Statistical Inference and Learning Methods for Research

Longhai Li

2025-11-20

Table of contents

1 Preface 1

Preface 3
- Audience and Prerequisites 3
- Key Features 3
- Structure of the Book 4

2 Data Science with R and Quarto 5
- 2.1 Basic R Objects and Operations 5
- 2.2 Import a dataset into R environment and Simple Operation 8
- 2.3 Create your own function 13
- 2.4 Include Images Saved in An External File 14

3 Simple Linear Regression 17
- 3.1 Overview of Simple Linear Regression 17
  - 3.1.1 Least Squares Estimation 18
  - 3.1.2 Residual and Sum of Squares Definitions 19
  - 3.1.3 Coefficient of Determination (R^2) 20
  - 3.1.4 F-test for Overall Significance 20
  - 3.1.5 t-test for the Slope β_1 22
  - 3.1.6 Prediction for a New Case x_0 23
- 3.2 Example 1: Vehicle Insurance Premium (warm-up) 23
  - 3.2.1 Input data 23
  - 3.2.2 Estimating regression coefficients 25
  - 3.2.3 Residuals and fitted values (geometry picture) 25
  - 3.2.4 SST, SSR, SSE and their meanings 27
  - 3.2.5 Visual ANOVA on an RSS plot 28
  - 3.2.6 R^2, F and a compact ANOVA table 29
  - 3.2.7 Sampling distributions via animation 30
- 3.3 Example 2: Oxygen Purity Data 31
  - 3.3.1 Data 31
  - 3.3.2 Fit and quick summary 32
  - 3.3.3 Scatter with fitted line 33
  - 3.3.4 Coefficient CIs and ANOVA 34
  - 3.3.5 Mean-response and prediction bands 35
  - 3.3.6 Residual diagnostics (assumptions check) 36
- 3.4 Correlation analysis (for comparison, not causation) 37
  - 3.4.1 Data and scatter 37

3.4.2 Pearson correlation and test . . . 38
3.5 What to report (checklist) . . . 39

4 Multiple Linear Regression 41
4.1 An Example: Wire Bond Strength Dataset . . . 41
4.1.1 Loading Data and Visualization . . . 41
4.1.2 Model Fitting and Summary . . . 44
4.1.3 Confidence Intervals and Model Components . . . 45
4.2 RSS-based Inference: F-test, and adjusted R^2 . . . 46
4.2.1 RSS-Based Quantities . . . 47
4.2.2 Remarks . . . 47
4.2.3 A Simulation Study to Understand the Distributions of RSS . . . 49
4.2.4 Example: Modelling Children Weight with Height and Age . . . 54
4.2.5 Example: Wire bond strength . . . 57
4.2.6 Relationship between t-test and partial F-test . . . 59
4.3 Predictions for Mean Response and a Future Observation . . . 59
4.3.1 Confidence Interval for Mean Response . . . 59
4.3.2 Prediction Interval for a New Observation . . . 59
4.4 Model Diagnostics . . . 60
4.4.1 Residual Calculations . . . 60
4.4.2 Residual Plots . . . 61
4.5 Influential Observations . . . 62
4.5.1 Plotting with the `olsrr` Package . . . 63
4.6 Polynomial Regression . . . 66
4.7 Handling Categorical Variables with Dummy Variables . . . 68
4.7.1 Four Models Involving "sex" . . . 70
4.7.2 Orders of Terms Matters in ANOVA and Warnings in Interpreting t-test Tables . . . 83
4.8 Model Building . . . 87
4.8.1 All Possible Regression . . . 87
4.8.2 Automated Stepwise Procedures . . . 88
4.9 Multicollinearity . . . 91
4.9.1 A Simple Example . . . 91
4.9.2 VIFs in the Wine Quality Data . . . 93
4.9.3 VIFs in the Children Height Data . . . 93

5 Residual Diagnostics for Regression Modelling 95
5.1 Introduction . . . 95
5.2 Introduction . . . 95
5.3 The Linear Model . . . 95
5.4 Residuals for OLS . . . 96
5.4.1 Our Notations . . . 96
5.4.2 Non-studentized Residuals . . . 96
5.4.3 Studentized Residuals . . . 97
5.4.4 List of Residuals . . . 99
5.4.5 Example of Various Residuals . . . 99

5.5 Cook's Distance 108
5.5.1 Definition from the change in coefficients 108
5.5.2 Example for Cook's Distance: 111
Appendix: Key Identities 115
Finding the LOOCV Residual ($e_{i,-i}$) from the Ordinary Residual (e_i) 115
Finding the LOOCV Standard Error from the Full-Model Standard Error 115

6 Logistic Regression 117
6.1 Odds as a Function of Probability 117
6.2 Logistic Regression 119
6.3 A Dataset Simulated from Logistic Regression 120
6.3.1 Fit a logistic model to the simulated data 120
6.4 Example: Coronary Heart Disease Data 122
6.4.1 Load a dataset 122
6.4.2 Fit Logistic Regression Model for a Single Variable 123
6.4.3 Fit Logistic Regression Model with all variables 128
6.5 Inference for Coefficients: Confidence Intervals and Covariance Matrix 129
6.6 Inference for Odds Ratios 130
6.6.1 Interpretation of Odds Ratios in Logistic Regression 130
6.6.2 Examples of Finding ORs and Their CIs for the CHD Dataset 134
6.7 Assessing Statistical Significance with Wilks' Theorem (Analogue of F-test for OLS) 135
6.8 Assessing Predictive Effect-Size (Anologue to R^2_{adj}) 142
6.8.1 Understanding the Confusion Matrix and Metrics 142
6.8.2 Illustration with the Simulated Dataset 143
6.8.3 Application to the CHD Dataset 151

7 Randomized Complete Block Design 157
7.1 Completely Randomized Design 157
7.1.1 Design on R 157
7.1.2 Plasma Etching Experiment 158
7.2 Unbalanced Designs with Unequal Sample Sizes 175
7.3 Randomized Complete Block Design 177
7.3.1 Vascular Graft Experiment 177

8 Two-Factor Factorial Design 185
8.1 Battery Design Experiment 185
8.2 Data Setup and Preparation 185
8.3 Exploratory Data Analysis and Visualization 186
8.4 Boxplots of Main Effects 187
8.5 Interaction Plot 187
8.6 Model Fitting and Analysis of Variance (ANOVA) 189
8.7 Model Adequacy Checks 190
8.8 Post-Hoc Analysis: Pairwise Comparisons 191
8.9 Tukey's HSD Test 191
8.10 Fisher's LSD Method 193

1 Preface

Preface

This book has evolved from the lecture notes for *STAT 845: Statistical Methods for Research*, a graduate-level course taught at the University of Saskatchewan. It is born out of a recognition that for many graduate students, statistics is not merely a theoretical subject, but a vital tool required to unlock the meaning behind their research data.

Audience and Prerequisites

This text is designed specifically for graduate students who possess an introductory background in statistics but find themselves facing complex research problems that require more robust analytical tools. Whether you are designing an experiment for an agricultural field trial, analyzing patient data in epidemiology, or optimizing processes in engineering, this book aims to bridge the gap between basic statistical literacy and the practical application of advanced methods.

Key Features

To support the transition from theory to practice, this book incorporates several distinct pedagogical features:

- **Data Science Technologies:** We leverage the modern `R` ecosystem, moving beyond basic command-line usage. This includes using Quarto for dynamic reporting, `ggplot2` for publication-quality visualization, and modern libraries for efficient data tabulation. These tools ensure that students are equipped with the current industry standards for data science.
- **Statistical Inference and Learning:** A core theme of the book is embedding concepts of statistical learning to distinguish between statistical significance (p-values) and practical significance (effect size and predictive power). We aim to train researchers to look beyond simple "pass/fail" metrics and evaluate the meaningful impact of their findings.
- **Simulation and Animation for Visualizing Probability:** Abstract concepts such as sampling distributions, p-values, and confidence intervals can be difficult to grasp without mathematical training. However, they can be quickly visualized with simulation and animation. We utilize animations to illustrate the probabilistic interpretation of these concepts, allowing readers to "see" the randomness and convergence that underlie statistical inference.
- **Real-World Datasets:** The messy reality of research cannot be captured by perfect, artificial data. We employ real datasets throughout the text to demonstrate the specific challenges and pitfalls encountered when applying statistical methods in practice, from handling outliers to addressing violations of assumptions.

Structure of the Book

The material is organized to guide the reader from foundational tools to complex experimental designs:

- **Chapters 1 and 2** lay the groundwork, introducing the philosophy of statistical research and providing a crash course in `R` for data analysis.
- **Chapters 3 and 4** cover the cornerstone of modeling: Linear Regression. We move from Simple Linear Regression to Multiple Linear Regression, allowing students to handle multi-variable relationships.
- **Chapter 5** delves into the diagnostics of these models, specifically understanding leverage and adjusting residuals in Ordinary Least Squares (OLS) to ensure model validity.
- **Chapter 6** introduces Logistic Regression, equipping researchers to handle categorical and binary outcomes.
- **Chapters 7 and 8** shift focus to Experimental Design. We explore Randomized Complete Block Design and Two-Factor Factorial Design, essential methodologies for controlling variability and understanding interaction effects in controlled experiments.

2 Data Science with R and Quarto

2.1 Basic R Objects and Operations

```r
## create a vector
x <- 1:10
x <- seq (30,3, by = -2)
a <- c(66.32, 69.87, 70.12, 90.37, 50.08, 61.20, 65.00, 57.65)
d <- a [1]
a [1] <- 85.34

mean (a)
```

```
[1] 68.70375
```

```r
ma <- mean (a)
## read a vector of numbers from a file
x <- scan("numbers.txt")
x2 <- scan("number2.txt")

## one can also read number withoug saving to a file
y <- scan(text = "7  8  9 10 11 12 13 13 14 17 17 45")

## create a matrix
A <- matrix (0, 4, 2)

A <- matrix (1:8, 4,2)

A
```

```
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
```

```r
D <- matrix (a, 4, 2, byrow=T)

D <- matrix(1:8, 2, 4)
D
```

```
     [,1] [,2] [,3] [,4]
[1,]    1    3    5    7
[2,]    2    4    6    8
```

```r
## create another matrix with all entry 0
B <- matrix (1:5000, 100, 50)

## assign a number to B
B[2,4] <- 45
B[1,]
```

```
 [1]    1  101  201  301  401  501  601  701  801  901 1001 1101 1201 1301 1401
[16] 1501 1601 1701 1801 1901 2001 2101 2201 2301 2401 2501 2601 2701 2801 2901
[31] 3001 3101 3201 3301 3401 3501 3601 3701 3801 3901 4001 4101 4201 4301 4401
[46] 4501 4601 4701 4801 4901
```

```r
B[,1]
```

```
  [1]   1   2   3   4   5   6   7   8   9  10  11  12  13  14  15  16  17  18
 [19]  19  20  21  22  23  24  25  26  27  28  29  30  31  32  33  34  35  36
 [37]  37  38  39  40  41  42  43  44  45  46  47  48  49  50  51  52  53  54
 [55]  55  56  57  58  59  60  61  62  63  64  65  66  67  68  69  70  71  72
 [73]  73  74  75  76  77  78  79  80  81  82  83  84  85  86  87  88  89  90
 [91]  91  92  93  94  95  96  97  98  99 100
```

```r
B[1,] <- 1:50


## create a list
E <- list (newa = a, newA = A)
## list the names of components
names (E)
```

```
[1] "newa" "newA"
```

```
## to look at the component of E
E$newA
```

```
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
```

```
E$newa <- 10:17

## create a dataframe
scores <- c (30, 45, 50)
names <- c("Peter", "John", "Alice")
stat245_scores <- data.frame (names, scores)
stat245_scores
```

```
  names scores
1 Peter     30
2  John     45
3 Alice     50
```

```
stat245_scores$names
```

```
[1] "Peter" "John"  "Alice"
```

```
stat245_scores$scores [1] <- 40
stat245_scores
```

```
  names scores
1 Peter     40
2  John     45
3 Alice     50
```

```
stat245_scores$perc <- stat245_scores$scores/50 * 100
stat245_scores
```

```
  names scores perc
1 Peter     40   80
2  John     45   90
3 Alice     50  100
```

```r
stat245_scores$adj <- stat245_scores$perc + 10
stat245_scores
```

```
  names scores perc adj
1 Peter     40   80  90
2  John     45   90 100
3 Alice     50  100 110
```

```r
################################################################################
```

2.2 Import a dataset into R environment and Simple Operation

```r
################################################################################

## import myagpop.csv into an R data frame called 'myagpop'
agpop <- read.csv("agpop.csv")

## Now, we can use the data:

## preview agpop
head (agpop)
```

```
                 county state acres92 acres87 acres82 farms92 farms87 farms82
1 ALEUTIAN ISLANDS AREA    AK  683533  726596  764514      26      27      28
2        ANCHORAGE AREA    AK   47146   59297  256709     217     245     223
3        FAIRBANKS AREA    AK  141338  154913  204568     168     175     170
4           JUNEAU AREA    AK     210     214     127       8       8      12
5  KENAI PENINSULA AREA    AK   50810   85712   98035      93     119     137
6        AUTAUGA COUNTY    AL  107259  116050  145044     322     388     453
  largef92 largef87 largef82 smallf92 smallf87 smallf82 region
1       14       16       20        6        4        1      W
2        9       10       11       41       52       38      W
3       25       28       21       12       18       25      W
4        0        0        0        5        4        8      W
5        9       18       17       12       18       19      W
6       25       32       32        8       19       17      S
```

```r
## look at the variable name
colnames (agpop)
```

```
 [1] "county"   "state"    "acres92"  "acres87"  "acres82"  "farms92"
 [7] "farms87"  "farms82"  "largef92" "largef87" "largef82" "smallf92"
[13] "smallf87" "smallf82" "region"
```

```
## find number of cols
ncol (agpop)
```

```
[1] 15
```

```
## find number of rows
nrow (agpop)
```

```
[1] 3078
```

```
## access a certain row
agpop [2, ]
```

```
          county state acres92 acres87 acres82 farms92 farms87 farms82 largef92
2 ANCHORAGE AREA    AK   47146   59297  256709     217     245     223        9
  largef87 largef82 smallf92 smallf87 smallf82 region
2       10       11       41       52       38      W
```

```
## access a certain column
agpop [1:20, "acres92"] ## equivalent to
```

```
 [1] 683533  47146 141338    210  50810 107259 167832 177189  48022 137426
[11] 144799  96427  73841 109555 121504  99466  67950  61426  68478  47200
```

```
agpop$acres92[1:20]
```

```
 [1] 683533  47146 141338    210  50810 107259 167832 177189  48022 137426
[11] 144799  96427  73841 109555 121504  99466  67950  61426  68478  47200
```

```
agpop$largef92[1:20]
```

```
 [1] 14  9 25  0  9 25 24 40  6  9 29 18  4 22 24  8  9 13  4  5
```

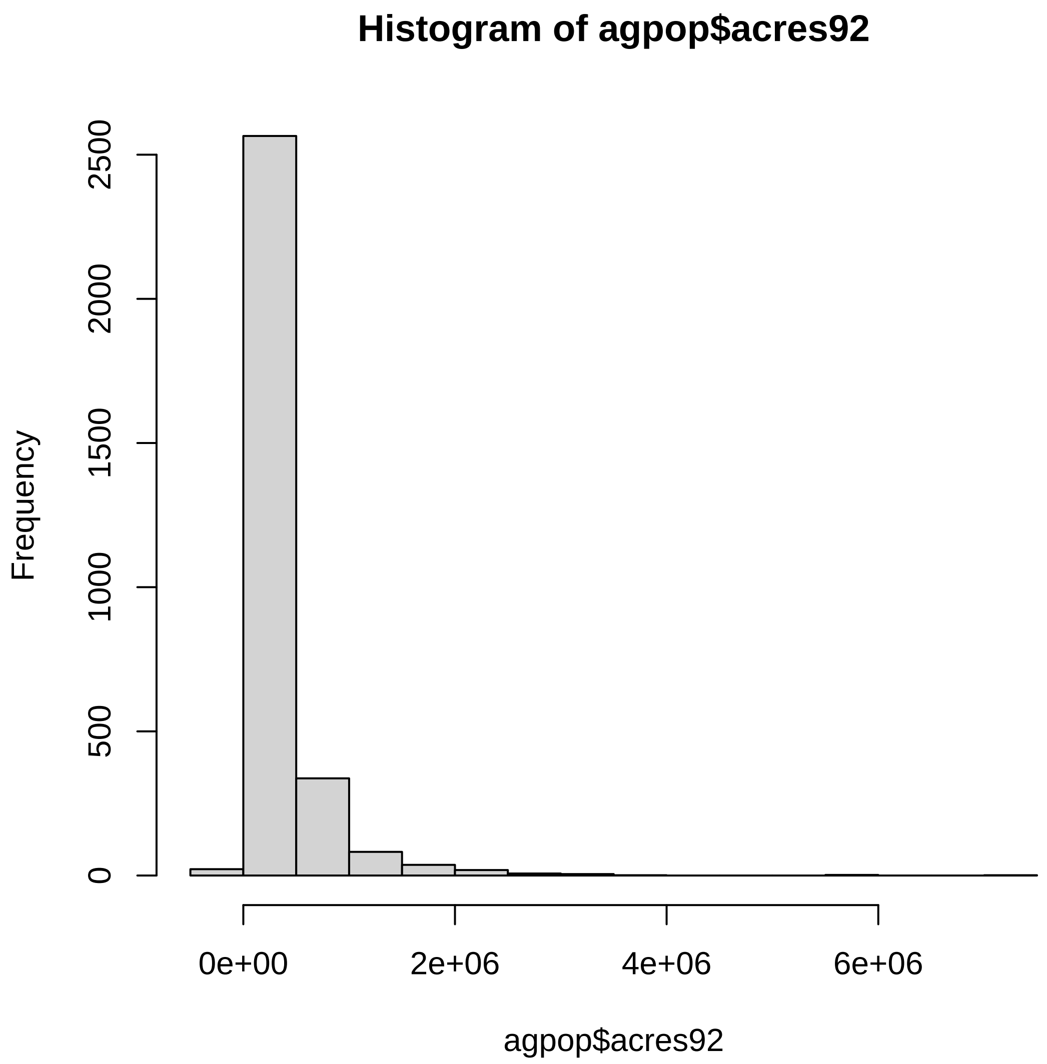
```
## find mean of acres92
mean (agpop $acres92)
```

```
[1] 306677
```

```r
## find sd of acres92
sd (agpop $acres92)
```

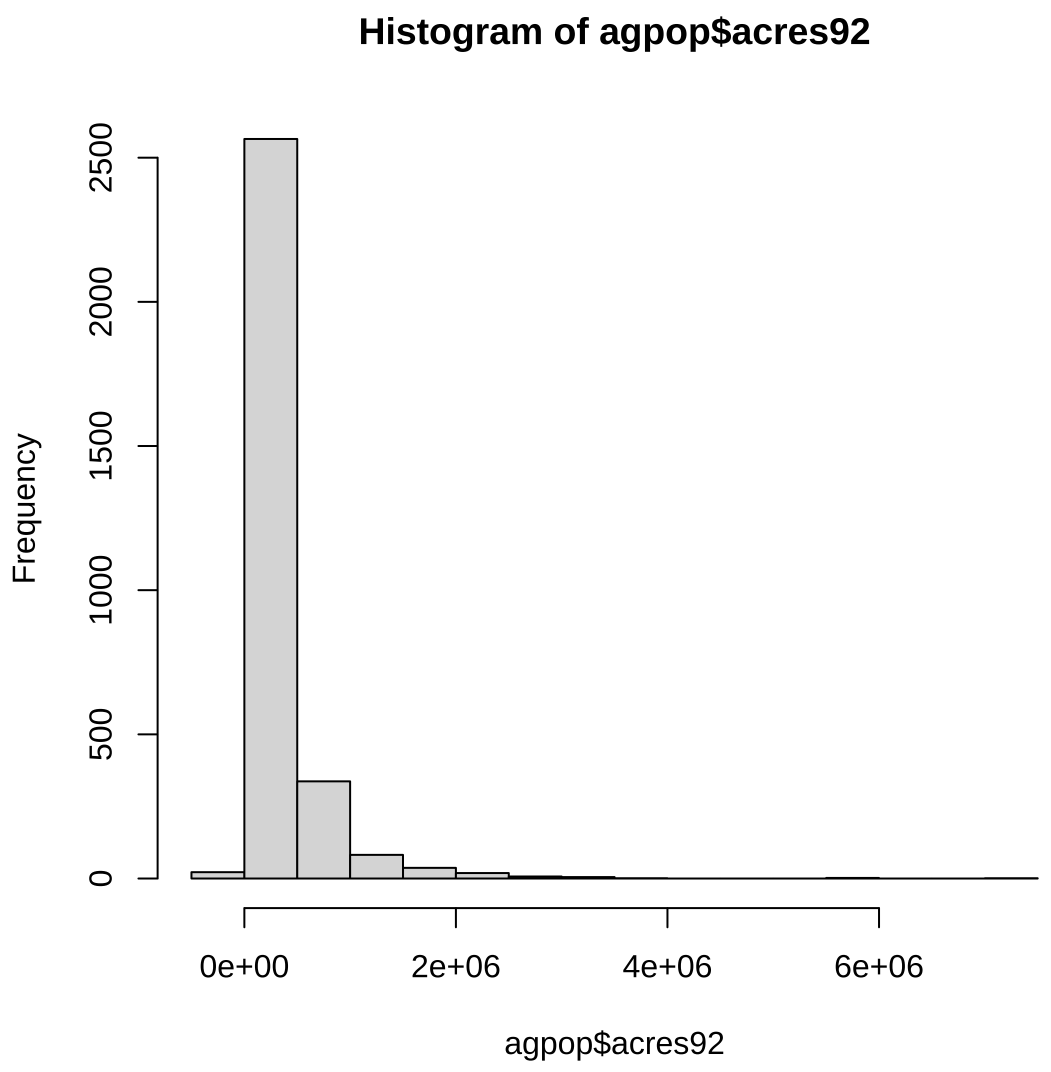
```
[1] 424686.7
```

```r
agpop_AK  <- agpop [agpop$state == "AK", ]

agpop_AK <- subset (agpop, state == "AK")

agpop_W <- subset (agpop, region == "W")

agpop_largefarm <- subset (agpop, largef92 > 10)


hist (agpop$acres92)
```

