = \sigma_2^2/\sigma_1^2 = 1$.

Importance: Recall that when we had two **independent** random samples (not matched pairs), how we formed a confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ depended on which assumption we made regarding σ_1^2 and σ_2^2. There are two cases:

- $\sigma_1^2 = \sigma_2^2 \longrightarrow$ the two population variances are equal
- $\sigma_1^2 \neq \sigma_2^2 \longrightarrow$ the two population variances are not equal.

Therefore, inference for the population variance ratio Λ can be useful in helping us select the preferred confidence interval for the population mean difference Δ with independent samples.

Result: Under the assumptions outlined above, the quantity

$$Q = \frac{S_1^2/\sigma_1^2}{S_2^2/\sigma_2^2} \sim F(n_1 - 1, n_2 - 1),$$

an F **distribution** with (numerator) $n_1 - 1$ and (denominator) $n_2 - 1$ degrees of freedom. This describes the sampling distribution of Q, that is, how Q will vary probabilistically when sampling from two (independent) normal populations.

Facts: The F distribution has the following characteristics:

- Its pdf is continuous, skewed right, and its support is positive values only (no negative values); see Figure 8.9 (next page).
- It is indexed by two **degree of freedom** parameters ν_1 and ν_2. These are usually integers which depend on sample sizes.
- the **mean** of an F distribution is close to 1 regardless of the values of ν_1 and ν_2.
- The F pdf formula is unnecessary for our purposes. R will compute probabilities and quantiles from any F distribution.

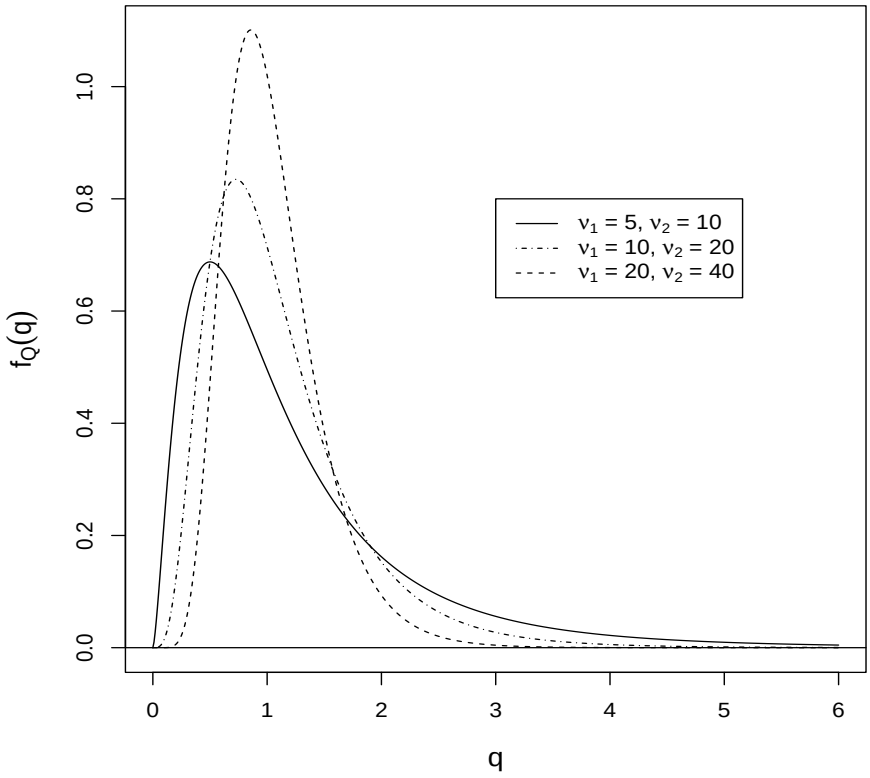


Figure 8.9: F pdfs with different degrees of freedom.

F **R CODE:** Suppose $Q \sim F(\nu_1, \nu_2)$.

$F_Q(q) = P(Q \leq q)$	ϕ_p
`pf(q,`ν_1, ν_2`)`	`qf(p,`ν_1, ν_2`)`

Notation: We introduce notation that identifies quantiles from an $F(n_1 - 1, n_2 - 1)$ distribution. Define

$$\begin{aligned} F_{n_1-1,n_2-1,1-\alpha/2} &= \textbf{upper } \alpha/2 \text{ quantile from } F(n_1 - 1, n_2 - 1) \text{ pdf} \\ F_{n_1-1,n_2-1,\alpha/2} &= \textbf{lower } \alpha/2 \text{ quantile from } F(n_1 - 1, n_2 - 1) \text{ pdf.} \end{aligned}$$

For example, if $n_1 = 10$, $n_2 = 10$, and $\alpha = 0.05$, then

$$\begin{aligned} F_{9,9,0.975} &\approx 4.03 \\ F_{9,9,0.025} &\approx 0.248 \end{aligned}$$

We can obtain quantiles like these using the `qf` function in R:

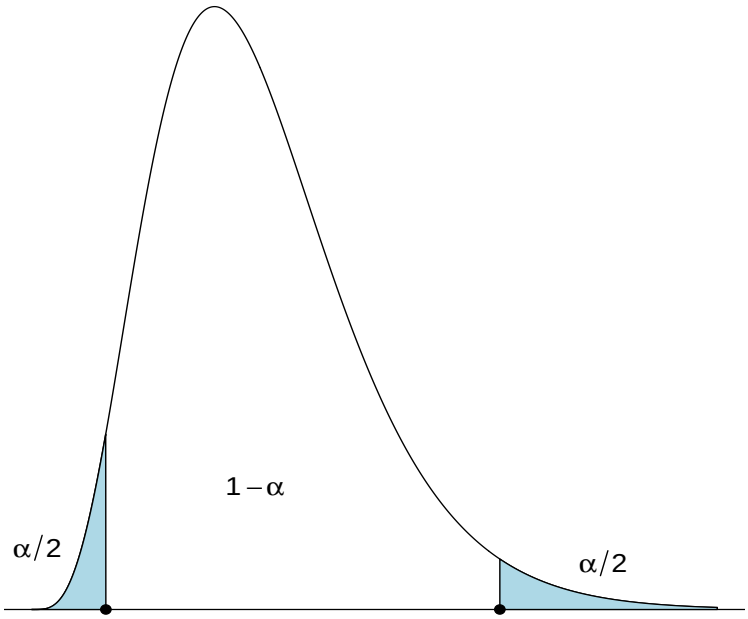


Figure 8.10: $F(n_1-1, n_2-1)$ pdf. The lower $\alpha/2$ quantile $F_{n_1-1,n_2-1,\alpha/2}$ and the upper $\alpha/2$ quantile $F_{n_1-1,n_2-1,1-\alpha/2}$ are shown using solid circles.

```
> options(digits=3)
> qf(0.975,9,9)
[1] 4.03
> qf(0.025,9,9)
[1] 0.248
```

Derivation: For any value of α, $0 < \alpha < 1$, we can write

$$\begin{aligned} 1-\alpha &= P(F_{n_1-1,n_2-1,\alpha/2} < Q < F_{n_1-1,n_2-1,1-\alpha/2}) \quad \longleftarrow \text{ this comes from Figure 8.10.} \\ &= P\left(F_{n_1-1,n_2-1,\alpha/2} < \frac{S_1^2/\sigma_1^2}{S_2^2/\sigma_2^2} < F_{n_1-1,n_2-1,1-\alpha/2}\right) \\ &= P\left(\frac{S_2^2}{S_1^2}\, F_{n_1-1,n_2-1,\alpha/2} < \frac{\sigma_2^2}{\sigma_1^2} < \frac{S_2^2}{S_1^2}\, F_{n_1-1,n_2-1,1-\alpha/2}\right). \end{aligned}$$

This shows

$$\left(\frac{S_2^2}{S_1^2}\, F_{n_1-1,n_2-1,\alpha/2},\ \frac{S_2^2}{S_1^2}\, F_{n_1-1,n_2-1,1-\alpha/2}\right)$$

is a $100(1-\alpha)\%$ **confidence interval** for the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$. We interpret the interval in the usual way:

> "We are $100(1-\alpha)\%$ confident the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$ is in this interval."

Important: Here is how we use the confidence interval to compare the population variances σ_1^2 and σ_2^2 when a $100(1-\alpha)\%$ confidence level is used:

- If the confidence interval for Λ consists entirely of values larger than 1; e.g., (1.4, 5.7), we would infer
$$\Lambda = \frac{\sigma_2^2}{\sigma_1^2} > 1 \implies \sigma_2^2 > \sigma_1^2.$$
- If the confidence interval for Λ consists entirely of values smaller than 1; e.g., (0.3, 0.6), we would infer
$$\Lambda = \frac{\sigma_2^2}{\sigma_1^2} < 1 \implies \sigma_2^2 < \sigma_1^2.$$
- If the confidence interval for Λ contains "1;" e.g., (0.6, 1.4), we cannot infer an ordering between σ_1^2 and σ_2^2. What this would suggest is that
$$\Lambda = \frac{\sigma_2^2}{\sigma_1^2} = 1$$
is a plausible value for the population variance ratio. In other words, we don't have sufficient evidence that one population variance is larger than the other.

Example 8.4. A plant uses two automated filling systems in the production of automobile paint: one rotary system and one inline system. The target volume of each system is 128.0 fluid ounces (1 gallon) for each can. There has been recent concern that the fill volume variability levels may be different for the two systems. To test this, industrial engineers took independent random samples of cans from each system and measured the fill volume of each can (in fluid ounces).

Rotary ($n_1 = 24$)	127.75	127.87	127.86	127.92	128.03	127.94	127.91	128.10
	128.01	128.11	127.79	127.93	127.89	127.96	127.80	127.94
	128.02	127.82	128.11	127.92	127.74	127.78	127.85	127.96
Inline ($n_2 = 24$)	127.90	127.90	127.74	127.93	127.62	127.76	127.63	127.93
	127.86	127.73	127.82	127.84	128.06	127.88	127.85	127.60
	128.02	128.05	127.95	127.89	127.82	127.92	127.71	127.78

Boxplots of the two samples are shown in Figure 8.11 (next page).

Q: Find a 95% confidence interval for the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$.
A: We can use the `var.test` function in R to calculate the confidence interval directly:

```
> options(digits=2)
> var.test(inline,rotary,conf.level=0.95)$conf.int  #inline = pop 2
[1] 0.59 3.14
```

A 95% confidence interval for the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$ is

$$(0.59, 3.14).$$

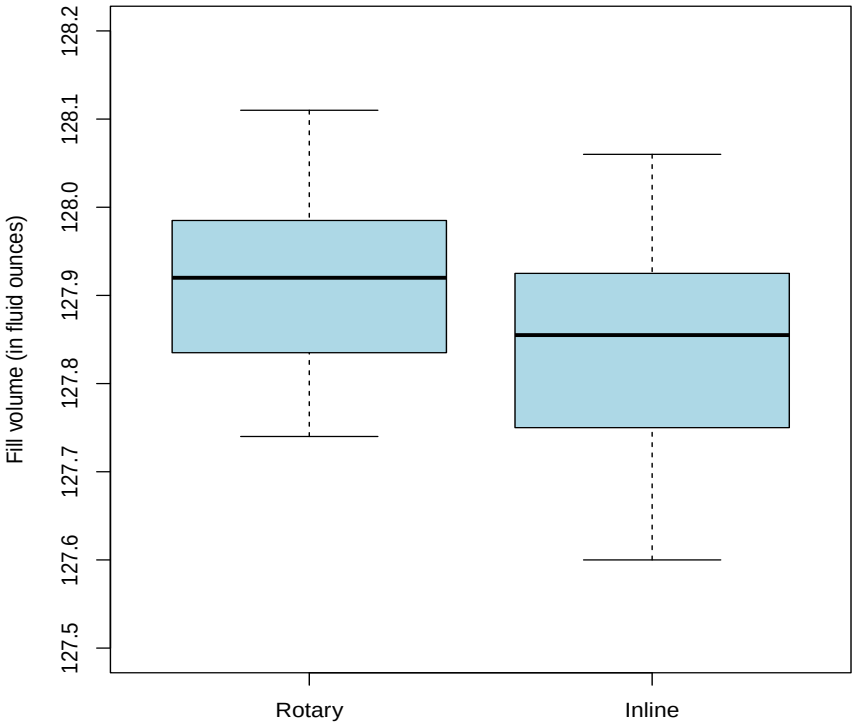


Figure 8.11: Paint fill volume data. Boxplots of fill volumes (in fluid ounces) for independent samples of cans from rotary and inline filling systems.

Interpretation: We are 95% confident the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$ is between 0.59 and 3.14. Because this interval contains "1," we cannot conclude the population variance fill volume for the rotary system (σ_1^2) is different than the population variance fill volume for the inline system (σ_2^2).

Remark: The analysis above could be used to justify the use of the equal population variance confidence interval for $\Delta = \mu_1 - \mu_2$ if you wanted to compare the population mean fill volumes for the two systems.

Assumptions: The confidence interval

$$\left(\frac{S_2^2}{S_1^2} \, F_{n_1-1,n_2-1,\alpha/2}, \; \frac{S_2^2}{S_1^2} \, F_{n_1-1,n_2-1,1-\alpha/2} \right)$$

for the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$ is created using three assumptions:

1. We have random samples from each population.
2. The two samples are independent.
3. The population distributions are normal.

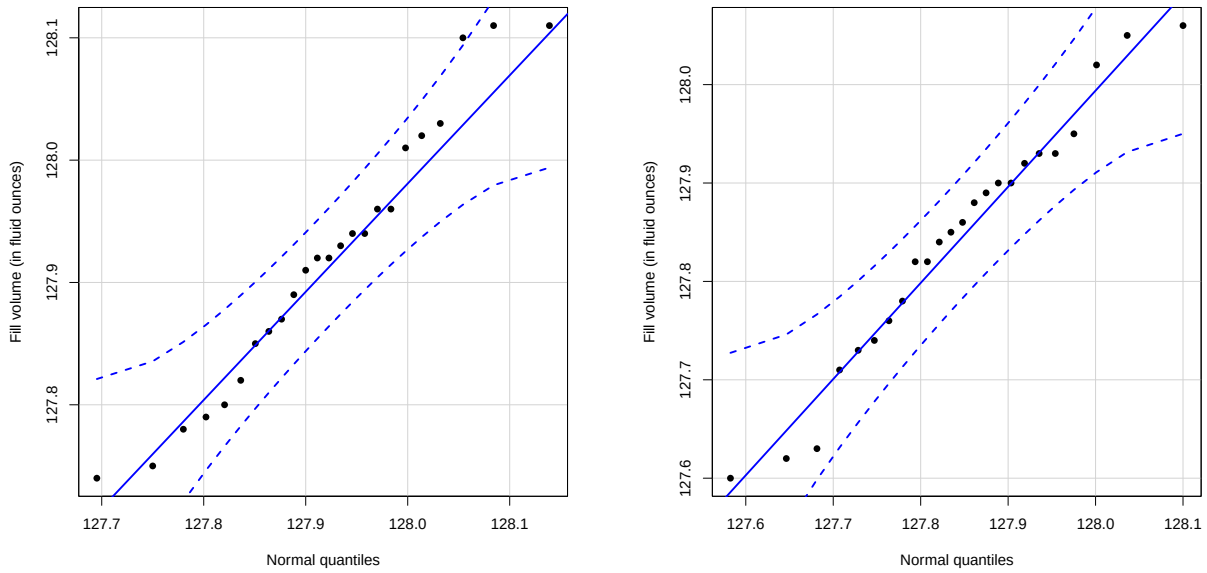


Figure 8.12: Paint fill volume data. Normal qq plots for rotary (left) and inline (right) fill volumes.

Discussion: The confidence interval for the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$ is **not robust** to departures of any of these assumptions.

- In particular, the normality assumption for both populations is especially critical. Why? The sampling distribution result

$$Q = \frac{S_1^2/\sigma_1^2}{S_2^2/\sigma_2^2} \sim F(n_1 - 1, n_2 - 1)$$

  depends on it heavily, and we used this sampling distribution as a "starting point" to derive the interval. Departures from normality in either population could cause the confidence interval for Λ to be misleading.

- The same authors who advise not to use the equal population variance confidence interval for the population mean difference $\Delta = \mu_1 - \mu_2$ also recommend the interval for Λ not be used. To them, mandating normal populations is too restrictive.

Summary: By now, you should be starting to see that

- confidence intervals created for **population means** using the t distribution are robust to normality departures. This includes intervals for a single population mean μ (Chapter 7) and the population mean difference $\Delta = \mu_1 - \mu_2$.

- confidence intervals for **population variances** (using the χ^2 or F distributions) are not robust to normality departures. This includes intervals for a single population variance σ^2 (Chapter 7) and the population variance ratio $\Lambda = \sigma_2^2/\sigma_1^2$.

8.4 Comparing two population proportions with independent samples

Goal: We now extend our confidence interval procedure for one population proportion p in Section 7.3 to two populations. Define

$$\begin{aligned} p_1 &= \text{population proportion in Population 1} \\ p_2 &= \text{population proportion in Population 2.} \end{aligned}$$

For example, we might want to compare the population proportion of

- defective circuit boards for two different suppliers
- patients who respond to two different treatments
- on-time payments for two customer groups
- covid-19 cases for rural and urban areas.

Point estimators: We assume there are two **independent** random samples of individuals; one sample from each population to be compared. Define

$$\begin{aligned} X_1 &= \text{number of "successes" in Sample 1} \sim b(n_1, p_1) \\ X_2 &= \text{number of "successes" in Sample 2} \sim b(n_2, p_2). \end{aligned}$$

The point estimators for p_1 and p_2 are the **sample proportions**

$$\begin{aligned} \widehat{p}_1 &= \frac{X_1}{n_1} \\ \widehat{p}_2 &= \frac{X_2}{n_2}. \end{aligned}$$

We would like to construct a $100(1-\alpha)\%$ confidence interval for $\Delta = p_1 - p_2$, the **population proportion difference**, using $\widehat{\Delta} = \widehat{p}_1 - \widehat{p}_2$ as a point estimator. The following approximate sampling distribution is used to do this.

Result: When the sample sizes n_1 and n_2 are large,

$$Z = \frac{(\widehat{p}_1 - \widehat{p}_2) - (p_1 - p_2)}{\sqrt{\dfrac{p_1(1-p_1)}{n_1} + \dfrac{p_2(1-p_2)}{n_2}}} \sim \mathcal{AN}(0,1).$$

This result can be used to show

$$(\widehat{p}_1 - \widehat{p}_2) \pm z_{\alpha/2}\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1} + \frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}$$

is an approximate $100(1-\alpha)\%$ **confidence interval** for $\Delta = p_1 - p_2$.

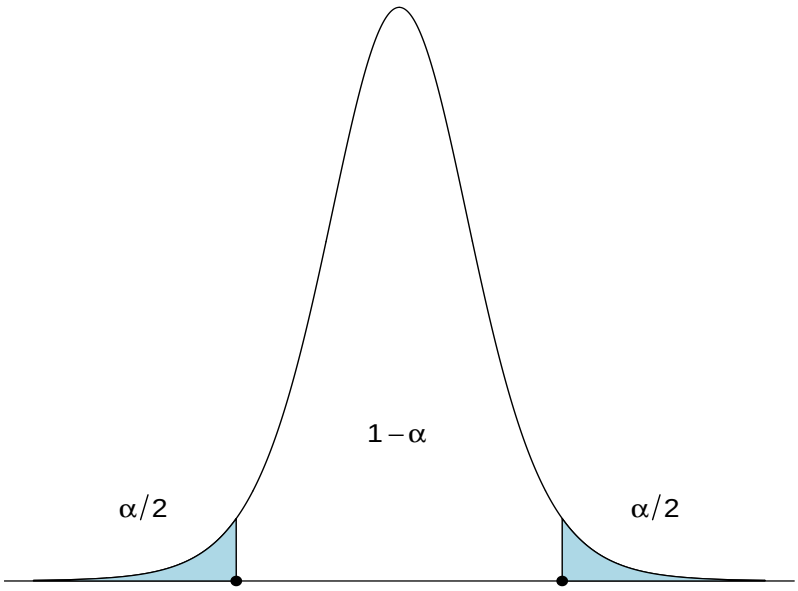


Figure 8.13: $\mathcal{N}(0,1)$ pdf. The lower $\alpha/2$ quantile $-z_{\alpha/2}$ and the upper $\alpha/2$ quantile $z_{\alpha/2}$ are shown using solid circles.

- Note again the form of the interval:

$$\underbrace{\text{point estimate}}_{\widehat{p}_1-\widehat{p}_2} \pm \underbrace{\text{quantile}}_{z_{\alpha/2}} \times \underbrace{\text{standard error}}_{\sqrt{\frac{\widehat{p}_1(1-\widehat{p}_1)}{n_1}+\frac{\widehat{p}_2(1-\widehat{p}_2)}{n_2}}}.$$

  We interpret the interval in the same way:

  > "We are $100(1-\alpha)\%$ confident the population proportion difference $\Delta = p_1 - p_2$ is in this interval."

- The value $z_{\alpha/2}$ is the upper $\alpha/2$ quantile from the $\mathcal{N}(0,1)$ distribution.

Important: Here is how we use the confidence interval to compare the population proportions p_1 and p_2 when a $100(1-\alpha)\%$ confidence level is used:

- If the confidence interval for Δ consists entirely of positive values; e.g., (0.08, 0.34), we would infer
$$\Delta = p_1 - p_2 > 0 \implies p_1 > p_2.$$
- If the confidence interval for Δ consists entirely of negative values; e.g., $(-0.34, -0.08)$, we would infer
$$\Delta = p_1 - p_2 < 0 \implies p_1 < p_2.$$
- If the confidence interval for Δ contains "0;" e.g., $(-0.34, 0.08)$, we cannot infer an ordering between p_1 and p_2. What this would suggest is that
$$\Delta = p_1 - p_2 = 0$$

is a plausible value for the population proportion difference. In other words, we don't have sufficient evidence that one population proportion is larger than the other.

Remark: As in the one-sample problem (Section 7.3), this interval should be used only when the sample sizes n_1 and n_2 are "large." A common **rule of thumb** is to require

$$\begin{array}{rclrcl} n_1\widehat{p}_1 & \geq & 5 & n_1(1-\widehat{p}_1) & \geq & 5 \\ n_2\widehat{p}_2 & \geq & 5 & n_2(1-\widehat{p}_2) & \geq & 5. \end{array}$$

Under these conditions, the sampling distribution approximation for Z on the previous page should be adequate, thereby making the confidence interval formula for $\Delta = p_1 - p_2$ approximately valid. This approximation is a consequence of the CLT.

Example 8.5. Researchers performed a study to assess the effectiveness of administering xylitol to prevent acute otitis media (AOM, infection behind the eardrum) in children attending daycare centers in Finland. Xylitol, an artificial sweetener which has antibacterial properties in dental care, was administered to the children in syrup form.

- $n_1 = 165$ children were randomized to receive a "control" syrup (containing no xylitol). Sixty-eight (68) of these children developed AOM.
- $n_2 = 159$ children were randomized to receive xylitol syrup. Forty-six (46) of these children developed AOM.

Let p_1 and p_2 denote the population proportions of children who develop AOM for the two groups (control and xylitol, respectively). Point estimates for p_1 and p_2 based on this study are

$$\widehat{p}_1 = \frac{68}{165} \approx 0.412 \quad \text{and} \quad \widehat{p}_2 = \frac{46}{159} \approx 0.289,$$

and a 95% confidence interval for $\Delta = p_1 - p_2$ is

$$(0.412 - 0.289) \pm 1.96\sqrt{\frac{0.412(1-0.412)}{165} + \frac{0.289(1-0.289)}{159}} \longrightarrow (0.020, 0.226).$$

Interpretation: We are 95% confident the population proportion difference $\Delta = p_1 - p_2$ is between 0.020 and 0.226. Because this interval consists entirely of positive values, we can infer the population proportion of children who develop AOM in the control group (p_1) is larger than the population proportion of children who develop AOM in the xylitol group (p_2). This analysis would support the use of xylitol in reducing the population proportion of AOM cases.

Implementation in R: We can use the `prop.test` function in R to calculate the confidence interval directly:

```
> options(digits=3)
> prop.test(c(68,46),c(165,159),conf.level=0.95,correct=FALSE)$conf.int
[1] 0.0198 0.2258
```

9 One-Way Classification and Analysis of Variance

Recall: In the last chapter, we discussed writing confidence intervals for the population mean difference $\Delta = \mu_1 - \mu_2$ with two independent random samples. The resulting confidence interval allowed us to compare two population means μ_1 and μ_2.

Q: What if there are more than two populations we would like to compare? For example,

- In Example 8.1, we compared the population mean breaking strength of two types of fabric. What if we wanted to compare the breaking strength of four types of fabric: wool, polyester, nylon, and acrylic? How do we compare four population means?
- In Example 8.2, we compared the population mean hatching weight of commercial and transgenic chickens. Suppose there are two different types of transgenic chickens we would like to include in the comparison with commercial chickens. How would we compare the three population means?

Goals: In this chapter, we discuss how to make comparisons among more than two population means. Our first goal is to develop a statistical procedure to assess if multiple population means could be equal. If the evidence shows they aren't equal, we then develop a follow-up procedure to determine which population means might be different and how they are different.

Example 9.1. Mortar is a paste-like substance which binds building blocks like bricks and concrete units. Different mortar mixes are usually classified on the basis of compressive strength and their bonding properties to prevent cracking. In a building project, engineers want to compare the population mean flexural bond strength of four types of mortars:

1. ordinary cement mortar (OCM)
2. polymer impregnated mortar (PIM)
3. resin mortar (RM)
4. polymer cement mortar (PCM).

Random samples of mortar specimens were taken, and each specimen was subjected to a compression test to measure its flexural bond strength (in psi). Here are the measurements that were collected:

OCM ($n_1 = 8$):	51.45	42.96	41.11	48.06	38.27	38.88	42.74	49.62		
PIM ($n_2 = 10$):	64.97	64.21	57.39	52.79	64.87	53.27	51.24	55.87	61.76	67.15
RM ($n_3 = 10$):	48.95	62.41	52.11	60.45	58.07	52.16	61.71	61.06	57.63	56.80
PCM ($n_4 = 8$):	35.28	38.59	48.64	50.99	51.52	52.85	46.75	48.31		

Side-by-side boxplots of these samples are shown in Figure 9.1 (next page).