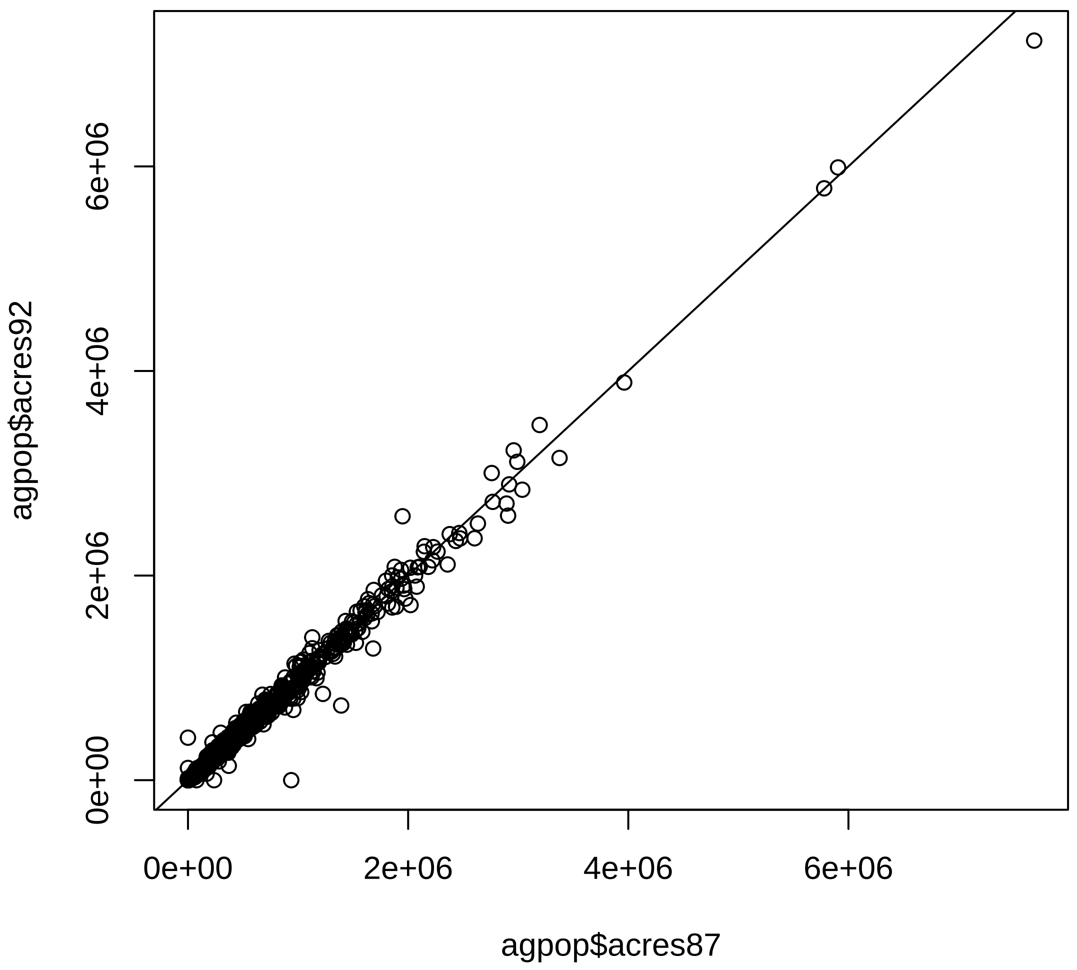


Produce Plots

```
#pdf ("hist_acres92.pdf") ## use this command and dev.off to save the output to a file
hist (agpop$acres92)
```



```
#dev.off()

#jpeg ("agpop_acres_87v92.jpg")

plot (agpop$acres87, agpop$acres92)
abline (a = 0, b = 1)
```



```
#dev.off()## this is used to close the jpeg file
```

2.3 Create your own function

```
### data is a matrix or data.frame
means_col <- function (data)
{
    n <- ncol (data)
    cmeans <- rep (NA, n)
    for (j in 1:n)
    {
        cmeans[j] <- mean (data[,j])

    }
    cmeans
```

```r
}

### apply function
means_col (agpop[, 3:13])
```

```
 [1] 306676.97141 313016.37817 320193.69298    625.50357    678.28428
 [6]    728.06238     56.17674     54.86160     52.62248     54.09227
[11]     59.53769
```

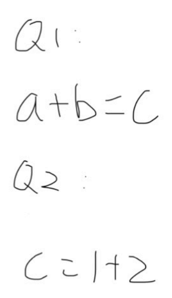
```r
### R built-in function
colMeans (agpop[, 3:13])
```

```
     acres92      acres87      acres82      farms92      farms87      farms82 
306676.97141 313016.37817 320193.69298    625.50357    678.28428    728.06238 
    largef92     largef87     largef82     smallf92     smallf87 
    56.17674     54.86160     52.62248     54.09227     59.53769 
```

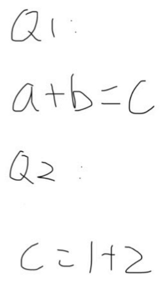
2.4 Include Images Saved in An External File

Using the following R code to include your images saved in an external file.

```r
knitr::include_graphics("handwriting.png")
```



You can hide the above R code by setting "echo=FALSE" for the r chunk. For example, I will include the image once again as follows:



Q1:

$a+b=c$

Q2:

$c=1+2$

Figure 2.1: This is a figure inserted from the file called “handwriting.png”

3 Simple Linear Regression

A Simulation Illustration with R

```r
require("knitr")
knitr::opts_chunk$set(
  comment = "#",
  fig.width = 6,
  fig.height = 6,
  cache = TRUE
)
set.seed(47)

options(sim_rebuild=FALSE)
```

3.1 Overview of Simple Linear Regression

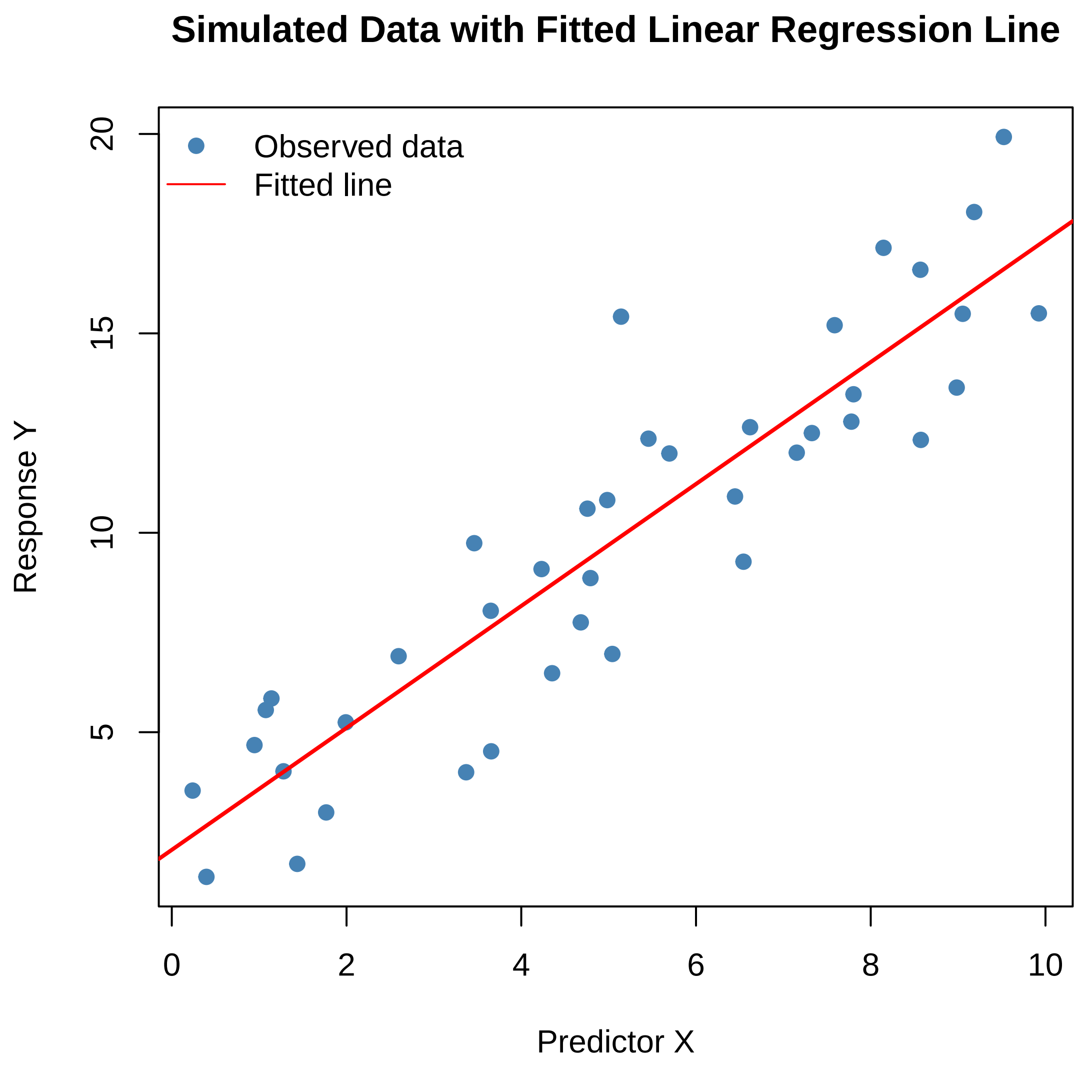
To make the simple linear regression model concrete, let's first visualize a simulated dataset that follows

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma^2).$$

Here, β_0 is the intercept, β_1 is the slope, and ε_i represents random noise.

```r
set.seed(2025)
n <- 40
beta0 <- 2; beta1 <- 1.5; sigma <- 2
x <- runif(n, 0, 10)
y <- beta0 + beta1 * x + rnorm(n, 0, sigma)
dat <- data.frame(x, y)

fit <- lm(y ~ x, data = dat)

plot(x, y, pch = 19, col = "steelblue",
     xlab = "Predictor X", ylab = "Response Y",
     main = "Simulated Data with Fitted Linear Regression Line")
```

```r
abline(fit, col = "red", lwd = 2)
legend("topleft", legend = c("Observed data", "Fitted line"),
       pch = c(19, NA), lty = c(NA, 1), col = c("steelblue", "red"), bty = "n")
```



The scatterplot shows data points scattered around a line — the red line is the fitted regression model.

3.1.1 Least Squares Estimation

Goal: Find $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize

$$\text{SSE} = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2.$$

Solutions:

$$\widehat{\beta}_1 = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\sum_i (x_i - \bar{x})^2} = \frac{S_{xy}}{S_{xx}}, \qquad \widehat{\beta}_0 = \bar{y} - \widehat{\beta}_1\,\bar{x}.$$

Here

$$S_{xy} = \sum_i (x_i - \bar{x})(y_i - \bar{y}), \qquad S_{xx} = \sum_i (x_i - \bar{x})^2.$$

Shortcut (computational) formulas:

$$S_{xy} = \sum_i x_i y_i - n\,\bar{x}\,\bar{y}, \qquad S_{xx} = \sum_i x_i^2 - n\,\bar{x}^2.$$

Interpretation:
- $\widehat{\beta}_1$ measures the estimated change in Y for each unit increase in X.
- $\widehat{\beta}_0$ represents the fitted value of Y when $X = 0$.

3.1.2 Residual and Sum of Squares Definitions

Let $\widehat{y}_i = \widehat{\beta}_0 + \widehat{\beta}_1 x_i$ and $e_i = y_i - \widehat{y}_i$.

Symbol	Definition	Computing Formula (in terms of S_{xx}, S_{xy}, etc.)
SST	Total Sum of Squares	$\sum_i (y_i - \bar{y})^2 = S_{yy} = \sum_i y_i^2 - n\,\bar{y}^2$
SSR	Regression Sum of Squares	$\sum_i (\widehat{y}_i - \bar{y})^2 = \widehat{\beta}_1^2 S_{xx} = \frac{S_{xy}^2}{S_{xx}}$
SSE	Error (Residual) Sum of Squares	$\sum_i (y_i - \widehat{y}_i)^2 = S_{yy} - \frac{S_{xy}^2}{S_{xx}}$

Identity:

$$\text{SST} = \text{SSR} + \text{SSE}.$$

Here,

$$S_{xx} = \sum_i (x_i - \bar{x})^2 = \sum_i x_i^2 - n\bar{x}^2, \qquad S_{yy} = \sum_i (y_i - \bar{y})^2 = \sum_i y_i^2 - n\bar{y}^2, \qquad S_{xy} = \sum_i (x_i - \bar{x})(y_i - \bar{y}) = \sum_i x_i y_i - n$$

3.1.3 Coefficient of Determination (R^2)

Measures the proportion of total variation in Y explained by X:

$$R^2 = \frac{\text{SSR}}{\text{SST}} = 1 - \frac{\text{SSE}}{\text{SST}}.$$

Interpretation:

- $R^2 = 1$ means perfect linear fit;
- $R^2 = 0$ means the model explains none of the variation.

3.1.4 F-test for Overall Significance

Tests whether X is linearly related to Y.

Hypotheses:

$$H_0 : \beta_1 = 0 \quad \text{vs.} \quad H_A : \beta_1 \neq 0.$$

Test Statistic:

$$F = \frac{\text{MSR}}{\text{MSE}} = \frac{\text{SSR}/1}{\text{SSE}/(n-2)} \sim F_{1,n-2} \quad (H_0).$$

p-value approach for observe F^{obs}:

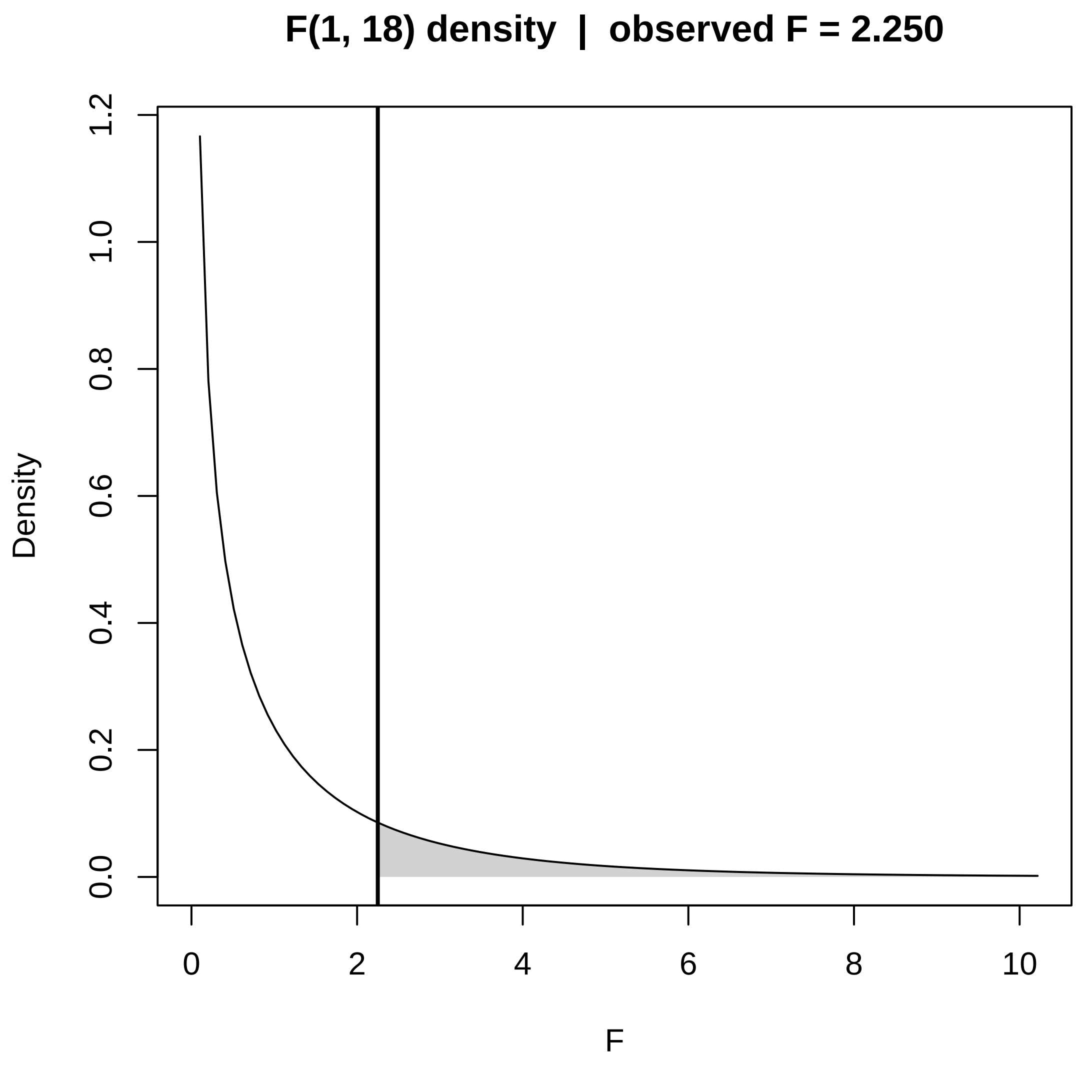
Given the observed statistic F^{obs} with $(1,\, n-2)$ df,

$$p-\text{value} \;=\; \Pr\big(F_{1,\,n-2} \geq F^{\text{obs}}\big) \;=\; \text{pf}\big(F^{\text{obs}},\, 1,\, n-2,\, \text{lower.tail} = \text{FALSE}\big).$$

```r
## -- Inputs (provide these from your analysis context) -------------------------
## n   <- ...    # sample size
## SSR <- ...    # regression sum of squares
## SSE <- ...    # error sum of squares
n   <- 20
SSR <- 5
SSE <- 40





df1  <- 1
df2  <- n - 2
Fobs <- (SSR/df1) / (SSE/df2)         # observed F
pval <- pf(Fobs, df1 = df1, df2 = df2, lower.tail = FALSE)
pval
```

```
[1] 0.1509505
```

```r
## -- Plot F density and shade the p-value tail (with proper annotations) -------
xmax <- max(qf(0.995, df1, df2), Fobs * 1.2)  # extra space for labels
peak <- max(df(seq(0, xmax, length.out = 500), df1, df2))

## Density curve
curve(df(x, df1, df2), from = 0, to = xmax,
      xlab = "F", ylab = "Density",
      main = sprintf("F(%d, %d) density  |  observed F = %.3f", df1, df2, Fobs))

## Shade right tail (p-value region)
xs <- seq(Fobs, xmax, length.out = 300)
ys <- df(xs, df1, df2)
polygon(c(Fobs, xs, xmax), c(0, ys, 0),
        col = rgb(0, 0, 0, 0.18), border = NA)

## Vertical line at Fobs (optional visual aid)
abline(v = Fobs, lwd = 2)

## ---- Annotation for F^obs pointing to the x-axis value (Fobs, 0) -------------
x_txt_F <- Fobs + 0.06 * xmax
y_txt_F <- 0.45 * peak
arrows(x0 = x_txt_F, y0 = y_txt_F, x1 = Fobs, y1 = 0,
       length = 0.08, lwd = 1.5)
text(x_txt_F, y_txt_F,
     labels = bquote(F^{obs} == .(format(Fobs, digits = 3))),
     pos = 4)

## ---- Annotation for p-value pointing into the shaded tail --------------------
x_tip_p <- (Fobs + xmax) / 1.7
y_tip_p <- df(x_tip_p, df1, df2)
x_txt_p <- Fobs + 0.08 * xmax
y_txt_p <- 0.80 * peak
arrows(x0 = x_txt_p, y0 = y_txt_p, x1 = x_tip_p, y1 = y_tip_p,
       length = 0.08, lwd = 1.5)
text(x_txt_p, y_txt_p,
     labels = bquote(p == .(format(pval, digits = 4, scientific = TRUE))),
     pos = 4)
```



3.1.5 t-test for the Slope β_1

Equivalent to the F-test in simple regression since $t^2 = F$.

Formula:

$$t = \frac{\hat{\beta}_1}{\mathrm{SE}(\hat{\beta}_1)}, \qquad \mathrm{SE}(\hat{\beta}_1) = \sqrt{\frac{\hat{\sigma}^2}{\sum_i (x_i - \bar{x})^2}}, \qquad \hat{\sigma}^2 = \frac{\mathrm{SSE}}{n-2}.$$

Distribution:

$$t \sim t_{n-2} \quad (H_0 : \beta_1 = 0).$$

3.1.6 Prediction for a New Case x_0

Predicted mean response:

$$\hat{y}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0.$$

95% Confidence interval for mean response:

$$\hat{y}(x_0) \pm t_{1-\alpha/2,,n-2}, \hat{\sigma}, \sqrt{\frac{1}{n} + \frac{(x_0 - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}}.$$

95% Prediction interval for a new observation:

$$\hat{y}(x_0) \pm t_{1-\alpha/2,,n-2}, \hat{\sigma}, \sqrt{1 + \frac{1}{n} + \frac{(x_0 - \bar{x})^2}{\sum_i (x_i - \bar{x})^2}}.$$

Summary Cheat Sheet

Concept	Key Formula
Model	$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$
LS Estimates	$\hat{\beta}_1 = S_{xy}/S_{xx}, \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$
Decomposition	$\text{SST} = \text{SSR} + \text{SSE}$
R^2	$R^2 = 1 - \text{SSE}/\text{SST}$
F-test	$F = (\text{SSR}/1)/(\text{SSE}/(n-2))$
t-test	$t = \hat{\beta}_1 / \text{SE}(\hat{\beta}_1)$
Prediction	$\hat{y}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$

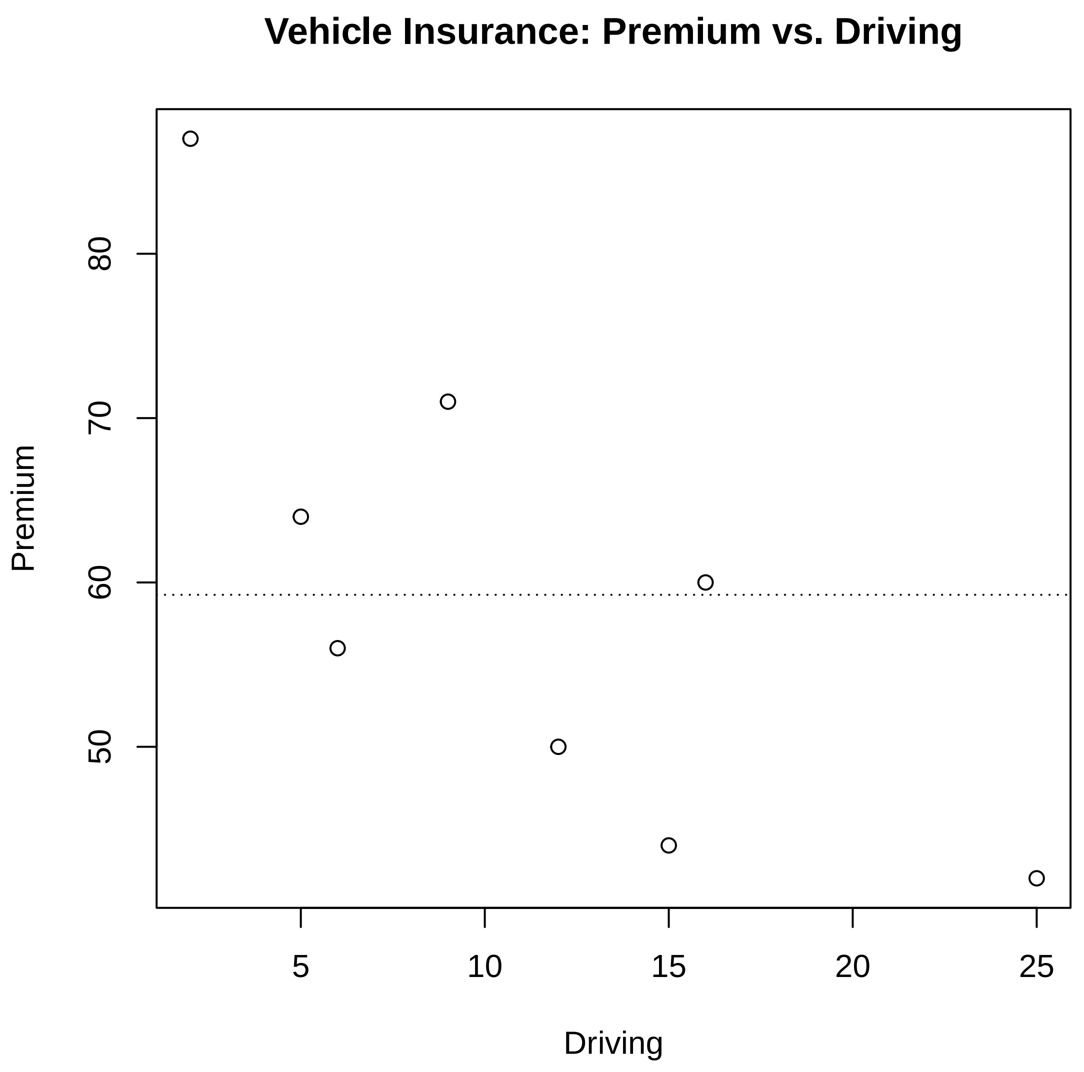
3.2 Example 1: Vehicle Insurance Premium (warm-up)

We examine premiums y vs. driving amount x. The scatterplot hints at a **downward** trend.

3.2.1 Input data

```r
issu <- data.frame(
  driving = c(5, 2, 12, 9, 15, 6, 25, 16),
  premium = c(64, 87, 50, 71, 44, 56, 42, 60)
)
```

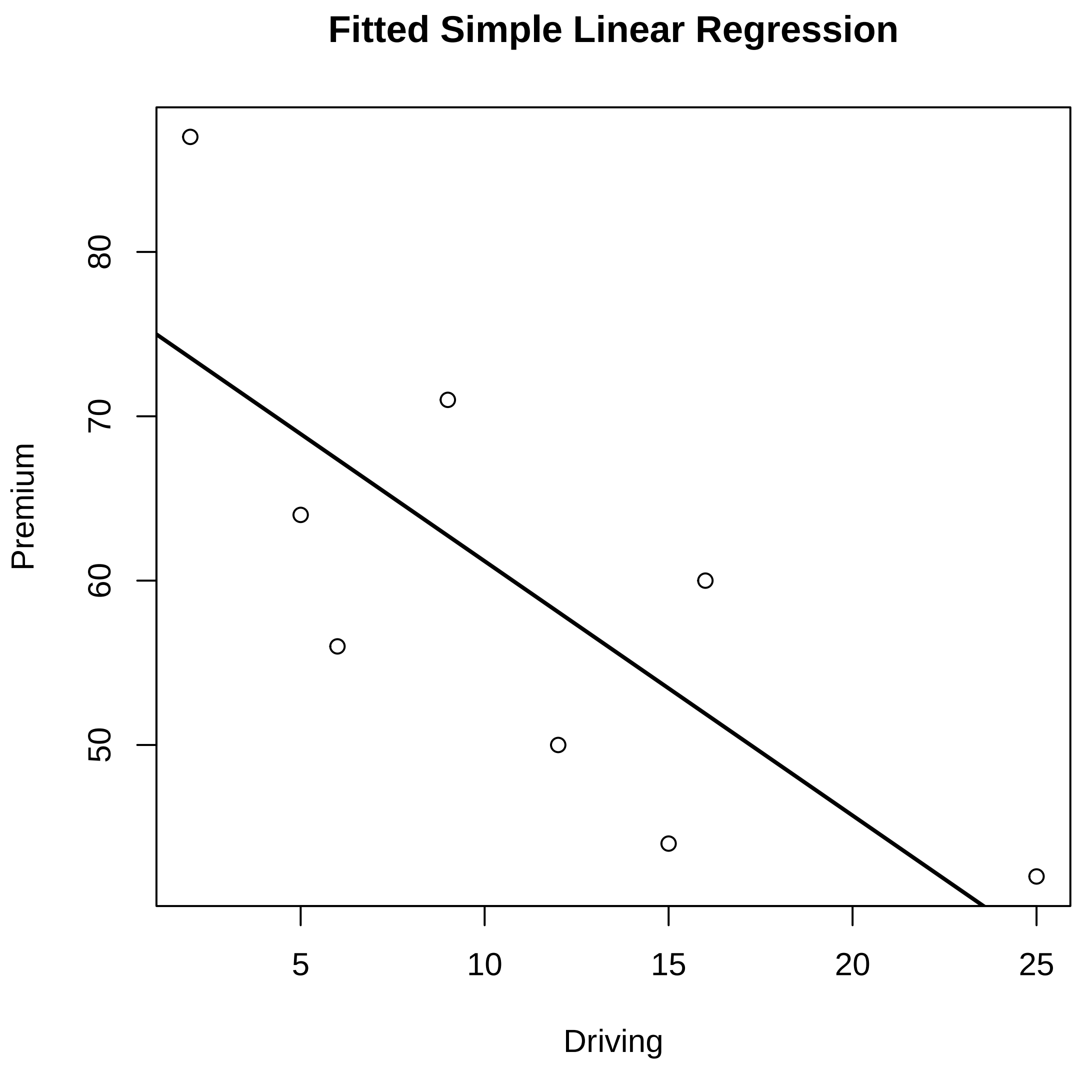
```r
y <- issu$premium
x <- issu$driving
xbar <- mean(x); ybar <- mean(y); n <- length(y)

plot(x, y, xlab = "Driving", ylab = "Premium",
     main = "Vehicle Insurance: Premium vs. Driving")
abline(h = ybar, lty = 3)
```



Narrative. The horizontal line at $\bar{y}$ represents the intercept-only model. Any fitted line that tilts away from this must earn its keep by reducing residual variation enough to offset the loss of one degree of freedom.

3.2.2 Estimating regression coefficients

```r
fit.issu <- lm(y ~ x)
plot(x, y, xlab = "Driving", ylab = "Premium",
     main = "Fitted Simple Linear Regression")
abline(fit.issu, lwd = 2)
```



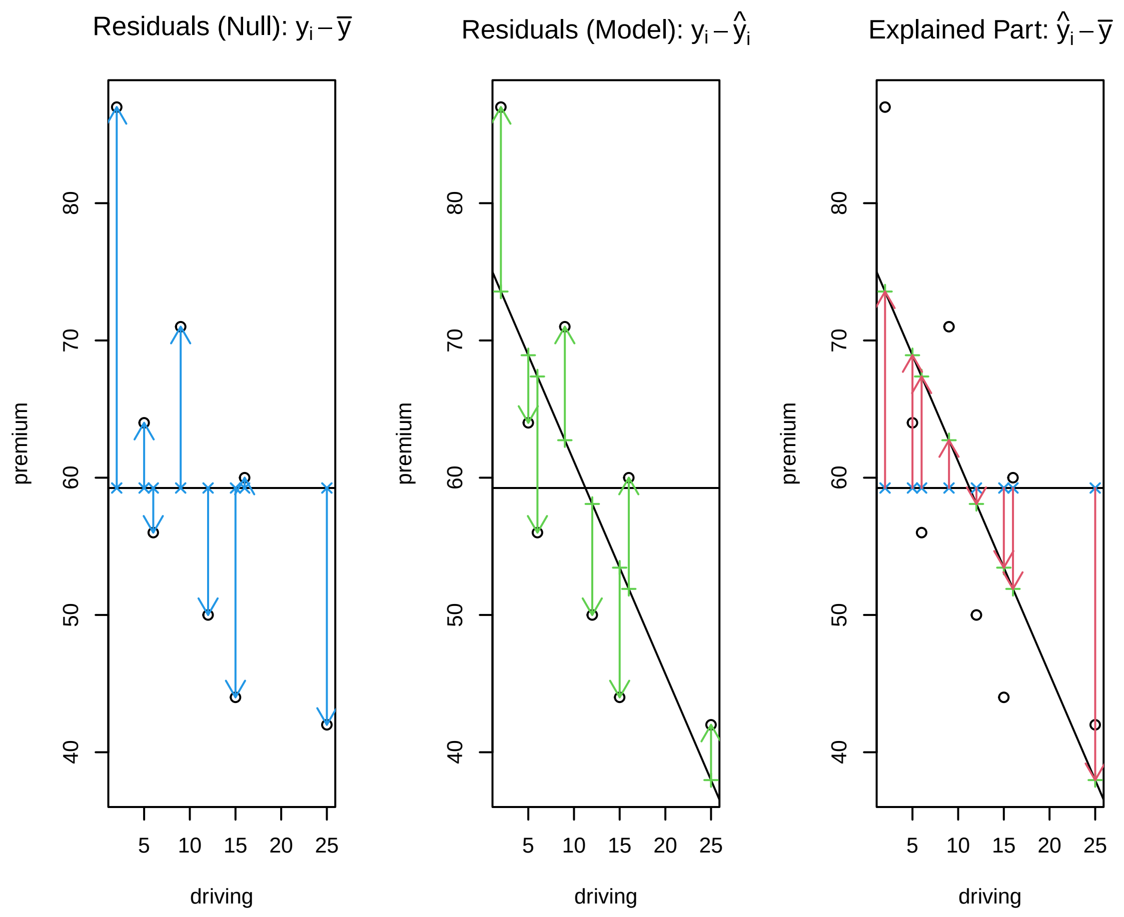
The slope estimate $\hat{\beta}_1$ captures the **marginal change in premium per unit of driving** (units of y per unit of x). Inference on β_1 tells us whether the pattern rises above noise.

3.2.3 Residuals and fitted values (geometry picture)

Let $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i$ and $\tilde{y}_i = \bar{y}$. Residuals are $e_i = y_i - \hat{y}_i$ (model) and $y_i - \bar{y}$ (null). Visualizing all three clarifies the ANOVA identity.

```r
beta0 <- coef(fit.issu)[1]
beta1 <- coef(fit.issu)[2]
fitted1 <- beta0 + beta1 * x
fitted0 <- rep(ybar, n)
residual1 <- y - fitted1
residual0 <- y - fitted0

data.frame(y, fitted0, residual0, fitted1, residual1,
           diff.fitted = fitted1 - fitted0)
```

```
   y fitted0 residual0  fitted1  residual1 diff.fitted
1 64   59.25      4.75 68.92243  -4.922425    9.672425
2 87   59.25     27.75 73.56519  13.434811   14.315189
3 50   59.25     -9.25 58.08931  -8.089309   -1.160691
4 71   59.25     11.75 62.73207   8.267927    3.482073
5 44   59.25    -15.25 53.44654  -9.446545   -5.803455
6 56   59.25     -3.25 67.37484 -11.374837    8.124837
7 42   59.25    -17.25 37.97066   4.029335  -21.279335
8 60   59.25      0.75 51.89896   8.101043   -7.351043
```



3.2.4 SST, SSR, SSE and their meanings

- SST $= \sum(y_i - \bar{y})^2$ quantifies **total** variability around the mean.
- SSR $= \sum(\hat{y}_i - \bar{y})^2$ is the part **explained by** x.
- SSE $= \sum(y_i - \hat{y}_i)^2$ is the **leftover** (unexplained) variability.

```
SST <- sum((y - fitted0)^2); SST
```

```
[1] 1557.5
```

```
SSE <- sum((y - fitted1)^2); SSE
```

```
[1] 639.0065
```

```
SSR <- SST - SSE; SSR
```

```
[1] 918.4935
```

Direct check: $\text{SSR} = \sum(\hat{y}_i - \bar{y})^2$.

```r
sum((fitted1 - fitted0)^2)
```

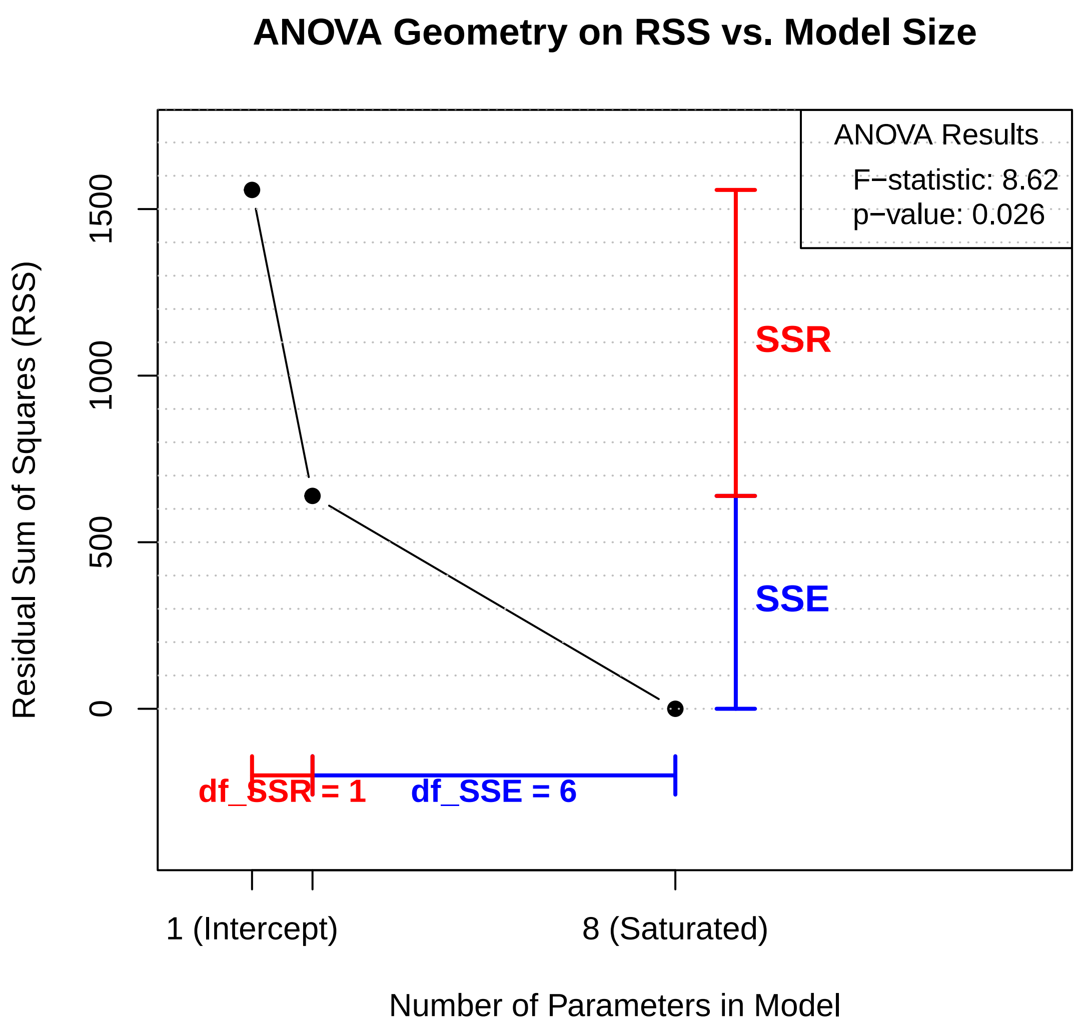
```
[1] 918.4935
```

3.2.5 Visual ANOVA on an RSS plot

We place the **residual sum of squares** against model dimension to show the trade-off between fit and df.

```r
## Recompute cleanly
SST <- sum((y - mean(y))^2)
SSE <- sum(resid(fit.issu)^2)
SSR <- SST - SSE
df_SSR <- 1
df_SSE <- n - 2

par(mar = c(6, 4, 4, 2) + 0.1)
plot(c(1, 2, n), c(SST, SSE, 0), type = "b", pch = 19,
     xlab = "Number of Parameters in Model",
     ylab = "Residual Sum of Squares (RSS)",
     main = "ANOVA Geometry on RSS vs. Model Size",
     xlim = c(0, 14), ylim = c(-400, SST * 1.1), xaxt = "n")
axis(1, at = c(1, 2, n), labels = c("1 (Intercept)", "2 (+Slope)", paste(n, "(Saturated)")))
abline(h = seq(0, 2000, by = 100), lty = 3, col = "grey")

par(xpd = TRUE)
arrows(9, 0, 9, SSE, col = "blue", code = 3, angle = 90, length = 0.1, lwd = 2)
text(9, SSE/2, "SSE", col = "blue", pos = 4, font = 2, cex = 1.2)

arrows(9, SSE, 9, SST, col = "red", code = 3, angle = 90, length = 0.1, lwd = 2)
text(9, (SST + SSE)/2, "SSR", col = "red", pos = 4, font = 2, cex = 1.2)

arrows(2, -200, n, -200, col = "blue", code = 3, angle = 90, length = 0.1, lwd = 2)
text((2 + n)/2, -250, paste("df_SSE =", df_SSE), col = "blue", font = 2)

arrows(1, -200, 2, -200, col = "red", code = 3, angle = 90, length = 0.1, lwd = 2)
text(1.5, -250, paste("df_SSR =", df_SSR), col = "red", font = 2)
par(xpd = FALSE)

f_value <- (SSR/df_SSR) / (SSE/df_SSE)
```

```r
p_value <- pf(f_value, df1 = df_SSR, df2 = df_SSE, lower.tail = FALSE)
legend("topright",
       legend = c(sprintf("F-statistic: %.2f", f_value),
                  sprintf("p-value: %.3f", p_value)),
       title = "ANOVA Results", bty = "o", cex = 0.9)
```



3.2.6 R^2, F and a compact ANOVA table

```r
R2 <- SSR / SST; R2
```

```
[1] 0.5897229
```

```r
f  <- (SSR/1) / (SSE/(n-2)); f
```

```
[1] 8.624264
```

```r
pvf <- pf(f, df1 = 1, df2 = n-2, lower.tail = FALSE); pvf
```

```
[1] 0.0260588
```

```r
Ftable <- data.frame(
  Source = c("Regression", "Error"),
  df     = c(1, n - 2),
  SS     = c(SSR, SSE),
  MS     = c(SSR/1, SSE/(n-2)),
  F      = c(f, NA),
  pvalue = c(pvf, NA),
  R2part = c(SSR, SSE) / SST
)
Ftable
```

```
      Source df       SS       MS        F    pvalue    R2part
1 Regression  1 918.4935 918.4935 8.624264 0.0260588 0.5897229
2      Error  6 639.0065 106.5011       NA        NA 0.4102771
```

A call to `anova()` reproduces the same test:

```r
anova(fit.issu)
```

```
Analysis of Variance Table

Response: y
          Df Sum Sq Mean Sq F value  Pr(>F)
x          1 918.49  918.49  8.6243 0.02606 *
Residuals  6 639.01  106.50
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

3.2.7 Sampling distributions via animation

Under $H_0 : \beta_1 = 0$, F follows $F_{1,n-2}$. Under H_A, the distribution shifts right (noncentral F).

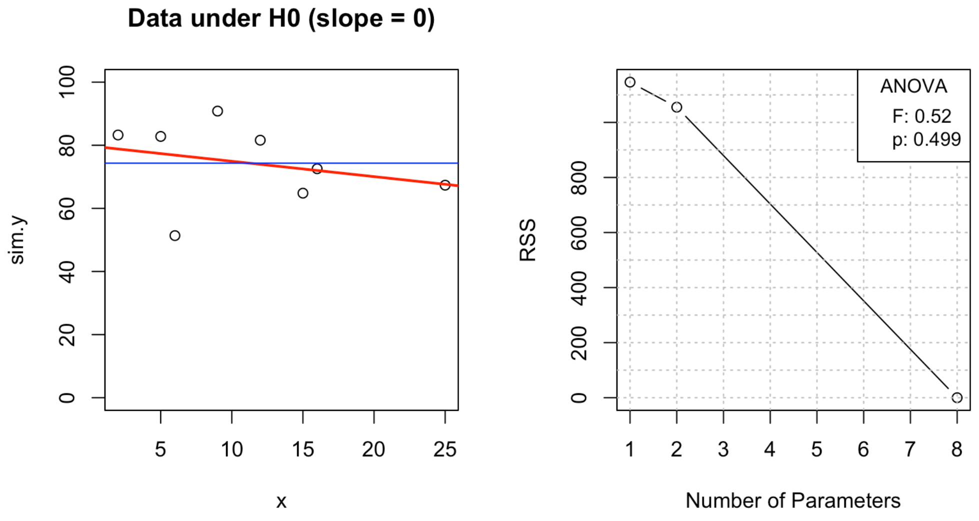


Figure 3.1: Simulation under H0: animated GIF (HTML) and static PNG (PDF).

3.2.7.1 Null world (H_0 true)

3.2.7.2 Alternative world (H_1 true)

3.3 Example 2: Oxygen Purity Data

We model oxygen purity y as a function of hydrocarbon level x and report both **mean response** and **prediction** uncertainty.

3.3.1 Data

```
x <- c(0.99, 1.02, 1.15, 1.29, 1.46, 1.36, 0.87, 1.23, 1.55, 1.40, 1.19,
       1.15, 0.98, 1.01, 1.11, 1.20, 1.26, 1.32, 1.43, 0.95)
y <- c(90.01, 89.05, 91.43, 93.74, 96.73, 94.45, 87.59, 91.77, 99.42, 93.65,
       93.54, 92.52, 90.56, 89.54, 89.85, 90.39, 93.25, 93.41, 94.98, 87.33)
n <- length(x); n
```

```
[1] 20
```

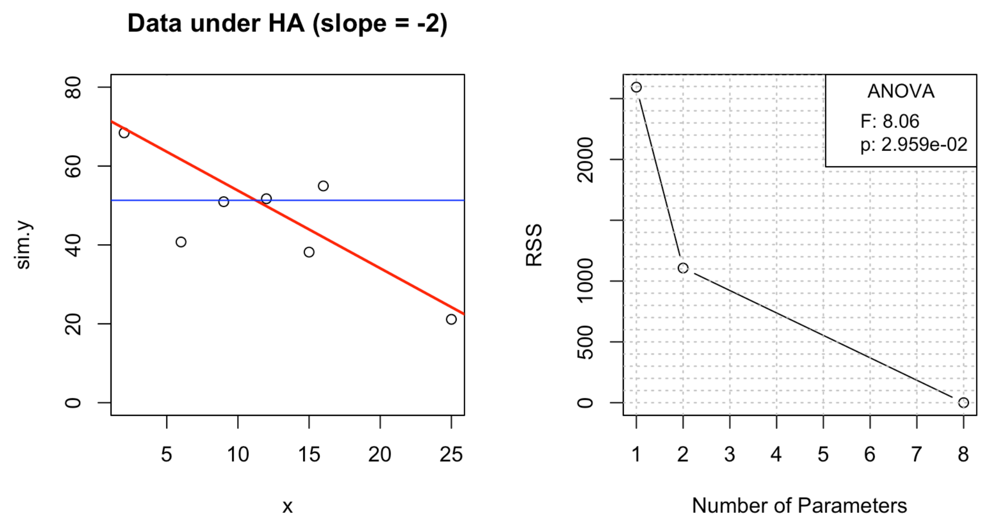


Figure 3.2: Simulation under HA (slope = -2): animated GIF for HTML, static PNG for PDF.