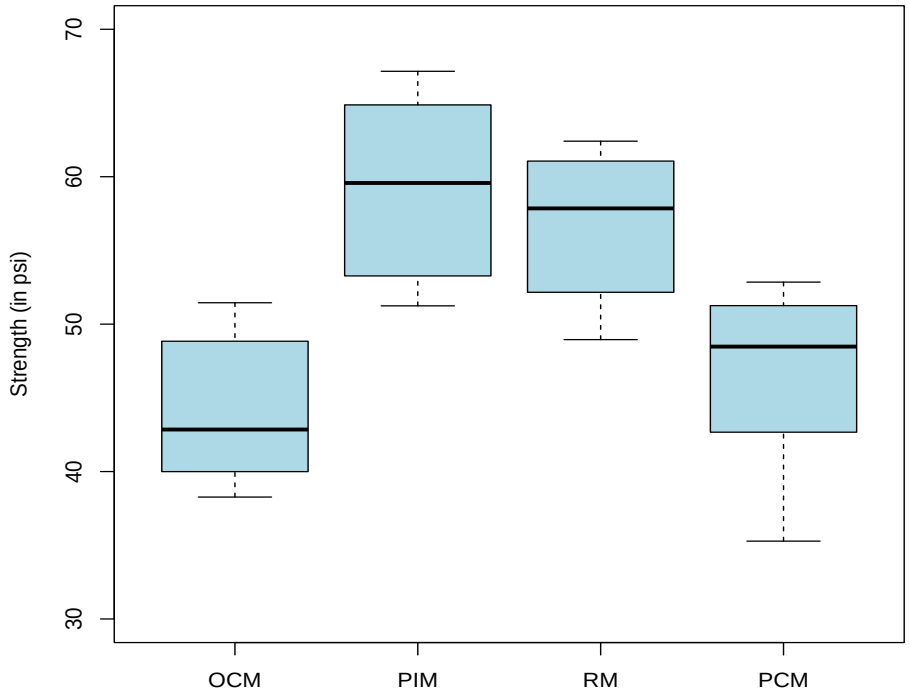


Figure 9.1: Mortar strength data. Boxplots of flexural bond strengths (in psi) for four types of mortar.

Discussion: An initial question one might have is the following:

> *"Is it possible the four population mean mortar strengths are equal? Or, does the evidence suggest the population means are different?*

This question can be framed statistically as a **hypothesis test**:

$$H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$$

versus

$$H_1 : \text{the population means are not all equal.}$$

Under the assumptions we will make, the hypothesis H_0 implies there is one population distribution with mean μ that is producing the four samples we see in Figure 9.1. The hypothesis H_1 says multiple population distributions (with different means) are producing the samples. Our first goal is to determine which hypothesis is more credible based on the observed data. This is the focus of Section 9.1. If it is subsequently determined that H_1 is more credible, our efforts will then turn to finding where the population mean differences are. This is the focus of Section 9.2.

Remark: When we say "one-way classification," what we mean is that there is only one characteristic (or **factor**) which is being considered for comparison.

- In Example 9.1, we are comparing the flexural bond strength of four mortar types. The only characteristic which distinguishes one specimen from another is what type of mortar it is.
- Some studies might investigate more than one factor. For example, suppose the engineers in Example 9.1 wanted to determine how flexural bond strength depended on
  - Factor 1: mortar type (OCM, PIM, RM, and PCM)
  - Factor 2: temperature (10 deg C, 20 deg C, and 30 deg C).

  This would be a two-way classification. That is, we would classify a single specimen according to which type of mortar it is and at what temperature the flexural bond strength is being measured.
- This chapter considers only one-way classification analyses. Analyses for two or more factors is discussed in Chapter 12.

9.1 Overall F test for equality of population means

Setting: In general, suppose we have t **independent** random samples:

$$\begin{aligned}
&\text{Sample 1}: X_{11}, X_{12}, ..., X_{1n_1} \text{ is a random sample from a } \mathcal{N}(\mu_1, \sigma^2) \text{ population} \\
&\text{Sample 2}: X_{21}, X_{22}, ..., X_{2n_2} \text{ is a random sample from a } \mathcal{N}(\mu_2, \sigma^2) \text{ population} \\
&\quad \vdots \qquad\qquad\qquad\qquad\qquad\qquad \vdots \\
&\text{Sample } t: X_{t1}, X_{t2}, ..., X_{tn_t} \text{ is a random sample from a } \mathcal{N}(\mu_t, \sigma^2) \text{ population.}
\end{aligned}$$

Goal: Our goal is to formulate a statistical inference procedure which allows us to test

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_t$$

versus

$$H_1 : \text{the population means are not all equal.}$$

We will make a decision on which hypothesis, H_0 or H_1, is more supported by the data (evidence) we see in the samples. In statistical inference, we call H_0 the **null hypothesis**. We call H_1 the **alternative hypothesis**.

Assumptions: The statistical inference procedure we will develop to test H_0 versus H_1 is based on four assumptions:

1. We have random samples from each population.
2. The t samples are independent.

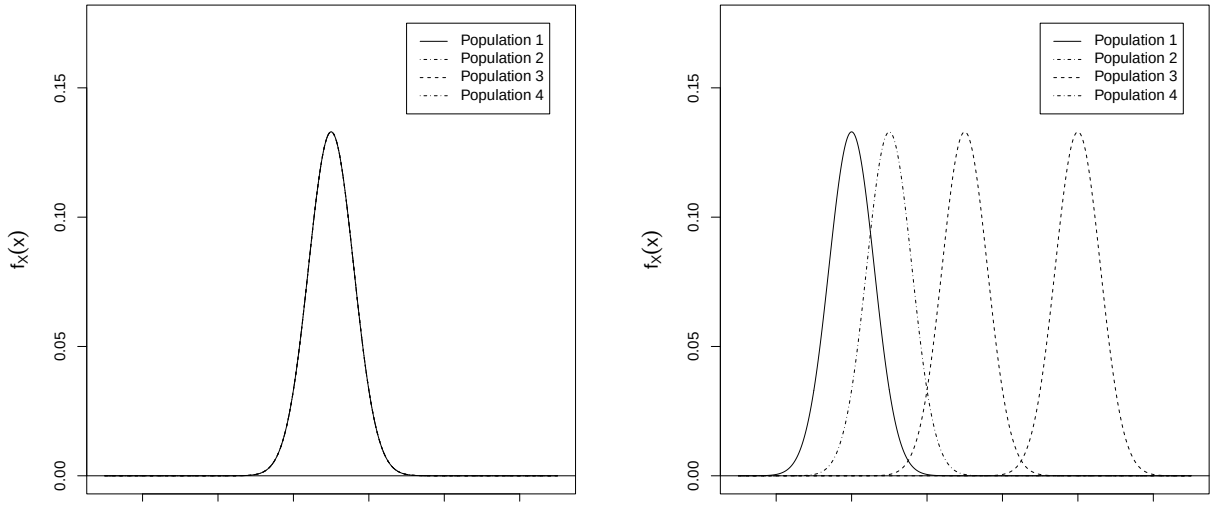


Figure 9.2: Left: All the population means are equal (H_0). Right: At least one of the population means is different than the others (H_1).

3. The population distributions are normal.
4. The population variances are all equal, that is, $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_t^2 = \sigma^2$.

Observation: If $H_0 : \mu_1 = \mu_2 = \cdots = \mu_t$ is true (i.e., all the population means are equal), this implies there is a single population distribution

$$\mathcal{N}(\mu, \sigma^2)$$

which produces the t different samples; see Figure 9.2 (above, left). The value μ is the common value of $\mu_1, \mu_2, ..., \mu_t$. Therefore, the question becomes, "Is this hypothesis more consistent with the data? Or, does the evidence suggest there are two or more normal distributions producing the samples?"

Q: If we are trying to learn about how the population means compare, why is the statistical inference procedure designed to do this called "the analysis of variance?"
A: Because the procedure is built on estimating the common population variance σ^2 in two different ways:

- one way which estimates σ^2 within the samples, and
- one way which estimates σ^2 across the samples.
- **Important:** These two estimates tend to be close to each other when H_0 is true. The second estimate tends to be larger than the first estimate when H_1 is true.
- The ratio of the two estimates has an F distribution when H_0 is true. That's why it's called "the overall F test."

"Within" estimator of σ^2: The sample variance of each sample

$$S_i^2 = \frac{1}{n_i - 1}\sum_{j=1}^{n_i}(X_{ij} - \overline{X}_{i+})^2, \quad i = 1, 2, ..., t,$$

is an unbiased estimator of the common population variance σ^2 (from Chapter 6). Therefore, take the t sample variances $S_1^2, S_2^2, ..., S_t^2$ and combine them to form

$$\text{SS}_\text{E} = (n_1 - 1)S_1^2 + (n_2 - 1)S_2^2 + \cdots + (n_t - 1)S_t^2.$$

If we divide SS_E by $N - t$, where

$$N = \sum_{i=1}^{t} n_i$$

is the total number of observations across the t samples, then we get

$$\text{MS}_\text{E} = \frac{(n_1 - 1)S_1^2 + (n_2 - 1)S_2^2 + \cdots + (n_t - 1)S_t^2}{N - t} = \frac{\text{SS}_\text{E}}{N - t}.$$

This is simply a weighted average of the t sample variances $S_1^2, S_2^2, ..., S_t^2$. Each sample variance is an unbiased estimator of σ^2. The weighted average MS_E is too, that is,

$$E(\text{MS}_\text{E}) = \sigma^2.$$

MS_E is our "within" estimator of σ^2.

"Across" estimator of σ^2: When we say "across," we mean that we are assessing the variability in the sample means $\overline{X}_{1+}, \overline{X}_{2+}, ..., \overline{X}_{t+}$ across the samples. Intuitively,

- if the population means are all equal (H_0 true), then the sample means $\overline{X}_{1+}, \overline{X}_{2+}, ..., \overline{X}_{t+}$ should be close to each other and therefore the variability among them should be small.
- if the population means are not all equal (H_1 true), then the variability among the sample means $\overline{X}_{1+}, \overline{X}_{2+}, ..., \overline{X}_{t+}$ could be very large.

We will form a second unbiased estimator of σ^2 under the assumption H_0 is true. To make the exposition (and derivation) easier to follow, suppose the sample sizes are equal; i.e.,

$$n_1 = n_2 = \cdots = n_t = n.$$

We know from Chapter 6 that

$$\underbrace{\overline{X}_{1+} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)}_{\text{Sample 1}}, \quad \underbrace{\overline{X}_{2+} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)}_{\text{Sample 2}}, \quad ..., \quad \underbrace{\overline{X}_{t+} \sim \mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)}_{\text{Sample } t},$$

where μ is the common value of $\mu_1, \mu_2, ..., \mu_t$ when H_0 is true. In other words, when H_0 is true, we can conceptualize $\overline{X}_{1+}, \overline{X}_{2+}, ..., \overline{X}_{t+}$ as a "random sample" from a

$$\mathcal{N}\left(\mu, \frac{\sigma^2}{n}\right)$$

distribution. Therefore, the "sample variance" of $\overline{X}_{1+}, \overline{X}_{2+}, ..., \overline{X}_{t+}$, which is

$$\frac{1}{t-1}\sum_{i=1}^{t}(\overline{X}_{i+} - \overline{X}_{++})^2,$$

is an unbiased estimator of σ^2/n, that is,

$$E\left[\frac{1}{t-1}\sum_{i=1}^{t}(\overline{X}_{i+} - \overline{X}_{++})^2\right] = \frac{\sigma^2}{n} \implies E\left[\frac{1}{t-1}\sum_{i=1}^{t} n(\overline{X}_{i+} - \overline{X}_{++})^2\right] = \sigma^2.$$

The quantity

$$\text{MS}_\text{T} = \frac{1}{t-1}\underbrace{\sum_{i=1}^{t} n(\overline{X}_{i+} - \overline{X}_{++})^2}_{=\text{ SS}_\text{T}} = \frac{\text{SS}_\text{T}}{t-1}$$

is an unbiased estimator of σ^2 when H_0 is true. MS_T is our "across" estimator of σ^2.

Remark: Our derivation of the "across" estimator assumed a balanced design where the sample sizes $n_1 = n_2 = \cdots = n_t = n$. If we have different sample sizes n_i (like in Example 9.1), we simply adjust MS_T to

$$\text{MS}_\text{T} = \frac{1}{t-1}\underbrace{\sum_{i=1}^{t} n_i(\overline{X}_{i+} - \overline{X}_{++})^2}_{=\text{ SS}_\text{T}}.$$

This is still an unbiased estimator for σ^2 when H_0 is true.

Summary: The following summarizes what we have learned so far:

1. **When H_0 is true** (i.e., the population means are equal), then

$$\begin{aligned} E(\text{MS}_\text{T}) &= \sigma^2 \\ E(\text{MS}_\text{E}) &= \sigma^2. \end{aligned}$$

   These two facts suggest that when H_0 is true,

$$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}}$$

   should be close to 1.

2. **When H_1 is true** (i.e., at least one population mean is different), then

$$\begin{aligned} E(\text{MS}_\text{T}) &> \sigma^2 \\ E(\text{MS}_\text{E}) &= \sigma^2. \end{aligned}$$

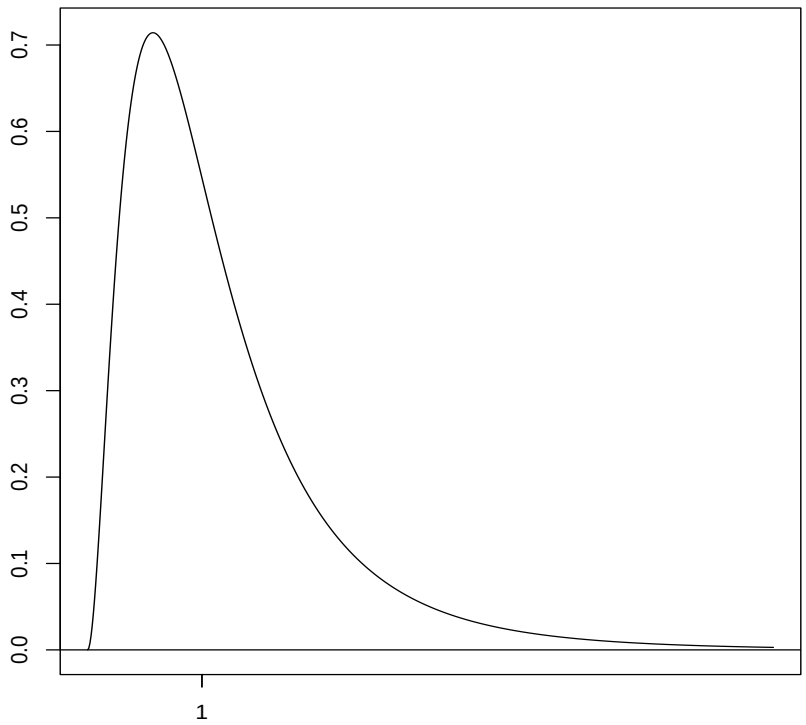


Figure 9.3: $F(t-1, N-t)$ pdf. This represents the sampling distribution of F when H_0 is true.

These two facts suggest that when H_1 is true,

$$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}}$$

should be larger than 1. It could be a lot larger than 1 depending on how different the population means are. The more different they are, the larger F tends to be. *Therefore, the larger F is, the more evidence we have against H_0.*

Sampling distribution: When H_0 is true,

$$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}} \sim F(t-1, N-t),$$

an F sampling distribution with $t-1$ (numerator) and $N-t$ (denominator) degrees of freedom. We can therefore gauge "how much evidence we have against H_0" by seeing where F falls on this distribution; see Figure 9.3 above.

- Values of F close to 1 are consistent with H_0.
- Values of F out in the right tail (i.e., much larger than 1) are consistent with H_1.

Example 9.1 (continued). We calculate the F statistic for the mortar strength data to see which hypothesis, H_0 or H_1, is more supported. Here are the data again:

OCM ($n_1 = 8$):	51.45	42.96	41.11	48.06	38.27	38.88	42.74	49.62		
PIM ($n_2 = 10$):	64.97	64.21	57.39	52.79	64.87	53.27	51.24	55.87	61.76	67.15
RM ($n_3 = 10$):	48.95	62.41	52.11	60.45	58.07	52.16	61.71	61.06	57.63	56.80
PCM ($n_4 = 8$):	35.28	38.59	48.64	50.99	51.52	52.85	46.75	48.31		

We have

$$\begin{aligned} t &= 4 \longleftarrow \text{number of "treatments" (or groups to compare)} \\ N &= 36 \longleftarrow \text{total number of observations.} \end{aligned}$$

Therefore, if H_0 is true,

$$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}} \sim F(t-1, N-t) \longrightarrow F(3, 32).$$

We will gauge the strength of evidence against H_0 by seeing where F falls on this distribution. Remember, values of F close to 1 are consistent with H_0.

Implementation in R: We use R's `lm` function to "fit" a linear model which relates the strength data to the mortar type. The `anova` function is used to produce an **analysis of variance table**. This table contains the F statistic (`F value`).

```
> options(digits=6)
> fit = lm(Strength ~ Mortar)
> anova(fit)
Analysis of Variance Table

Response: Strength
          Df Sum Sq Mean Sq F value   Pr(>F)
Mortar     3 1520.9   507.0   16.85 9.58e-07 ***
Residuals 32  962.9    30.1
```

Analysis: Figure 9.4 (next page) shows the $F(3, 32)$ pdf, which represents the sampling distribution of F when H_0 is true (i.e., all the population means are equal). The F statistic $F \approx 16.85$ is far out in the right tail.

- This isn't a value of F we would expect to see from this distribution (i.e., the distribution of F if H_0 was true).
- Because F is so far out in the tail, this means we have very strong evidence against H_0 in favor of H_1.
- Our conclusion here is at least one of the mortar strength population means is different than the others. This "overall" assessment does not give information about which one(s) may be different. We will pursue this question in Section 9.2.

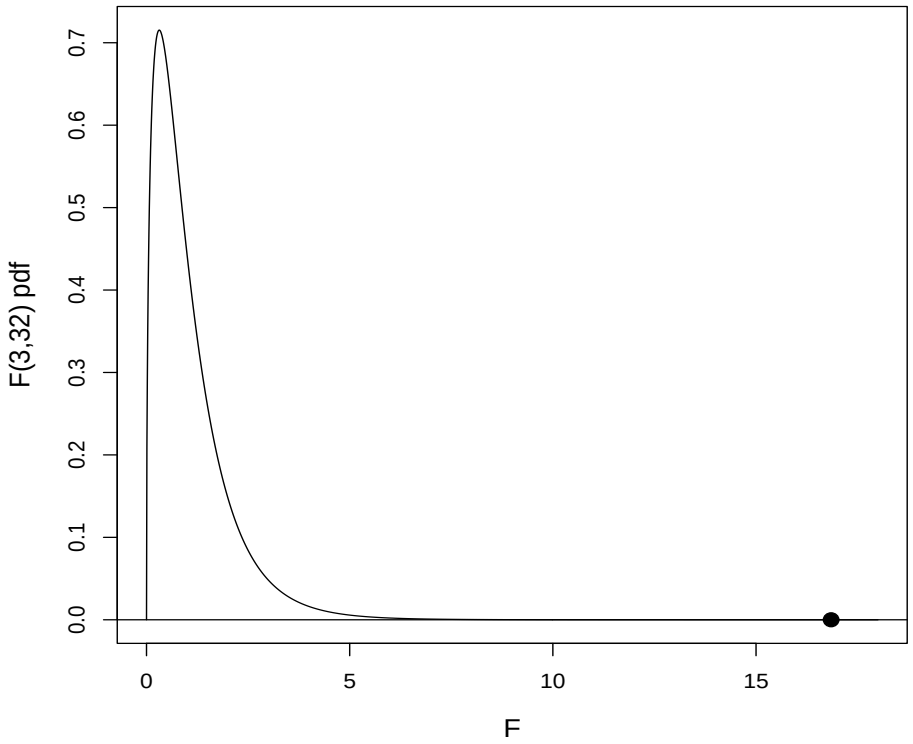


Figure 9.4: Mortar strength data. $F(3, 32)$ pdf. This is the distribution of F when H_0 is true. The F statistic $F \approx 16.85$ is shown using a solid circle.

Discussion: We have just performed a data analysis where there is overwhelming evidence the population means are not all equal. Section 9.2 will help us determine which population means are different and how they are different. We have three items for discussion first:

- Analysis of variance (ANOVA) tables
- Probability values (p-values)
- a review of the assumptions underpinning the overall F test and how to check them.

9.1.1 ANOVA table for one-way classification

Terminology: An **analysis of variance** (ANOVA) **table** is a table which shows how data variation is partitioned into different sources. In a one-way classification, there are only two such sources:

1. variation due to the differences in the "treatments" (i.e., the groups we are comparing)
2. variation that is "left over" after explaining how the treatment groups are different.

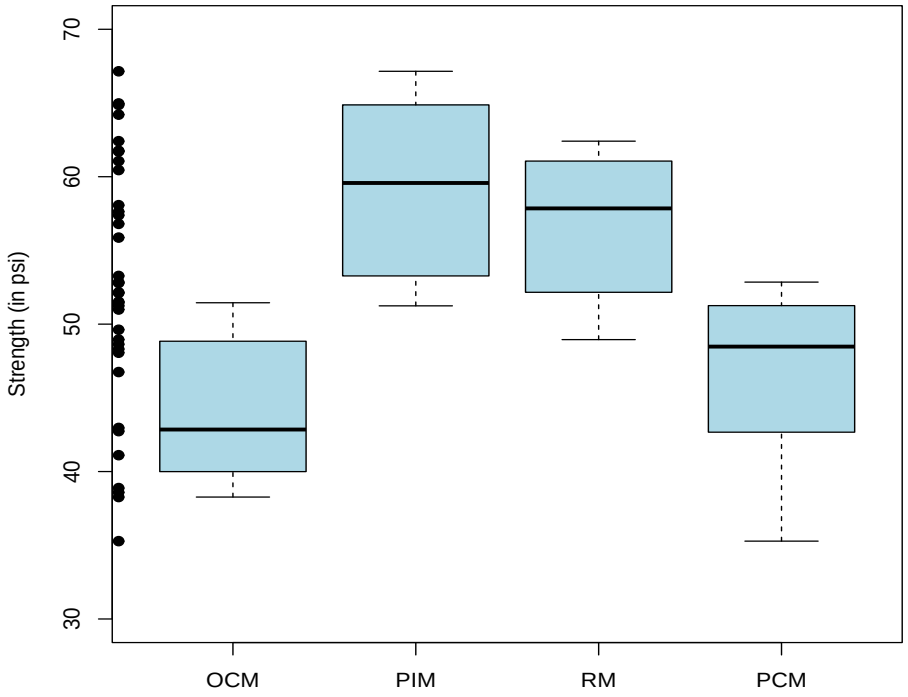


Figure 9.5: Mortar strength data. Boxplots of flexural bond strengths (in psi) for four types of mortar. All observations are shown using dots on the vertical axis.

This partition of variability can be written out mathematically as

$$\underbrace{\sum_{i=1}^{t}\sum_{j=1}^{n_i}(X_{ij}-\overline{X}_{++})^2}_{\text{SS}_{\text{TOT}}} = \underbrace{\sum_{i=1}^{t} n_i(\overline{X}_{i+}-\overline{X}_{++})^2}_{\text{SS}_{\text{T}}} + \underbrace{\sum_{i=1}^{t}\sum_{j=1}^{n_i}(X_{ij}-\overline{X}_{i+})^2}_{\text{SS}_{\text{E}}},$$

or, in other words,

$$\text{SS}_{\text{TOT}} = \text{SS}_{\text{T}} + \text{SS}_{\text{E}}.$$

We call

- SS_{TOT} is the **total sum of squares**. This measures how much variability there is in all the data combined.
- SS_{T} is the **treatment sum of squares**. This measures how much variability there is in the treatment group means.
- SS_{E} is the **error (residual) sum of squares**. This measures how much variability is "left over" after accounting for differences among the treatment groups.

ANOVA table: The general form of an ANOVA table for a one-way classification analysis is shown below:

Source	df	SS	MS	F
Treatments	$t-1$	SS_T	$\text{MS}_\text{T} = \frac{\text{SS}_\text{T}}{t-1}$	$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}}$
Residuals	$N-t$	SS_E	$\text{MS}_\text{E} = \frac{\text{SS}_\text{E}}{N-t}$	
Total	$N-1$	SS_TOT		

Notes:

- The **degrees of freedom** (df) column lists $t-1$ and $N-t$, which are the degrees of freedom in the sampling distribution of F when H_0 is true; recall

$$F = \frac{\text{MS}_\text{T}}{\text{MS}_\text{E}} \sim F(t-1, N-t).$$

  The degrees of freedom add down.

- We have already seen

$$\text{SS}_\text{TOT} = \text{SS}_\text{T} + \text{SS}_\text{E}$$

  for the **sum of squares** column (SS). The sum of squares add down.

- The **mean squares** (MS) are the sum of squares divided by their degrees of freedom. Recall

$$\begin{aligned} E(\text{MS}_\text{T}) &= \sigma^2 \\ E(\text{MS}_\text{E}) &= \sigma^2 \end{aligned}$$

  when H_0 is true. These were the two unbiased estimators of σ^2 we derived initially (assuming H_0 is true).

- The F **statistic** is the ratio of the mean squares.

Mortar strength data: We have already seen the ANOVA table for the mortar strength data in Example 9.1:

```
Analysis of Variance Table

Response: Strength
          Df Sum Sq Mean Sq F value   Pr(>F)
Mortar     3 1520.9   507.0   16.85 9.58e-07 ***
Residuals 32  962.9    30.1
```

Note: R does not include the SS_TOT row for the total sum of squares.

9.1.2 Probability values

Remark: When we perform a hypothesis test like

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_t$$

versus

$$H_1 : \text{the population means are not all equal,}$$

we are ultimately making a decision between two competing hypotheses. Are the data more consistent with H_0 or H_1? The probability value (p-value) is a widely used concept that helps investigators make a decision.

Terminology: The **probability value** (**p-value**) for a hypothesis test measures how much evidence we have against H_0. It is important to remember the following:

$$\text{the smaller the p-value} \implies \text{the more evidence against } H_0.$$

This decision rule is written in a way that reminds us how we should think about hypothesis testing. The p-value quantifies the strength of the evidence we have against H_0. If the strength of this evidence is judged to be sufficient, then we reject H_0 in favor of H_1.

Mortar strength data: The p-value `Pr(>F)` provided in the ANOVA table (see previous page) is

$$\text{p-value} = 9.58 \times 10^{-7} = 0.000000958.$$

By any reasonable definition of "small," this p-value is small. In fact, this p-value is incredibly small.