```r
purity.data <- data.frame(x = x, y = y)
head(purity.data)
```

```
     x     y
1 0.99 90.01
2 1.02 89.05
3 1.15 91.43
4 1.29 93.74
5 1.46 96.73
6 1.36 94.45
```

3.3.2 Fit and quick summary

```r
fit <- lm(y ~ x, data = purity.data)
summary(fit)
```

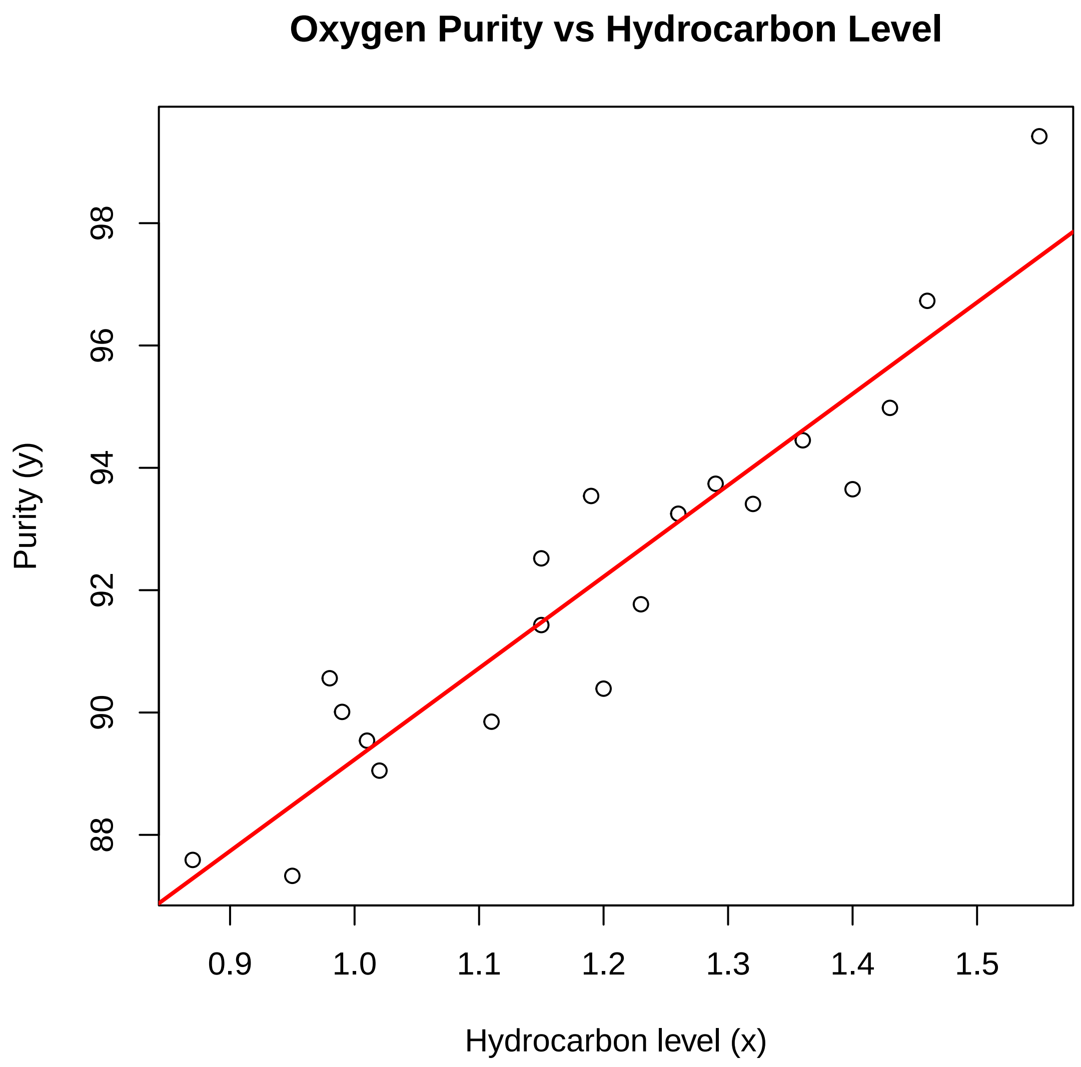
```
Call:
lm(formula = y ~ x, data = purity.data)

Residuals:
     Min       1Q   Median       3Q      Max
```

```
-1.83029 -0.73334  0.04497  0.69969  1.96809

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)   74.283      1.593   46.62  < 2e-16 ***
x             14.947      1.317   11.35 1.23e-09 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.087 on 18 degrees of freedom
Multiple R-squared:  0.8774,    Adjusted R-squared:  0.8706 
F-statistic: 128.9 on 1 and 18 DF,  p-value: 1.227e-09
```

Interpretation. The slope's sign gives the direction of association; its t test (or F with 1 df) assesses evidence for a trend. Look at $\hat{\sigma}$ for noise scale and R^2 for variance explained.

3.3.3 Scatter with fitted line

```r
plot(purity.data$x, purity.data$y,
     xlab = "Hydrocarbon level (x)", ylab = "Purity (y)",
     main = "Oxygen Purity vs Hydrocarbon Level")
abline(fit, col = "red", lwd = 2)
```



3.3.4 Coefficient CIs and ANOVA

```r
confint(fit, level = 0.95)
```

```
                2.5 %   97.5 %
(Intercept) 70.93555 77.63108
x           12.18107 17.71389
```

```r
anova(fit)
```

```
Analysis of Variance Table
```

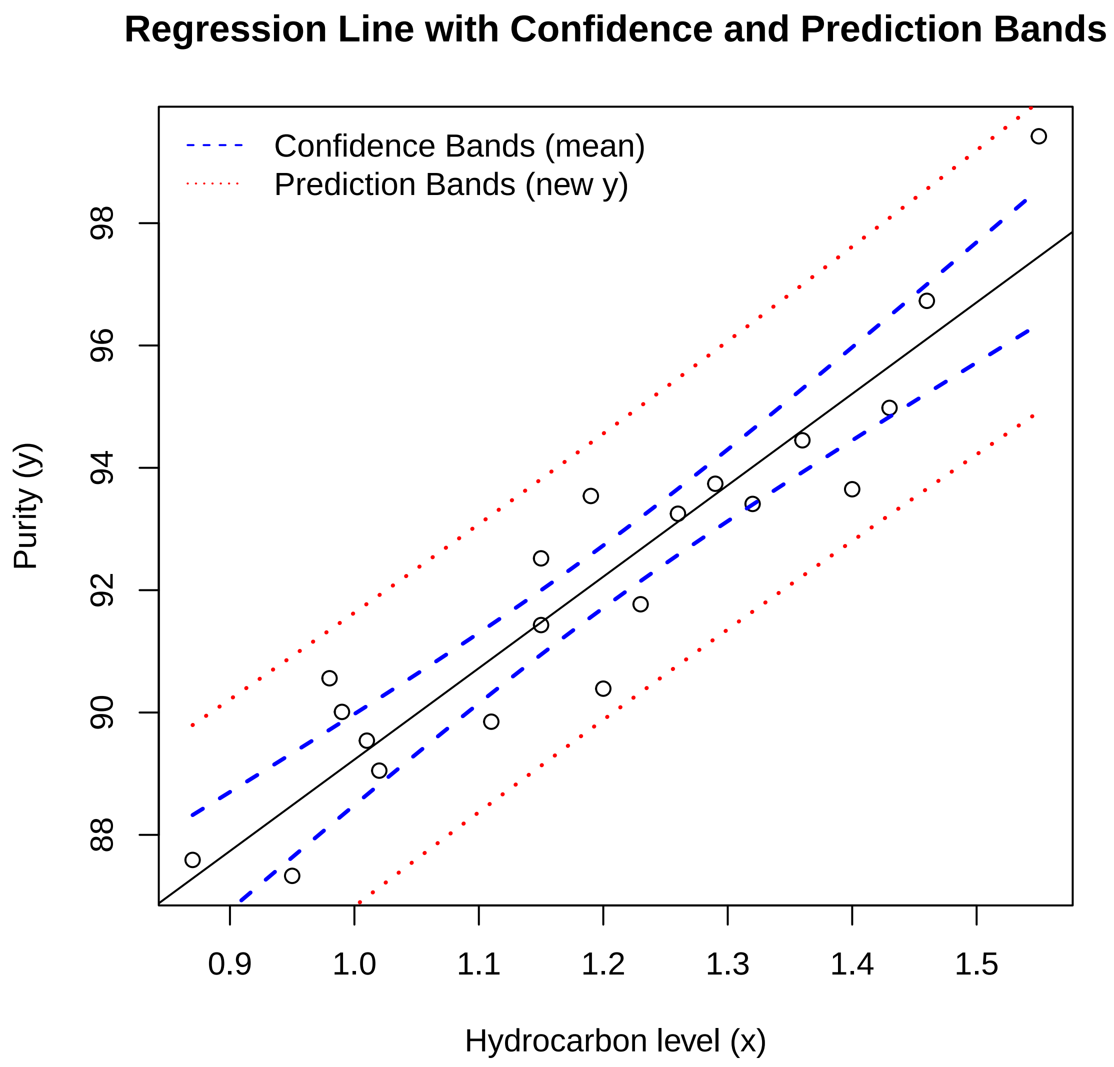
```
Response: y
          Df Sum Sq Mean Sq F value    Pr(>F)
x          1 152.13 152.127  128.86 1.227e-09 ***
Residuals 18  21.25   1.181
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

3.3.5 Mean-response and prediction bands

The **mean-response CI** narrows near $\bar{x}$ and widens at the extremes; the **prediction band** is wider by the irreducible noise term.

```
x0 <- seq(min(purity.data$x), max(purity.data$x), length = 50)
newdata <- data.frame(x = x0)

est.mean <- predict(fit, newdata = newdata, interval = "confidence", level = 0.95)
pred.new <- predict(fit, newdata = newdata, interval = "prediction", level = 0.95)
```

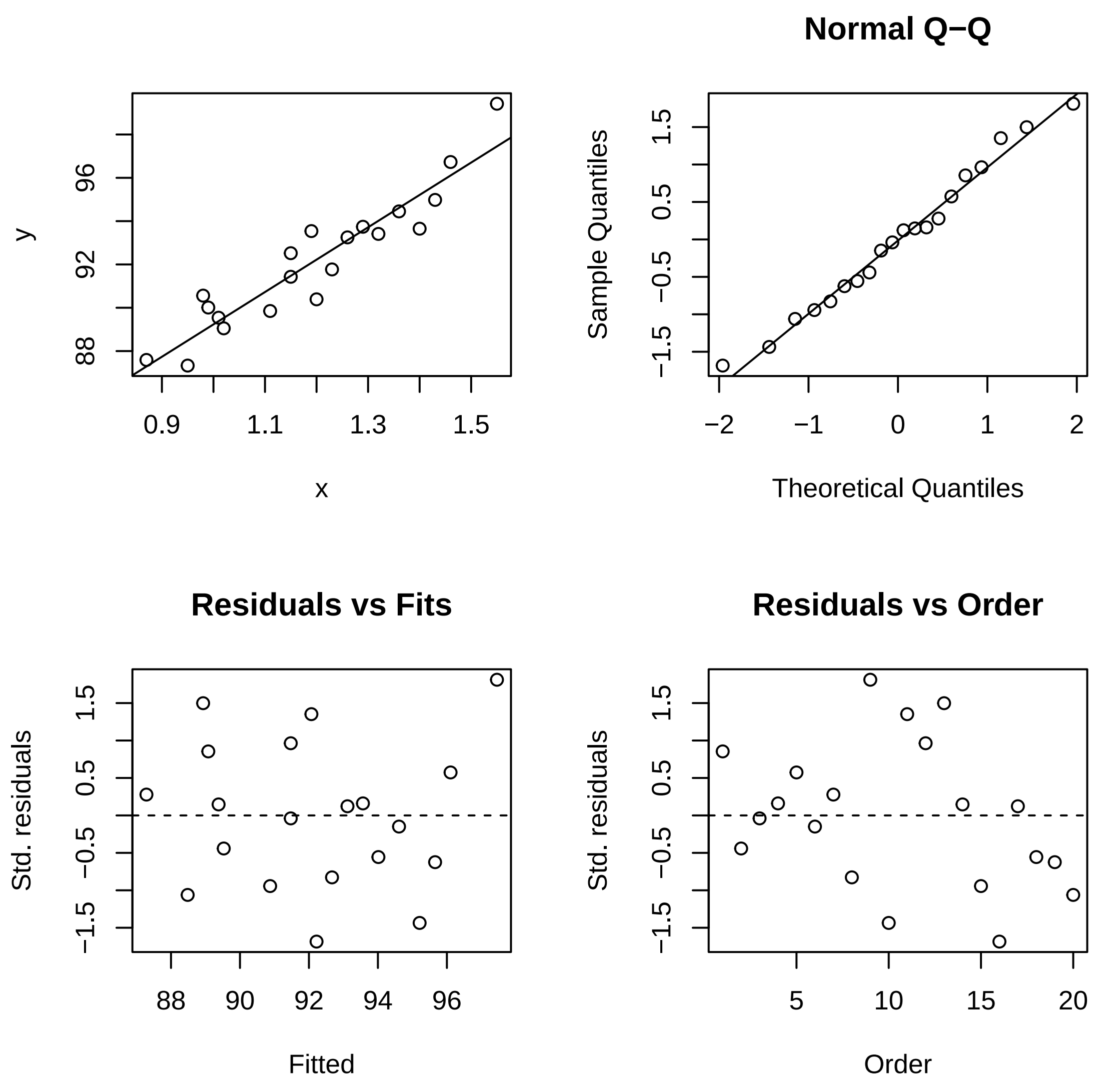
```
plot(purity.data$x, purity.data$y,
     xlab = "Hydrocarbon level (x)", ylab = "Purity (y)",
     main = "Regression Line with Confidence and Prediction Bands")
abline(fit)
matlines(x0, est.mean[, 2:3], col = "blue", lty = 2, lwd = 2)
matlines(x0, pred.new[, 2:3], col = "red",  lty = 3, lwd = 2)
legend("topleft", c("Confidence Bands (mean)", "Prediction Bands (new y)"),
       col = c("blue", "red"), lty = 2:3, bty = "n")
```



3.3.6 Residual diagnostics (assumptions check)

We look for **no pattern** in residuals vs. fits and **approximate straightness** in the Q–Q plot.

```r
pred <- fitted.values(fit)
e <- resid(fit)
d <- e / summary(fit)$sigma

par(mfrow = c(2,2))
plot(purity.data$x, purity.data$y, xlab = "x", ylab = "y"); abline(fit)
qqnorm(d, main = "Normal Q-Q"); qqline(d)
plot(pred, d, xlab = "Fitted", ylab = "Std. residuals", main = "Residuals vs Fits"); abline(h
plot(1:n, d, xlab = "Order", ylab = "Std. residuals", main = "Residuals vs Order"); abline(h =
```



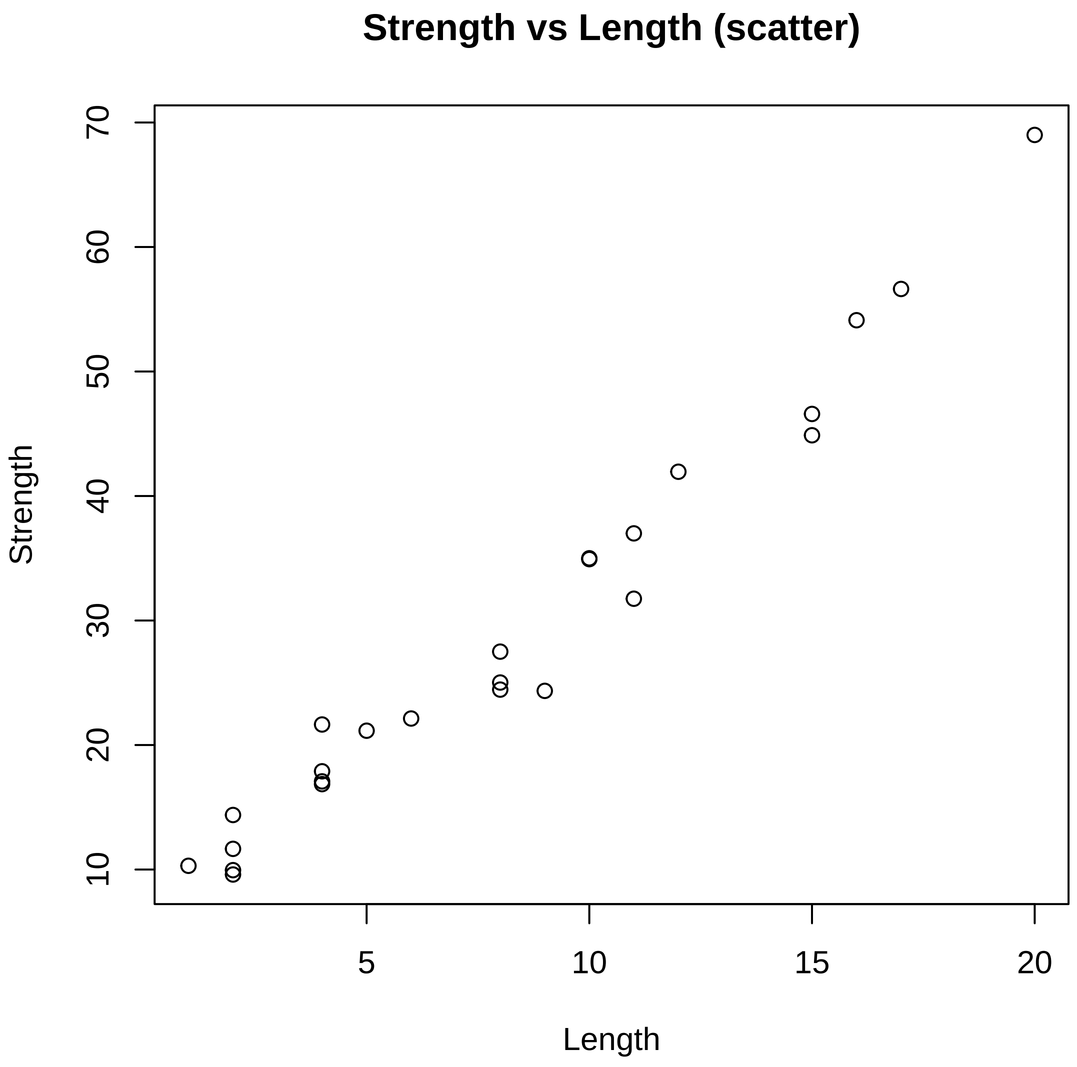
```
par(mfrow = c(1,1))
```

3.4 Correlation analysis (for comparison, not causation)

Correlation summarizes linear association without fitting a line or making model assumptions.

3.4.1 Data and scatter

```r
strength <- c(9.95,24.45,31.75,35.00,25.02,16.86,14.38,9.60,24.35,
              27.50,17.08,37.00,41.95,11.66,21.65,17.89,69.00,10.30,
              34.93,46.59,44.88,54.12,56.63,22.13,21.15)
length <- c(2,8,11,10,8,4,2,2,9,8,4,11,12,2,4,4,20,1,10,
            15,15,16,17,6,5)
plot(length, strength, xlab = "Length", ylab = "Strength",
     main = "Strength vs Length (scatter)")
```



3.4.2 Pearson correlation and test

```r
cor(strength, length)
```

```
[1] 0.9818118
```

```r
cor.test(strength, length)
```

```

	Pearson's product-moment correlation

data:  strength and length
t = 24.801, df = 23, p-value < 2.2e-16
alternative hypothesis: true correlation is not equal to 0
95 percent confidence interval:
 0.9585414 0.9920735
sample estimates:
      cor 
0.9818118 
```

Note. A large $|r|$ and small p indicate linear association; regression further quantifies the slope and supports prediction, with diagnostics to check assumptions.

3.5 What to report (checklist)

- Estimated line $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$ with units.
- t/F test for slope, p-value and CI for β_1.
- R^2 and $\hat{\sigma}$ (RMSE) for fit quality.
- Mean-response and prediction intervals at substantively relevant x_0.
- Residual diagnostics and any remedies (transformations, robust methods) if needed.

4 Multiple Linear Regression

4.1 An Example: Wire Bond Strength Dataset

4.1.1 Loading Data and Visualization

Note: You must change the file paths in the `read.csv()` functions below to match the location of the files on your computer (for example `C:\\Users\\<YourUsername>\\Documents` on Windows).

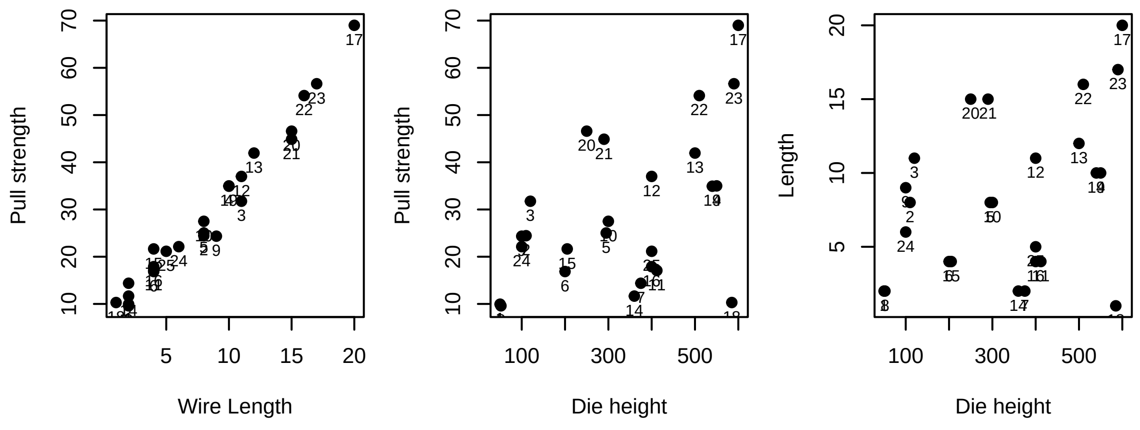
```
## Read data. Change the path as necessary.
## Example: bond.data <- read.csv("wire-bond.csv")
bond.data <- read.csv("wire-bond.csv")

## This will now be automatically rendered as a paged table
bond.data
```

```
   strength length height
1      9.95      2     50
2     24.45      8    110
3     31.75     11    120
4     35.00     10    550
5     25.02      8    295
6     16.86      4    200
7     14.38      2    375
8      9.60      2     52
9     24.35      9    100
10    27.50      8    300
11    17.08      4    412
12    37.00     11    400
13    41.95     12    500
14    11.66      2    360
15    21.65      4    205
16    17.89      4    400
17    69.00     20    600
18    10.30      1    585
19    34.93     10    540
20    46.59     15    250
21    44.88     15    290
```

```
22     54.12      16     510
23     56.63      17     590
24     22.13       6     100
25     21.15       5     400
```

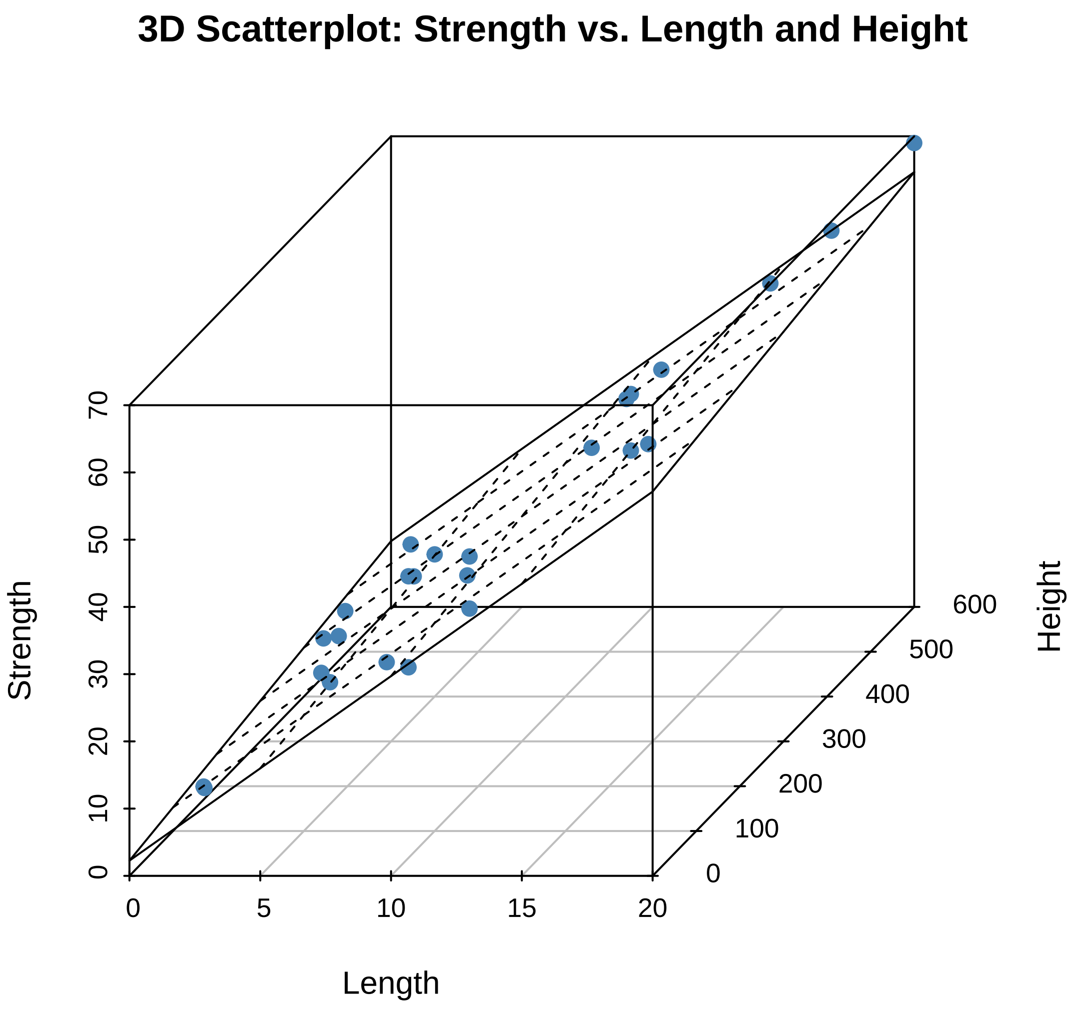
2D Visualization

```r
par(mfrow = c(1, 3), mar = c(5, 4, 2, 1))

## 1) length vs strength
i1 <- which(!is.na(bond.data$length) & !is.na(bond.data$strength))
plot(bond.data$length[i1], bond.data$strength[i1],
     xlab = "Wire Length", ylab = "Pull strength", pch = 19)
text(bond.data$length[i1], bond.data$strength[i1],
     labels = i1, pos = 1, offset = 0.4, cex = 0.75)

## 2) height vs strength
i2 <- which(!is.na(bond.data$height) & !is.na(bond.data$strength))
plot(bond.data$height[i2], bond.data$strength[i2],
     xlab = "Die height", ylab = "Pull strength", pch = 19)
text(bond.data$height[i2], bond.data$strength[i2],
     labels = i2, pos = 1, offset = 0.4, cex = 0.75)

## 3) height vs length
i3 <- which(!is.na(bond.data$height) & !is.na(bond.data$length))
plot(bond.data$height[i3], bond.data$length[i3],
     xlab = "Die height", ylab = "Length", pch = 19)
text(bond.data$height[i3], bond.data$length[i3],
     labels = i3, pos = 1, offset = 0.4, cex = 0.75)
```



3D Visualize

```
library(scatterplot3d)

par(mfrow = c(1,1))
s3d <- with(bond.data, scatterplot3d(
  x = length,
  y = height,
  z = strength,
  pch = 19,
  color = "steelblue",
  main = "3D Scatterplot: Strength vs. Length and Height",
  xlab = "Length",
  ylab = "Height",
  zlab = "Strength",
  angle = 60
))

fit <- lm(strength ~ length + height, data = bond.data)
s3d$plane3d(fit, lty.box = "solid")
```



4.1.2 Model Fitting and Summary

We fit a multiple linear regression model with `strength` as the response variable and `length` and `height` as predictors.

```r
fit <- lm(strength ~ length + height, data = bond.data)
summary(fit)
```

```

Call:
lm(formula = strength ~ length + height, data = bond.data)

Residuals:
   Min     1Q Median     3Q    Max 
-3.865 -1.542 -0.362  1.196  5.841 
```

```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.263791   1.060066   2.136 0.044099 *
length      2.744270   0.093524  29.343  < 2e-16 ***
height      0.012528   0.002798   4.477 0.000188 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.288 on 22 degrees of freedom
Multiple R-squared:  0.9811,    Adjusted R-squared:  0.9794
F-statistic: 572.2 on 2 and 22 DF,  p-value: < 2.2e-16
```

The summary provides the ANOVA F-test for overall significance, R^2, adjusted R^2, and t-tests for individual coefficients.

4.1.3 Confidence Intervals and Model Components

```r
## Confidence intervals
confint(fit)
```

```
                  2.5 %     97.5 %
(Intercept) 0.065348613 4.46223426
length      2.550313061 2.93822623
height      0.006724246 0.01833138
```

```r
## Fitted values and residuals
pred <- fitted.values(fit)
e <- resid(fit)
data.frame(y = bond.data$strength, y.hat = pred, e = e)
```

```
       y     y.hat           e
1   9.95  8.378721  1.57127871
2  24.45 25.596008 -1.14600783
3  31.75 33.954095 -2.20409488
4  35.00 36.596784 -1.59678413
5  25.02 27.913653 -2.89365294
6  16.86 15.746432  1.11356772
7  14.38 12.450260  1.92974001
8   9.60  8.403777  1.19622309
9  24.35 28.214999 -3.86499936
10 27.50 27.976292 -0.47629200
```

```
11 17.08 18.402328 -1.32232830
12 37.00 37.461882 -0.46188206
13 41.95 41.458933  0.49106715
14 11.66 12.262343 -0.60234282
15 21.65 15.809071  5.84092866
16 17.89 18.251995 -0.36199456
17 69.00 64.665871  4.33412887
18 10.30 12.336831 -2.03683074
19 34.93 36.471506 -1.54150602
20 46.59 46.559789  0.03021107
21 44.88 47.060901 -2.18090138
22 54.12 52.561290  1.55871047
23 56.63 56.307784  0.32221591
24 22.13 19.982190  2.14780957
25 21.15 20.996264  0.15373580
```

```
## Covariance matrix and standard errors
cov.mat <- vcov(fit)
cov.mat
```

```
             (Intercept)        length        height
(Intercept)  1.123740429 -3.921612e-02 -1.781991e-03
length      -0.039216122  8.746709e-03 -9.903775e-05
height      -0.001781991 -9.903775e-05  7.831149e-06
```

```
data.frame(std.error = sqrt(diag(cov.mat)))
```

```
              std.error
(Intercept) 1.060066238
length      0.093523844
height      0.002798419
```

4.2 RSS-based Inference: F-test, and adjusted R^2

The General Linear Model

The general linear model is:

$$y = X\beta + \epsilon$$

- y: $n \times 1$ vector of responses
- X: $n \times p$ design matrix (first column often ones)
- β: $p \times 1$ parameter vector, where $p = k + 1$
- ϵ: $n \times 1$ error vector

4.2.1 RSS-Based Quantities

4.2.1.1 RSS-Based Quantities

Source	Sum of Squares	R^2	df	Mean Squares	F	SS_{adj}	$\hat{\sigma}^2$	R^2_{adj}
$x^\top\beta$	$\text{SSR} = \sum_{i=1}^{n}(\hat{y}_i - \bar{y})^2$	$\frac{\text{SSR}}{\text{SST}}$	k	$\text{MSR} = \frac{\text{SSR}}{k}$	$\frac{\text{MSR}}{\text{MSE}}$	SSR_{adj}	$\hat{\sigma}^2_{x^\top\beta} = \frac{\text{SSR}_{\text{adj}}}{n-1}$	$\frac{\text{SSR}_{\text{adj}}}{\text{SST}} = 1 - \frac{\text{MSE}}{\text{MST}}$
ϵ	$\text{SSE} = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$	—	$n-p$	$\text{MSE} = \frac{\text{SSE}}{n-p}$	—	SSE	$\hat{\sigma}^2_\epsilon = \text{MSE}$	—
y	$\text{SST} = \sum_{i=1}^{n}(y_i - \bar{y})^2$	—	$n-1$	$\text{MST} = \frac{\text{SST}}{n-1}$	—	SST	$\hat{\sigma}^2_y = \text{MST}$	—

Interpretation of the $\hat{\sigma}^2$ Column

The $\hat{\sigma}^2$ column highlights how each sum of squares corresponds to an estimated variance.
This view makes the adjusted coefficient of determination clear:

$$R^2_{\text{adj}} = 1 - \frac{\hat{\sigma}^2_\epsilon}{\hat{\sigma}^2_y} = \frac{\hat{\sigma}^2_{x^\top\beta}}{\hat{\sigma}^2_y}.$$

Hence, the adjusted R^2 simply expresses the **proportion of total estimated variance** attributable to the fitted model $X\beta$ rather than the residual noise ϵ.

4.2.2 Remarks

4.2.2.1 Fundamental Identities

$$\text{SST} = \text{SSR} + \text{SSE},$$
$$\text{MST} = \text{MSE} + \frac{\text{SSR}_{\text{adj}}}{n-1}.$$

where

$$\text{SSR}_{\text{adj}} = (n-1)MST - (n-p+k)\text{MSE} = \text{SST} - \text{SSE} - k\,\text{MSE} = \text{SSR} - k\,\text{MSE}.$$

4.2.2.2 Difference of $\hat{\sigma}^2$ and Mean Squares

The quantity $\hat{\sigma}^2$ represents the **estimated variance** associated with each component of the model. MSE and MST are the estimated variances of the ϵ and y itself. However, the MSR, although called **Mean Square for Regression (MSR)** is *NOT* an estimate of the variance or sample variance of $x^\top \beta$. The name of "mean" here is used to indicate a different thing. Its name "Mean Square" reflects that it is also an estimate estimate of noise variance σ^2 under $H_0\colon\ \beta = 0$:

$$E[\text{MSR} \mid H_0] = \sigma^2, \qquad E[\text{MSR} \mid H_1] > \sigma^2.$$

Hence the F-statistic

$$F = \frac{\text{MSR}}{\text{MSE}}$$

is approximately equal to 1 subject to the variability as characterized with F-distribution with degree freedoms of k and $n-p$. This test is to test whether any regression coefficients are not equal to 0.

4.2.2.3 $\hat{\sigma}^2_{x^\top\beta} = \frac{\text{SSR}_{\text{adj}}}{n-1}$

$\hat{\sigma}^2_{x^\top\beta}$ is an unbiased estimator of the variance of linear signal when x is a regarded as a random variable. This can be seen from the following equations:

$$E[\text{SSR}] = k\,\sigma^2 + \beta^\top X^\top (I - J/n)\,X\,\beta, \qquad E[\text{MSE}] = \sigma^2.$$

Hence,

$$\begin{aligned} E[\text{SSR}_{\text{adj}}] &= E[\text{SSR}] - k\,E[\text{MSE}] \\ &= \beta^\top X^\top (I - J/n)\,X\,\beta \\ &= \sum_{i=1}^{n} (\mu_i - \bar{\mu})^2, \end{aligned}$$

where

$$\begin{aligned} \mu_i &= x_i^\top \beta \\ \bar{\mu} &= \tfrac{1}{n} \sum_{i=1}^{n} \mu_i \end{aligned}$$

For fixed X, $\text{SSR}_{\text{adj}}/(n-1)$ equals the **sample variance** of the true means $\{\mu_i\}$ over the observed design points. If the rows of X are independently sampled with covariance matrix Σ_X (the random-X model), then

$$\mathbb{E}_X\left[\frac{\text{SSR}_{\text{adj}}}{n-1}\right] = \beta^\top \Sigma_X \beta = \text{Var}(x^\top \beta),$$

4.2.2.4 Connection to Rao-Blackwell Formula

The decomposition of $\hat{\sigma}^2$ is consistent with the **Rao–Blackwell formula** for total variance:

$$\text{Var}(y) = \text{Var}\big(E[y \mid x]\big) + E\big(\text{Var}[y \mid x]\big).$$

Here,

- $\text{Var}\big(E[y \mid x]\big)$ corresponds to the **explained variation** due to the regression component $x^\top \beta$, and
- $E\big(\text{Var}[y \mid x]\big)$ corresponds to the **residual variation** due to ϵ.

4.2.3 A Simulation Study to Understand the Distributions of RSS

Data Generating Model

For $n = 30$ and $p_{max} = 20$, simulate with either $H_0 : \beta = \mathbf{0}$ or H_1 where only $\beta_1 \neq 0$; $\epsilon_i \sim N(0, 1)$.

Sequence of Fitted Models

Model Name	# of Predictors (k)	# of Parameters (p)	R Formula
Model 0	0	1	`y ~ 1`
Model 1	2	3	`y ~ x_1 + x_2`
…	…	…	…
Final Model	20	21	`y ~ x_1 + ... + x_20`

4.2.3.1 When H_0 is true

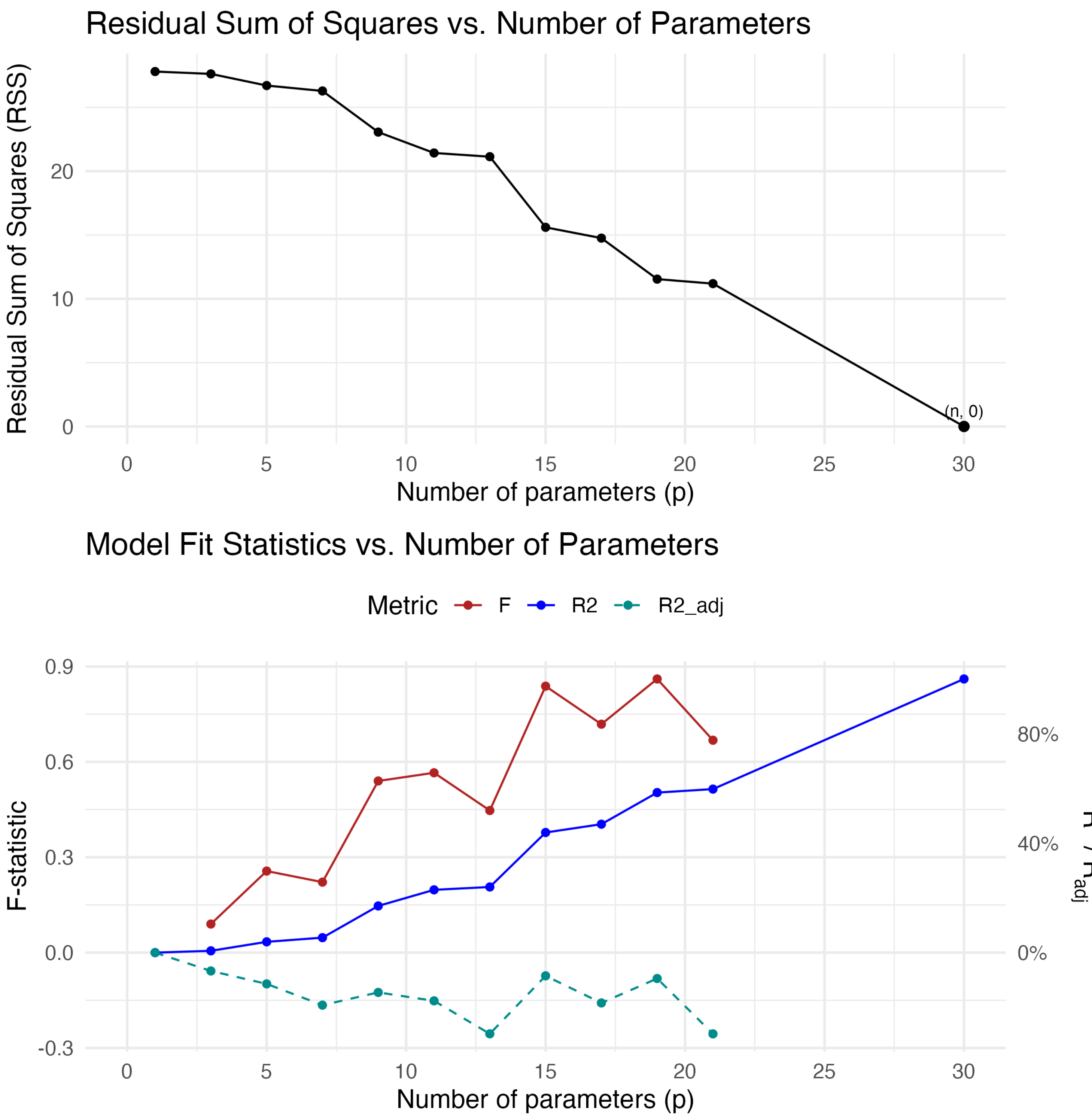


Figure 4.1: When H_0 is true: MP4 animation (HTML) or a representative static frame (PDF).