- P-values in one-way classification analyses are calculated as **areas to the right** of F under its sampling distribution when H_0 is true. This is what `Pr(>F)` means in the R output.
- The area to the right of $F = 16.85$ under the $F(3, 32)$ pdf is 0.000000958; see Figure 9.4.
- This number (probability) being so small means that $F \geq 16.85$ would be incredibly unlikely to see when H_0 is true.
- Therefore, our decision is to reject

  $$H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$$

  in favor of

  $$H_1 : \text{the population means are not all equal.}$$

Q: In general, how small does the p-value have to be before we attain "sufficient evidence" to reject H_0 in favor of H_1?

A: There is no "right" answer to this question. A common strategy adopted by practitioners is the following:

- Before data collection and analysis, adopt a **significance level** α for any inference that is to be performed (like testing H_0 versus H_1). The significance level is related to the confidence level in confidence intervals (Chapters 7-8).
- Specifically, α is the probability one rejects H_0 when it is true; i.e.,

$$\alpha = P(\text{Reject } H_0 | H_0 \text{ true}).$$

  Therefore, when an investigator specifies what α is, s/he is eliciting the percentage of times in the long run a true H_0 will be rejected (a mistake). Clearly, one wants this percentage to be small.
- Common values of α are $\alpha = 0.10$, $\alpha = 0.05$ (the most common), and $\alpha = 0.01$.
- The smaller the α is chosen to be, the more evidence one requires to reject H_0. This is a true because

$$\textbf{p-value} < \alpha \Longrightarrow \textbf{reject } H_0\textbf{.}$$

- Therefore, the value of α chosen by the investigator determines what "sufficient evidence" means. It is how small the p-value must be to reject H_0.

Q: How large would the F statistic have to be in Example 9.1 to have "sufficient evidence" against H_0 if we used $\alpha = 0.05$ as a significance level?
A: If $\alpha = 0.05$, then we need to find the 95th percentile of the $F(3, 32)$ distribution, the sampling distribution of F when H_0 is true; see Figure 9.6 (next page). This percentile is

$$F_{3,32,0.95} \approx 2.901.$$

```
> options(digits=4)
> qf(0.95,3,32)
[1] 2.901
```

Therefore, we would reject

$$H_0 : \mu_1 = \mu_2 = \mu_3 = \mu_4$$

in favor of

$$H_1 : \text{the population means are not all equal}$$

whenever

$$F > 2.901 \iff \text{p-value} < 0.05.$$

Recall the F statistic in Example 9.1 was $F = 16.85$! This is why the p-value was so small.

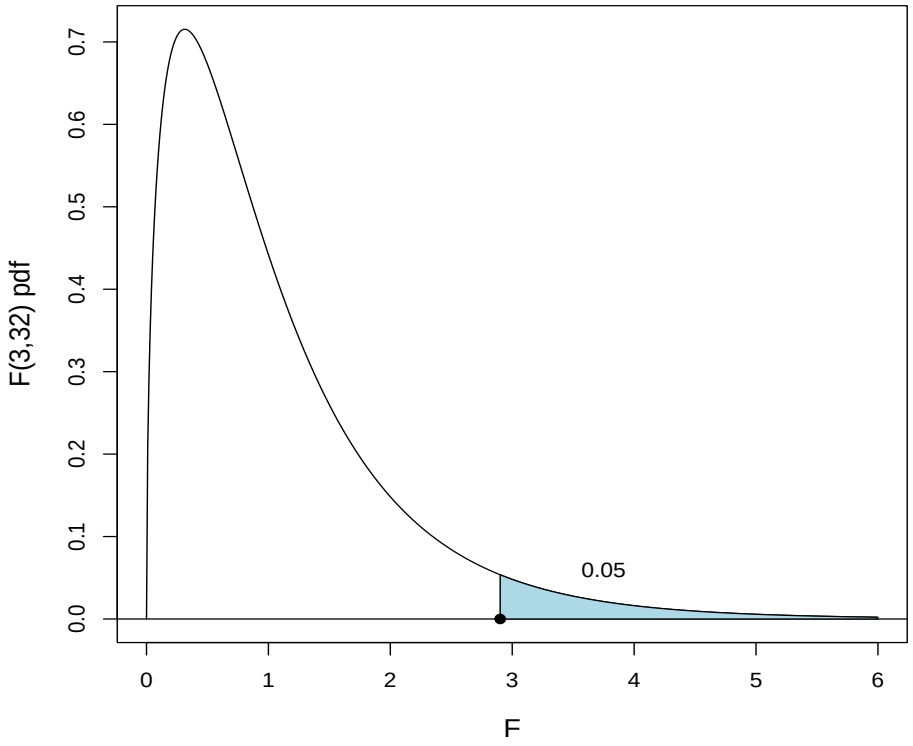


Figure 9.6: $F(3, 32)$ pdf. This is the distribution of F when H_0 is true in Example 9.1. When $\alpha = 0.05$, values of F larger than $F_{3,32,0.95} \approx 2.901$ lead to rejecting H_0.

Discussion: Suppose in Example 9.1 the value of the F statistic was $F = 3.04$ instead.

- Using $\alpha = 0.05$, we would reject H_0 because

$$F > F_{3,32,0.95} \approx 2.901 \iff \text{p-value} = 0.043 < 0.05.$$

- Using $\alpha = 0.01$, we would not reject H_0 because

$$F < F_{3,32,0.99} \approx 4.459 \iff \text{p-value} = 0.043 > 0.01.$$

Therefore, two different people who analyze the **same data** could reach different conclusions about H_0 and H_1. Is this a contradiction?

```
> options(digits=2)
> 1-pf(3.04,3,32) # p-value
[1] 0.043
> options(digits=4)
> qf(0.99,3,32) # 99th percentile
[1] 4.459
```

9.1.3 Assumptions for one-way classification analyses

Recall: The overall F test for H_0 versus H_1 is based on four assumptions:

1. We have **random samples** from each population.

2. The t samples are **independent**.

These assumptions are critical and are usually valid when the study is performed properly. This means selecting samples independently (in observational studies) or using randomization to assign individuals to different treatment groups (in designed experiments).

3. The population distributions are **normal**.

We can use normal qq plots with each sample to check this assumption. Of course, with small samples (like in Example 9.1), these plots may not be all that helpful. Like other statistical inference procedures involving means, the overall F test is robust to minor to moderate departures from normality.

4. **Equal population variances**, that is, $\sigma_1^2 = \sigma_2^2 = \cdots = \sigma_t^2 = \sigma^2$.

This assumption is extremely critical. Recall the entire idea behind the F test was coming up with two unbiased estimates of σ^2 when H_0 is true, that is,

$$\begin{aligned} E(\text{MS}_\text{T}) &= \sigma^2 \\ E(\text{MS}_\text{E}) &= \sigma^2. \end{aligned}$$

If the t population variances are not equal, then we have no idea what MS_T and MS_E are even estimating.

- We can do empirical checks using side-by-side boxplots with the samples, but these graphs offer only sample information. If we notice substantially different amounts of variability in the samples, it's probably a good idea not to even do the F test. It could be misleading.

- There is a nonparametric procedure for one-way classification analyses called the **Kruskal-Wallis test** which does not require normality or equal population variances. It is a better test to use when both assumptions are in doubt.

- There is also a procedure which formally tests the equality of t population variances, that is,

$$H_0 : \sigma_1^2 = \sigma_2^2 = \cdots = \sigma_t^2$$

versus

$$H_1 : \text{the population variances are not all equal.}$$

The procedure is called **Bartlett's test**. However, this test depends critically on the normality assumption (like the test for the equality of population variances in Section 8.3). A nonparametric version of Bartlett's test that does not assume normality is available; it is called **Levene's test**.

9.2 Multiple comparisons following the overall F test

Recall: In a one-way classification, the overall F test is used to test

$$H_0 : \mu_1 = \mu_2 = \cdots = \mu_t$$

versus

$$H_1 : \text{the population means are not all equal.}$$

If we reject H_0 in favor of H_1, as we did in Example 9.1 with the mortar strength data, we conclude at least one population mean is different than the others. However, we do not know which ones are different or how they are different. Therefore, rejecting H_0 and concluding "the evidence supports H_1" is not all that informative.

Follow-up analysis: If H_0 is rejected, the obvious task becomes determining which population means are different from the others. We will do this by writing confidence intervals for all **pairwise population mean differences**

$$\Delta_{ii'} = \mu_i - \mu_{i'},$$

for $1 \leq i < i' \leq t$, and seeing which intervals exclude "0" like we did in Chapter 8. If there are t treatment groups in H_0, there are

$$\binom{t}{2} = \frac{t(t-1)}{2}$$

pairwise confidence intervals to construct. For example, in Example 9.1, there are $t = 4$ treatment groups (OCM, PIM, RM, and PCM) and therefore 6 pairwise population mean differences:

$$\Delta_{12} = \mu_1 - \mu_2 \qquad \Delta_{13} = \mu_1 - \mu_3 \qquad \Delta_{14} = \mu_1 - \mu_4$$
$$\Delta_{23} = \mu_2 - \mu_3 \qquad \Delta_{24} = \mu_2 - \mu_4 \qquad \Delta_{34} = \mu_3 - \mu_4,$$

where

$$\begin{aligned} \mu_1 &= \text{population mean strength for OCM} \\ \mu_2 &= \text{population mean strength for PIM} \\ \mu_3 &= \text{population mean strength for RM} \\ \mu_4 &= \text{population mean strength for PCM.} \end{aligned}$$

Constructing confidence intervals for the 6 pairwise population mean differences above will allow us to determine which population means are different and how they are different.

Problem: We have a new statistical challenge to confront. Suppose we write 95% confidence intervals for each pairwise population mean difference above. What is the confidence level associated with the 6 intervals combined as a group? Is it larger than 95%? smaller than 95%, or equal to 95%?

A: It's smaller than 95%. In fact, it's potentially *a lot* smaller than 95%. In statistics, this is known as the **multiple comparisons problem**.

Discussion: There is an inequality in probability called **Bonferroni's Inequality**, which states that if we have events $A_1, A_2, ..., A_K$, the probability each event occurs

$$P\left(\bigcap_{k=1}^{K} A_k\right) \geq \sum_{k=1}^{K} P(A_k) - (K-1).$$

To see how this inequality can be used in our current discussion on making multiple population-level comparisons, define the event

$$A_k = \{k\text{th confidence interval includes its population mean difference}\},$$

for $k = 1, 2, ..., K$. The intersection

$$\bigcap_{k=1}^{K} A_k = \{\text{each of the } K \text{ intervals includes its population mean difference}\}$$

is the event we are interested in because we would like all confidence intervals to include their population mean difference with a given level of confidence. How small can

$$P\left(\bigcap_{k=1}^{K} A_k\right)$$

be? This probability is the confidence level for all K intervals **combined**. Consider the following table which uses Bonferroni's Inequality to find a lower bound for this probability. We assume each of the K intervals has been constructed using a 95% confidence level individually so that $P(A_1) = P(A_2) = \cdots = P(A_K) = 0.95$.

Number of treatment groups t	Number of pairwise intervals K	Lower bound
3	3	$3(0.95) - 2 = 0.85$
4	6	$6(0.95) - 5 = 0.70$
5	10	$10(0.95) - 9 = 0.50$
6	15	$15(0.95) - 14 = 0.25$
$\vdots$	$\vdots$	$\vdots$
10	45	$45(0.95) - 44 = -1.25$!!

Therefore, with just $t = 4$ treatment groups (populations), like in Example 9.1, the probability each of the six 95% confidence intervals will contain its population mean difference can be as low as 0.70. For studies with more treatment groups, this combined confidence level can be much lower! Clearly, this is a problem which has to be addressed. If we do not address it, then we run the risk of having very low confidence in our assessment of how the population means are different.

Goal: Following a rejection of H_0 using the overall F test for one-way classification, we would like to construct confidence intervals for all pairwise population mean differences

$$\Delta_{ii'} = \mu_i - \mu_{i'},$$

for $1 \leq i < i' \leq t$. We would like our **family-wise confidence level** to be $100(1-\alpha)\%$. By "family-wise," we mean that our confidence level $100(1-\alpha)\%$ applies to the collection of all $\binom{t}{2}$ intervals combined.

Solution: If we want to promise the family-wise confidence level is $100(1-\alpha)\%$ for the $\binom{t}{2}$ intervals combined, then we have to increase the confidence level associated with each individual interval. **Tukey's multiple comparisons method** is designed to do this for all pairwise population mean differences. Family-wise $100(1-\alpha)\%$ confidence intervals for $\Delta_{ii'} = \mu_i - \mu_i'$ are

$$(\overline{X}_{i+} - \overline{X}_{i'+}) \pm q_{t,N-t,\alpha}\sqrt{\text{MS}_\text{E}\left(\frac{1}{n_i} + \frac{1}{n_{i'}}\right)},$$

where $q_{t,N-t,\alpha}$ is the quantile that guarantees a family-wise confidence level of $100(1-\alpha)\%$ for all pairwise population mean differences.

- We see these intervals have the familiar form:

$$\underbrace{\text{point estimate}}_{\overline{X}_{i+}-\overline{X}_{i'+}} \pm \underbrace{\text{quantile}}_{q_{t,N-t,\alpha}} \times \underbrace{\text{standard error}}_{\sqrt{\text{MS}_\text{E}\left(\frac{1}{n_i}+\frac{1}{n_{i'}}\right)}}.$$

- The quantile $q_{t,N-t,\alpha}$ comes from **Tukey's studentized range distribution**, which describes the difference between the largest and smallest sample means.
- We can use these confidence intervals to determine which population means are different as we did before:
  - a confidence interval excluding "0" suggests that pair of population means is different.
  - a confidence interval including "0" does not suggest that pair of population means is different.

Example 9.1 (continued). We use R to construct 95% Tukey confidence intervals for all 6 pairwise population mean differences. The family-wise confidence level in the collection of intervals below is 95%.

```
> options(digits=3)
> TukeyHSD(aov(fit),conf.level=0.95)
  Tukey multiple comparisons of means
    95% family-wise confidence level
```

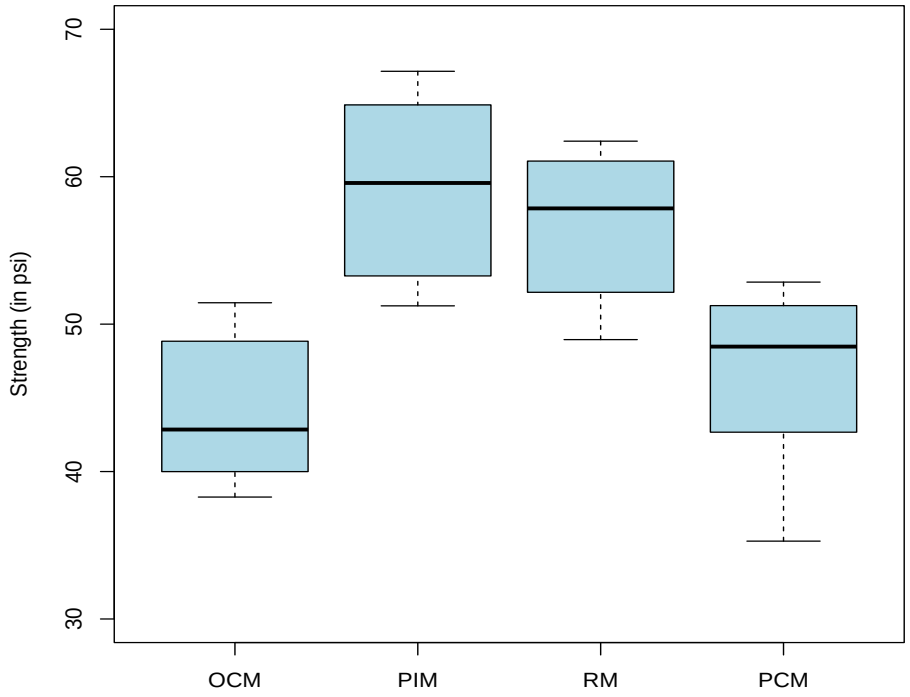


Figure 9.7: Mortar strength data. Boxplots of flexural bond strengths (in psi) for four types of mortar.

```
$Mortar
         diff   lwr   upr p adj
PCM-OCM  2.48 -4.95  9.91 0.803
PIM-OCM 15.22  8.17 22.27 0.000
RM-OCM  13.00  5.95 20.05 0.000
PIM-PCM 12.74  5.69 19.79 0.000
RM-PCM  10.52  3.47 17.57 0.002
RM-PIM  -2.22 -8.86  4.43 0.803
```

Interpretation: In the R output above, the columns labeled `lwr` and `upr` give, respectively, the lower and upper limits of the pairwise confidence intervals.

- `PCM-OCM`: We are 95% confident the population mean difference between PCM and OCM mortar strength is between -4.95 and 9.91 psi.
  - This confidence interval includes "0," so we cannot conclude these two population means are different.
  - This same conclusion is also identified by the **adjusted p-value** for these two mortars in the `p adj` column. This p-value is large ($0.803 > 0.05$), meaning we would not reject the hypothesis these two population mean strengths are equal.

- `PIM-OCM`: We are 95% confident the population mean difference between PIM and OCM mortar strength is between 8.17 and 22.27 psi.
  - This confidence interval does not include "0" and contains only positive values. This suggests the population mean PIM mortar strength is larger than the population mean OCM mortar strength.
  - This same conclusion is also identified by the **adjusted p-value** for these two mortars in the `p adj` column. This p-value is very small (< 0.001), meaning we would reject the hypothesis these two population mean strengths are equal.
- Interpretations for the remaining four confidence intervals are written similarly.

Remark: The R output in this example allows us to make 6 comparisons for each pair of population mean mortar strengths. Each comparison we make has a "protected" confidence level of 95%, and this confidence level applies to all 6 comparisons as a group. This is the reason we make corrections for multiple comparisons.

- In general, if you do not correct for multiple comparisons, there is a good chance you will conclude two population means are different when, in fact, they are not. This is called a **false discovery**.
- When one compares a large number of treatment groups, the probability an uncorrected analysis will produce at least one false discovery approaches 1 very quickly.
- This is why the multiple comparisons issue is so critical−to prevent false discoveries in our conclusions.

Mortar strength data: From the R output, the following pairs of population means are declared to be different:

`PIM-OCM` `RM-OCM` `PIM-PCM` `RM-PCM`.

The following pairs of population means are not declared to be different:

`PCM-OCM` `RM-PIM`.

We can therefore conclude:

- The `PIM` and `RM` population mean strengths are larger than the `OCM` and `PCM` population mean strengths.
- We cannot conclude the `PCM` and `OCM` population mean strengths are different.
- We cannot conclude the `RM` and `PIM` population mean strengths are different.

These conclusions carry with them an overall (family-wise) confidence level of 95%. That is, we are 95% confident that **all of these conclusions** are correct.

10 Simple Linear Regression

10.1 Introduction

Big picture: A problem often arising in engineering, business, medicine, and other areas, is that of investigating the mathematical relationship between two (or more) variables. The goal is often to model a continuous **response variable** Y as a function of one or more independent variables, say, $x_1, x_2, ..., x_k$. One can express this model as

$$Y = g(x_1, x_2, ..., x_k) + \epsilon,$$

where $g : \mathbb{R}^k \to \mathbb{R}$ and ϵ is a random error term that satisfies certain assumptions. This is called a **regression model**.

- The presence of the error term ϵ reminds us that the relationship between Y and the independent variables through $g(x_1, x_2, ..., x_k)$ is not perfect. If it was perfect, this would be a deterministic model.
- The independent variables $x_1, x_2, ..., x_k$ are assumed to be fixed (not random) and measured without error.

There are different types of regression models. A **nonparametric model** would leave the form of g unspecified, essentially regarding the relationship between Y and the independent variables $x_1, x_2, ..., x_k$ to be characterized by an unknown function. A **parametric model** would specify the form of g, for example,

$$Y = \underbrace{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k}_{g(x_1, x_2, ..., x_k)} + \epsilon,$$

where $\beta_0, \beta_1, ..., \beta_k$ are unknown regression parameters. This is called a **linear regression model**. The adjective "linear" does not refer to the form of $g(x_1, x_2, ..., x_k)$. Instead, it refers to the manner in which the regression parameters $\beta_0, \beta_1, ..., \beta_k$ appear in the g function. With the g function above, note that

$$\begin{aligned}
\frac{\partial g(x_1, x_2, ..., x_k)}{\partial \beta_0} &= 1 \\
\frac{\partial g(x_1, x_2, ..., x_k)}{\partial \beta_1} &= x_1 \\
&\vdots \\
\frac{\partial g(x_1, x_2, ..., x_k)}{\partial \beta_k} &= x_k.
\end{aligned}$$

All of these partial derivatives are free of $\beta_0, \beta_1, ..., \beta_k$, meaning g is a linear function of these parameters. With this definition in mind, we see all of the following models are linear in the

regression parameters:

$$\begin{aligned}
Y &= \underbrace{\beta_0 + \beta_1 x}_{g(x)} + \epsilon \\
Y &= \underbrace{\beta_0 + \beta_1 x + \beta_2 x^2}_{g(x)} + \epsilon \\
Y &= \underbrace{\beta_0 + \beta_1 x_1 + \beta_2 x_2}_{g(x_1,x_2)} + \epsilon \\
Y &= \underbrace{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2}_{g(x_1,x_2)} + \epsilon \\
Y &= \underbrace{\beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \beta_6 x_2 x_3 + \beta_7 x_1 x_2 x_3}_{g(x_1,x_2,x_3)} + \epsilon.
\end{aligned}$$

These are all examples of linear regression models. An example of a **nonlinear regression model** is

$$Y = \underbrace{\frac{\beta_0}{1 + \beta_1 e^{\beta_2 x}}}_{g(x)} + \epsilon.$$

This model is not linear in its parameters β_0, β_1, and β_2. For example,

$$\frac{\partial g(x)}{\partial \beta_0} = \frac{1}{1 + \beta_1 e^{\beta_2 x}},$$

which is not free of β_1 and β_2.

Preview: This chapter is about **simple linear regression**, which involves population-level models of the form

$$Y = \beta_0 + \beta_1 x + \epsilon.$$

We will examine the following questions:

1. The regression parameters β_0 and β_1 are best regarded as unknown because they describe how Y and x are related in a **population** of individuals. How do we estimate them with a sample from the population?

2. How do we perform **statistical inference**, for example, writing confidence intervals β_0 and β_1? Note that a confidence interval for β_1 would be especially useful. It would allow us to assess whether Y and x are linearly related in the population.

3. How do we use our estimated model to make **predictions** while quantifying the uncertainty in these predictions?

This chapter answers these questions for simple linear regression, that is, when there is one independent variable x. Chapter 11 moves to **multiple linear regression** where there are multiple independent variables $x_1, x_2, ..., x_k$. Multiple linear regression models are presented using vectors and matrices because it makes things easier.

10.2 Simple linear regression model

Terminology: A **simple linear regression model** is of the form

$$Y = \beta_0 + \beta_1 x + \epsilon.$$

The population regression function $g(x) = \beta_0 + \beta_1 x$ is a straight line with intercept β_0 and slope β_1. These parameters describe the population of individuals for which this model is assumed. The error term ϵ is assumed to be random, making this a statistical model.

Interpretation: If $E(\epsilon) = 0$, then

$$\begin{aligned} E(Y) &= E(\beta_0 + \beta_1 x + \epsilon) \\ &= \beta_0 + \beta_1 x + E(\epsilon) \\ &= \beta_0 + \beta_1 x. \end{aligned}$$

Therefore, we have the following interpretations for the regression parameters β_0 and β_1:

- β_0 represents the population mean of Y when $x = 0$.
- β_1 is the population-level change in $E(Y)$ brought about by a one-unit change in x.

Example 10.1. A study was conducted involving a sample of $n = 24$ "middle-aged" men (all aged 45-64 years) to determine the relationship between

$$\begin{aligned} Y &= \text{maximum oxygen uptake (in mL/kg/min)} \\ x &= \text{time to run a two-minute mile (in seconds).} \end{aligned}$$

A person's maximum oxygen uptake is the highest amount of oxygen the body can take in and use during intense exercise and is the gold standard for measuring cardiorespiratory fitness (the higher the better). Here are the data from the study:

Subject	Max O_2	Time	Subject	Max O_2	Time	Subject	Max O_2	Time
1	27.33	1218	9	21.23	1345	17	38.29	1043
2	38.10	1105	10	34.66	1110	18	32.18	1103
3	27.08	1191	11	26.49	1227	19	41.91	983
4	35.06	1262	12	31.17	1113	20	32.80	1144
5	27.45	1268	13	31.18	1158	21	33.65	1055
6	27.46	1207	14	28.21	1160	22	38.67	1000
7	32.82	1070	15	36.81	1060	23	45.62	1048
8	34.92	1043	16	38.28	1047	24	41.76	1075

A scatterplot of the sample is shown in Figure 10.1. Based on the appearance of the data in the plot, a simple linear regression model (for the population of "middle-aged" men) seems appropriate.

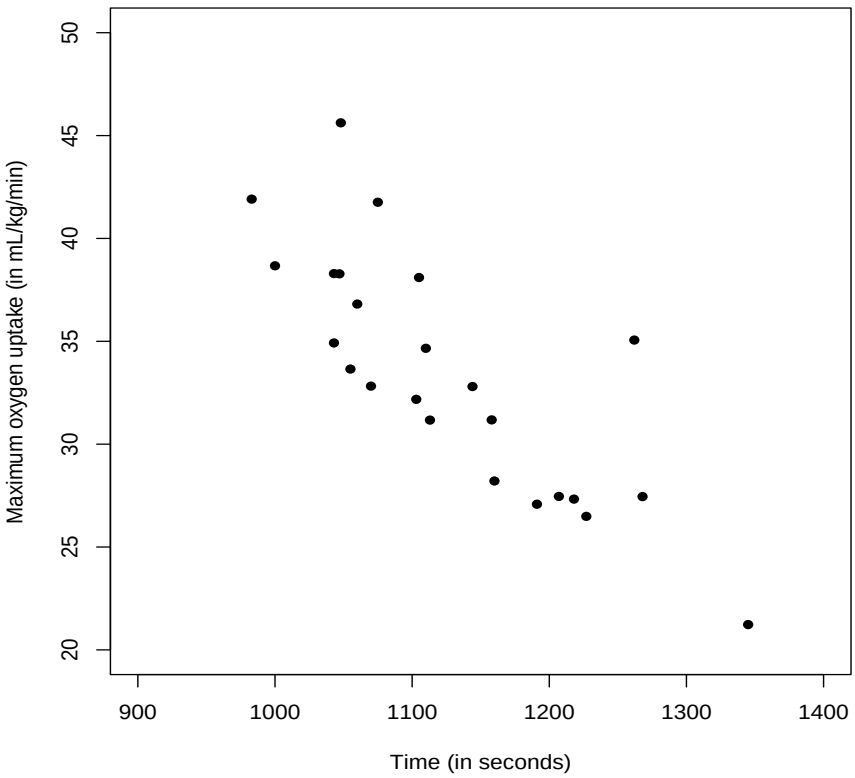


Figure 10.1: Max O_2 uptake data. Scatterplot of maximum oxygen uptake (Y) and the time to run a two-minute mile (x) for $n = 24$ middle-aged men.