4.2.3.2 When H_1 is true

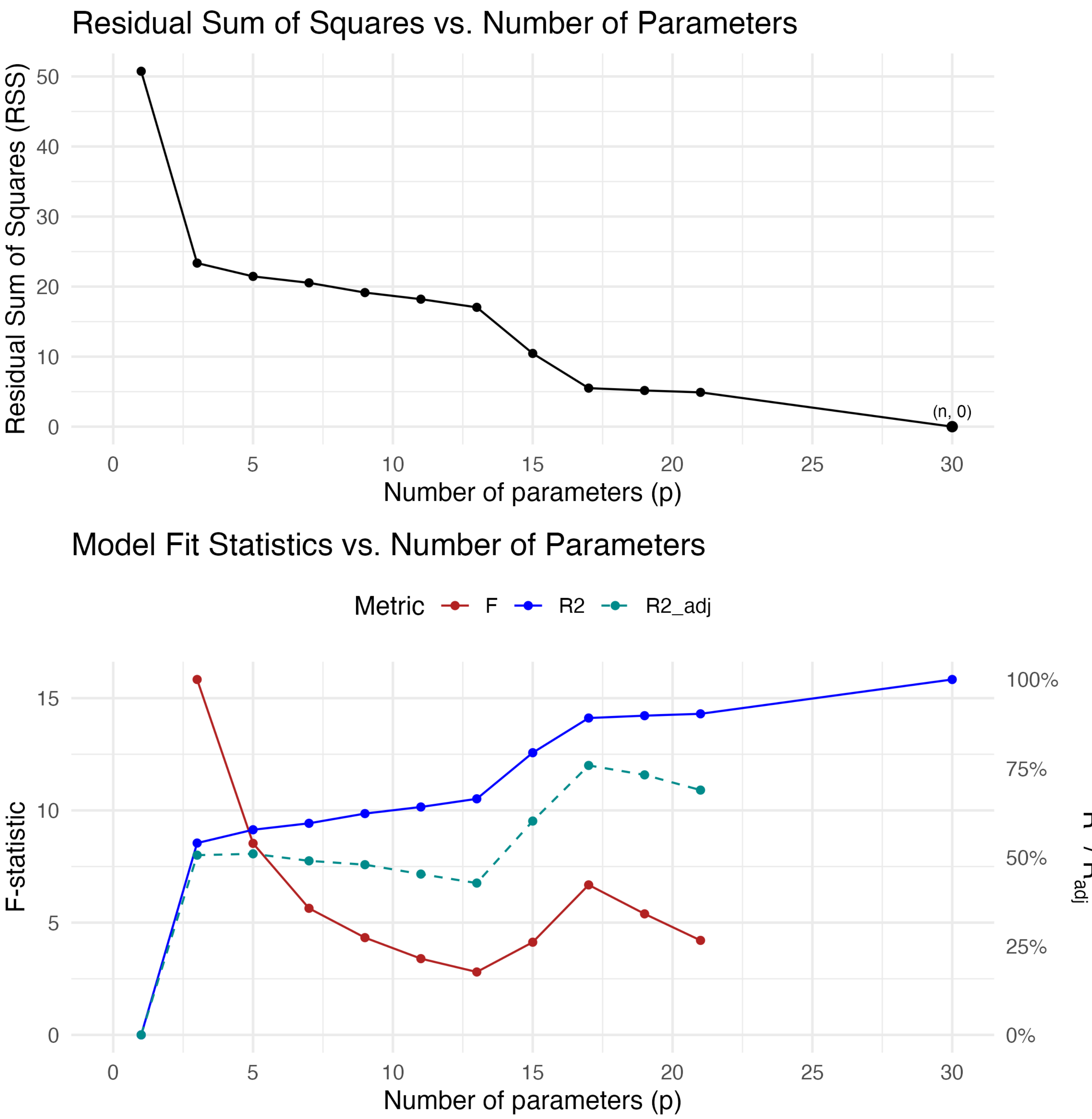


Figure 4.2: When H_1 is true: MP4 animation (HTML) or a representative static frame (PDF).

4.2.4 Example: Modelling Children Weight with Height and Age

```r
## Data: Weight, height and age of children
wgt <- c(64, 71, 53, 67, 55, 58, 77, 57, 56, 51, 76, 68)
hgt <- c(57, 59, 49, 62, 51, 50, 55, 48, 42, 42, 61, 57)
age <- c(8, 10, 6, 11, 8, 7, 10, 9, 10, 6, 12, 9)
child.data <- data.frame(wgt, hgt, age)
```

4.2.4.1 Problem 1: Height then Age

```r
fit_hgt_age <- lm(wgt ~ hgt + age, data = child.data)
summary(fit_hgt_age)
```

```

Call:
lm(formula = wgt ~ hgt + age, data = child.data)

Residuals:
    Min      1Q  Median      3Q     Max 
-6.8708 -1.7004  0.3454  1.4642 10.2336 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)  
(Intercept)   6.5530    10.9448   0.599   0.5641  
hgt           0.7220     0.2608   2.768   0.0218 *
age           2.0501     0.9372   2.187   0.0565 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.66 on 9 degrees of freedom
Multiple R-squared:   0.78, Adjusted R-squared:  0.7311 
F-statistic: 15.95 on 2 and 9 DF,  p-value: 0.001099
```

```r
fit_hgt <- lm(wgt ~ hgt, data = child.data)
summary(fit_hgt)
```

```

Call:
lm(formula = wgt ~ hgt, data = child.data)
```

```
Residuals:
    Min      1Q  Median      3Q     Max 
-5.8736 -3.8973 -0.4402  2.2624 11.8375 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)   
(Intercept)   6.1898    12.8487   0.482  0.64035   
hgt           1.0722     0.2417   4.436  0.00126 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 5.471 on 10 degrees of freedom
Multiple R-squared:  0.663,	Adjusted R-squared:  0.6293 
F-statistic: 19.67 on 1 and 10 DF,  p-value: 0.001263
```

```r
anova(fit_hgt, fit_hgt_age)
```

```
Analysis of Variance Table

Model 1: wgt ~ hgt
Model 2: wgt ~ hgt + age
  Res.Df    RSS Df Sum of Sq      F  Pr(>F)  
1     10 299.33                              
2      9 195.43  1     103.9 4.7849 0.05649 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
anova(fit_hgt_age)
```

```
Analysis of Variance Table

Response: wgt
          Df Sum Sq Mean Sq F value    Pr(>F)    
hgt        1 588.92  588.92 27.1216 0.0005582 ***
age        1 103.90  103.90  4.7849 0.0564853 .  
Residuals  9 195.43   21.71                      
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.2.4.2 Problem 2: Age then Height

```r
fit_age <- lm(wgt ~ age, data = child.data)
summary(fit_age)
```

```

Call:
lm(formula = wgt ~ age, data = child.data)

Residuals:
    Min      1Q  Median      3Q     Max 
-11.000  -3.911   1.143   4.071  10.000 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)   
(Intercept)  30.5714     8.6137   3.549  0.00528 **
age           3.6429     0.9551   3.814  0.00341 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 6.015 on 10 degrees of freedom
Multiple R-squared:  0.5926,	Adjusted R-squared:  0.5519 
F-statistic: 14.55 on 1 and 10 DF,  p-value: 0.003407
```

```r
fit_age_hgt <- lm(wgt ~ age + hgt, data = child.data)
summary(fit_age_hgt)
```

```

Call:
lm(formula = wgt ~ age + hgt, data = child.data)

Residuals:
    Min      1Q  Median      3Q     Max 
-6.8708 -1.7004  0.3454  1.4642 10.2336 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)  
(Intercept)   6.5530    10.9448   0.599   0.5641  
age           2.0501     0.9372   2.187   0.0565 .
hgt           0.7220     0.2608   2.768   0.0218 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 4.66 on 9 degrees of freedom
Multiple R-squared:   0.78,	Adjusted R-squared:  0.7311 
```

```
F-statistic: 15.95 on 2 and 9 DF,  p-value: 0.001099
```

```
anova(fit_age, fit_age_hgt)
```

```
Analysis of Variance Table

Model 1: wgt ~ age
Model 2: wgt ~ age + hgt
  Res.Df    RSS Df Sum of Sq      F  Pr(>F)
1     10 361.86
2      9 195.43  1    166.43 7.6646 0.02181 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
anova(fit_age_hgt)
```

```
Analysis of Variance Table

Response: wgt
          Df Sum Sq Mean Sq F value    Pr(>F)
age        1 526.39  526.39 24.2419 0.0008205 ***
hgt        1 166.43  166.43  7.6646 0.0218070 *
Residuals  9 195.43   21.71
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.2.5 Example: Wire bond strength

```
fit_len_hgt <-  lm(strength ~ length + height, data = bond.data)
fit_hgt_len <-  lm(strength ~ height+length, data = bond.data)
anova(fit_len_hgt)
```

```
Analysis of Variance Table

Response: strength
          Df Sum Sq Mean Sq  F value    Pr(>F)
length     1 5885.9  5885.9 1124.293 < 2.2e-16 ***
height     1  104.9   104.9   20.041 0.0001883 ***
Residuals 22  115.2     5.2
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
anova(fit_hgt_len)
```

```
Analysis of Variance Table

Response: strength
          Df Sum Sq Mean Sq F value    Pr(>F)
height     1 1483.2  1483.2  283.32 4.731e-14 ***
length     1 4507.5  4507.5  861.01 < 2.2e-16 ***
Residuals 22  115.2     5.2
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
summary(fit_hgt_len)
```

```
Call:
lm(formula = strength ~ height + length, data = bond.data)

Residuals:
   Min     1Q Median     3Q    Max
-3.865 -1.542 -0.362  1.196  5.841

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.263791   1.060066   2.136 0.044099 *
height      0.012528   0.002798   4.477 0.000188 ***
length      2.744270   0.093524  29.343  < 2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.288 on 22 degrees of freedom
Multiple R-squared:  0.9811,    Adjusted R-squared:  0.9794
F-statistic: 572.2 on 2 and 22 DF,  p-value: < 2.2e-16
```

```r
summary(fit_len_hgt)
```

```
Call:
lm(formula = strength ~ length + height, data = bond.data)

Residuals:
   Min     1Q Median     3Q    Max
```

```
-3.865 -1.542 -0.362  1.196  5.841

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) 2.263791   1.060066   2.136 0.044099 *
length      2.744270   0.093524  29.343  < 2e-16 ***
height      0.012528   0.002798   4.477 0.000188 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.288 on 22 degrees of freedom
Multiple R-squared:  0.9811,    Adjusted R-squared:  0.9794
F-statistic: 572.2 on 2 and 22 DF,  p-value: < 2.2e-16
```

4.2.6 Relationship between t-test and partial F-test

- A t-test for a single coefficient is a special case of the partial F-test; the relationship is $F = t^2$ for 1 df in the numerator.
- The p-value from t-test (output of *summary(lm())*) is the same as anova test for: $H_0 : \beta_j = 0$ vs H_1: all covaraites have non-zero effects.

4.3 Predictions for Mean Response and a Future Observation

4.3.1 Confidence Interval for Mean Response

```r
predict(fit, newdata = data.frame(length = 8, height = 275),
        interval = "confidence", level = 0.95)
```

```
      fit      lwr      upr
1 27.6631 26.66324 28.66296
```

4.3.2 Prediction Interval for a New Observation

```r
predict(fit, newdata = data.frame(length = 8, height = 275),
        interval = "prediction", level = 0.95)
```

```
      fit      lwr      upr
1 27.6631 22.81378 32.51241
```

4.4 Model Diagnostics

4.4.1 Residual Calculations

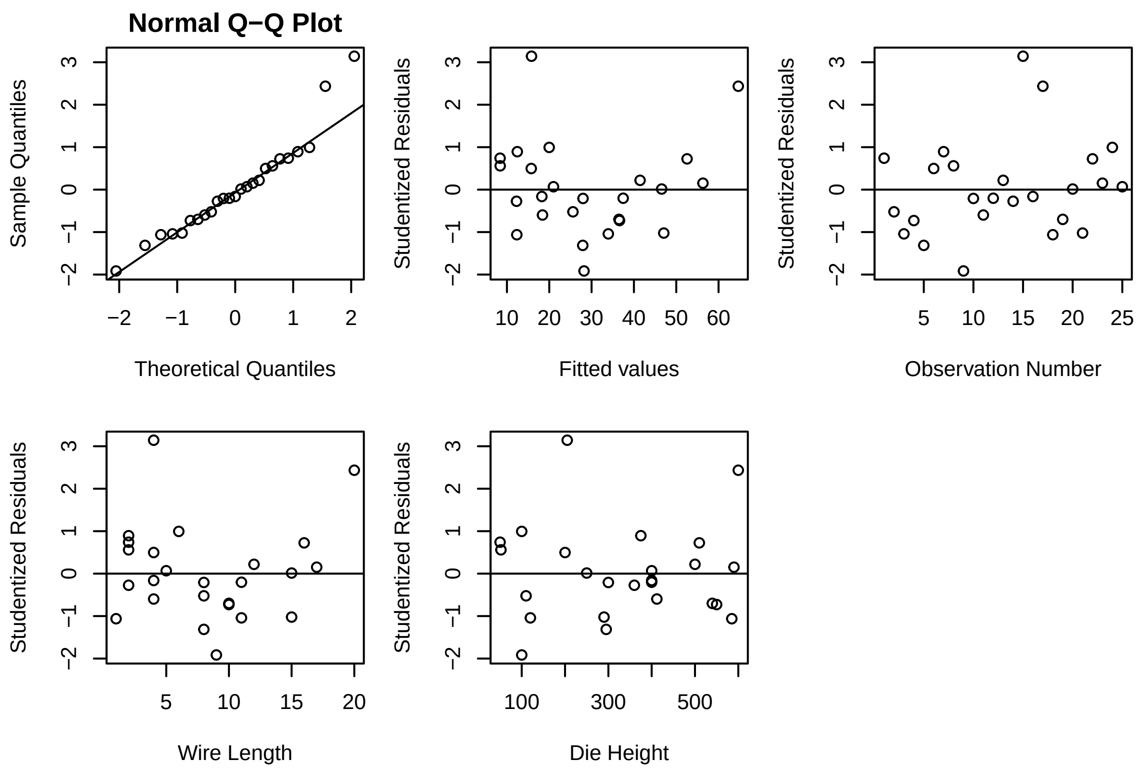
```
residuals_df <- data.frame(
  hat_values = hatvalues(fit),
  ordinary_resid = resid(fit),
  standardized_resid = resid(fit) / sigma(fit),
  studentized_internal = rstandard(fit),
  studentized_external = rstudent(fit)
)
residuals_df
```

```
   hat_values ordinary_resid standardized_resid studentized_internal
1  0.15728923     1.57127871         0.68673363           0.74808172
2  0.11164598    -1.14600783        -0.50086730          -0.53140990
3  0.14191905    -2.20409488        -0.96330846          -1.03992315
4  0.10188923    -1.59678413        -0.69788088          -0.73640435
5  0.04178381    -2.89365294        -1.26468257          -1.29196212
6  0.07486842     1.11356772         0.48668921           0.50599936
7  0.11806106     1.92974001         0.84340057           0.89807919
8  0.15608149     1.19622309         0.52281407           0.56911105
9  0.12797685    -3.86499936        -1.68921340          -1.80892479
10 0.04131672    -0.47629200        -0.20816532          -0.21260369
11 0.09253979    -1.32232830        -0.57792886          -0.60668127
12 0.05256700    -0.46188206        -0.20186740          -0.20739197
13 0.08202675     0.49106715         0.21462286           0.22400668
14 0.11291577    -0.60234282        -0.26325633          -0.27950939
15 0.07373697     5.84092866         2.55280118           2.65246601
16 0.08794942    -0.36199456        -0.15821117          -0.16566382
17 0.25934228     4.33412887         1.89424832           2.20104100
18 0.29287870    -2.03683074        -0.89020500          -1.05862725
19 0.09617553    -1.54150602        -0.67372136          -0.70866056
20 0.14726101     0.03021107         0.01320387           0.01429859
21 0.12963943    -2.18090138        -0.95317165          -1.02169558
22 0.13580052     1.55871047         0.68124063           0.73281364
23 0.18237610     0.32221591         0.14082575           0.15574183
24 0.10908869     2.14780957         0.93870874           0.99452024
25 0.07287021     0.15373580         0.06719084           0.06978142
   studentized_external
1            0.74035927
2           -0.52255660
3           -1.04194550
```

```
4           -0.72850799
5           -1.31305171
6            0.49726770
7            0.89397096
8            0.56016499
9           -1.91552083
10          -0.20792931
11          -0.59775404
12          -0.20282206
13           0.21910643
14          -0.27356920
15           3.14216850
16          -0.16195600
17           2.43521394
18          -1.06168251
19          -0.70040768
20           0.01396991
21          -1.02276424
22           0.72486668
23           0.15224503
24           0.99426154
25           0.06818458
```

4.4.2 Residual Plots

```r
n <- nrow(bond.data)
r <- rstudent(fit)
y.hat <- fitted.values(fit)

par(mfrow = c(2, 3), mar = c(4, 4, 2, 1))
qqnorm(r, main = "Normal Q-Q Plot"); qqline(r)
plot(y.hat, r, xlab = "Fitted values", ylab = "Studentized Residuals"); abline(h = 0)
plot(1:n, r, xlab = "Observation Number", ylab = "Studentized Residuals"); abline(h = 0)
plot(bond.data$length, r, xlab = "Wire Length", ylab = "Studentized Residuals"); abline(h = 0)
plot(bond.data$height, r, xlab = "Die Height", ylab = "Studentized Residuals"); abline(h = 0)
```



4.5 Influential Observations

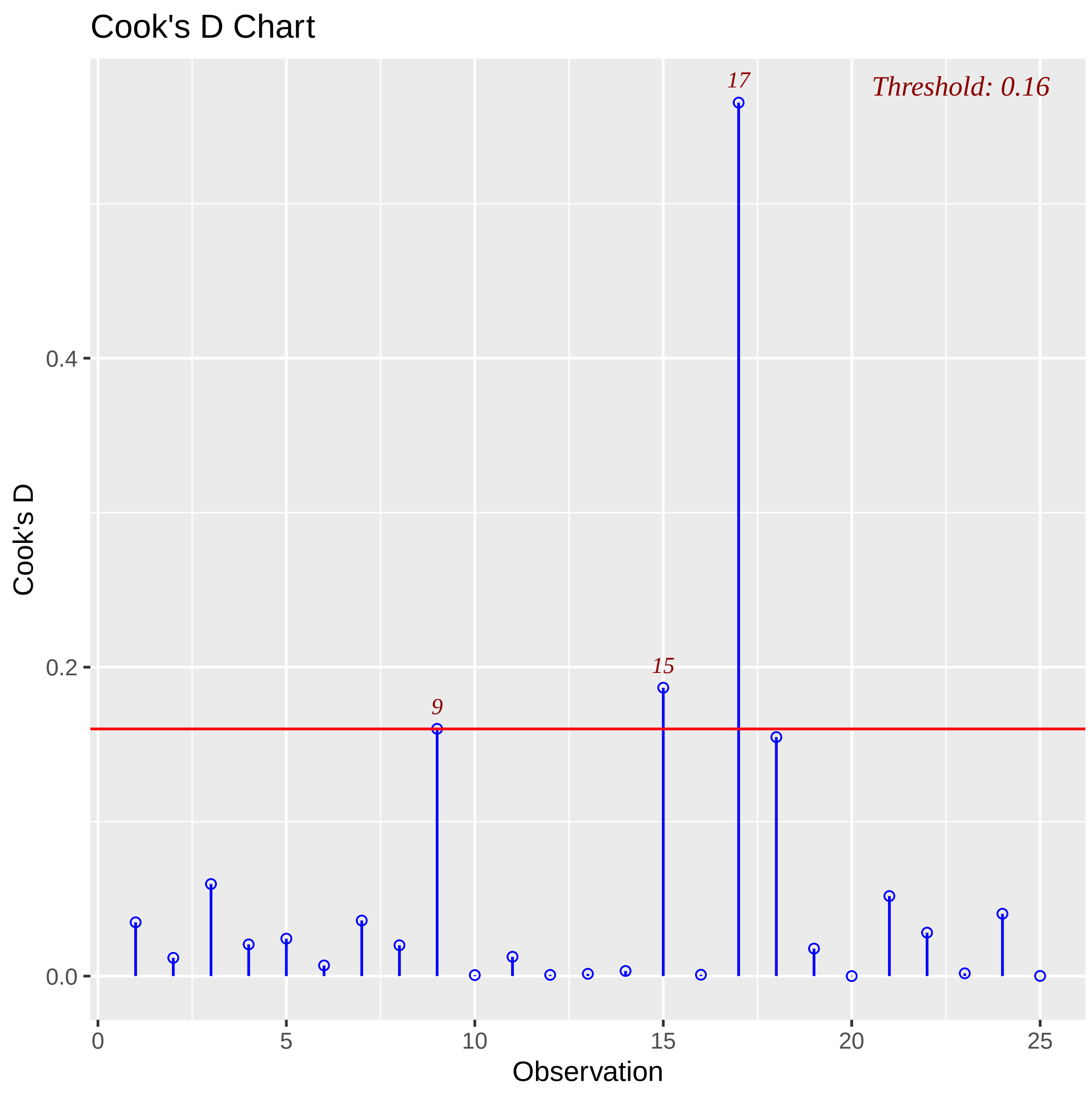
```
influence_df <- data.frame(dffits = dffits(fit),
                           cook.D = cooks.distance(fit),
                           dfbetas(fit))
influence_df
```

```
         dffits       cook.D  X.Intercept.       length       height
1   0.319854702 3.481748e-02  0.3179493921 -0.100534181 -0.200085326
2  -0.185251548 1.183028e-02 -0.1403477437 -0.051464370  0.148315370
3  -0.423741713 5.962023e-02 -0.2219151046 -0.237135616  0.339340552
4  -0.245376811 2.050736e-02  0.0787635526  0.022343842 -0.184260891
5  -0.274191565 2.426179e-02 -0.1572410603 -0.009662357  0.055328303
6   0.141461363 6.906752e-03  0.1301249135 -0.058073567 -0.049408295
7   0.327082639 3.598953e-02  0.1479853099 -0.261848970  0.142220906
8   0.240902557 1.996750e-02  0.2394962591 -0.076575387 -0.149787102
9  -0.733818383 1.600749e-01 -0.5011686139 -0.283749099  0.605559181
10 -0.043165927 6.493384e-04 -0.0241138520 -0.001038287  0.007460760
11 -0.190885522 1.251125e-02 -0.0602003847  0.132053762 -0.102733745
12 -0.047774650 7.954763e-04  0.0017554145 -0.016926531 -0.008495572
```