Discussion: If we assume

$$Y = \beta_0 + \beta_1 x + \epsilon \quad \Longleftrightarrow \quad E(Y) = \beta_0 + \beta_1 x$$

holds for the population of all middle-aged men, then what does ϵ represent?

A: It captures everything not explained by the population regression function $g(x) = \beta_0 + \beta_1 x$. This includes

- Sampling variability. The study included a sample of $n = 24$ middle-aged men. This is a small part of the population of "all middle-aged men." Different samples of men will produce different measurements. The variability among different sets of measurements from the same population is absorbed into the error term.
- What are all the additional factors that influence maximum oxygen uptake?
  - Age, genetics, health factors, behavioral factors (e.g., smoking status, exercise frequency, etc.), environmental factors, etc.

- None of these factors are in the population-level model $E(Y) = \beta_0 + \beta_1 x$, so any influence they have on the maximum oxygen uptake gets absorbed into the error term.

- Measurement error in the response variable Y. This includes any error that is introduced when measuring the maximum oxygen uptake on the individual men.

10.3 Least-squares estimation

Terminology: For simple linear regression, when we say we want to "fit the model" or "estimate the model," we mean we would like to estimate the population-level parameters

$$\beta_0 \text{ and } \beta_1$$

with the observed data like those in Figure 10.1. Suppose we observe a random sample of individuals from a larger population and the pairs

$$(x_1, Y_1), (x_2, Y_2), ..., (x_n, Y_n)$$

are obtained which follow

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i,$$

for $i = 1, 2, ..., n$. Formal assumptions on the error terms ϵ_i will be needed later when we investigate sampling distributions and statistical inference.

Least-squares estimation: A widely accepted method of estimating the population parameters β_0 and β_1 is to use least squares, which says to choose the values of β_0 and β_1 that minimize

$$Q(\beta_0, \beta_1) = \sum_{i=1}^{n} [Y_i - (\beta_0 + \beta_1 x_i)]^2.$$

That is, in least-squares estimation, one seeks to minimize the sum of squared vertical distances between

$$Y_i \text{ and } \beta_0 + \beta_1 x_i.$$

Taking partial derivatives of $Q(\beta_0, \beta_1)$, we obtain

$$\begin{aligned} \frac{\partial Q(\beta_0, \beta_1)}{\partial \beta_0} &= -2 \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 x_i) \stackrel{\text{set}}{=} 0 \\ \frac{\partial Q(\beta_0, \beta_1)}{\partial \beta_1} &= -2 \sum_{i=1}^{n} (Y_i - \beta_0 - \beta_1 x_i) x_i \stackrel{\text{set}}{=} 0. \end{aligned}$$

Solving these equations simultaneously for β_0 and β_1 gives

$$\widehat{\beta}_0 = \overline{Y} - \widehat{\beta}_1 \overline{x}$$

and

$$\widehat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \overline{x})(Y_i - \overline{Y})}{\sum_{i=1}^n (x_i - \overline{x})^2}.$$

These are the **least-squares estimators** of β_0 and β_1, respectively. The estimated model is written as follows:

$$\widehat{Y} = \widehat{\beta}_0 + \widehat{\beta}_1 x.$$

This is the equation of the line which minimizes $Q(\beta_0, \beta_1)$, the sum of squared vertical distances. We call this the **least-squares regression line**, the so-called "line of best fit."

Example 10.1 (continued). For the maximum oxygen uptake data in Example 10.1, we use R to calculate the least-squares estimates of β_0 and β_1 in the model

$$Y = \beta_0 + \beta_1 x + \epsilon \quad \Longleftrightarrow \quad \texttt{max.O2} = \beta_0 + \beta_1 \texttt{(time)} + \epsilon.$$

```
> options(digits=3)
> fit = lm(max.O2 ~ time)
> fit

Coefficients:
(Intercept)         time
    91.3003      -0.0513
```

From the R output, we identify

$$\begin{aligned} \widehat{\beta}_0 &\approx 91.3003 \\ \widehat{\beta}_1 &\approx -0.0513. \end{aligned}$$

The equation of the least-squares regression line is

$$\widehat{Y} = 91.3003 - 0.0513x \quad \Longleftrightarrow \quad \widehat{\texttt{max.O2}} = 91.3003 - 0.0513\texttt{(time)}.$$

This line is shown in Figure 10.2 (next page) superimposed over the scatterplot. The equation above is our **estimate** of how maximum oxygen uptake (Y) and the time to run a two-minute mile (x) are linearly related in the population of all middle-aged men.

Curiosity: What would happen if we sampled another $n = 24$ individuals from the population of all middle-aged men?

- We would get different individuals, different observations of Y and x, and different least-squares estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$.
- That is, the least-squares estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$ will vary from sample to sample.
- We therefore need to examine the properties of $\widehat{\beta}_0$ and $\widehat{\beta}_1$ as estimators and their **sampling distributions**. This will inform us how to perform statistical inference for β_0 and β_1 in the population.

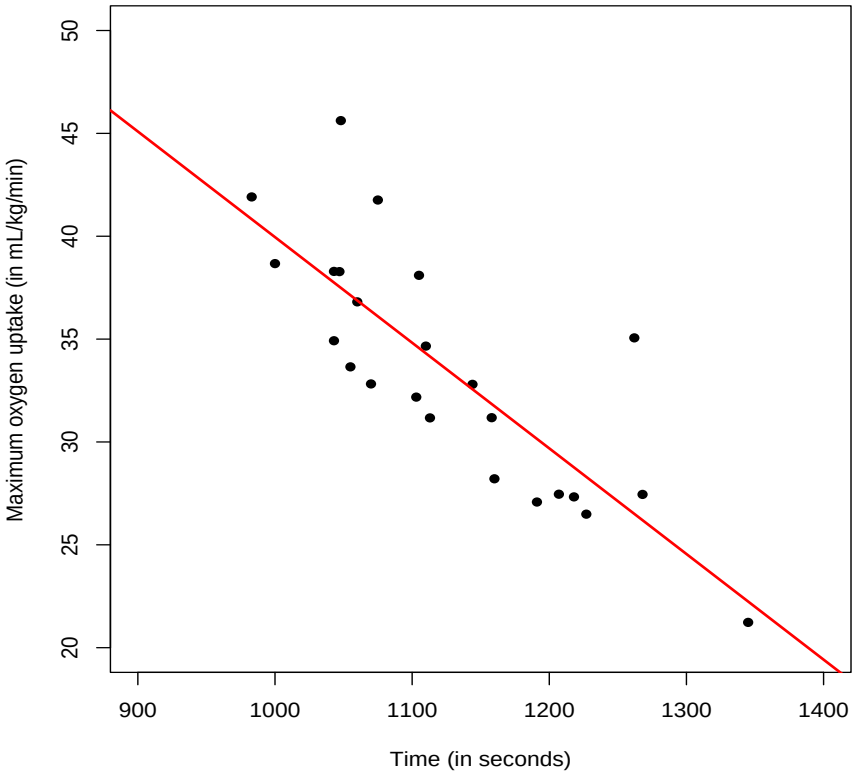


Figure 10.2: Max O_2 uptake data. Scatterplot of maximum oxygen uptake (Y) and the time to run a two-minute mile (x) for $n = 24$ middle-aged men. The least-squares regression line has been superimposed.

10.4 Model assumptions and sampling distributions

Importance: Our goal is to perform statistical inference for the population-level parameters β_0 and β_1 in the simple linear regression model

$$Y_i = \beta_0 + \beta_1 x_i + \epsilon_i,$$

for $i = 1, 2, ..., n$. To do this, we first need to state statistical assumptions on the (random) error terms ϵ_i.

Assumptions: We will assume

- $E(\epsilon_i) = 0$, for $i = 1, 2, ..., n$, that is, the errors have zero mean
- $V(\epsilon_i) = \sigma^2$, for $i = 1, 2, ..., n$, that is, the errors have constant variance
- the errors ϵ_i are independent
- the errors ϵ_i are normally distributed.

Simple linear regression results: Under the assumptions stated on the previous page, mathematics shows the following for the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon.$$

Result 1:

$$Y \sim \mathcal{N}(\beta_0 + \beta_1 x, \sigma^2).$$

In other words, the response variable Y is normally distributed with mean $\beta_0 + \beta_1 x$ and variance σ^2. Note the population mean of Y is a linear function of x. The population variance of Y does not depend on x.

Result 2: The least-squares estimators $\widehat{\beta}_0$ and $\widehat{\beta}_1$ are **unbiased**, that is,

$$\begin{aligned} E(\widehat{\beta}_0) &= \beta_0 \\ E(\widehat{\beta}_1) &= \beta_1. \end{aligned}$$

Result 3: The least-squares estimators $\widehat{\beta}_0$ and $\widehat{\beta}_1$ have **normal sampling distributions**, specifically,

$$\widehat{\beta}_0 \sim \mathcal{N}(\beta_0, c_{00}\sigma^2) \quad \text{and} \quad \widehat{\beta}_1 \sim \mathcal{N}(\beta_1, c_{11}\sigma^2),$$

where

$$c_{00} = \frac{1}{n} + \frac{\overline{x}^2}{S_{xx}} \quad \text{and} \quad c_{11} = \frac{1}{S_{xx}}$$

and $S_{xx} = \sum_{i=1}^{n}(x_i - \overline{x})^2$.

Remark: We see the **standard errors** of the least-squares estimators

$$\begin{aligned} \text{se}(\widehat{\beta}_0) &= \sqrt{c_{00}\sigma^2} \\ \text{se}(\widehat{\beta}_1) &= \sqrt{c_{11}\sigma^2} \end{aligned}$$

both depend on σ^2, the population variance of Y, which is unknown. This creates a problem. If we don't know what σ^2 is, we can't calculate the standard errors above. If we can't calculate the standard errors, we can't quantify uncertainty. This means we can't write confidence intervals for β_0 and β_1 or perform hypothesis tests for them. Therefore, if we want to perform statistical inference for either parameter, we have to estimate σ^2 first.

Result 4: An unbiased estimator of σ^2, the population variance of Y, is given by

$$\widehat{\sigma}^2 = \frac{1}{n-2}\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2,$$

where

$$\widehat{Y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_i.$$

We will use $\widehat{\sigma}^2$ as an estimate of σ^2 so that we can estimate $\text{se}(\widehat{\beta}_0)$ and $\text{se}(\widehat{\beta}_1)$ above. This will allow us to quantify the uncertainty in the least-squares estimates of β_0 and β_1.

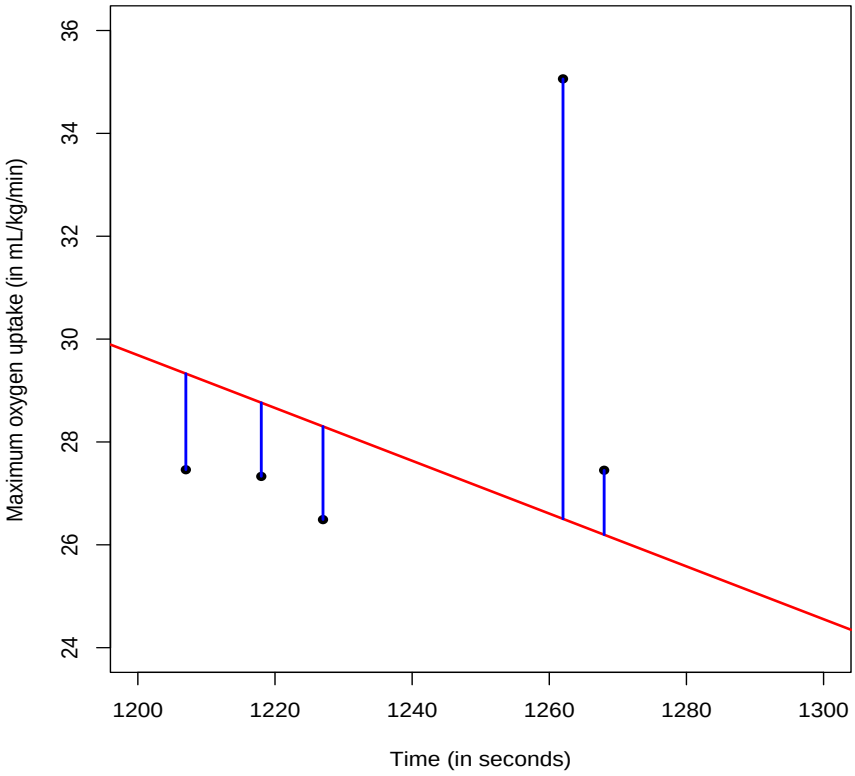


Figure 10.3: Max O_2 uptake data. Residuals and fitted values for 5 observations.

Terminology: After estimating a simple linear regression model, the **fitted value** associated with the ith observation (x_i, Y_i) is

$$\widehat{Y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_i$$

and the ith **residual** is

$$e_i = Y_i - \widehat{Y}_i.$$

Each observation has its own fitted value and residual. Figure 10.3 (above) shows the residuals and fitted values for men in Example 10.1 whose two-minute mile times are between 1200 and 1300 seconds. Note that

- If an individual's Y value is above the least squares regression line, then $Y_i > \widehat{Y}_i$ and its residual e_i is positive.
- If an individual's Y value is below the least squares regression line, then $Y_i < \widehat{Y}_i$ and its residual e_i is negative.
- If an individual's Y value is on the least squares regression line, then $Y_i = \widehat{Y}_i$ and its residual e_i is zero.

Example 10.1 (continued). For the maximum oxygen uptake data in Example 10.1, we use R to calculate the residuals and fitted values (to 2 dp). Recall the equation of the least-squares regression line is

$$\widehat{Y} = 91.3003 - 0.0513x \quad \Longleftrightarrow \quad \widehat{\texttt{max.O2}} = 91.3003 - 0.0513\texttt{(time)}.$$

Residuals and fitted values can be obtained using `residuals(fit)` and `predict(fit)` in R, respectively; see our R code online.

Subject	Max O_2 (Y_i)	Time (x_i)	Fitted value ($\widehat{Y}_i$)	Residual (e_i)
1	27.33	1218	28.76	−1.43
2	38.10	1105	34.57	3.53
3	27.08	1191	30.15	−3.07
4	35.06	1262	26.50	8.56
5	27.45	1268	26.20	1.25
6	27.46	1207	29.33	−1.87
7	32.82	1070	36.36	−3.54
8	34.92	1043	37.75	−2.83
9	21.23	1345	22.24	−1.01
10	34.66	1110	34.31	0.35
11	26.49	1227	28.30	−1.81
12	31.17	1113	34.15	−2.98
13	31.18	1158	31.84	−0.66
14	28.21	1160	31.74	−3.53
15	36.81	1060	36.88	−0.07
16	38.28	1047	37.54	0.74
17	38.29	1043	37.75	0.54
18	32.18	1103	34.67	−2.49
19	41.91	983	40.83	1.08
20	32.80	1144	32.56	0.24
21	33.65	1055	37.13	−3.48
22	38.67	1000	39.96	−1.29
23	45.62	1048	37.49	8.13
24	41.76	1075	36.11	5.65

Interesting fact: The sum of the residuals from any least-squares regression fit equals 0, that is,

$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (Y_i - \widehat{Y}_i) = 0.$$

This is true as long as the regression model contains an intercept term (β_0). For the maximum oxygen uptake data in Example 10.1, we see this holds (up to rounding error):

```
> options(digits=3)
> sum(residuals(fit))
[1] -1.33e-15
```

Our estimate of σ^2, the population variance of Y, is

$$\widehat{\sigma}^2 = \frac{1}{24-2}\sum_{i=1}^{24}(Y_i - \widehat{Y}_i)^2 \approx 12.23.$$

```
> options(digits=4)
> sum((residuals(fit)^2))/(24-2)
[1] 12.23
```

10.5 Statistical inference for β_0 and β_1

Importance: In the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon \quad \Longleftrightarrow \quad E(Y) = \beta_0 + \beta_1 x,$$

we now discuss how to perform statistical inference for β_0 and β_1, the intercept and slope parameters in the model. Remember, this model describes how Y and x are related in a population of individuals, so β_0 and β_1 are (unknown) population parameters.

- Inference for β_1 is usually more important. The value of β_1 describes the strength and direction of the linear relationship between $E(Y)$ and x in the **population** of individuals (we estimate the model using only a sample).
- Therefore, writing a confidence interval or performing a hypothesis test for β_1 allows us to characterize whether $E(Y)$ and x are linearly related in the population.
- Inference for β_0 is also possible, but it usually isn't practically relevant. For example, in Example 10.1 with

  $$\begin{aligned} Y &= \text{maximum oxygen uptake (in mL/kg/min)} \\ x &= \text{time to run a two-minute mile (in seconds)}, \end{aligned}$$

  the model

  $$Y = \beta_0 + \beta_1 x + \epsilon \quad \Longleftrightarrow \quad E(Y) = \beta_0 + \beta_1 x,$$

  so β_0 would represent the population mean maximum oxygen uptake $E(Y)$ for all men who run the two-minute mile in $x = 0$ seconds! Intercept terms in linear regression often have nonsensical interpretations like this.

Result: Under the assumptions stated earlier for simple linear regression,

$$T = \frac{\widehat{\beta}_1 - \beta_1}{\sqrt{c_{11}\widehat{\sigma}^2}} \sim t(n-2),$$

where recall $c_{11} = 1/S_{xx}$ and $S_{xx} = \sum_{i-1}^{n}(x_i - \overline{x})^2$. This describes the sampling distribution of T, that is, how T will vary probabilistically when sampling from a population where the simple linear model and its assumptions are correct.

Confidence intervals: This previous sampling distribution result can be used to derive a $100(1-\alpha)\%$ confidence interval for β_1, which is

$$\widehat{\beta}_1 \pm t_{n-2,\alpha/2}\sqrt{c_{11}\widehat{\sigma}^2}.$$

- The value $t_{n-2,\alpha/2}$ is the upper $\alpha/2$ quantile from the $t(n-2)$ distribution.
- Note the familiar form of the interval:

$$\underbrace{\text{point estimate}}_{\widehat{\beta}_1} \pm \underbrace{\text{quantile}}_{t_{n-2,\alpha/2}} \times \underbrace{\text{standard error}}_{\sqrt{c_{11}\widehat{\sigma}^2}}.$$

- We interpret the interval in the usual way:

  > "We are $100(1-\alpha)\%$ confident the population slope parameter β_1 is in this interval."

  Or, in other words,

  > "For a one-unit increase in x, we are $100(1-\alpha)\%$ confident the change in the population mean $E(Y)$ is in this interval.

  This alternative interpretation is directed towards interpreting what β_1 represents in the population-level model

$$Y = \beta_0 + \beta_1 x + \epsilon \quad \Longleftrightarrow \quad E(Y) = \beta_0 + \beta_1 x.$$

- Note that if
  - the confidence interval for β_1 consists entirely of positive values; e.g., (1.5, 4.3), we would infer $\beta_1 > 0$ meaning that $E(Y)$ and x are **positively** linearly related in the population.
  - the confidence interval for β_1 consists entirely of negative values; e.g., $(-4.3, -1.5)$, we would infer $\beta_1 < 0$ meaning that $E(Y)$ and x are **negatively** linearly related in the population.
  - the confidence interval for β_1 contains "0;" e.g., $(-1.5, 4.3)$, we cannot infer that $E(Y)$ and x are linearly related in the population.

Example 10.1 (continued). For the maximum oxygen uptake data in Example 10.1, we use R to calculate confidence intervals for β_0 and β_1. Confidence intervals can be calculated directly using R's `confint` function:

```
> options(digits=2)
> confint(fit,level=0.95)
             2.5 %  97.5 %
(Intercept) 72.857 109.744
time        -0.068  -0.035
```

Interpretation: Again, the confidence interval for β_0 is meaningless because this represents the population mean maximum oxygen uptake $E(Y)$ for all men who run the two-minute mile in zero seconds. The confidence interval $(-0.068, -0.035)$ for β_1 is more meaningful:

> "For a one-second increase in the time to run a two-minute mile, we are 95% confident the change in the population mean maximum oxygen uptake $E(Y)$ is between -0.068 and -0.035 mL/kg/min."

Because this interval consists entirely of negative values, we would infer that $\beta_1 < 0$. This would mean the mean maximum oxygen uptake and the time to run a two-minute mile are negatively related in the population of all middle-aged men.

Hypothesis tests: Under our simple linear regression model and its assumptions, if we wanted to formally test

$$H_0 : \beta_1 = 0$$
versus
$$H_1 : \beta_1 \neq 0,$$

we would calculate

$$T = \frac{\widehat{\beta}_1 - \beta_1}{\sqrt{c_{11}\widehat{\sigma}^2}}$$

under the assumption H_0 is true (i.e., $\beta_1 = 0$) and then reject H_0 if the corresponding p-value was small. P-values would be calculated as areas under the $t(n-2)$ pdf because this is the sampling distribution of T when H_0 is true.

Example 10.1 (continued). For the maximum oxygen uptake data in Example 10.1, we use R to perform a hypothesis test for β_1. Test statistics and p-values can be calculated directly using R's `summary` function:

```
> summary(fit)
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 91.30032    8.89317   10.27  7.5e-10 ***
time        -0.05134    0.00787   -6.52  1.5e-06 ***

Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.5 on 22 degrees of freedom
Multiple R-squared:  0.659,     Adjusted R-squared:  0.644
F-statistic: 42.6 on 1 and 22 DF,  p-value: 1.46e-06
```

Interpretation: The value of the test statistic (`t value`) is

$$T = \frac{\widehat{\beta}_1}{\sqrt{c_{11}\widehat{\sigma}^2}} = \frac{-0.05134}{0.00787} = -6.52.$$

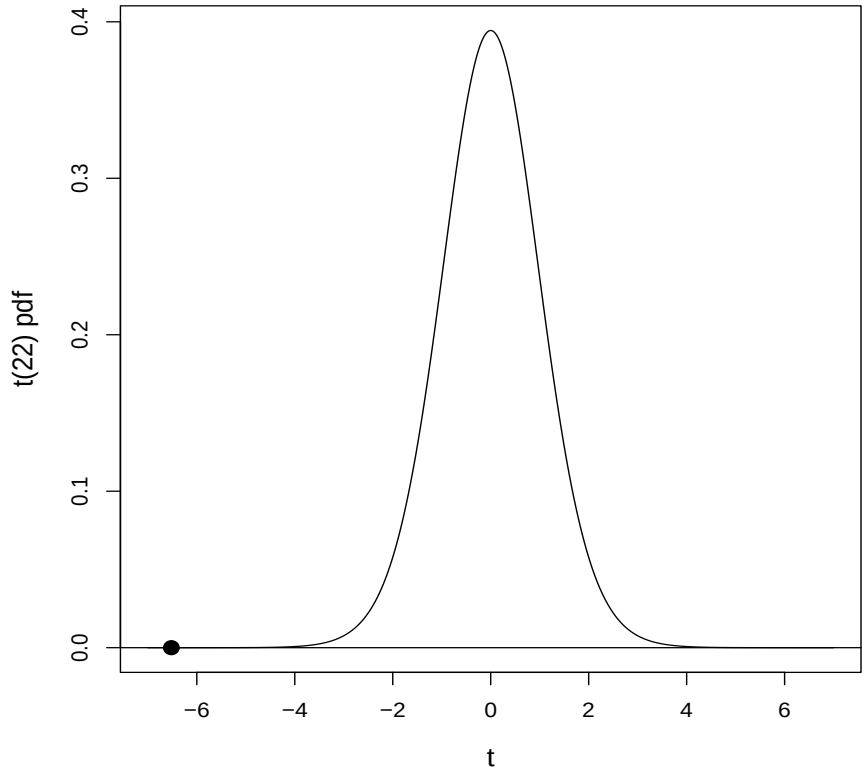


Figure 10.4: Max O_2 uptake data. Sampling distribution of T when $H_0 : \beta_1 = 0$ is true. The value of the test statistic $T \approx -6.52$ is shown using a solid circle.

For reference, I have graphed the $t(22)$ pdf in Figure 10.4 (above) and identified where the test statistic (`t value = -6.52`) falls on this distribution.

- This is not a value of T we would expect to see if $H_0 : \beta_1 = 0$ was true.
- The probability value (p-value) for the test

$$H_0 : \beta_1 = 0$$
$$\text{versus}$$
$$H_1 : \beta_1 \neq 0$$

  is

$$\text{p-value} = 1.5 \times 10^{-6} = 0.0000015.$$

- This is calculated by finding the area to the **left** of -6.52 under the $t(22)$ pdf above and then doubling it. This is what `Pr(>|t|)` means. The area is doubled because H_1 doesn't specify which direction β_1 differs from 0.
- At any reasonably chosen significance level α (e.g., $\alpha = 0.05$), we would reject H_0 because the p-value is so small.

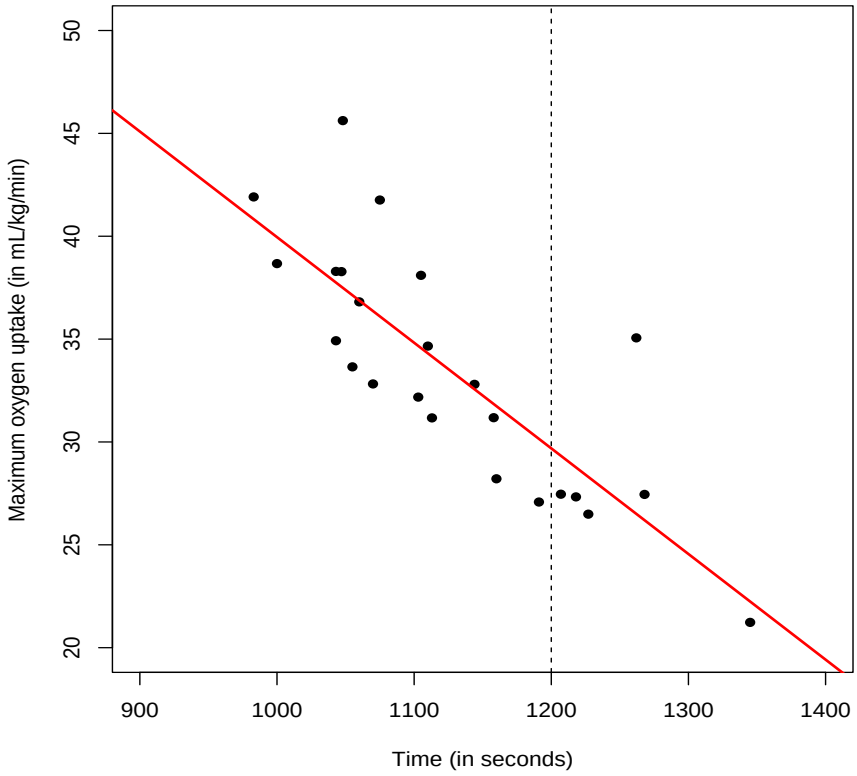


Figure 10.5: Max O_2 uptake data. Scatterplot of maximum oxygen uptake (Y) and the time to run a two-minute mile (x) for $n = 24$ middle-aged men. The least-squares regression line has been superimposed. A dotted vertical line at $x = x_0 = 1200$ seconds has been added.