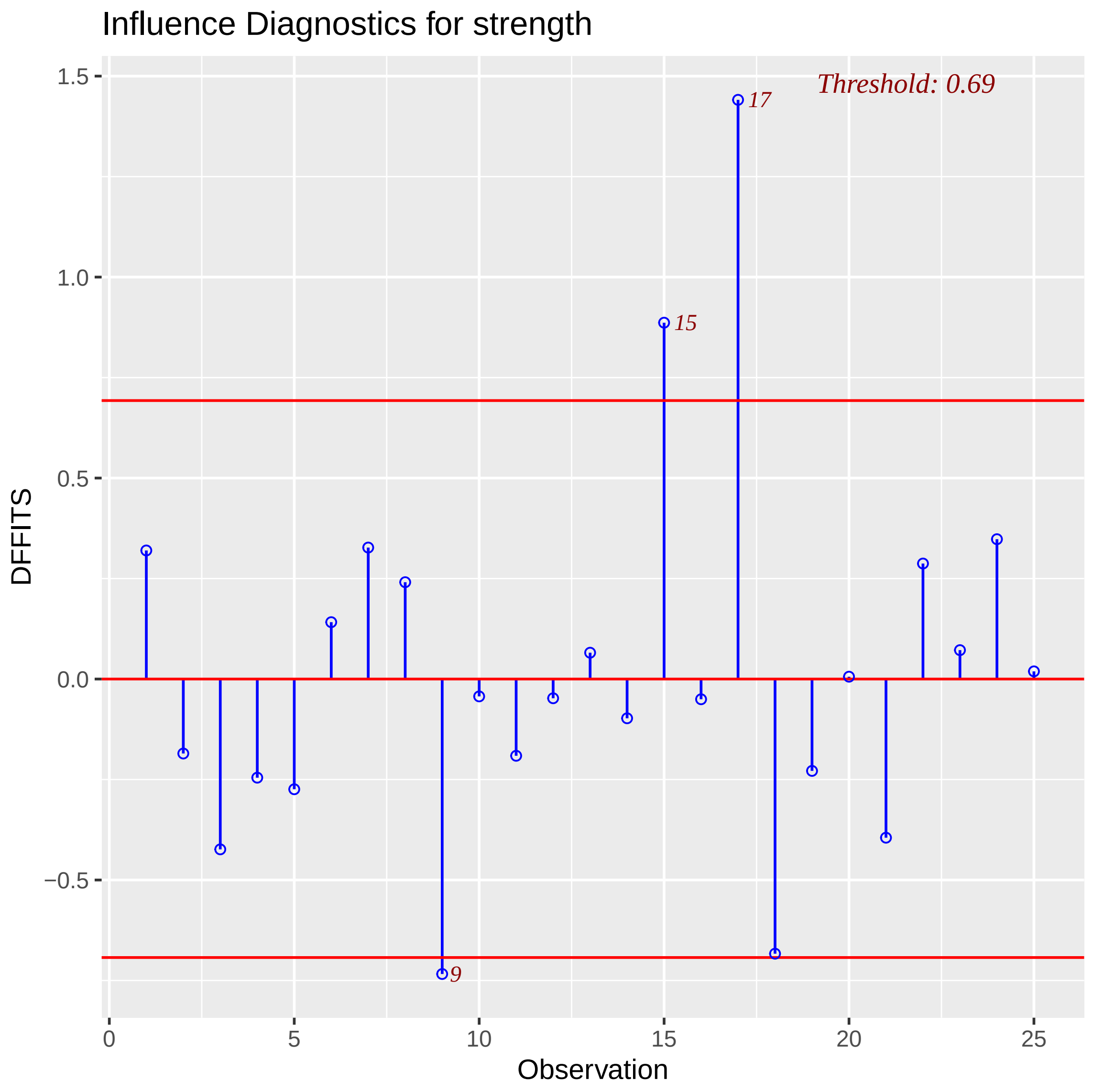
```
13  0.065496465 1.494604e-03 -0.0224255162  0.017340091  0.033756253
14 -0.097602753 3.314830e-03 -0.0483552961  0.077880727 -0.038066705
15  0.886553487 1.866936e-01  0.8097463528 -0.374290156 -0.292048214
16 -0.050292599 8.821617e-04 -0.0177647675  0.034746758 -0.025275682
17  1.441003392 5.654455e-01 -0.8513738015  1.008880052  0.413618783
18 -0.683268805 1.547244e-01 -0.0218935465  0.521608456 -0.532432956
19 -0.228476293 1.781295e-02  0.0700729860  0.018004228 -0.167581999
20  0.005805362 1.176892e-05  0.0005613509  0.004752581 -0.003094588
21 -0.394724862 5.182743e-02 -0.0084618169 -0.324109965  0.170622396
22  0.287343813 2.812893e-02 -0.1326208213  0.183002776  0.076391058
23  0.071903545 1.803448e-03 -0.0412553376  0.040164093  0.030365108
24  0.347915085 4.036930e-02  0.3084561584  0.016541769 -0.262089402
25  0.019115733 1.275757e-04  0.0062730782 -0.011614674  0.009459029
```

4.5.1 Plotting with the `olsrr` Package

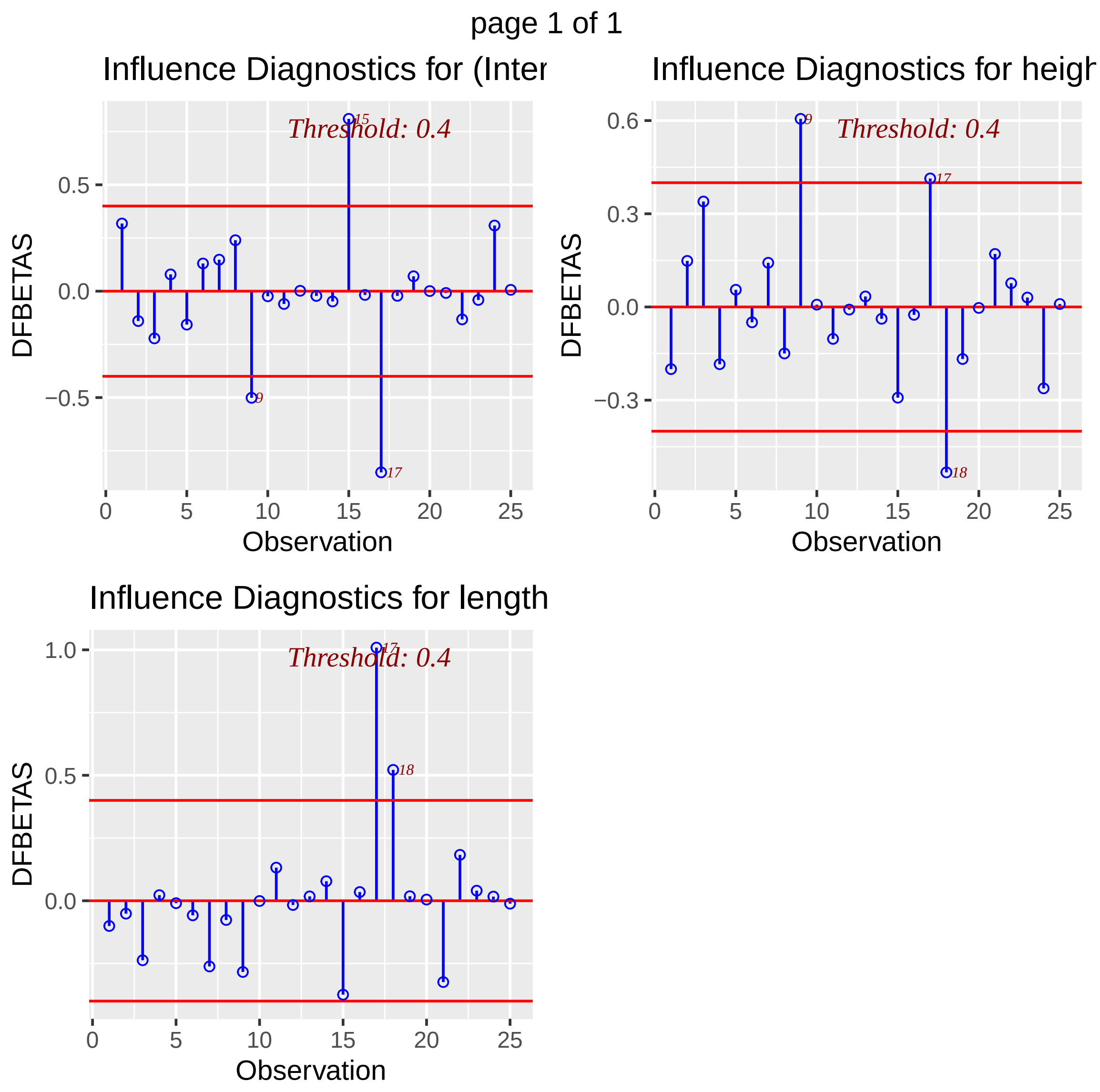
```r
## install.packages("olsrr") # Run once if needed
library(olsrr)

ols_plot_cooksd_chart(fit)
```



```
ols_plot_dffits(fit)
```



```r
ols_plot_dfbetas(fit)
```



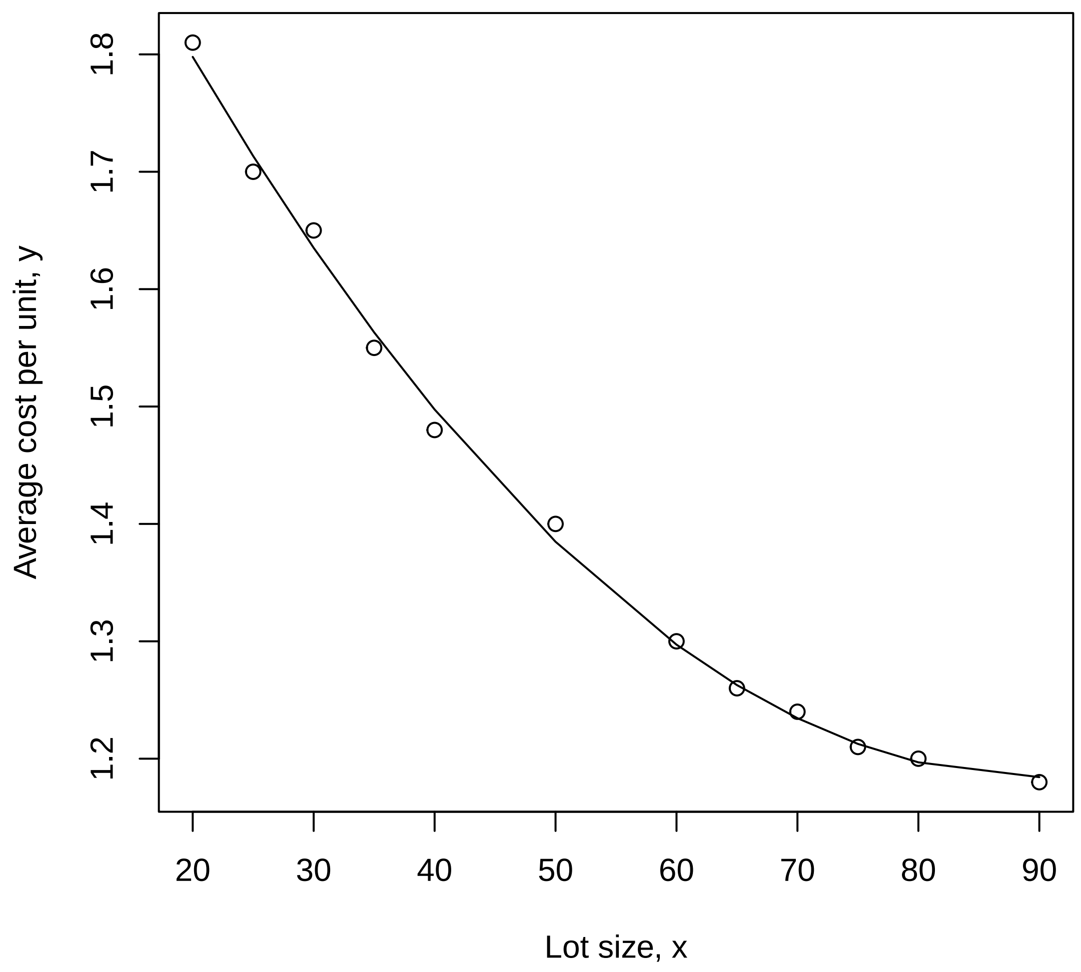
4.6 Polynomial Regression

```
y <- c(1.81, 1.70, 1.65, 1.55, 1.48, 1.40, 1.30, 1.26, 1.24, 1.21, 1.20, 1.18)
x <- c(20, 25, 30, 35, 40, 50, 60, 65, 70, 75, 80, 90)
fit_poly <- lm(y ~ x + I(x^2))
summary(fit_poly)
```

```
Call:
lm(formula = y ~ x + I(x^2))
```

```
Residuals:
       Min         1Q     Median         3Q        Max
-0.0174763 -0.0065087  0.0001297  0.0071482  0.0151887

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.198e+00  2.255e-02   97.48 6.38e-15 ***
x           -2.252e-02  9.424e-04  -23.90 1.88e-09 ***
I(x^2)       1.251e-04  8.658e-06   14.45 1.56e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.01219 on 9 degrees of freedom
Multiple R-squared:  0.9975,    Adjusted R-squared:  0.9969
F-statistic:  1767 on 2 and 9 DF,  p-value: 2.096e-12
```

```r
plot(x, y, xlab = "Lot size, x", ylab = "Average cost per unit, y")
lines(x, predict(fit_poly, newdata = data.frame(x = x)), type = "l")
```



```r
fit1 <- lm(y ~ x)
anova(fit1, fit_poly)
```

```
Analysis of Variance Table

Model 1: y ~ x
Model 2: y ~ x + I(x^2)
  Res.Df      RSS Df Sum of Sq      F    Pr(>F)
1     10 0.032340
2      9 0.001337  1  0.031002 208.67 1.564e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.7 Handling Categorical Variables with Dummy Variables

Investigate the common observation that males tend to have higher blood pressure than females of similar age.

```r
## Note: Update this path to your local file location
sbpdata <- read.csv("sbpdata.csv")
sbpdata
```

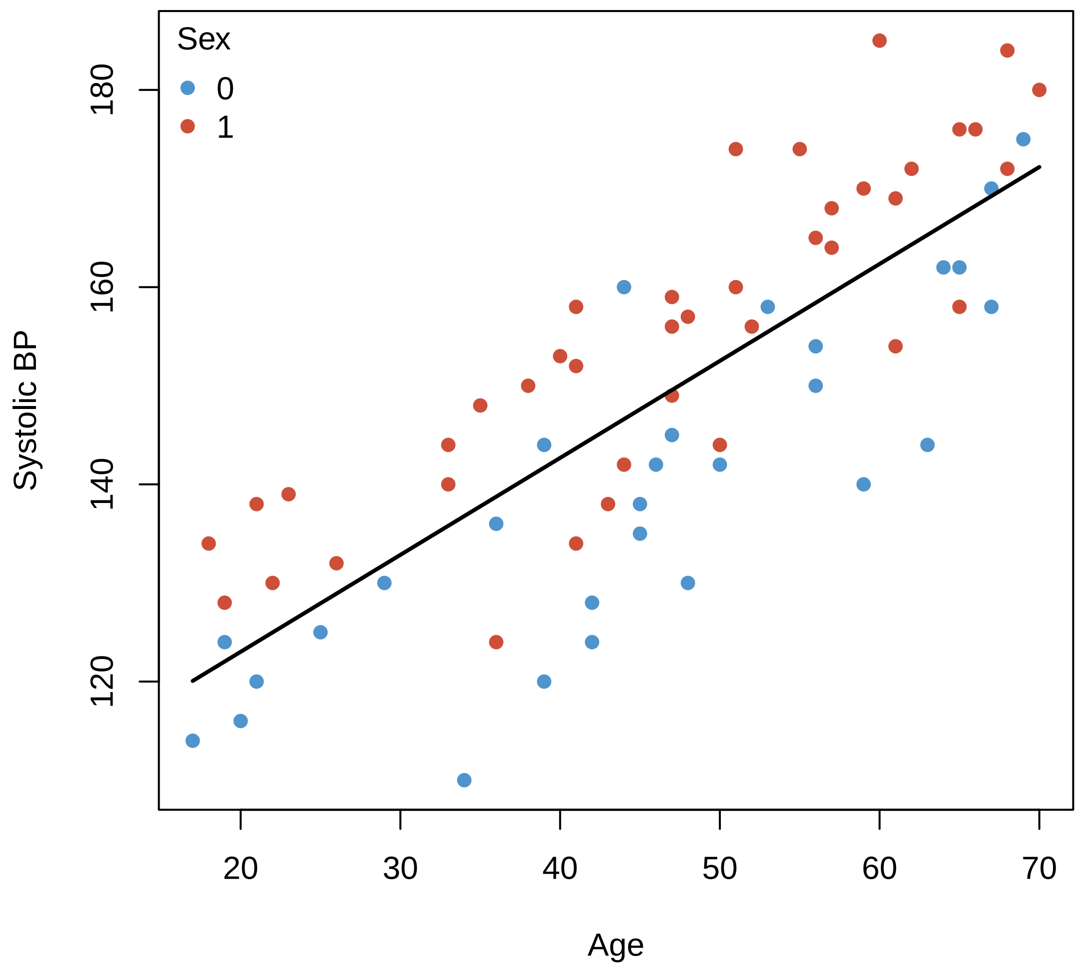
```
   sex sbp age
1    0 144  39
2    0 138  45
3    0 145  47
4    0 162  65
5    0 142  46
6    0 170  67
7    0 124  42
8    0 158  67
9    0 154  56
10   0 162  64
11   0 150  56
12   0 140  59
13   0 110  34
14   0 128  42
15   0 130  48
16   0 135  45
17   0 114  17
18   0 116  20
19   0 124  19
20   0 136  36
21   0 142  50
22   0 120  39
23   0 120  21
24   0 160  44
25   0 158  53
26   0 144  63
27   0 130  29
28   0 125  25
29   0 175  69
30   1 158  41
31   1 185  60
32   1 152  41
33   1 159  47
34   1 176  66
35   1 156  47
36   1 184  68
37   1 138  43
38   1 172  68
39   1 168  57
```

```
40    1 176  65
41    1 164  57
42    1 154  61
43    1 124  36
44    1 142  44
45    1 144  50
46    1 149  47
47    1 128  19
48    1 130  22
49    1 138  21
50    1 150  38
51    1 156  52
52    1 134  41
53    1 134  18
54    1 174  51
55    1 174  55
56    1 158  65
57    1 144  33
58    1 139  23
59    1 180  70
60    1 165  56
61    1 172  62
62    1 160  51
63    1 157  48
64    1 170  59
65    1 153  40
66    1 148  35
67    1 140  33
68    1 132  26
69    1 169  61
```

4.7.1 Four Models Involving "sex"

4.7.1.1 Coincidence Model (Age Only)

```r
## Ensure sex is a factor (labels will appear in the legend)
sbpdata$sex <- as.factor(sbpdata$sex)

## Fit (you already have this)
fit.age <- lm(sbp ~ age, data = sbpdata)

## Generate predictions over the observed age range
new_age <- seq(min(sbpdata$age, na.rm = TRUE),
               max(sbpdata$age, na.rm = TRUE),
               length.out = 200)
pred <- predict(fit.age, newdata = data.frame(age = new_age))

## Simple palette for the sex levels (works for 1-3 levels; expand if needed)
lev  <- levels(sbpdata$sex)
cols <- setNames(c("steelblue3", "tomato3", "darkorchid3")[seq_along(lev)], lev)

## Scatter plot with colored points by sex
plot(sbp ~ age, data = sbpdata,
     col = cols[sbpdata$sex], pch = 16,
     xlab = "Age", ylab = "Systolic BP")

## Add predicted line
lines(new_age, pred, lwd = 2)

## Legend
legend("topleft", legend = lev, col = cols[lev], pch = 16, bty = "n", title = "Sex")
```



```
data.frame(model.matrix(fit.age))
```

```
   X.Intercept. age
1             1  39
2             1  45
3             1  47
4             1  65
5             1  46
6             1  67
7             1  42
8             1  67
9             1  56
10            1  64
11            1  56
12            1  59
13            1  34
14            1  42
```

```
15                1  48
16                1  45
17                1  17
18                1  20
19                1  19
20                1  36
21                1  50
22                1  39
23                1  21
24                1  44
25                1  53
26                1  63
27                1  29
28                1  25
29                1  69
30                1  41
31                1  60
32                1  41
33                1  47
34                1  66
35                1  47
36                1  68
37                1  43
38                1  68
39                1  57
40                1  65
41                1  57
42                1  61
43                1  36
44                1  44
45                1  50
46                1  47
47                1  19
48                1  22
49                1  21
50                1  38
51                1  52
52                1  41
53                1  18
54                1  51
55                1  55
56                1  65
57                1  33
58                1  23
59                1  70
```

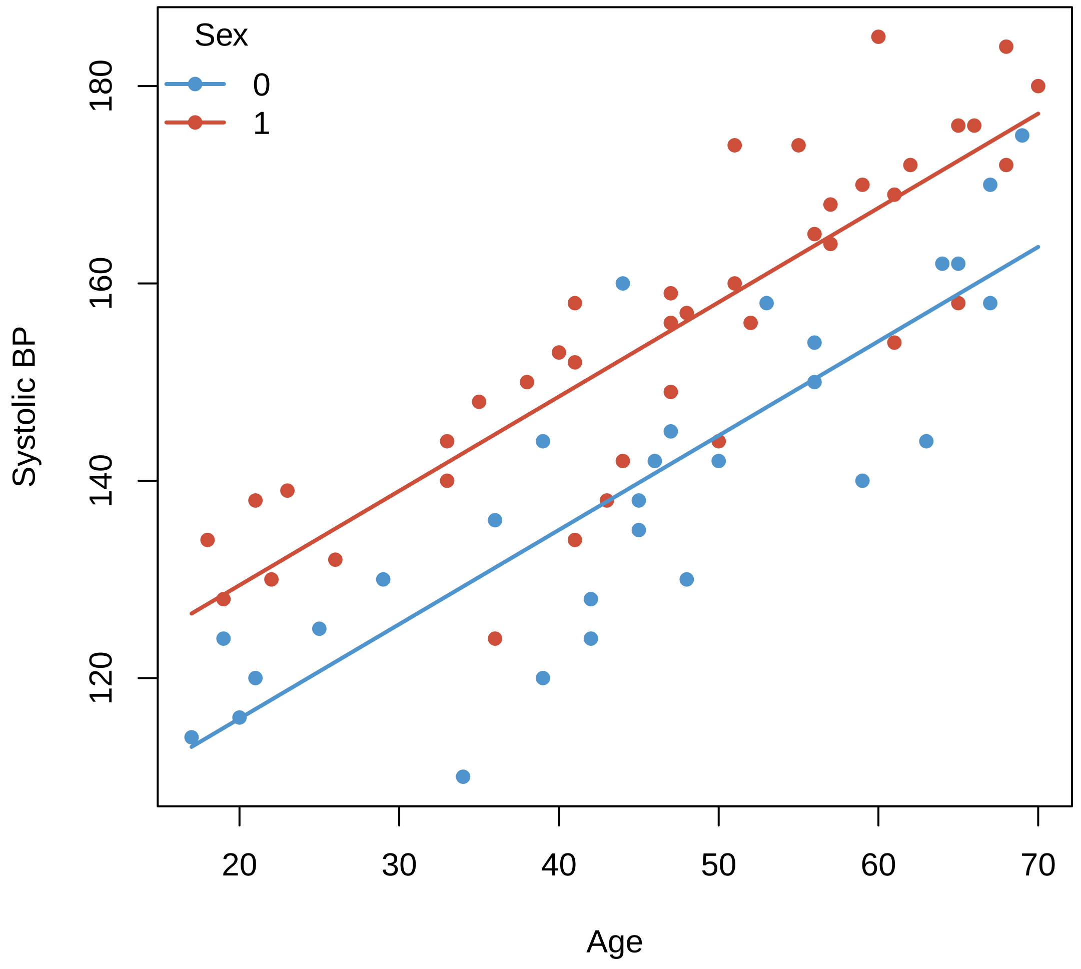
```
60             1  56
61             1  62
62             1  51
63             1  48
64             1  59
65             1  40
66             1  35
67             1  33
68             1  26
69             1  61
```