10.6 Confidence intervals for $E(Y)$ and prediction intervals for Y^*

Discussion: After we estimate the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon,$$

we can learn about how the response variable Y behaves at a certain setting of the independent variable x, say when $x = x_0$. For example, in Example 10.1, suppose we are interested in the population of all middle-age men who run the two-minute mile in $x_0 = 1200$ seconds; see Figure 10.5 above. Two statistical inference questions emerge:

1. How do we **estimate** the mean maximum oxygen uptake $E(Y)$ for this population?
2. How do we **predict** the maximum oxygen uptake for one individual in this population?

Upon first glance, these questions may sound the same, but they are very different. The first question deals with estimating a population mean, specifically, the mean maximum oxygen uptake of the population of all middle-aged men who run the two-minute mile in

1200 seconds. The second question deals with predicting the maximum oxygen uptake of one middle-aged man in this population.

Recall: Under our simple linear regression model assumptions, we know from Result 1 that

$$Y \sim \mathcal{N}(\beta_0 + \beta_1 x, \sigma^2),$$

for all x. Therefore, when $x = x_0$, we have

$$Y \sim \mathcal{N}(\beta_0 + \beta_1 x_0, \sigma^2).$$

Referring to this probability distribution,

- our goal in the estimation problem is to write a $100(1-\alpha)\%$ **confidence interval** for

$$E(Y|x_0) = \beta_0 + \beta_1 x_0,$$

  the population mean of Y when $x = x_0$.

- our goal in the prediction problem is write a $100(1-\alpha)\%$ **prediction interval** for $Y^*(x_0)$, which represents a single observation from the $\mathcal{N}(\beta_0 + \beta_1 x_0, \sigma^2)$ distribution.

Your intuition should suggest that inference for a population mean (the first problem) should be much more precise than predicting where one observation will fall (the second problem), especially when there is a large amount of variability in the distribution of the response variable Y.

Confidence interval: A $100(1-\alpha)\%$ confidence interval for the population mean $E(Y|x_0)$ is

$$(\widehat{\beta}_0 + \widehat{\beta}_1 x_0) \pm t_{n-2,\alpha/2} \sqrt{\widehat{\sigma}^2 \left[\frac{1}{n} + \frac{(x_0 - \overline{x})^2}{S_{xx}}\right]}.$$

Prediction interval: A $100(1-\alpha)\%$ prediction interval for $Y^*(x_0)$ is

$$(\widehat{\beta}_0 + \widehat{\beta}_1 x_0) \pm t_{n-2,\alpha/2} \sqrt{\widehat{\sigma}^2 \left[1 + \frac{1}{n} + \frac{(x_0 - \overline{x})^2}{S_{xx}}\right]}.$$

Comparison: The two intervals have the same form and are nearly identical.

- The extra "1" in the prediction interval's standard error arises from the additional uncertainty associated with predicting a new response from the $\mathcal{N}(\beta_0 + \beta_1 x_0, \sigma^2)$ distribution.

- Therefore, at the same value of x_0, a $100(1-\alpha)\%$ prediction interval for $Y^*(x_0)$ will necessarily be **longer** than the corresponding $100(1-\alpha)\%$ confidence interval for $E(Y|x_0)$.

- Prediction is always less precise than estimation.

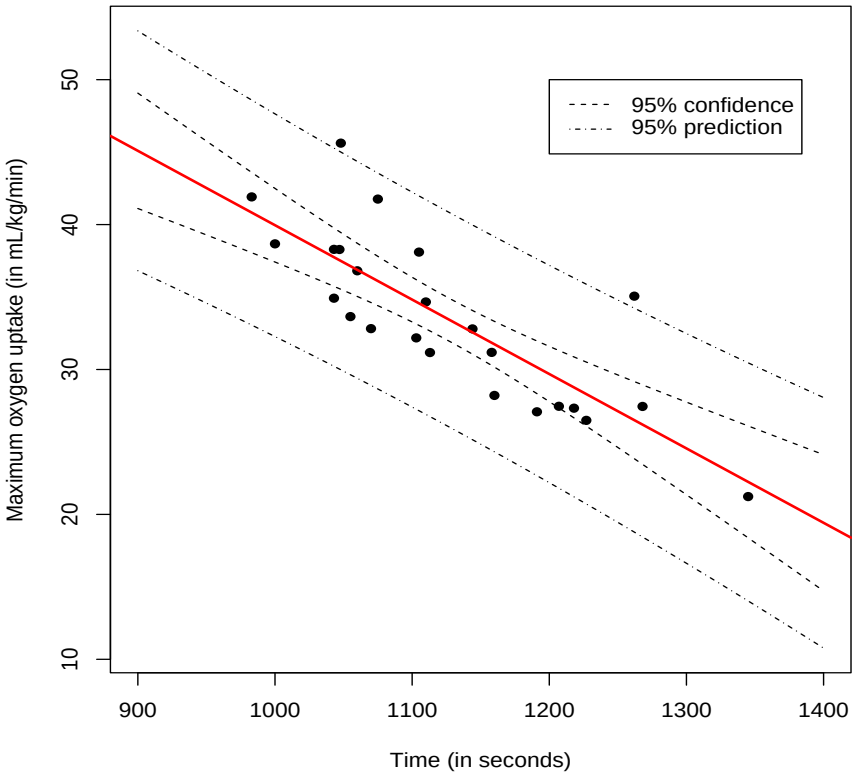


Figure 10.6: Max O_2 uptake data. Scatterplot of maximum oxygen uptake (Y) and the time to run a two-minute mile (x) for $n = 24$ middle-aged men. The least-squares regression line has been superimposed. Ninety-five percent (95%) confidence and prediction bands have been added.

Interval length: The length of both intervals depends on the value of x_0.

- The standard error for both intervals will be smallest when $x_0 = \overline{x}$ and will get larger the farther x_0 is from $\overline{x}$ in either direction.
- This implies the precision with which we estimate $E(Y|x_0)$ or predict $Y^*(x_0)$ decreases the further we get away from $\overline{x}$.
- This makes intuitive sense, namely, we would expect to have the most "confidence" in our estimated model near the "center" of the observed data.
- For the maximum oxygen uptake data in Example 10.1, confidence intervals and prediction intervals will be at their smallest length when $x_0 = 1126$ seconds; see Figure 10.6 above.

```
> mean(time)
[1] 1126
```

Example 10.1 (continued). For the maximum oxygen uptake data in Example 10.1, we use R to calculate

1. a 95% confidence interval for $E(Y)$ when $x = 1200$ seconds
2. a 95% prediction interval for Y^* when $x = 1200$ seconds.

Both intervals are found using R's `predict` function:

```
> options(digits=4)
> predict(fit,data.frame(time=1200),level=0.95,interval="confidence")
    fit   lwr   upr
1 29.69 27.78 31.59
> predict(fit,data.frame(time=1200),level=0.95,interval="prediction")
    fit   lwr   upr
1 29.69 22.19 37.19
```

Interpretation: The value `fit` in the R output (to 2 dp) is

$$\widehat{\beta}_0 + \widehat{\beta}_1 x_0 = 91.30032 - 0.05134(1200) = 29.69.$$

The values `lwr` and `upr` give the lower and upper limits of the intervals. Here is how they are interpreted:

- We are 95% confident the population mean maximum oxygen uptake $E(Y)$ for middle-aged men who run a two-minute mile in 1200 seconds is between 27.78 and 31.59 mL/kg/min.
- For an individual man who runs the two-minute mile in 1200 seconds, we would predict his maximum oxygen uptake is between 22.19 and 37.19 mL/kg/min with probability 0.95.

These interpretations must be written carefully! The main point is that the confidence interval is estimating the mean of a population. The prediction interval is for one individual in this population.

Warning: Investigators sometimes try to estimate $E(Y|x_0)$ or predict $Y^*(x_0)$ for values of x_0 outside the range of x values used in the study. This is called **extrapolation**.

- In order for inferences to be valid, one must believe the regression model is still suitable for x values outside the range where there are observed data. In some situations, this might be reasonable. In others, we may have no theoretical basis for making such a claim without data to support it.
- In Example 10.1 (see Figure 10.6), I would be nervous estimating or predicting anything outside the range of 1000-1300 seconds or thereabouts. There is little or no data outside this range to support any meaningful inference, and common sense tells us there are natural limits to how large or small maximum oxygen uptake can be.

11 Multiple Linear Regression

11.1 Introduction

Preview: In the last chapter, we considered the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon.$$

We now extend this model to include multiple independent variables $x_1, x_2, ..., x_k$. This is useful because the response Y can depend on more than one independent variable. Specifically, we consider models of the form

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon.$$

We call this a **multiple linear regression model**.

- There are now k independent (predictor) variables and $p = k+1$ regression parameters $\beta_0, \beta_1, \beta_2, ..., \beta_k$.
  - in simple linear regression, $k = 1$ and $p = 2$.
- The regression parameters describe the **population** for which this model is applicable. They are unknown and are to be estimated with the observed data; i.e., based on a sample from the population.
- We continue to assume the independent variables $x_1, x_2, ..., x_k$ are fixed and are measured without error.
- We continue to assume that $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Methods to diagnose regression assumptions will be discussed later.

Example 11.1. An article by Liu et al. (1996) in *Journal of Air and Waste Management Association* described a study motivated by the waste disposal problems in Kaohsiung City, Taiwan. The goal was to describe how

$$Y = \text{ energy content of solid waste specimen when incinerated (kcal/kg)}$$

was related to $k = 4$ independent variables measured on each waste specimen

$$\begin{aligned} x_1 &= \text{plastic by weight (measured as \% of total weight)} \\ x_2 &= \text{paper by weight (measured as \% of total weight)} \\ x_3 &= \text{garbage by weight (measured as \% of total weight)} \\ x_4 &= \text{moisture percentage.} \end{aligned}$$

The authors wanted to estimate a multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon$$

using a sample of solid waste specimens whose measurements are shown on the next page.

Specimen	Energy (Y)	Plastic (x_1)	Paper (x_2)	Garbage (x_3)	Moisture (x_4)
1	947	18.69	15.65	45.01	58.21
2	1407	19.43	23.51	39.69	46.31
3	1452	19.24	24.23	43.16	46.63
4	1553	22.64	22.20	35.76	45.85
5	989	16.54	23.56	41.20	55.14
6	1162	21.44	23.65	35.56	54.24
7	1466	19.53	24.45	40.18	47.20
8	1656	23.97	19.39	44.11	43.82
9	1254	21.45	23.84	35.41	51.01
10	1336	20.34	26.50	34.21	49.06
11	1097	17.03	23.46	32.45	53.23
12	1266	21.03	26.99	38.19	51.78
13	1401	20.49	19.87	41.35	46.69
14	1223	20.45	23.03	43.59	53.57
15	1216	18.81	22.62	42.20	52.98
16	1334	18.28	21.87	41.50	47.44
17	1155	21.41	20.47	41.20	54.68
18	1453	25.11	22.59	37.02	48.74
19	1278	21.04	26.27	38.66	53.22
20	1153	17.99	28.22	44.18	53.37
21	1225	18.73	29.39	34.77	51.06
22	1237	18.49	26.58	37.55	50.66
23	1327	22.08	24.88	37.07	50.72
24	1229	14.28	26.27	35.80	48.24
25	1205	17.74	23.61	37.36	49.92
26	1221	20.54	26.58	35.40	53.58
27	1138	18.25	13.77	51.32	51.38
28	1295	19.09	25.62	39.54	50.13
29	1391	21.25	20.63	40.72	48.67
30	1372	21.62	22.71	36.22	48.19

Discussion: In this chapter, we pursue many of the same questions we did for simple linear regression in the last chapter:

- We used **least squares** to estimate β_0 and β_1 in simple linear regression. How does this estimation method generalize for multiple linear regression like in Example 11.1, that is, how do we estimate β_0, β_1, β_2, β_3, and β_4?
- How do we perform **statistical inference** for the regression parameters? What do these inferences mean about the population?
- How do we use our estimated model to make **predictions** while quantifying the uncertainty in these predictions?
- How do we **assess model fit**? That is, how do we check if the underlying statistical assumptions are satisfied?

11.2 Least squares estimation

Data: Suppose we have a random sample of n individuals from a population. In multiple linear regression, we can envision the observed data as follows:

Individual	Y	x_1	x_2	$\cdots$	x_k
1	Y_1	x_{11}	x_{12}	$\cdots$	x_{1k}
2	Y_2	x_{21}	x_{22}	$\cdots$	x_{2k}
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$
n	Y_n	x_{n1}	x_{n2}	$\cdots$	x_{nk}

Each of the n individuals contributes a response Y and a value of each of the independent variables $x_1, x_2, ..., x_k$. For the ith individual in the sample, we write

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i,$$

for $i = 1, 2, ..., n$.

Matrix representation: To estimate the population parameters $\beta_0, \beta_1, \beta_2, ..., \beta_k$ with the random sample, we again use least squares. In doing so, it is advantageous to express multiple linear regression models in terms of matrices and vectors. This streamlines notation and makes the presentation easier. Define

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix}, \quad \boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{pmatrix}.$$

With these definitions, the model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i,$$

for $i = 1, 2, ..., n$, can be written as

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}.$$

In this representation,

- $\mathbf{Y}$ is an $n \times 1$ (random) vector of responses
- $\mathbf{X}$ is an $n \times p$ (fixed) matrix of independent variable measurements ($p = k + 1$)
- $\boldsymbol{\beta}$ is a $p \times 1$ (fixed) vector of unknown population regression parameters
- $\boldsymbol{\epsilon}$ is an $n \times 1$ (random) vector of unobserved errors.

Example 11.1 (continued). Here are $\mathbf{Y}$, $\mathbf{X}$, $\boldsymbol{\beta}$, and $\boldsymbol{\epsilon}$ for the waste incineration data in Example 11.1. There are $n = 30$ individuals (specimens) and $k = 4$ independent variables.

$$\mathbf{Y} = \begin{pmatrix} 947 \\ 1407 \\ \vdots \\ 1372 \end{pmatrix}_{30\times 1} \quad \mathbf{X} = \begin{pmatrix} 1 & 18.69 & 15.65 & 45.01 & 58.21 \\ 1 & 19.43 & 23.51 & 39.69 & 46.31 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 21.62 & 22.71 & 36.22 & 48.19 \end{pmatrix}_{30\times 5} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix}_{5\times 1} \quad \boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_{30} \end{pmatrix}_{30\times 1}.$$

Least Squares: The idea of least squares is the same in multiple linear regression as it was in simple linear regression. We now want to find the values of $\beta_0, \beta_1, \beta_2, ..., \beta_k$ that minimize

$$Q(\beta_0, \beta_1, \beta_2, ..., \beta_k) = \sum_{i=1}^{n} [Y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik})]^2.$$

With

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}, \quad \mathbf{X} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix}, \quad \text{and} \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{pmatrix},$$

first note that

$$\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik}$$

is the dot product of $\boldsymbol{\beta}$ and the ith row of $\mathbf{X}$. Therefore,

$$\mathbf{X}\boldsymbol{\beta} = \begin{pmatrix} \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \cdots + \beta_k x_{1k} \\ \beta_0 + \beta_1 x_{21} + \beta_2 x_{22} + \cdots + \beta_k x_{2k} \\ \vdots \\ \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \cdots + \beta_k x_{nk} \end{pmatrix}$$

and

$$Y_i - (\beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik})$$

is the ith entry of the vector

$$\mathbf{Y} - \mathbf{X}\boldsymbol{\beta} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} - \begin{pmatrix} \beta_0 + \beta_1 x_{11} + \beta_2 x_{12} + \cdots + \beta_k x_{1k} \\ \beta_0 + \beta_1 x_{21} + \beta_2 x_{22} + \cdots + \beta_k x_{2k} \\ \vdots \\ \beta_0 + \beta_1 x_{n1} + \beta_2 x_{n2} + \cdots + \beta_k x_{nk} \end{pmatrix}.$$

Therefore, the objective function Q above can be written as

$$Q(\boldsymbol{\beta}) = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})'(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}),$$

the dot product of $\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$ with itself; i.e., the squared length of the vector $\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$. Mathematically, least squares selects the value of $\boldsymbol{\beta}$ that minimizes the squared length of $\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}$ among all vectors $\boldsymbol{\beta} \in \mathbb{R}^p$.

Solution: Because $Q(\boldsymbol{\beta})$ is a scalar function of the p elements of $\boldsymbol{\beta}$, we can use calculus to determine the values of the p elements that minimize it. Formally, we can take p partial derivatives, one with respect to each of $\beta_0, \beta_1, \beta_2, ..., \beta_k$, and set these equal to zero. Using the calculus of matrices, we can write this resulting system of p equations (and p unknowns) as follows:

$$\mathbf{X}'\mathbf{X}\boldsymbol{\beta} = \mathbf{X}'\mathbf{Y}.$$

These are called the **normal equations**. Provided that $\mathbf{X}'\mathbf{X}$ has a unique inverse, the solution is

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta}_1 \\ \widehat{\beta}_2 \\ \vdots \\ \widehat{\beta}_k \end{pmatrix}.$$

This is the **least squares estimator** of $\boldsymbol{\beta}$. It is the value of $\boldsymbol{\beta}$ that makes $Q(\boldsymbol{\beta})$ as small as possible.

Technical note: For the least squares estimator

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

to be unique, we need $\mathbf{X}$ to be of **full column rank**; i.e., $r(\mathbf{X}) = p = k+1$. This will occur when there are no linear dependencies among the columns of $\mathbf{X}$. If $r(\mathbf{X}) < p$, then $\mathbf{X}'\mathbf{X}$ does not have a unique inverse, and the normal equations can not be solved uniquely. R will alert the user when $\mathbf{X}'\mathbf{X}$ does not have a unique inverse.

Example 11.1 (continued). We now use R's `lm` function to calculate the least squares estimate $\widehat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ for the waste incineration data in Example 11.1:

```
> options(digits=3)
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> fit

Coefficients:
(Intercept)      plastic        paper      garbage     moisture
    2244.92        28.93         7.64         4.30       -37.35
```

This output gives the value of the least squares estimate

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta}_1 \\ \widehat{\beta}_2 \\ \widehat{\beta}_3 \\ \widehat{\beta}_4 \end{pmatrix} = \begin{pmatrix} 2244.92 \\ 28.93 \\ 7.64 \\ 4.30 \\ -37.35 \end{pmatrix}.$$

Therefore, the estimated regression model for the waste incineration data in Example 11.1 is

$$\widehat{Y} = 2244.92 + 28.93x_1 + 7.64x_2 + 4.30x_3 - 37.35x_4,$$

or, in other words,

$$\widehat{\texttt{energy}} = 2244.92 + 28.93\texttt{plastic} + 7.64\texttt{paper} + 4.30\texttt{garbage} - 37.35\texttt{moisture}.$$

In more modern regression language, this might also be called a **prediction equation**. It is the equation we would use to predict the energy content for a new waste specimen.

11.3 Analysis of variance for (multiple) linear regression

Importance: When we estimate a linear regression model (simple or multiple), we are really partitioning the variation in the response data

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix}$$

into one of two parts:

1. the variation in $Y_1, Y_2, ..., Y_n$ that is explained by the regression model
2. the variation in $Y_1, Y_2, ..., Y_n$ that is *not* explained by the regression model.

This partition can be written mathematically as

$$\underbrace{\sum_{i=1}^{n}(Y_i - \overline{Y})^2}_{\text{SS}_{\text{TOT}}} = \underbrace{\sum_{i=1}^{n}(\widehat{Y}_i - \overline{Y})^2}_{\text{SS}_{\text{R}}} + \underbrace{\sum_{i=1}^{n}(Y_i - \widehat{Y}_i)^2}_{\text{SS}_{\text{E}}},$$

where

$$\widehat{Y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_{i1} + \widehat{\beta}_2 x_{i2} + \cdots + \widehat{\beta}_k x_{ik}$$

is the ith **fitted value** and

$$e_i = Y_i - \widehat{Y}_i$$

is the ith **residual**. Fitted values and residuals have the same interpretation in multiple regression as they did in simple linear regression:

- Fitted value $(\widehat{Y}_i) \longrightarrow$ Value of Y that is predicted by the model fit
- Residual $(e_i) \longrightarrow$ Difference between the observed Y_i and the fitted $\widehat{Y}_i$.

Interpretation: The equation

$$\text{SS}_{\text{TOT}} = \text{SS}_{\text{R}} + \text{SS}_{\text{E}}$$

is a mathematical description of how variability is partitioned:

- SS_{TOT} is the **total sum of squares**. This measures how much variability there is in the response data $Y_1, Y_2, ..., Y_n$.
- SS_{R} is the **regression (model) sum of squares**. This measures how much variability in the response data is explained by the estimated linear regression model.
- SS_{E} is the **error (residual) sum of squares**. This measures how much variability is "left over" after estimating the linear regression model.

ANOVA table: The general form of an ANOVA table for linear regression (simple or multiple) is shown below:

Source	df	SS	MS	F
Regression	$p-1$	SS_{R}	$\text{MS}_{\text{R}} = \frac{\text{SS}_{\text{R}}}{p-1}$	$F = \frac{\text{MS}_{\text{R}}}{\text{MS}_{\text{E}}}$
Residuals	$n-p$	SS_{E}	$\text{MS}_{\text{E}} = \frac{\text{SS}_{\text{E}}}{n-p}$	
Total	$n-1$	SS_{TOT}		

Notes:

- The **degrees of freedom** (df) add down.
  - The degrees of freedom for SS_{TOT} is the divisor in the sample variance
  $$S^2 = \frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \overline{Y})^2 = \frac{\text{SS}_{\text{TOT}}}{n-1}.$$
  - The degrees of freedom for SS_{R} is $k = p-1$, the number of independent variables in the model.
  - The degrees of freedom for SS_{E} is the divisor needed to create an unbiased estimator of σ^2, the error variance in $\epsilon \sim \mathcal{N}(0, \sigma^2)$. That is,
  $$\text{MS}_{\text{E}} = \frac{\text{SS}_{\text{E}}}{n-p}$$
  is an unbiased estimator of σ^2.
- **Mean squares** (MS) are the sums of squares divided by their degrees of freedom.
- The F **statistic** is formed by taking the ratio of MS_{R} and MS_{E}.

Example 11.1 (continued). We now use R to produce the ANOVA table for the waste incineration data in Example 11.1:

```
> Model = cbind(plastic,paper,garbage,moisture)
> fit = lm(energy ~ Model)
> anova(fit)

Analysis of Variance Table

Response: energy
          Df  Sum Sq   Mean Sq  F value     Pr(>F)
Model      4  664931  166232.7  167.714 < 2.22e-16
Residuals 25   24779     991.2
```

Overall *F* test: In the multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon \iff E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$, the F statistic in the ANOVA table tests

$$H_0 : \beta_1 = \beta_2 = \cdots = \beta_k = 0$$

versus

$$H_1 : \text{at least one of the } \beta_j\text{'s is nonzero.}$$

That is, H_0 says none of the independent variables are linearly related to $E(Y)$ in the population, whereas H_1 says at least one independent variable is. If H_0 is rejected, we do not know which one or how many of the population regression parameters are nonzero; only that at least one is.

Sampling distribution: When H_0 is true, both MS_R and MS_E are unbiased estimators of σ^2. Therefore,

$$F = \frac{\text{MS}_\text{R}}{\text{MS}_\text{E}}$$

should be close to 1, and, under our regression assumptions,

$$F = \frac{\text{MS}_\text{R}}{\text{MS}_\text{E}} \sim F(p-1, n-p).$$

Recall that the mean of an F distribution is around 1. Therefore,

- Values of F in the center of this distribution (close to 1) are consistent with H_0.
- Large values of F (i.e., out in the right tail) are consistent with H_1.
- Unusually small values of F (i.e., closer to 0) could indicate there is a violation of our statistical assumptions or we have fit a poor model.

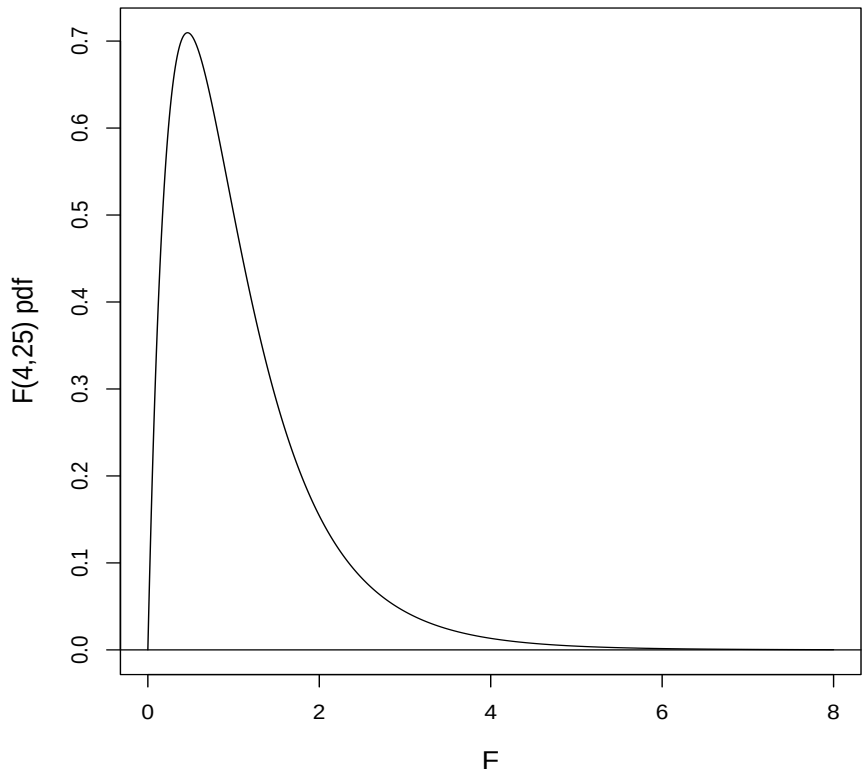


Figure 11.1: Waste incineration data. $F(4, 25)$ pdf. This is the sampling distribution of F when H_0 is true.

Example 11.1 (continued). We now perform the overall F test for the waste incineration data in Example 11.1. In the multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon \iff E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$$

the F statistic tests

$$H_0 : \beta_1 = \beta_2 = \beta_3 = \beta_4 = 0$$

versus

$$H_1 : \text{at least one of } \beta_1, \beta_2, \beta_3, \beta_4 \text{ is nonzero.}$$

The F statistic $F = 167.714$ conveys an obvious decision to reject H_0 in favor of H_1; see Figure 11.1 above. The p-value `Pr(>F)` is extremely small:

$$\text{p-value} = 2.22 \times 10^{-16} = 0.00000000000000222.$$

We conclude at least one of the independent variables (among `paper`, `plastic`, `garbage`, and `moisture`) is linearly related to the mean energy content $E(Y)$ in the population.

Terminology: After a linear regression model (simple or multiple) is fit, we know that variation is partitioned according to

$$\text{SS}_{\text{TOT}} = \text{SS}_{\text{R}} + \text{SS}_{\text{E}}.$$

The proportion of variation in the response data explained by the model fit is

$$R^2 = \frac{\text{SS}_{\text{R}}}{\text{SS}_{\text{TOT}}}.$$

This is called the **coefficient of determination**. Clearly,

$$0 \leq R^2 \leq 1.$$

In general, the larger the R^2, the better the estimated regression model explains the variability in the response.

Example 11.1 (continued). For the waste incineration data in Example 11.1, recall the ANOVA table presented earlier:

```
Analysis of Variance Table

Response: energy
          Df  Sum Sq   Mean Sq  F value     Pr(>F)
Model      4  664931  166232.7  167.714 < 2.22e-16
Residuals 25   24779     991.2
```

Therefore, the coefficient of determination

$$R^2 = \frac{\text{SS}_{\text{R}}}{\text{SS}_{\text{TOT}}} = \frac{664931}{664931 + 24779} \approx 0.964.$$

Interpretation: About 96.4% of the variability in the energy content data is explained by the multiple linear regression model that includes `paper`, `plastic`, `garbage`, and `moisture`. The remaining 3.6% of the variability is explained by other sources.

Warning: It is important to understand what R^2 measures and what it does not. Its value is calculated under the assumption that the regression model you have just fit is the **correct** model for the population. It assesses how much of the variation in the response is attributed to the relationship in that particular model.

- If R^2 is small, it could be that there is just a lot of inherent variation in the response data. Although the estimated regression model is reasonable for the population, it can explain only so much of the overall variation.
- Alternatively, R^2 may be large (e.g., close to 1) but for an estimated model that is not appropriate for the data. A better model may exist. We will see an example of this later.
- Investigators should be careful not to give R^2 more attention than it deserves.

Sequential sums of squares: We know the partition

$$\text{SS}_{\text{TOT}} = \text{SS}_{\text{R}} + \text{SS}_{\text{E}}$$

describes how much variation in the response data is explained by the model (SS_{R}) and how much variation is not explained by the model (SS_{E}). Upon request, R will take

$$\text{SS}_{\text{R}}$$

and break it down further. Specifically, we can further partition SS_{R} into individual sources that are attributable to each independent variable separately. To illustrate this, recall the ANOVA table for the waste incineration data in Example 11.1:

```
Analysis of Variance Table

Response: energy
          Df  Sum Sq   Mean Sq  F value     Pr(>F)
Model      4  664931  166232.7  167.714 < 2.22e-16
Residuals 25   24779     991.2
```

The regression (model) sum of squares $\text{SS}_{\text{R}} = 664931$ can be broken down into four sources in the following order:

- the part due to the regression on x_1 (i.e., simple linear regression)
- the part due to adding x_2 to the model which includes x_1
- the part due to adding x_3 to the model which includes x_1 and x_2
- the part due to adding x_4 to the model which includes x_1, x_2, and x_3.

In notation,

$$\text{SS}_{\text{R}} = \text{SS}(x_1) + \text{SS}(x_2|x_1) + \text{SS}(x_3|x_1, x_2) + \text{SS}(x_4|x_1, x_2, x_3).$$

These are called **sequential sums of squares**. They quantify the relative contribution of each independent variable as it is added to the model in sequence.

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> anova(fit)
Analysis of Variance Table

          Df Sum Sq Mean Sq F value  Pr(>F)
plastic    1 239735  239735  241.87 2.3e-14
paper      1  11239   11239   11.34  0.0025
garbage    1   2888    2888    2.91  0.1002
moisture   1 411069  411069  414.73 < 2e-16
Residuals 25  24779     991
```

Interpretation: The first thing we notice is

$$\begin{aligned} \text{SS}_\text{R} = 664931 &= 239735 + 11239 + 2888 + 411069 \\ &= \text{SS}(x_1) + \text{SS}(x_2|x_1) + \text{SS}(x_3|x_1, x_2) + \text{SS}(x_4|x_1, x_2, x_3). \end{aligned}$$

What do these four sequential sums of squares tell us in terms of the relative contribution of each independent variable? On their own, not much very much because it is hard to discern how large each contribution is. However, when we scale them, we can form F statistics

$$\begin{aligned} F_1 &= \frac{\text{SSR}(x_1)}{\text{MS}_\text{E}} = \frac{239735}{991} \approx 241.87 \\ F_2 &= \frac{\text{SSR}(x_2|x_1)}{\text{MS}_\text{E}} = \frac{11239}{991} \approx 11.34 \\ F_3 &= \frac{\text{SSR}(x_3|x_1, x_2)}{\text{MS}_\text{E}} = \frac{2888}{991} \approx 2.91 \\ F_4 &= \frac{\text{SSR}(x_4|x_1, x_2, x_3)}{\text{MS}_\text{E}} = \frac{411069}{991} \approx 414.73. \end{aligned}$$

We can use these F statistics (and their corresponding p-values) to assess the importance of each variable as it is added to the regression model. Specifically, each F statistic tests

$$H_0 : \text{the predictor variable does not contribute to the model}$$

versus

$$H_1 : \text{the predictor variable does contribute to the model.}$$

Recall that "large" F statistics ("small" p-values; i.e., smaller than the significance level α) are evidence against H_0. Using $\alpha = 0.05$, we would conclude

- the predictor x_1 (`paper`) is linearly related to mean energy content in the population (p-value $= 2.3 \times 10^{-14}$)
- the predictor x_2 (`plastic`) contributes to the model which already includes x_1 (p-value $= 0.0025$)
- the predictor x_3 (`garbage`) does not contribute to the model which already includes x_1 and x_2 (p-value $= 0.1002$)
- the predictor x_4 (`moisture`) contributes to the model which already includes x_1, x_2, and x_3 (p-value $< 2 \times 10^{-16}$).

Interesting: Sequential sums of squares are used to assess the relative contribution of each independent (predictor) variable as it is added to the model in a particular order. Therefore, if you change the ordering of the independent variables x_1, x_2, x_3, x_4, you change the partition of SS_R.

Illustration: Before, we used

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
```

which adds the independent variables x_1, x_2, x_3, and x_4 in this order. Suppose instead we specified

```
> fit = lm(energy ~ garbage + moisture + paper + plastic)
```

which adds x_3, x_4, x_2, and x_1 in this order. Here is the partition of the regression (model) sums of squares SS_R for this ordering:

```
> anova(fit)
Analysis of Variance Table

          Df Sum Sq Mean Sq F value Pr(>F)
garbage    1   5245    5245   5.292   0.0301
moisture   1 555276  555276 560.223  < 2e-16
paper      1    402     402   0.406   0.5298
plastic    1 104007  104007 104.934 1.97e-10
Residuals 25  24779     991
```

For this partition (up to rounding error), we note

$$\text{SS}_\text{R} = 664931 = 5245 + 555276 + 402 + 104007$$

as before. However, our assessment of the relative contributions of each independent variable changes to reflect this new ordering.

- In the first partition, x_3 (`garbage`) did not contribute significantly to a model that included x_1 (`plastic`) and x_2 (`paper`); p-value = 0.1002. However, in the second partition, there is strong evidence x_3 (`garbage`) is linearly related to $E(Y)$ in a simple linear regression; p-value = 0.0301.
- In the first partition, x_2 (`paper`) contributed significantly to a model that included x_1 (`plastic`); p-value = 0.0025. However, in the second partition, x_2 (`paper`) does not contribute significantly to a model that includes x_3 (`garbage`) and x_4 (`moisture`); p-value = 0.5298.

These are not contradictions. The differences in the conclusions are based entirely on the ordering of the independent variables; i.e., the F statistics (and p-values) for the two partitions are simply assessing different things.

Q: How many different sets of sequential sums of squares are there for the waste incineration data? That is, how many ways can one partition SS_R?
A: There are 4 independent variables. There are $4! = 24$ ways to order them.

11.4 Inference for individual regression parameters

Goal: In the multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon,$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$, our goal is to perform statistical inference for the population-level regression parameter β_j.

- This can help us assess the importance of using the independent variable x_j in a model that includes the other independent variables.
- That is, statistical inference regarding the population parameter β_j is **conditional** on the other independent variables being included in the model.

Result: Under our multiple linear regression model assumptions,

$$T_j = \frac{\widehat{\beta}_j - \beta_j}{\sqrt{c_{jj}\widehat{\sigma}^2}} \sim t(n-p),$$

where $\widehat{\beta}_j$ is the least squares estimate of β_j, $\widehat{\sigma}^2 = \text{MS}_\text{E}$ is the mean squared error, and $c_{jj} = (\mathbf{X}'\mathbf{X})^{-1}_{jj}$ is the corresponding diagonal element of the $(\mathbf{X}'\mathbf{X})^{-1}$ matrix. This describes the sampling distribution of T_j, that is, how T_j will vary probabilistically when sampling from a population where the multiple linear regression model and its assumptions are correct.

Confidence intervals: Under our multiple linear regression model assumptions, a $100(1-\alpha)\%$ confidence interval for β_j, for $j = 0, 1, 2, ..., k$, is

$$\widehat{\beta}_j \pm t_{n-p,\alpha/2}\sqrt{c_{jj}\widehat{\sigma}^2}.$$

- The value $t_{n-p,\alpha/2}$ is the upper $\alpha/2$ quantile from the $t(n-p)$ distribution.
- Note the familiar form of the interval:

$$\underbrace{\text{point estimate}}_{\widehat{\beta}_j} \pm \underbrace{\text{quantile}}_{t_{n-p,\alpha/2}} \times \underbrace{\text{standard error}}_{\sqrt{c_{jj}\widehat{\sigma}^2}}.$$

We interpret the interval in the usual way:

> "We are $100(1-\alpha)\%$ confident the population parameter β_j is in this interval."

Note that if

- the confidence interval for β_j consists entirely of positive values; e.g., (1.5, 4.3), we would infer $\beta_j > 0$ meaning that $E(Y)$ and x_j are **positively** linearly related in the population after accounting for the effects of the other independent variables.

- the confidence interval for β_j consists entirely of negative values; e.g., $(-4.3, -1.5)$, we would infer $\beta_j < 0$ meaning that $E(Y)$ and x_j are **negatively** linearly related in the population after accounting for the effects of the other independent variables.
- the confidence interval for β_j contains "0;" e.g., $(-1.5, 4.3)$, we cannot infer that $E(Y)$ and x_j are linearly related in the population after accounting for the effects of the other independent variables.
  - This is the same as saying "the independent variable x_j does not contribute to the model which includes the other independent variables."

Example 11.1 (continued). We now use R's `confint` function to write 95% confidence intervals for the individual regression parameters in the linear model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon \iff E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$$

for the waste incineration data in Example 11.1:

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> options(digits=3)
> confint(fit,conf.level=0.95)
              2.5 %  97.5 %
(Intercept) 1878.53 2611.32
plastic       23.11   34.74
paper          2.88   12.41
garbage        0.35    8.24
moisture     -41.13  -33.58
```

Here is how these confidence intervals are interpreted (separately):

- For a one-unit increase in `plastic` (measured as a % of total weight), we are 95% confident the increase in the population mean energy content $E(Y)$ is between 23.11 and 34.74 kcal/kg. This is after incorporating the effects of `paper`, `garbage`, and `moisture`.
- For a one-unit increase in `paper` (measured as a % of total weight), we are 95% confident the increase in the population mean energy content $E(Y)$ is between 2.88 and 12.41 kcal/kg. This is after incorporating the effects of `plastic`, `garbage`, and `moisture`.
- For a one-unit increase in `garbage` (measured as a % of total weight), we are 95% confident the increase in the population mean energy content $E(Y)$ is between 0.35 and 8.24 kcal/kg. This is after incorporating the effects of `plastic`, `paper`, and `moisture`.
- For a one-unit increase in `moisture` (measured as a %), we are 95% confident the **decrease** in the population mean energy content $E(Y)$ is between 33.58 and 41.13 kcal/kg. This is after incorporating the effects of `plastic`, `paper`, and `garbage`.

Hypothesis tests: Under our linear regression model and its assumptions, if we wanted to formally test

$$H_0 : \beta_j = 0$$
versus
$$H_1 : \beta_j \neq 0,$$

we would calculate

$$T_j = \frac{\widehat{\beta}_j - \beta_j}{\sqrt{c_{jj}\widehat{\sigma}^2}}$$

under the assumption H_0 is true (i.e., $\beta_j = 0$) and then reject H_0 if the corresponding p-value was small. P-values would be calculated as areas under the $t(n-p)$ pdf because this is the sampling distribution of T when H_0 is true. When we perform this test, we are assessing the relative importance of the predictor x_j **conditional** on the other independent variables being in the model.

Example 11.1 (continued). We now use R's `summary` function to perform hypothesis tests with individual regression parameters in the linear model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4 + \epsilon \iff E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$$

for the waste incineration data in Example 11.1:

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> summary(fit)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2244.92     177.90   12.62  2.4e-12 ***
plastic        28.93       2.82   10.24  2.0e-10 ***
paper           7.64       2.31    3.30   0.0029 **
garbage         4.30       1.92    2.24   0.0341 *
moisture      -37.35       1.83  -20.36  < 2e-16 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 31.5 on 25 degrees of freedom
Multiple R-squared:  0.964,     Adjusted R-squared:  0.958
F-statistic:  168 on 4 and 25 DF,  p-value: <2e-16
```

Assessment: At the $\alpha = 0.05$ level of significance, each independent variable is linearly related to the mean energy content $E(Y)$ in the population, after accounting for the effects of the other independent variables. All p-values are smaller than $\alpha = 0.05$. Note that we reached the same conclusions using the confidence intervals on the preceding page.

11.5 Confidence intervals for $E(Y)$ and prediction intervals for Y^*

Goal: For the multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon,$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$, we now want to perform statistical inference for a population of individuals at a specific setting of the independent variables which we denote by

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \end{pmatrix} = \begin{pmatrix} x_{10} \\ x_{20} \\ \vdots \\ x_{k0} \end{pmatrix} = \mathbf{x}_0.$$

- We would like to **estimate** the population mean of Y at this setting; i.e.,

  $$E(Y|\mathbf{x}_0) = \beta_0 + \beta_1 x_{10} + \beta_2 x_{20} + \cdots + \beta_k x_{k0}.$$

  We will write a $100(1-\alpha)\%$ confidence interval for $E(Y|\mathbf{x}_0)$.

- We would like to **predict** the value of an individual's response Y at the setting $\mathbf{x} = \mathbf{x}_0$. We will write a $100(1-\alpha)\%$ prediction interval for $Y^*(\mathbf{x}_0)$.

We considered both of these problems for simple linear regression in the last chapter (Section 10.6). For multiple linear regression, the ideas, implementation in R, and interpretation of the intervals are the same.

Example 11.1 (continued). For the waste incineration data, we use R's `predict` function to write a 95% confidence interval for the population mean energy content $E(Y)$ when

$$\mathbf{x}_0 = \begin{pmatrix} x_{10} \\ x_{20} \\ x_{30} \\ x_{40} \end{pmatrix} = \begin{pmatrix} 20 \\ 25 \\ 40 \\ 50 \end{pmatrix}.$$

We will also write a 95% prediction interval for $Y^*(\mathbf{x}_0)$, the energy content of an individual waste specimen with these values of x_1, x_2, x_3, and x_4.

Here is the R code to construct the **confidence interval**:

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> x.0 = data.frame(plastic=20,paper=25,garbage=40,moisture=50)
> predict(fit,x.0,conf.level=0.95,interval="confidence")
      fit     lwr     upr
1 1318.69 1303.33 1334.04
```

Recall the least-squares estimate of $\boldsymbol{\beta}$ is

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta}_1 \\ \widehat{\beta}_2 \\ \widehat{\beta}_3 \\ \widehat{\beta}_4 \end{pmatrix} = \begin{pmatrix} 2244.92 \\ 28.93 \\ 7.64 \\ 4.30 \\ -37.35 \end{pmatrix}.$$

The value for `fit` in the R output is

$$\begin{aligned} \widehat{Y} &= \widehat{\beta}_0 + \widehat{\beta}_1 x_{10} + \widehat{\beta}_2 x_{20} + \widehat{\beta}_3 x_{30} + \widehat{\beta}_4 x_{40} \\ &= 2244.92 + 28.93(20) + 7.64(25) + 4.30(40) - 37.35(50) \approx 1318.69 \text{ kcal/kg} \end{aligned}$$

(a small amount of error was introduced when rounding the least-squares estimates to 2 dp). A 95% confidence interval for $E(Y)$ at this setting of the independent variables is

$$(1303.33, 1334.04).$$

Interpretation: For the population of all waste specimens whose

`plastic` content is 20% of the total weight
`paper` content is 25% of the total weight
`garbage` content is 40% of the total weight
`moisture` content is 50%,

we are 95% confident the mean energy content $E(Y)$ is between 1303.33 and 1334.04 kcal/kg.

Here is the R code to construct the **prediction interval**:

```
> fit = lm(energy ~ plastic + paper + garbage + moisture)
> x.0 = data.frame(plastic=20,paper=25,garbage=40,moisture=50)
> predict(fit,x.0,conf.level=0.95,interval="prediction")
      fit     lwr     upr
1 1318.69 1252.05 1385.32
```

A 95% prediction interval for Y^* at this setting of the independent variables is

$$(1252.05, 1385.32).$$

Interpretation: For an individual waste specimen whose

`plastic` content is 20% of the total weight
`paper` content is 25% of the total weight
`garbage` content is 40% of the total weight
`moisture` content is 50%,

we would predict its energy content Y to be between 1252.05 and 1385.32 kcal/kg with probability 0.95.

11.6 Residual analysis (model diagnostics)

Importance: We now discuss model diagnostics for linear regression (both simple and multiple). The term "diagnostics" refers to the process of "checking the model assumptions." This is important because if the model assumptions are violated, then our analysis and all subsequent interpretations could be compromised.

Recall: We first recall the model assumptions on the error terms in the linear regression model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \epsilon_i,$$

for $i = 1, 2, ..., n$. These assumptions are

- $E(\epsilon_i) = 0$, for $i = 1, 2, ..., n$, that is, the errors have zero mean
- $V(\epsilon_i) = \sigma^2$, for $i = 1, 2, ..., n$, that is, the errors have constant variance
- the errors ϵ_i are independent
- the errors ϵ_i are normally distributed.

Residuals: To check these assumptions, we first have to deal with an obvious problem, namely, the error terms ϵ_i in the model are never actually observed. However, after fitting the model, we can calculate the residuals

$$e_i = Y_i - \widehat{Y}_i,$$

where the ith fitted value

$$\widehat{Y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_{i1} + \widehat{\beta}_2 x_{i2} + \cdots + \widehat{\beta}_k x_{ik}.$$

We can think of the residuals $e_1, e_2, ..., e_n$ as "proxies" for the errors $\epsilon_1, \epsilon_2, ..., \epsilon_n$. Therefore, we use the residuals to check our model assumptions instead. R will calculate the residuals (using the `resid` function) for any linear regression model fit.

Normality: To diagnose the normality assumption for the errors in linear regression, we can look at the (normal) qq plot of the residuals.

- We are looking for **general agreement** when plotting the residuals versus quantiles from a normal distribution.
- Substantial disagreement in the plot alerts us to a potential violation of normality.

If the normality assumption is violated in a linear regression analysis, this could affect population-level inferences for regression parameters, confidence intervals for $E(Y|\mathbf{x}_0)$, and prediction intervals for $Y^*(\mathbf{x}_0)$. All of these inference procedures are created under the normality assumption for the errors.

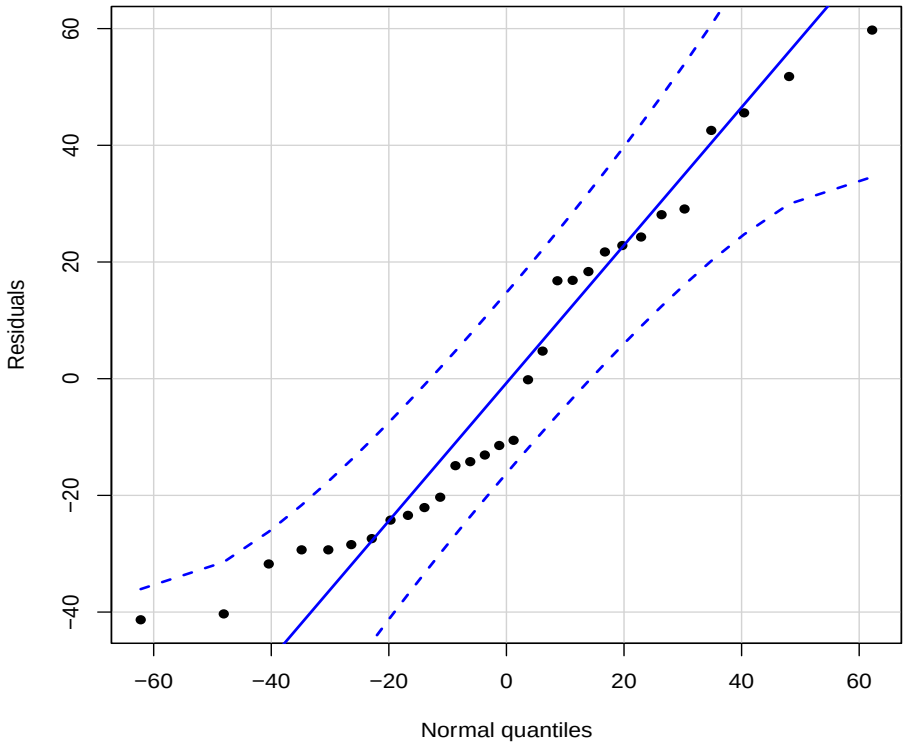


Figure 11.2: Waste incineration data. Normal qq plot for the residuals.

Example 11.1 (continued). We use R to construct a normal qq plot of the residuals from estimating

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \epsilon_i,$$

$i = 1, 2, ..., 30$, for the waste incineration data in Example 11.1. There are $n = 30$ individuals (specimens) in the data set, so there are 30 residuals. The qq plot in Figure 11.2 above shows general agreement between the residuals and the normal quantiles. There are no concerns with normality violations here.

Terminology: In linear regression analysis, a **residual plot** is a scatterplot of the residuals e_i (on the vertical axis) versus the fitted values $\widehat{Y}_i$ (on the horizontal axis). A residual plot can be useful in detecting the following violations:

- misspecifying the true regression function
  - i.e., a violation of the $E(\epsilon_i) = 0$ assumption
- non-constant variance (heteroscedasticity)
  - i.e., a violation of the $V(\epsilon_i) = \sigma^2$ assumption
- correlated observations; i.e., a violation of the assumption that the ϵ_i's are independent.

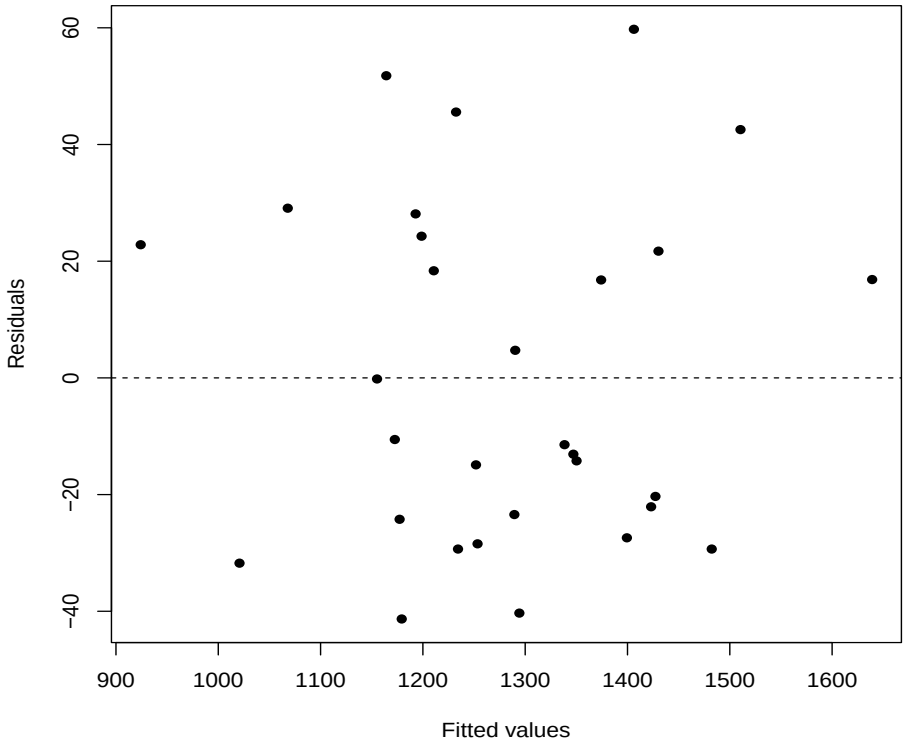


Figure 11.3: Waste incineration data. Residual plot.

Important: Mathematical arguments show if all of the linear regression model assumptions are satisfied, then the residuals and fitted values are **independent**.

- Therefore, if the residual plot looks random in appearance with no noticeable patterns (i.e., the plot looks like a random scatter of points), this suggests there are no violations in the model assumptions.
- On the other hand, if there are systematic (non-random) patterns in the residual plot, this suggests the model and its assumptions are inadequate in some way.
- Furthermore, a residual plot will often reveal what type of model violation is occurring. We will see examples of this later.

Example 11.1 (continued). We use R to construct the residual plot from estimating the model

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \beta_4 x_{i4} + \epsilon_i,$$

$i = 1, 2, ..., 30$, for the waste incineration data in Example 11.1. The residual plot in Figure 11.3 above shows a random scatter of points with no systematic patterns. There are no concerns with any model violations.

Example 11.2. Peak hour electricity demand refers to the times when electricity usage is at its highest, typically in the late afternoon and early evening on weekdays when people are home. During these periods, the strain on the electrical grid is greatest, so electricity is often more expensive. The engineering group at an electric company wants to describe the relationship between

$$\begin{aligned} Y &= \text{peak hour electricity demand (measured in kWh)} \\ x &= \text{total monthly energy usage (measured in kWh).} \end{aligned}$$

This is important for planning purposes because the generating system must be large enough to meet the maximum demand imposed by customers. They consider the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon$$

to describe the relationship for the population of all residential customers. A random sample of $n = 52$ customers is selected to estimate the model. The R output

```
> fit = lm(peak.demand ~ monthly.usage)
> fit

Coefficients:
  (Intercept)  monthly.usage
     -0.44756        0.00328
```

gives the least-squares estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$. The estimated model is

$$\widehat{Y} = -0.44756 + 0.00328x \iff \widehat{\texttt{peak.demand}} = -0.44756 + 0.00328(\texttt{monthly.usage}).$$

This estimate is shown in Figure 11.4 (next page, left) superimposed over the scatterplot. The residual plot from the least-squares fit is also shown (next page, right).

Observation: The residual plot in Figure 11.4 shows a classic "fanning out" shape, which is a telltale sign of non-constant variance in the errors. That is, the assumption

- $V(\epsilon_i) = \sigma^2$, for $i = 1, 2, ..., n$, that is, the errors have constant variance

appears to be violated in this example.

Q: What are the impacts of non-constant variance if we don't do anything to address it?
A: This will inflate the variance in our least squares estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$. This has negative downstream effects if we want to perform inference for β_0 and β_1, specifically, confidence intervals will be too wide and thus may not be informative. Confidence intervals for $E(Y|x_0)$ and prediction intervals for $Y^*(x_0)$ will also be too wide.

Remedy: A common strategy to handle non-constant variance is to **transform** the response variable Y in some way and then estimate the model again using the transformed response in place of Y.

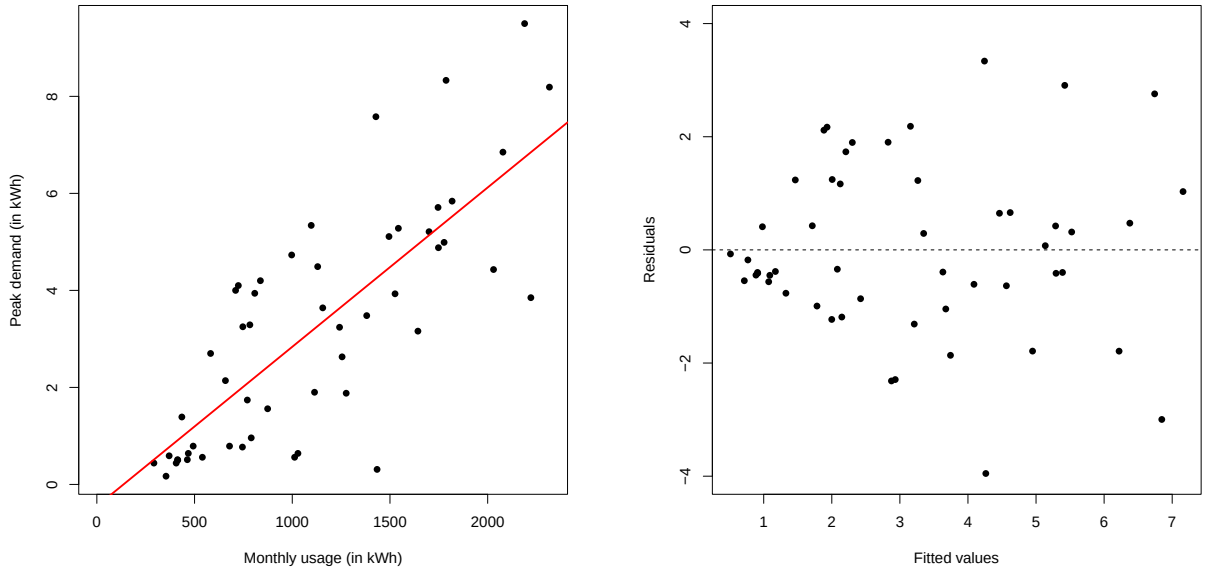


Figure 11.4: Electricity demand data. Left: Scatterplot of peak demand Y versus monthly usage x (both measured in kWh). The least-squares estimate has been superimposed. Right: Residual plot for the simple linear regression model fit.

Implementation: Common transformations to address non-constant variance are the logarithmic ($\ln Y$) and square root ($\sqrt{Y}$) transformations. Both of these functions keep small values of Y small and transform large values of Y into smaller values.

- A more advanced remedy is to use a model fitting technique known as **weighted least squares**; this involves weighting certain observations more/less depending on their level of variability. We will not pursue this.
- The advantage of using a transformation is that you can still use least squares without weighting. However, all inferences will pertain to the population model with the **transformed response**, not the response Y itself. That is, correct interpretations are on the transformed scale.

Analysis: I decided to use a square root transformation $W = \sqrt{Y}$. The R output

```
> sqrt.peak.demand = sqrt(peak.demand)
> fit.2 = lm(sqrt.peak.demand ~ monthly.usage)
> fit.2

Coefficients:
  (Intercept)  monthly.usage
     0.565034       0.000969
```

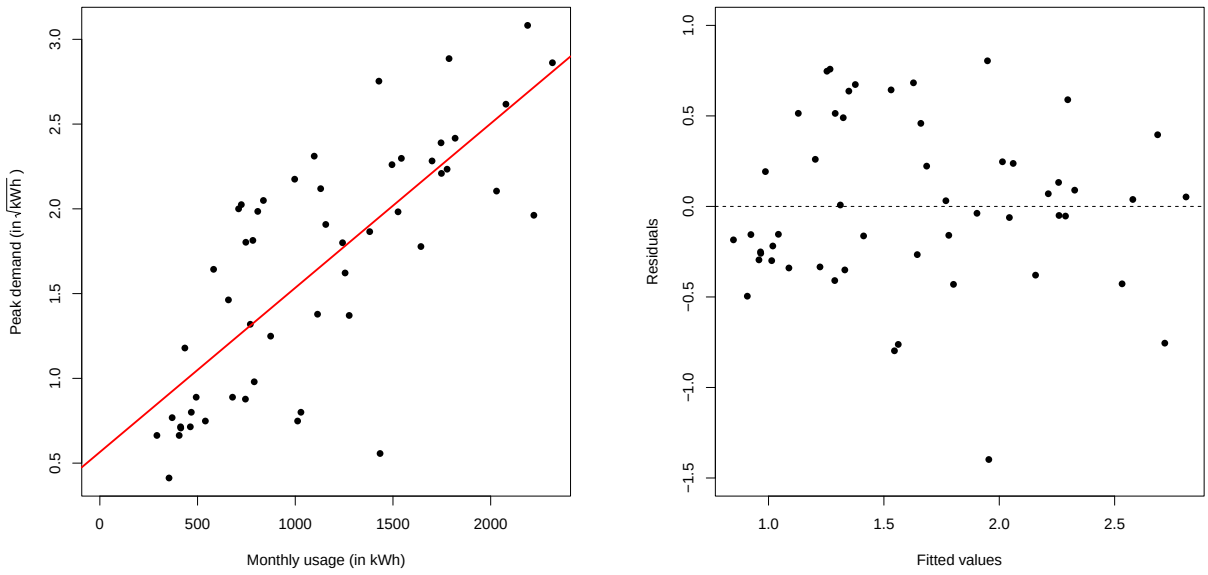


Figure 11.5: Electricity demand data. Left: Scatterplot of peak demand ($\sqrt{Y}$, measured in $\sqrt{\text{kWh}}$) versus monthly usage (x, measured in kWh) with the estimated simple linear regression line superimposed. Right: Residual plot for the simple linear regression model fit.

gives the least-squares estimates $\widehat{\beta}_0$ and $\widehat{\beta}_1$ for the transformed model

$$W = \beta_0 + \beta_1 x + \epsilon,$$

where

$$\begin{aligned} W &= \text{peak hour electricity demand (measured in } \sqrt{\text{kWh}}) \\ x &= \text{total monthly energy usage (measured in kWh).} \end{aligned}$$

The estimated model is

$$\widehat{W} = -0.565034 + 0.000969x$$

$$\Longleftrightarrow \quad \widehat{\sqrt{\texttt{peak.demand}}} = -0.565034 + 0.000969\texttt{(monthly.usage)}.$$

This estimate is shown in Figure 11.5 (above, left) superimposed over the scatterplot of $W = \sqrt{Y}$ versus x. The residual plot from the least-squares fit of the transformed model is also shown.

Observation: The residual plot in Figure 11.5 (above, right) shows a more random appearance which suggests the model assumptions are now satisfied. In particular, transforming the response appears to have "cured" the non-constant variance violation we saw in the untransformed analysis. The normal qq plot in Figure 11.6 (next page) shows good agreement between the residuals from estimating the transformed model and the normal quantiles.

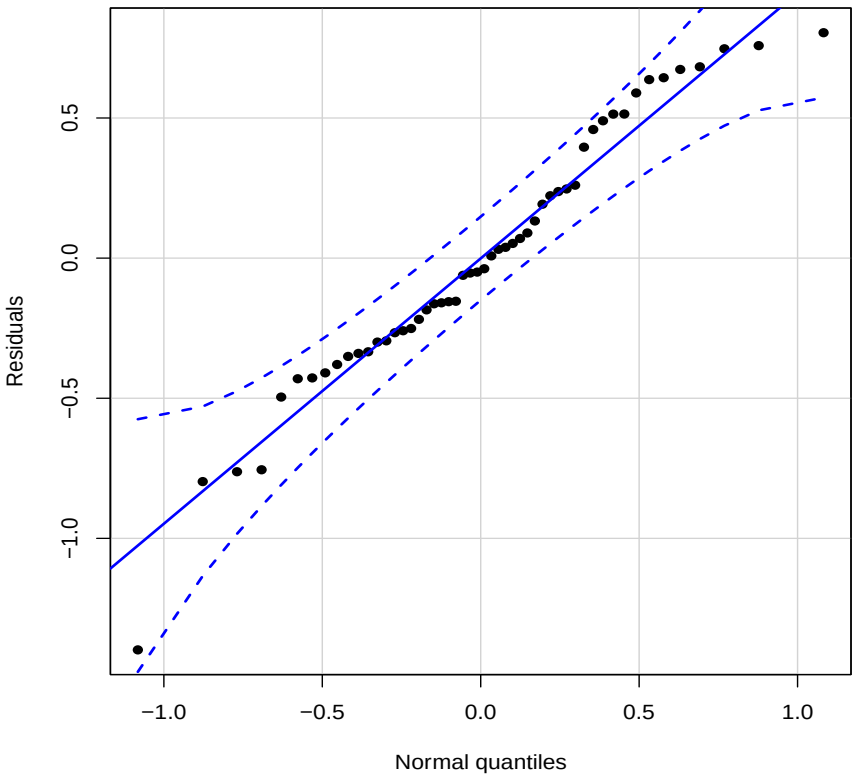


Figure 11.6: Electricity demand data. Normal qq plot of the residuals from the transformed model fit.

Statistical inference: I used R's `confint` function to write a 95% confidence interval for β_1 in the transformed model

$$W = \beta_0 + \beta_1 x + \epsilon \iff E(W) = \beta_0 + \beta_1 x.$$

Here is the output:

```
> confint(fit.2,conf.level=0.95)
                   2.5 %   97.5 %
(Intercept)    0.2778175 0.852250
monthly.usage 0.0007376 0.001201
```

Interpretation: We are 95% confident the population regression parameter β_1 (in the transformed model) is between 0.0007376 and 0.001201.

- Note this interval contains only positive values which suggests peak demand and monthly usage are positively related in the population of all residential customers.
- For every one kWh increase in monthly usage x, we are 95% confident the mean peak demand $E(W)$ will increase between 0.0007376 and 0.001201 $\sqrt{\text{kWh}}$.

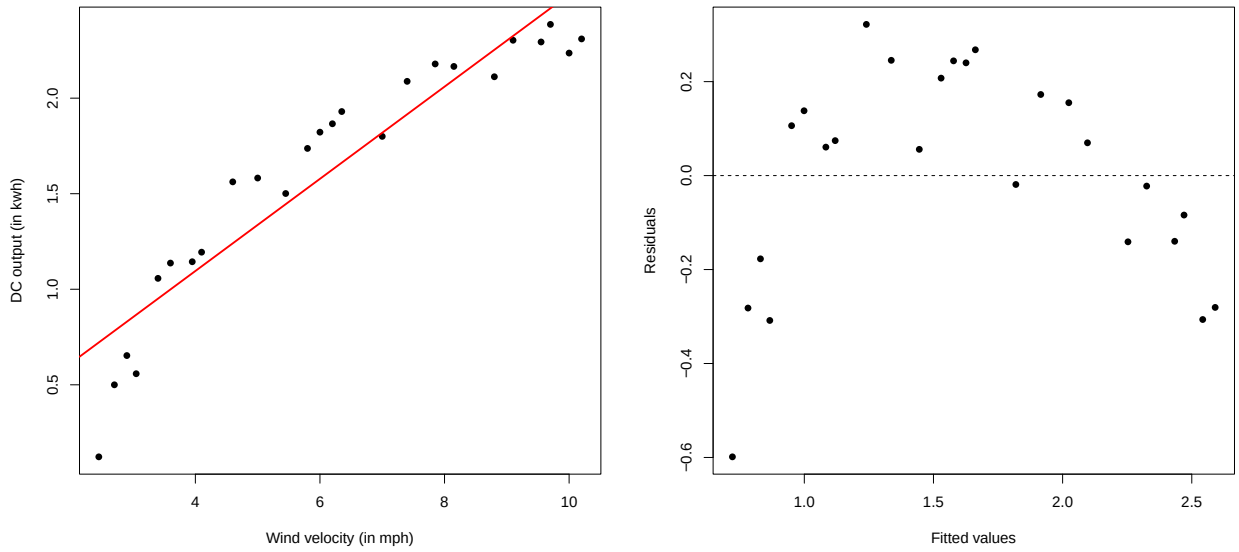


Figure 11.7: Wind turbine data. Left: Scatterplot of DC output (Y, measured in kWh) versus wind velocity (x, measured in mph) with the estimated simple linear regression line superimposed. Right: Residual plot for the simple linear regression model fit.

Example 11.3. An engineer is investigating the use of a wind turbine to generate electricity and has collected $n = 25$ measurements of

$$\begin{aligned} Y &= \text{direct current output (measured in kWh)} \\ x &= \text{wind velocity (measured in mph).} \end{aligned}$$

He initially assumes a simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon$$

to describe the relationship. The least squares estimate is shown in Figure 11.7 (above, left). The residual plot from the least squares fit is shown on the right. The ANOVA table from estimating the model is shown below:

```
> fit = lm(DC.output ~ velocity)
> anova(fit)
Analysis of Variance Table

Response: DC.output
          Df Sum Sq Mean Sq F value    Pr(>F)
velocity   1 8.9296  8.9296  160.26 7.546e-12 ***
Residuals 23 1.2816  0.0557
```

Observations: There is a **quadratic relationship** between DC output and wind velocity exhibited by these data. This is why the residual plot in Figure 11.7 (previous page, right) from the simple linear regression model fit shows a distinct quadratic pattern. This pattern is telling us the simple linear regression model

$$Y = \beta_0 + \beta_1 x + \epsilon$$

is inadequate. Interestingly, the coefficient of determination from estimating the simple linear regression model is

$$\frac{\text{SS}_{\text{R}}}{\text{SS}_{\text{TOT}}} = \frac{8.9296}{8.9296 + 1.2816} \approx 0.875.$$

A novice data analyst (e.g., one who doesn't even bother to look at the data, etc.) might think because this is pretty large, the simple linear regression model is a good model. However, even though 0.875 is "pretty large," its value refers to a model that is inappropriate. The data show a quadratic relationship between DC output and wind velocity−not a straight-line relationship.

Remedy: Fit a multiple linear regression model with two independent variables: wind velocity x and its square x^2. The model

$$Y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$$

is called a **quadratic regression model**. It is straightforward to fit this model in R. We simply regress Y on both x and x^2.

```
> velocity.sq = velocity^2
> fit.2 = lm(DC.output ~ velocity + velocity.sq)
> fit.2

Coefficients:
(Intercept)     velocity  velocity.sq
   -1.15590      0.72294     -0.03812
```

This output gives the value of the least squares estimate

$$\widehat{\boldsymbol{\beta}} = \begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta}_1 \\ \widehat{\beta}_2 \end{pmatrix} = \begin{pmatrix} -1.15590 \\ 0.72294 \\ -0.03812 \end{pmatrix}.$$

Therefore, the estimated quadratic regression model is

$$\widehat{Y} = -1.15590 + 0.72294x - 0.03812x^2,$$

or, in other words,

$$\widehat{\texttt{DC.output}} = -1.15590 + 0.72294\texttt{velocity} - 0.03812(\texttt{velocity})^2.$$

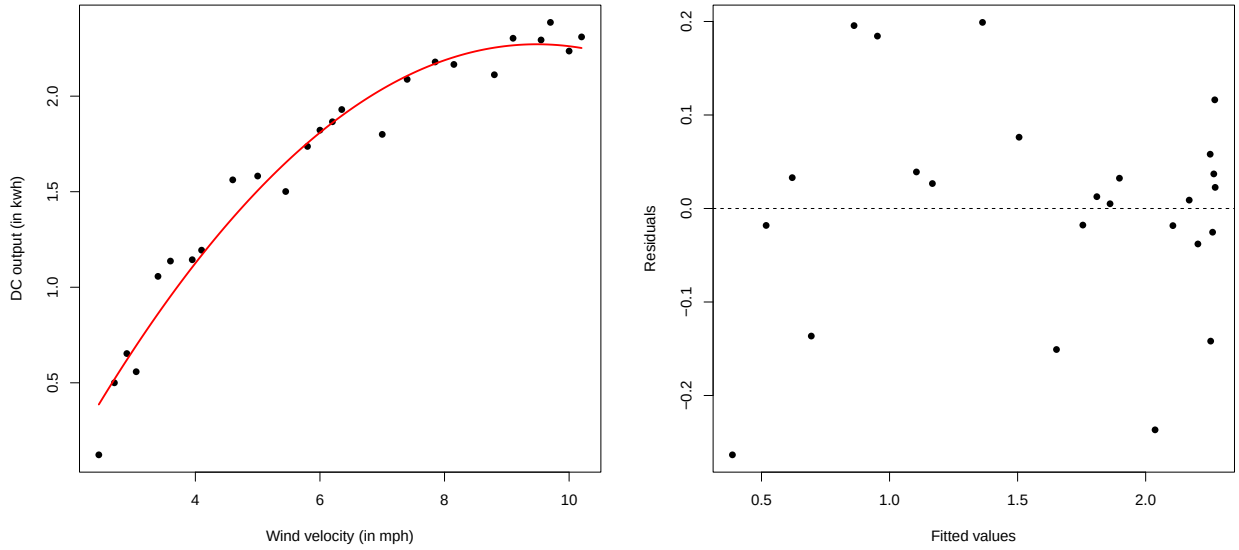


Figure 11.8: Wind turbine data. Left: Scatterplot of DC output (Y, measured in kWh) versus wind velocity (x, measured in mph) with the estimated quadratic fit superimposed. Right: Residual plot for the quadratic regression model fit.

Remark: The estimated quadratic regression model is shown in Figure 11.8 (above) accompanied by the residual plot from the model fit. The residual plot now looks more random. The quadratic pattern we saw in the residual plot from the simple linear regression model fit has now disappeared.

Inference: A relevant question to ask in this example is if the quadratic effect of wind velocity is significant for the population. We can answer this by writing a confidence interval for β_2 and seeing if this interval includes "0" or not.

- If the confidence interval for β_2 *does* include "0," this would suggest the quadratic term isn't needed and a simple linear regression model is appropriate for the population.

```
> options(digits=3)
> confint(fit.2,level=0.95)
              2.5 %  97.5 %
(Intercept) -1.5181 -0.7937
velocity     0.5955  0.8503
velocity.sq -0.0481 -0.0282
```

Interpretation: We are 95% confident the population regression parameter β_2 in the quadratic model is between -0.0481 and -0.0282. Note that this interval does not include "0" and includes only negative values. This suggests that quadratic effect between DC output and wind velocity is significant in the population.

12 Factorial Experiments

12.1 Introduction

Preview: In many engineering experiments, especially those in manufacturing settings, there are a number of independent variables (or **factors**) and the goal is to understand what effects these factors have on a continuous response variable Y, for example,

- Y = yield of a chemical process
- Y = lifetime of a part
- Y = fill volume or weight
- Y = bonding strength.

Terminology: A **factorial treatment structure** is an efficient way of defining treatments in an experiment where there are multiple factors. One example of a factorial treatment structure uses k factors, where each factor has two settings (or **levels**). This is called a 2^k factorial experiment.

Example 12.1. A nickel-titanium alloy is used to make components for jet turbine aircraft engines. Cracking is a potentially serious problem in one component as it can lead to nonrecoverable failure. An experiment is performed to understand how

$$Y = \text{largest component crack length (in mm)}$$

depends on four factors: pouring temperature (A), titanium content (B), heat treatment method (C), and amount of grain refiner used (D).

- Factor A has 2 levels: "low" temperature and "high" temperature
- Factor B has 2 levels: "low" content and "high" content
- Factor C has 2 levels: Method 1 and Method 2
- Factor D has 2 levels: "low" amount and "high" amount.

In this example, there are 4 factors, each with 2 levels. Thus, there are

$$2 \times 2 \times 2 \times 2 = 2^4 = 16$$

treatment combinations. These are listed here:

$$\begin{array}{cccc} a_1b_1c_1d_1 & a_1b_2c_1d_1 & a_2b_1c_1d_1 & a_2b_2c_1d_1 \\ a_1b_1c_1d_2 & a_1b_2c_1d_2 & a_2b_1c_1d_2 & a_2b_2c_1d_2 \\ a_1b_1c_2d_1 & a_1b_2c_2d_1 & a_2b_1c_2d_1 & a_2b_2c_2d_1 \\ a_1b_1c_2d_2 & a_1b_2c_2d_2 & a_2b_1c_2d_2 & a_2b_2c_2d_2 \end{array}$$

For example, the treatment combination $a_1b_1c_1d_1$ holds each factor at its "low" level, the treatment combination $a_1b_1c_2d_2$ holds Factors A and B at their "low" level and Factors C and D at their "high" level, and so on.

Terminology: In a 2^k factorial experiment, one **replicate** of the experiment requires 2^k runs, one at each of the treatment combinations.

- Therefore, in Example 12.1, one replicate of the experiment would require $2^4 = 16$ runs (one at each treatment combination listed on the previous page).
- Two replicates would require 32 runs, three replicates would require 48 runs, and so on.

Terminology: There are different types of effects in factorial experiments: **main effects** and **interaction effects**. For example, in a 2^4 factorial experiment,

- there is **1** "effect" that does not depend on any of the factors (an overall mean)
- there are **4** main effects: A, B, C, and D
- there are **6** two-way interaction effects: AB, AC, AD, BC, BD, and CD
- there are **4** three-way interaction effects: ABC, ABD, ACD, and BCD
- there is **1** four-way interaction effect: ABCD.

Note that

$$\begin{aligned} 2^4 = 16 &= 1 + 4 + 6 + 4 + 1 \\ &= \binom{4}{0} + \binom{4}{1} + \binom{4}{2} + \binom{4}{3} + \binom{4}{4}, \end{aligned}$$

that is, the binomial coefficients inform us how many effects there are of a given type.

Q: What do **main effects** mean? In Example 12.1,

- the main effect of A (temperature) estimates the difference in the mean response (largest crack length) between the 8 "high" levels of temperature and the 8 "low" levels of temperature, that is, between

$$\begin{array}{cc} a_2b_1c_1d_1 & a_2b_2c_1d_1 \\ a_2b_1c_1d_2 & a_2b_2c_1d_2 \\ a_2b_1c_2d_1 & a_2b_2c_2d_1 \\ a_2b_1c_2d_2 & a_2b_2c_2d_2 \end{array} \quad \text{and} \quad \begin{array}{cc} a_1b_1c_1d_1 & a_1b_2c_1d_1 \\ a_1b_1c_1d_2 & a_1b_2c_1d_2 \\ a_1b_1c_2d_1 & a_1b_2c_2d_1 \\ a_1b_1c_2d_2 & a_1b_2c_2d_2 \end{array}.$$

- this allows us to assess whether the mean response $E(Y)$ depends on factor A by itself (irrespective of the other factors)
- the other main effects (i.e., B, C, and D) are interpreted similarly.

Q: What do **interaction effects** mean? In Example 12.1,

- if the **two-way interaction** effect AB is significant, this means
  - the way the mean response $E(Y)$ depends on factor A is different for the two levels of B
  - the way $E(Y)$ depends on factor B is different for the two levels of A.
- This is what it means when we say that "two factors interact." Other two-way interaction effects are interpreted similarly.
- **Three-way interaction** effects are a little harder to interpret. For example, if the three-way interaction ABC is significant, this would mean the way two factors interact (e.g., AB, etc.) is different for the two levels of the other factor (e.g., C, etc.).
- Higher-order interaction effects become increasingly harder to interpret. For example, it is difficult to explain what the four-way interaction effect ABCD means. In experiments with a larger number of factors, any effect measuring really high-order interactions (e.g., ABCDEF, etc.) has little practical meaning.

Common goals: In most 2^k factorial experiments, investigators are interested in main effects and "lower-order" interaction effects. This means two-way interactions and occasionally three-way interactions. Higher-order interactions are often best regarded as "noise."

12.2 Example: A 2^2 experiment with replication

Remark: We start with the simplest factorial treatment structure−one where there are only $k = 2$ factors: A and B. We are interested in

- assessing the main effects of A and B separately
- assessing whether the two factors interact, that is, the interaction effect AB.

Example 12.2. Predicting corn yield prior to harvest is useful for making feed supply and marketing decisions. Corn must have an adequate amount of nitrogen (Factor A) and phosphorus (Factor B) for profitable production and also for environmental concerns.

Design: There are 2 factors in this example, each with two levels:

- Factor A: Nitrogen application amount: Level 1: 10 lbs/plot; Level 2: 15 lbs/plot
- Factor B: Phosphorous application amount: Level 1: 2 lbs/plot; Level 2: 4 lbs/plot.

There were 20 equally sized plots used in the experiment. Plots were randomly assigned to one of the $2^2 = 4$ treatment combinations (5 plots per treatment combination). On each plot, investigators measured the response variable

$$Y = \text{yield (measured in bushels per plot)}.$$

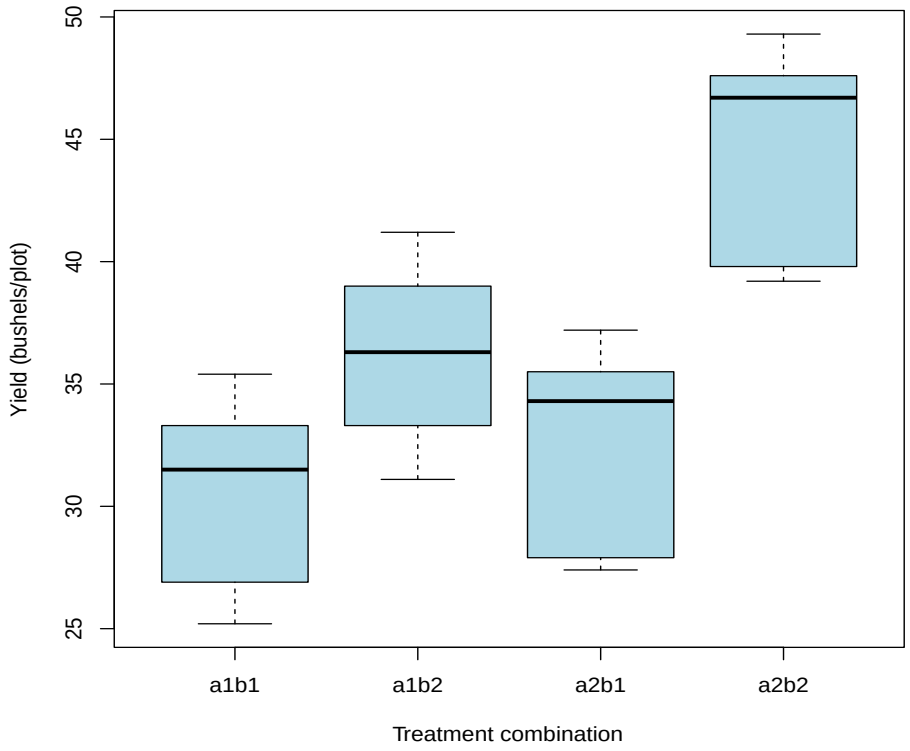


Figure 12.1: Corn yield data. Boxplots of yields (bushels/plot) for four treatment combinations.

Side-by-side boxplots of the data below are shown in Figure 12.1 (above).

Treatment combination	Yield (Y)	Treatment sample mean
a_1b_1	35.4, 26.9, 25.2, 33.3, 31.5	30.46
a_1b_2	39.0, 33.3, 41.2, 31.1, 36.3	36.18
a_2b_1	37.2, 27.9, 35.5, 27.4, 34.3	32.46
a_2b_2	49.3, 39.8, 39.2, 47.6, 46.7	44.52

Uninteresting analysis: One way to analyze these data would be to ignore the factorial treatment structure and simply regard each of the combinations a_1b_1, a_1b_2, a_2b_1, and a_2b_2 as a generic "treatment." We could then perform a one-way classification analysis with $t = 4$ treatment groups like we did in Chapter 9. This produces the following ANOVA table:

```
> fit = lm(Yield ~ Treatment)
> anova(fit)
Analysis of Variance Table

          Df Sum Sq Mean Sq F value   Pr(>F)
Treatment  3 579.05 193.017  9.9519 0.000609 ***
Residuals 16 310.32  19.395
```

Note: The value $F = 9.9519$ is not what we would expect from an $F(3, 16)$ distribution, the distribution of F when

$$H_0 : \mu_{11} = \mu_{12} = \mu_{21} = \mu_{22}$$

is true (p-value = 0.000609). Therefore, we would reject H_0 and conclude at least one of the four population mean yields is different.

Remark: The preceding analysis, although correct, isn't very interesting. Nowhere in this analysis are we accounting for the factorial treatment structure in the design. A more informative analysis would allow us to learn about the main effects of nitrogen (A) and phosphorous (B) and how these two factors potentially interact with each other. To see how this is done, note the treatment sum of squares from the one-way classification:

$$\text{SS}_\text{T} = 579.05.$$

The way we learn more about the specific effects is to partition SS_T. By "partition," I mean that we will write

$$\text{SS}_\text{T} = \text{SS}_\text{A} + \text{SS}_\text{B} + \text{SS}_\text{AB},$$

where

- SS_A = sum of squares due to the main effect of A (nitrogen)
- SS_B = sum of squares due to the main effect of B (phosphorus)
- SS_AB = sum of squares due to the interaction effect of A and B (nitrogen and phosphorus).

Two-way analysis: We can use R to write this partition in a richer ANOVA table:

```
> fit = lm(Yield ~ Nitrogen + Phosphorus + Nitrogen*Phosphorus)
> anova(fit)
Analysis of Variance Table

                    Df Sum Sq Mean Sq F value    Pr(>F)
Nitrogen             1 133.64  133.64  6.8907 0.0183819 *
Phosphorus           1 395.16  395.16 20.3743 0.0003533 ***
Nitrogen:Phosphorus  1  50.24   50.24  2.5906 0.1270504
Residuals           16 310.32   19.39
```

First, note that, up to rounding error,

$$\begin{aligned} \text{SS}_\text{T} = 579.05 &= 133.64 + 395.16 + 50.24 \\ &= \text{SS}_\text{A} + \text{SS}_\text{B} + \text{SS}_\text{AB}. \end{aligned}$$

Furthermore, the F statistics in the output above can be used to judge whether the effects A, B, and AB are significant.

Specifically, $F_{\text{A}} = 6.8907$ tests

$$H_0 : \text{the main effect of A is not significant}$$
$$\text{versus}$$
$$H_1 : \text{the main effect of A is significant,}$$

$F_{\text{B}} = 20.3743$ tests

$$H_0 : \text{the main effect of B is not significant}$$
$$\text{versus}$$
$$H_1 : \text{the main effect of B is significant,}$$

and $F_{\text{AB}} = 2.5906$ tests

$$H_0 : \text{the AB interaction effect is not significant}$$
$$\text{versus}$$
$$H_1 : \text{the AB interaction effect is significant.}$$

As usual, large F statistics (small p-values, e.g., p-value < 0.05) are evidence against H_0.

Conclusions: We have strong evidence the main effects of A (nitrogen) and B (phosphorous) are significant in the population of all plots. At the $\alpha = 0.05$ level of significance, we do not have sufficient evidence that nitrogen and phosphorous interact (that is, the AB interaction effect is not significant, p-value ≈ 0.127).

Terminology: An **interaction plot** is a graphical display that can help us assess (visually) whether two factors interact. In this plot, the levels of Factor A are marked on the horizontal axis. The sample means of the treatments are plotted against the levels of A, and the points corresponding to the same level of Factor B are joined by straight lines.

- If Factors A and B do not interact, the interaction plot should display approximately parallel lines.
  - That is, the effect of one factor on the mean response $E(Y)$ stays constant across the levels of the other factor. This is what it means to have no interaction.
- If the interaction plot displays a significant departure from parallelism (including an overwhelming case where the lines even cross), this is visual evidence of interaction.
  - That is, the effect of one factor on the response $E(Y)$ is different across the levels of the other factor.
- The F test that uses F_{AB} provides numerical evidence of interaction. The interaction plot provides visual evidence.
- *The larger F_{AB} is, the larger the departure from parallelism in the interaction plot.*

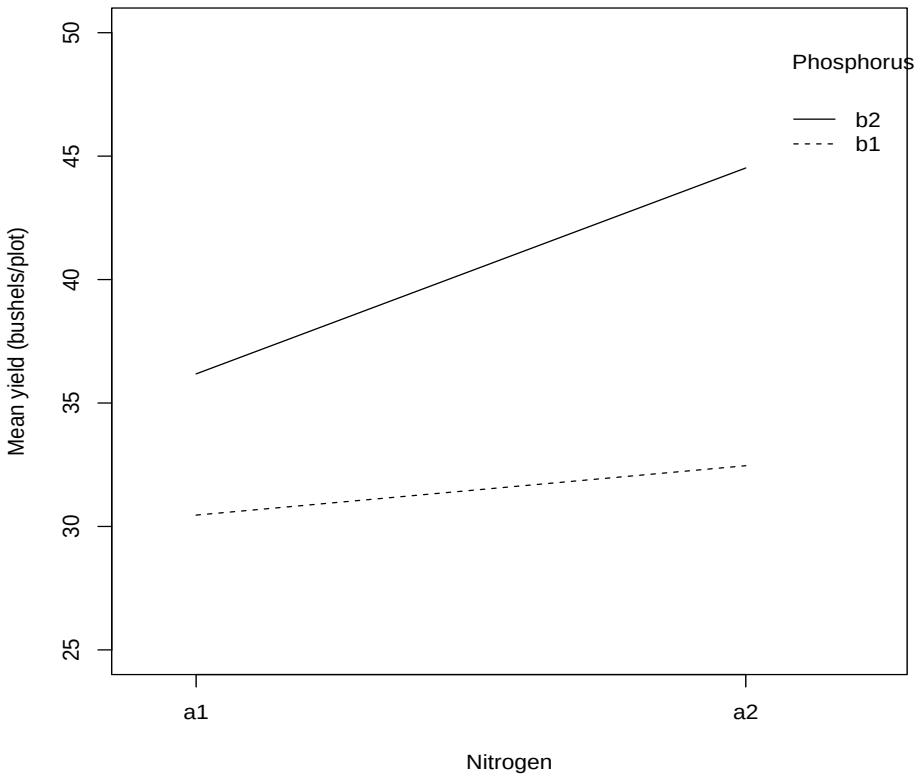


Figure 12.2: Corn yield data. Interaction plot of Nitrogen (A) and Phosphorous (B).

Example 12.2 (continued). We now use R to construct the interaction plot for the corn yield data in Example 12.2. We have already used the interaction test statistic F_{AB} to conclude that the interaction effect of nitrogen and phosphorus is not significant in the population; recall

$$F_{\text{AB}} \approx 2.59 \quad (\text{p-value} \approx 0.127).$$

In other words, the evidence for population-level interaction between nitrogen and phosphorous is not significant at the $\alpha = 0.05$ significance level. Therefore, although the interaction plot in Figure 12.2 (above) is not perfectly parallel, the departure from parallelism is not significant at the $\alpha = 0.05$ significance level.

Strategy for analyzing 2^2 factorial experiments:

1. Start by looking at whether the interaction effect is significant. This can be done by using an interaction plot and an F test that uses F_{AB}.

2. **If the interaction is significant**, then a formal analysis of main effects is not meaningful because their interpretations depend on the interaction.

- In this case, the best approach is to just ignore the factorial treatment structure and redo the entire analysis as a one-way ANOVA with 4 treatments.
- Tukey pairwise confidence intervals can be used to determine which means are different from the others and help to formulate an ordering among the 4 treatment population means.

3. **If the interaction is not significant**, I prefer to redo the analysis without the interaction term and then examine the main effects. This can be done by examining the sizes of F_{A} and F_{B}, respectively. Confidence intervals for population mean differences

$$\mu_{A1} - \mu_{A2} \quad \text{and} \quad \mu_{B1} - \mu_{B2}$$

can be used to quantify the size of these effects in the population.

Example 12.2 (continued). Because the nitrogen-phosphorous (AB) interaction was not significant, I redid the analysis leaving out the interaction term in the ANOVA:

```
> fit.2 = lm(Yield ~ Nitrogen + Phosphorus) # no interaction
> anova(fit.2)
Analysis of Variance Table

           Df Sum Sq Mean Sq F value    Pr(>F)
Nitrogen    1 133.64  133.64  6.3011 0.0224734 *
Phosphorus  1 395.16  395.16 18.6311 0.0004682 ***
Residuals  17 360.56   21.21
```

Observations: It's first insightful to note how this ANOVA partition compares to the one from the interaction analysis (see pp 224).

- The interaction sum of squares $\text{SS}_{\text{AB}} = 50.24$ from the interaction analysis has been "absorbed" into the error (residual) sum of squares in the no-interaction analysis.
- Because the no-interaction analysis does not specify an interaction for the population of all plots, any variation that explains interaction in the sample of 20 plots is regarded as "noise."
- The only sources of variation in the no-interaction analysis are the main effects of nitrogen (A) and phosphorous (B).
  - At the $\alpha = 0.05$ level of significance, the main effect of nitrogen (Factor A) is significant in the population ($F_{\text{A}} \approx 6.30$, p-value $\approx 0.0225 < 0.05$).
  - At the $\alpha = 0.05$ level of significance, the main effect of phosphorous (Factor B) is significant in the population ($F_{\text{B}} \approx 18.63$, p-value $\approx 0.0005 < 0.05$).

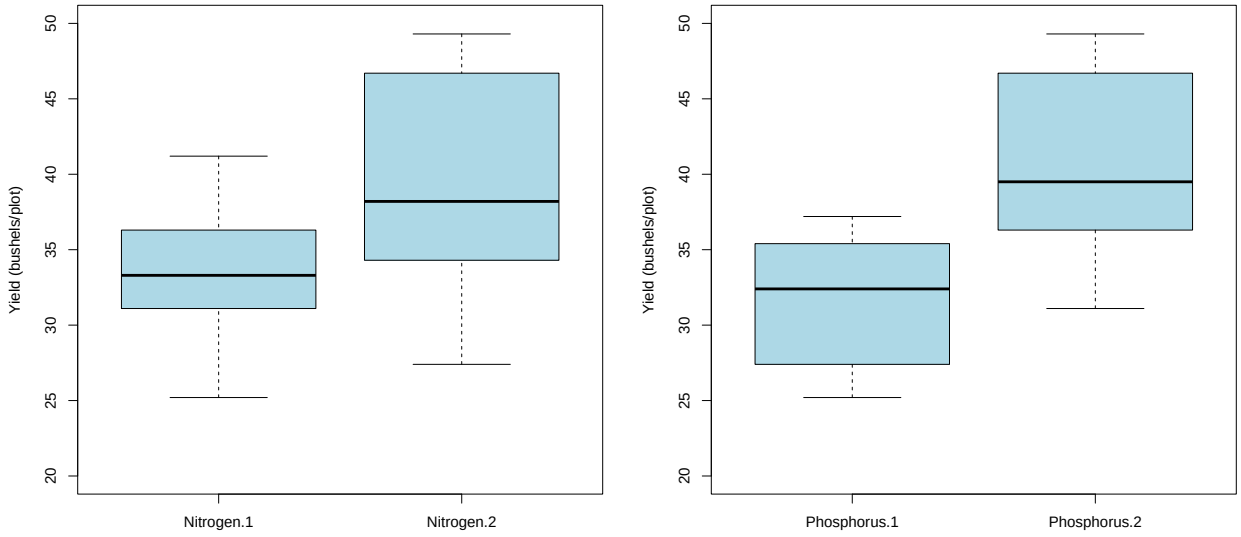


Figure 12.3: Corn yield data. Left: Boxplots of yields for nitrogen (Factor A). Right: Boxplots of yields for phosphorus (Factor B).

Confidence intervals: A 95% confidence interval for $\mu_{A1} - \mu_{A2}$, the difference in the population mean yields for the two levels of nitrogen (Factor A), is

$$(\overline{Y}_{A1} - \overline{Y}_{A2}) \pm t_{17,0.025}\sqrt{\text{MS}_\text{E}\left(\frac{1}{10} + \frac{1}{10}\right)}.$$

A 95% confidence interval for $\mu_{B1} - \mu_{B2}$, the difference in population mean yields for the two levels of phosphorus (Factor B), is

$$(\overline{Y}_{B1} - \overline{Y}_{B2}) \pm t_{17,0.025}\sqrt{\text{MS}_\text{E}\left(\frac{1}{10} + \frac{1}{10}\right)}.$$

The R code online can be used to calculate these intervals:

$$\begin{aligned} 95\%\text{ CI for } \mu_{A1} - \mu_{A2}: &\quad (-9.52, -0.82) \\ 95\%\text{ CI for } \mu_{B1} - \mu_{B2}: &\quad (-13.24, -4.54). \end{aligned}$$

Interpretation:

- We are 95% confident the difference in the population mean yields (low nitrogen minus high nitrogen) is between -9.52 and -0.82 bushels per acre.
  - Note this interval does not include "0" and includes only negative values.
  - This suggests the population mean yield at the high level of nitrogen is larger than the population mean yield at the low level of nitrogen.

- We are 95% confident the difference in the population mean yields (low phosphorus minus high phosphorus) is between -13.24 and -4.54 bushels per acre.
  - Note this interval does not include "0" and includes only negative values.
  - This suggests the population mean yield at the high level of phosphorus is larger than the population mean yield at the low level of phosphorus.

12.3 Example: A 2^4 experiment without replication

Example 12.3. A chemical product is produced in a pressure vessel. A factorial experiment is carried out to study the factors thought to influence

$$Y = \text{the filtration rate (in gallons per minute per square foot)}$$

of this product. The four factors are temperature (A), pressure (B), concentration of formaldehyde (C) and stirring rate (D). Each factor is present at two levels ("low" and "high"). A 2^4 experiment is performed with one replication; the data are shown below.

	Factor					Filtration rate
Run	A	B	C	D	Run label	(Y, gpm/ft^2)
1	$-$	$-$	$-$	$-$	$a_1b_1c_1d_1$	45
2	$+$	$-$	$-$	$-$	$a_2b_1c_1d_1$	71
3	$-$	$+$	$-$	$-$	$a_1b_2c_1d_1$	48
4	$+$	$+$	$-$	$-$	$a_2b_2c_1d_1$	65
5	$-$	$-$	$+$	$-$	$a_1b_1c_2d_1$	68
6	$+$	$-$	$+$	$-$	$a_2b_1c_2d_1$	60
7	$-$	$+$	$+$	$-$	$a_1b_2c_2d_1$	80
8	$+$	$+$	$+$	$-$	$a_2b_2c_2d_1$	65
9	$-$	$-$	$-$	$+$	$a_1b_1c_1d_2$	43
10	$+$	$-$	$-$	$+$	$a_2b_1c_1d_2$	100
11	$-$	$+$	$-$	$+$	$a_1b_2c_1d_2$	45
12	$+$	$+$	$-$	$+$	$a_2b_2c_1d_2$	104
13	$-$	$-$	$+$	$+$	$a_1b_1c_2d_2$	75
14	$+$	$-$	$+$	$+$	$a_2b_1c_2d_2$	86
15	$-$	$+$	$+$	$+$	$a_1b_2c_2d_2$	70
16	$+$	$+$	$+$	$+$	$a_2b_2c_2d_2$	96

Notation: When discussing factorial experiments, it is common to use the symbol "$-$" to denote the low level of a factor and the symbol "$+$" to denote the high level. For example, the first row of the table above indicates that each factor (A, B, C, and D) is at its "low" level. The response Y for this run is 45 gpm/ft^2.

Note: In Example 12.3, there are $k = 4$ factors, so there are 16 effects to estimate:

- 1 overall mean (an "effect" that doesn't depend on any of the factors)
- 4 main effects: A, B, C, and D
- 6 two-way interactions: AB, AC, AD, BC, BD, and CD
- 4 three-way interactions: ABC, ABD, ACD, BCD
- 1 four-way interaction: ABCD.

Analysis: Here is the R output from estimating the full model with all 15 main and interaction effects:

```
> fit = lm(filtration ~ A*B*C*D)
> anova(fit)

Analysis of Variance Table
          Df  Sum Sq Mean Sq F value Pr(>F)
A          1 1870.56 1870.56
B          1   39.06   39.06
C          1  390.06  390.06
D          1  855.56  855.56
A:B        1    0.06    0.06
A:C        1 1314.06 1314.06
B:C        1   22.56   22.56
A:D        1 1105.56 1105.56
B:D        1    0.56    0.56
C:D        1    5.06    5.06
A:B:C      1   14.06   14.06
A:B:D      1   68.06   68.06
A:C:D      1   10.56   10.56
B:C:D      1   27.56   27.56
A:B:C:D    1    7.56    7.56
Residuals  0    0.00
Warning message:
In anova.lm(fit) :
  ANOVA F-tests on an essentially perfect fit are unreliable
```

Terminology: A single replicate of a 2^k factorial experiment is called an **unreplicated factorial**. With only one replicate, there is no internal "error estimate," so we cannot perform F tests to judge significance. What do we do?

- One approach is to assume higher-order interactions are "negligible" and then combine their sum of squares to estimate the error.

- This is an appeal to the **sparsity of effects principle**, which states that most systems or processes are dominated by at most main effects and low-order interactions and that most high-order interactions are negligible.
- To learn about which effects may be negligible, we can fit the full ANOVA model and obtain the sum of squares (SS) for each effect (see previous page).
  - Effects with "large" SS can be retained.
  - Effects with "small" SS can be discarded.
- A smaller model with only the "large" effects can then be fit. This smaller model will have an error estimate formed by taking all of the effects with "small" SS and combining them together.

Analysis: From the full model table (on the last page), it is easy to see the effects

A, C, D, AC, AD

are the most relevant. The sum of squares associated with these effects are much larger than the other sum of squares. Therefore, we can estimate a smaller model with these 5 effects only (ostensibly regarding the other 10 effects to be "noise"). This will "free up" 10 degrees of freedom that can be used to estimate the error variance. In turn, this will allow us to perform F tests for the 5 effects we have identified above. Here is the R output from estimating the smaller model:

```
> fit.2 = lm(filtration ~ A + C + D + A*C + A*D)
> anova(fit.2)

Analysis of Variance Table
          Df  Sum Sq Mean Sq F value    Pr(>F)
A          1 1870.56 1870.56  95.865 1.928e-06 ***
C          1  390.06  390.06  19.990  0.001195 **
D          1  855.56  855.56  43.847 5.915e-05 ***
A:C        1 1314.06 1314.06  67.345 9.414e-06 ***
A:D        1 1105.56 1105.56  56.659 1.999e-05 ***
Residuals 10  195.13   19.51
```

Conclusion: Each effect is highly significant. The AC (temperature/concentration of formaldehyde) and AD (temperature/stirring rate) interaction plots in Figure 12.4 (next page) each show strong interaction.

Regression analysis: Even though there are no numerical values for the levels of temperature (Factor A), concentration of formaldehyde (Factor C), and stirring rate (Factor D) in Example 12.3, we can still use regression to estimate a population-level model. Specifically, we can introduce the following variables with numerical codings:

$$\begin{aligned} x_1 &= \text{temperature } (-1 = \text{low}; 1 = \text{high}) \\ x_2 &= \text{concentration of formaldehyde } (-1 = \text{low}; 1 = \text{high}) \\ x_3 &= \text{stirring rate } (-1 = \text{low}; 1 = \text{high}). \end{aligned}$$

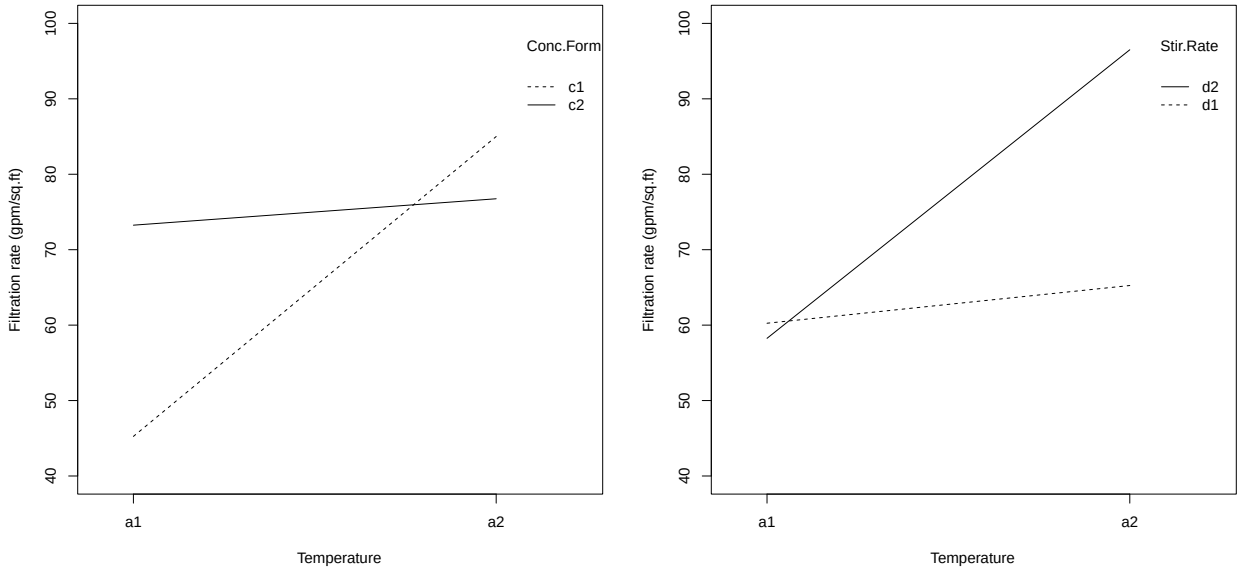


Figure 12.4: Filtration rate data. Interaction plots. Left: AC (temperature/concentration of formaldehyde). Right: AD (temperature/stirring rate).

With these values, we can fit the multiple linear regression model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_1 x_2 + \beta_5 x_1 x_3 + \epsilon.$$

Doing so in R gives

```
> fit = lm(filtration ~ temp + conc + stir + temp:conc + temp:stir)
> fit
Coefficients:
(Intercept)         temp         conc         stir    temp:conc    temp:stir
     70.062       10.812        4.938        7.313       -9.062        8.312
```

Therefore, the estimated regression model for the filtration rate data is

$$\widehat{Y} = 70.062 + 10.812x_1 + 4.938x_2 + 7.313x_3 - 9.062x_1x_2 + 8.312x_1x_3$$

or, in other words,

$$\widehat{\texttt{FILT}} = 70.062 + 10.812\ \texttt{TEMP} + 4.938\ \texttt{CONC} + 7.313\ \texttt{STIR} - 9.062\ \texttt{TEMP*CONC} + 8.312\ \texttt{TEMP*STIR}.$$

This equation can be used to predict the filtration rate at specific combinations of temperature (± 1), concentration (± 1), and stirring rate (± 1). Provided that our usual regression assumptions hold, confidence intervals for the population mean filtration rate $E(Y)$ and prediction intervals for Y are formed in the usual way.