```r
print(anova(fit.age))
```

```
Analysis of Variance Table

Response: sbp
          Df  Sum Sq Mean Sq F value    Pr(>F)    
age        1 14951.3 14951.3  121.27 < 2.2e-16 ***
Residuals 67  8260.5   123.3                      
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.7.1.2 Additive Effect Model (Age + Sex)

```r
## Parallelism: H0: beta3=0 (Sex has additive effect)
fit.agePLUSsex <- lm(sbp ~ age + sex, data = sbpdata)

## Ensure sex is a factor for labeling/colors
sbpdata$sex <- factor(sbpdata$sex)

## Fit (additive: parallelism)
fit.agePLUSsex <- lm(sbp ~ age + sex, data = sbpdata)

## X-range and palette
ages <- seq(min(sbpdata$age, na.rm = TRUE),
            max(sbpdata$age, na.rm = TRUE),
            length.out = 200)
lev  <- levels(sbpdata$sex)
cols <- setNames(c("steelblue3", "tomato3", "darkorchid3")[seq_along(lev)], lev)

## Scatter with colored points by sex
plot(sbp ~ age, data = sbpdata,
     col = cols[sbpdata$sex], pch = 16,
     xlab = "Age", ylab = "Systolic BP")

## Parallel fitted lines: one per sex (same slope, different intercepts)
for (sx in lev) {
  nd <- data.frame(age = ages, sex = factor(sx, levels = lev))
  yhat <- predict(fit.agePLUSsex, newdata = nd)
  lines(ages, yhat, col = cols[sx], lwd = 2)
}

## Legend
legend("topleft", legend = lev, col = cols[lev], pch = 16, lwd = 2, bty = "n", title = "Sex")
```



```
data.frame(model.matrix(fit.agePLUSsex))
```

```
   X.Intercept. age sex1
```

```
1              1  39     0
2              1  45     0
3              1  47     0
4              1  65     0
5              1  46     0
6              1  67     0
7              1  42     0
8              1  67     0
9              1  56     0
10             1  64     0
11             1  56     0
12             1  59     0
13             1  34     0
14             1  42     0
15             1  48     0
16             1  45     0
17             1  17     0
18             1  20     0
19             1  19     0
20             1  36     0
21             1  50     0
22             1  39     0
23             1  21     0
24             1  44     0
25             1  53     0
26             1  63     0
27             1  29     0
28             1  25     0
29             1  69     0
30             1  41     1
31             1  60     1
32             1  41     1
33             1  47     1
34             1  66     1
35             1  47     1
36             1  68     1
37             1  43     1
38             1  68     1
39             1  57     1
40             1  65     1
41             1  57     1
42             1  61     1
43             1  36     1
44             1  44     1
45             1  50     1
```

```
46             1  47    1
47             1  19    1
48             1  22    1
49             1  21    1
50             1  38    1
51             1  52    1
52             1  41    1
53             1  18    1
54             1  51    1
55             1  55    1
56             1  65    1
57             1  33    1
58             1  23    1
59             1  70    1
60             1  56    1
61             1  62    1
62             1  51    1
63             1  48    1
64             1  59    1
65             1  40    1
66             1  35    1
67             1  33    1
68             1  26    1
69             1  61    1
```

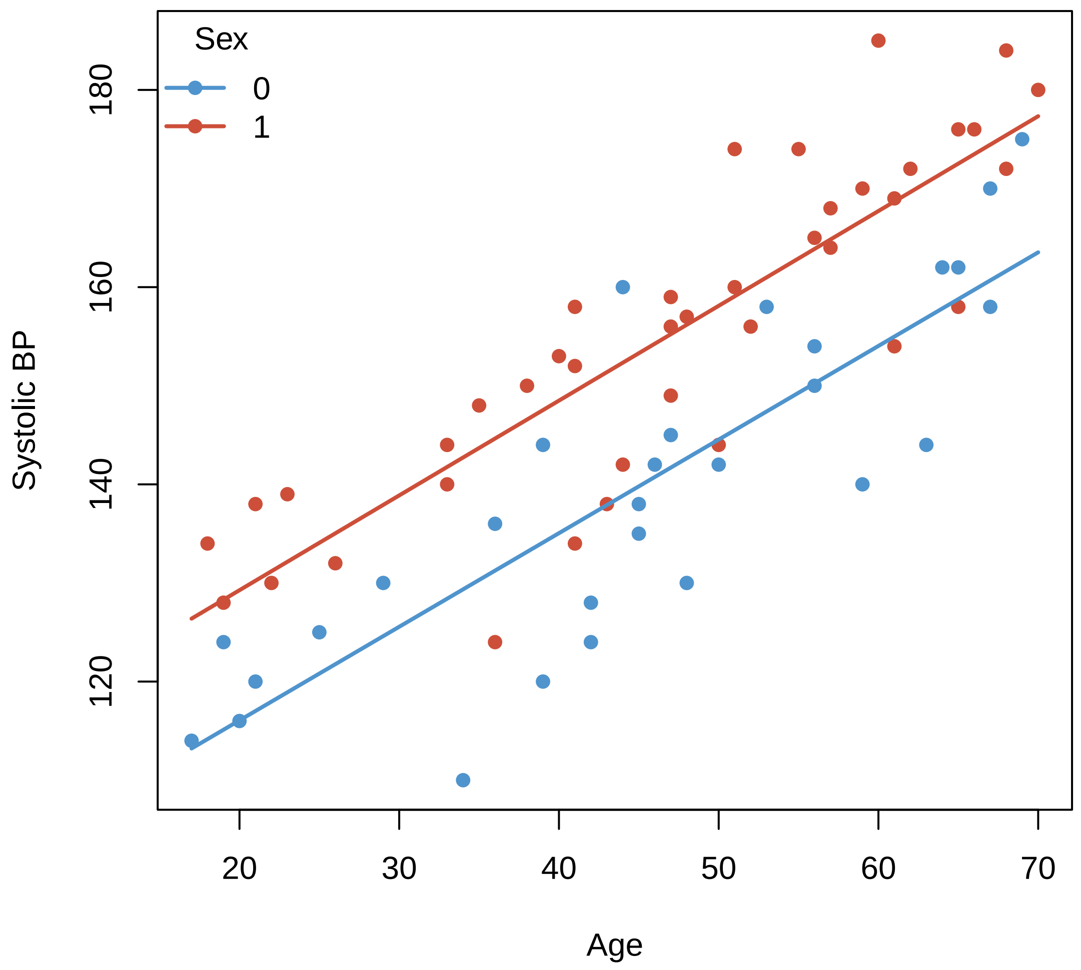
```
print(anova(fit.age, fit.agePLUSsex))
```

```
Analysis of Variance Table

Model 1: sbp ~ age
Model 2: sbp ~ age + sex
  Res.Df    RSS Df Sum of Sq      F    Pr(>F)
1     67 8260.5
2     66 5202.0  1    3058.5 38.805 3.701e-08 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.7.1.3 Varying Intercept and Varying Slope Model (Age + Sex + Age:Sex)

```
## Make sure sex is a factor (for colors/legend)
sbpdata$sex <- factor(sbpdata$sex)
```

```r
## Fit (interaction: different slopes by sex)
fit.age.TIMES.sex <- lm(sbp ~ age + sex + age:sex, data = sbpdata)

## Age grid and palette
ages <- seq(min(sbpdata$age, na.rm = TRUE),
            max(sbpdata$age, na.rm = TRUE),
            length.out = 200)
lev  <- levels(sbpdata$sex)
cols <- setNames(c("steelblue3", "tomato3", "darkorchid3")[seq_along(lev)], lev)

## Scatter: color points by sex
plot(sbp ~ age, data = sbpdata,
     col = cols[sbpdata$sex], pch = 16,
     xlab = "Age", ylab = "Systolic BP")

## Fitted lines: one per sex (different slopes allowed)
for (sx in lev) {
  nd <- data.frame(age = ages, sex = factor(sx, levels = lev))
  yhat <- predict(fit.age.TIMES.sex, newdata = nd)
  lines(ages, yhat, col = cols[sx], lwd = 2)
}

## Legend
legend("topleft", legend = lev, col = cols[lev], pch = 16, lwd = 2, bty = "n", title = "Sex")
```



Model Matrix and ANOVA

```
data.frame(model.matrix(fit.age.TIMES.sex))
```

```
   X.Intercept. age sex1 age.sex1
1             1  39    0        0
2             1  45    0        0
3             1  47    0        0
4             1  65    0        0
5             1  46    0        0
6             1  67    0        0
7             1  42    0        0
8             1  67    0        0
9             1  56    0        0
10            1  64    0        0
11            1  56    0        0
12            1  59    0        0
```

```
13            1  34     0         0
14            1  42     0         0
15            1  48     0         0
16            1  45     0         0
17            1  17     0         0
18            1  20     0         0
19            1  19     0         0
20            1  36     0         0
21            1  50     0         0
22            1  39     0         0
23            1  21     0         0
24            1  44     0         0
25            1  53     0         0
26            1  63     0         0
27            1  29     0         0
28            1  25     0         0
29            1  69     0         0
30            1  41     1        41
31            1  60     1        60
32            1  41     1        41
33            1  47     1        47
34            1  66     1        66
35            1  47     1        47
36            1  68     1        68
37            1  43     1        43
38            1  68     1        68
39            1  57     1        57
40            1  65     1        65
41            1  57     1        57
42            1  61     1        61
43            1  36     1        36
44            1  44     1        44
45            1  50     1        50
46            1  47     1        47
47            1  19     1        19
48            1  22     1        22
49            1  21     1        21
50            1  38     1        38
51            1  52     1        52
52            1  41     1        41
53            1  18     1        18
54            1  51     1        51
55            1  55     1        55
56            1  65     1        65
57            1  33     1        33
```

```
58             1  23    1       23
59             1  70    1       70
60             1  56    1       56
61             1  62    1       62
62             1  51    1       51
63             1  48    1       48
64             1  59    1       59
65             1  40    1       40
66             1  35    1       35
67             1  33    1       33
68             1  26    1       26
69             1  61    1       61
```

```
summary(fit.age.TIMES.sex)
```

```
Call:
lm(formula = sbp ~ age + sex + age:sex, data = sbpdata)

Residuals:
    Min      1Q  Median      3Q     Max 
-20.647  -3.410   1.254   4.314  21.153 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 97.07708    5.17046  18.775  < 2e-16 ***
age          0.94932    0.10864   8.738 1.43e-12 ***
sex1        12.96144    7.01172   1.849   0.0691 .  
age:sex1     0.01203    0.14519   0.083   0.9342    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.946 on 65 degrees of freedom
Multiple R-squared:  0.7759,	Adjusted R-squared:  0.7656 
F-statistic: 75.02 on 3 and 65 DF,  p-value: < 2.2e-16
```

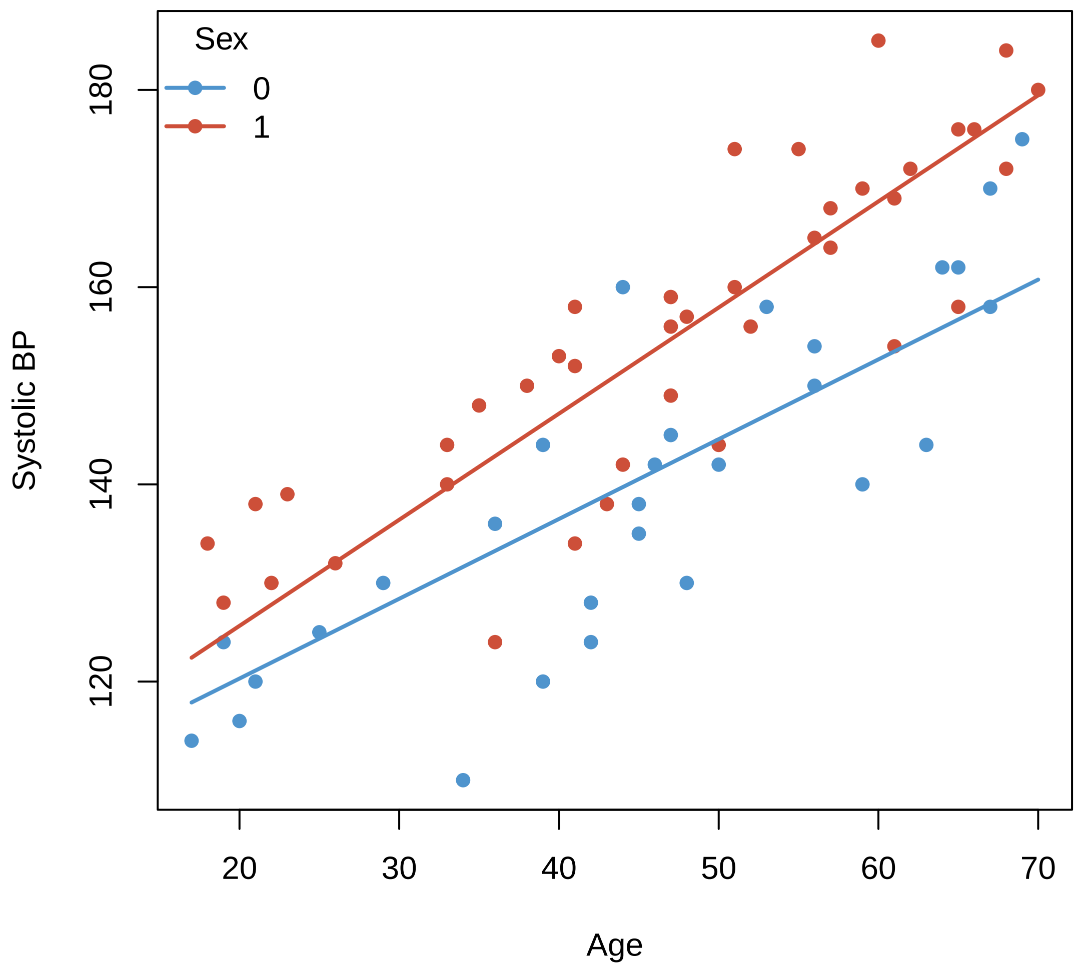
```
print(anova(fit.age,fit.agePLUSsex,fit.age.TIMES.sex))
```

```
Analysis of Variance Table

Model 1: sbp ~ age
Model 2: sbp ~ age + sex
Model 3: sbp ~ age + sex + age:sex
```

```
  Res.Df    RSS Df Sum of Sq       F    Pr(>F)    
1     67 8260.5                                   
2     66 5202.0  1   3058.52 38.2210 4.692e-08 ***
3     65 5201.4  1      0.55  0.0069    0.9342    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

4.7.1.4 Varying Slope, Equal Intercept Model (Age + Age:Sex)

```r
## Make sure sex is a factor (for colors/legend)
sbpdata$sex <- factor(sbpdata$sex)

## Fit (interaction: different slopes by sex)
fit.equal.intercept <- lm(sbp ~ age + age:sex, data = sbpdata)


## Age grid and palette
ages <- seq(min(sbpdata$age, na.rm = TRUE),
            max(sbpdata$age, na.rm = TRUE),
            length.out = 200)
lev  <- levels(sbpdata$sex)
cols <- setNames(c("steelblue3", "tomato3", "darkorchid3")[seq_along(lev)], lev)

## Scatter: color points by sex
plot(sbp ~ age, data = sbpdata,
     col = cols[sbpdata$sex], pch = 16,
     xlab = "Age", ylab = "Systolic BP")

## Fitted lines: one per sex (different slopes allowed)
for (sx in lev) {
  nd <- data.frame(age = ages, sex = factor(sx, levels = lev))
  yhat <- predict(fit.equal.intercept, newdata = nd)
  lines(ages, yhat, col = cols[sx], lwd = 2)
}

## Legend
legend("topleft", legend = lev, col = cols[lev], pch = 16, lwd = 2, bty = "n", title = "Sex")
```



4.7.2 Orders of Terms Matters in ANOVA and Warnings in Interpreting t-test Tables

```
fit.int <- lm(sbp ~ 1, data = sbpdata)
fit.sex <- lm(sbp ~ sex, data = sbpdata)

print(anova(fit.int,fit.age,fit.agePLUSsex, fit.age.TIMES.sex))
```

```
Analysis of Variance Table

Model 1: sbp ~ 1
Model 2: sbp ~ age
Model 3: sbp ~ age + sex
Model 4: sbp ~ age + sex + age:sex
  Res.Df     RSS Df Sum of Sq        F    Pr(>F)
1     68 23211.8
```

```
2      67  8260.5  1   14951.3 186.8390 < 2.2e-16 ***
3      66  5202.0  1    3058.5  38.2210 4.692e-08 ***
4      65  5201.4  1       0.5   0.0069    0.9342
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
print(anova(fit.int,fit.age,fit.equal.intercept, fit.age.TIMES.sex))
```

```
Analysis of Variance Table

Model 1: sbp ~ 1
Model 2: sbp ~ age
Model 3: sbp ~ age + age:sex
Model 4: sbp ~ age + sex + age:sex
  Res.Df     RSS Df Sum of Sq        F    Pr(>F)
1     68 23211.8
2     67  8260.5  1   14951.3 186.8390 < 2.2e-16 ***
3     66  5474.9  1    2785.6  34.8107 1.437e-07 ***
4     65  5201.4  1     273.4   3.4171   0.06907 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
print(anova(fit.int,fit.sex,fit.agePLUSsex, fit.age.TIMES.sex))
```

```
Analysis of Variance Table

Model 1: sbp ~ 1
Model 2: sbp ~ sex
Model 3: sbp ~ age + sex
Model 4: sbp ~ age + sex + age:sex
  Res.Df     RSS Df Sum of Sq        F    Pr(>F)
1     68 23211.8
2     67 19282.5  1    3929.2  49.1017 1.684e-09 ***
3     66  5202.0  1   14080.6 175.9583 < 2.2e-16 ***
4     65  5201.4  1       0.5   0.0069    0.9342
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
summary(fit.age)
```

```
Call:
```

```
lm(formula = sbp ~ age, data = sbpdata)

Residuals:
    Min      1Q  Median      3Q     Max 
-26.782  -7.632   1.968   8.201  22.651 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) 103.34905    4.33190   23.86   <2e-16 ***
age           0.98333    0.08929   11.01   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 11.1 on 67 degrees of freedom
Multiple R-squared:  0.6441,    Adjusted R-squared:  0.6388 
F-statistic: 121.3 on 1 and 67 DF,  p-value: < 2.2e-16
```

```r
summary(fit.equal.intercept)
```

```
Call:
lm(formula = sbp ~ age + age:sex, data = sbpdata)

Residuals:
     Min       1Q   Median       3Q      Max 
-21.6338  -4.3067   0.9922   4.9819  20.2753 

Coefficients:
             Estimate Std. Error t value Pr(>|t|)    
(Intercept) 104.12501    3.55578  29.283  < 2e-16 ***
age           0.80908    0.07918  10.219 3.14e-15 ***
age:sex1      0.26705    0.04608   5.795 2.09e-07 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 9.108 on 66 degrees of freedom
Multiple R-squared:  0.7641,    Adjusted R-squared:  0.757 
F-statistic: 106.9 on 2 and 66 DF,  p-value: < 2.2e-16
```

```r
summary(fit.agePLUSsex)
```

```
Call:
```

```
lm(formula = sbp ~ age + sex, data = sbpdata)

Residuals:
    Min      1Q  Median      3Q     Max 
-20.705  -3.299   1.248   4.325  21.160 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 96.77353    3.62085  26.727  < 2e-16 ***
age          0.95606    0.07153  13.366  < 2e-16 ***
sex1        13.51345    2.16932   6.229  3.7e-08 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.878 on 66 degrees of freedom
Multiple R-squared:  0.7759,	Adjusted R-squared:  0.7691 
F-statistic: 114.2 on 2 and 66 DF,  p-value: < 2.2e-16
```

```r
summary(fit.age.TIMES.sex)
```

```
Call:
lm(formula = sbp ~ age + sex + age:sex, data = sbpdata)

Residuals:
    Min      1Q  Median      3Q     Max 
-20.647  -3.410   1.254   4.314  21.153 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept) 97.07708    5.17046  18.775  < 2e-16 ***
age          0.94932    0.10864   8.738 1.43e-12 ***
sex1        12.96144    7.01172   1.849   0.0691 .  
age:sex1     0.01203    0.14519   0.083   0.9342    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 8.946 on 65 degrees of freedom
Multiple R-squared:  0.7759,	Adjusted R-squared:  0.7656 
F-statistic: 75.02 on 3 and 65 DF,  p-value: < 2.2e-16
```

4.8 Model Building

```r
library(olsrr)
## Note: Update this path to your local file location
wine <- read.csv("wine.csv")

model.wine <- lm(quality ~ ., data = wine)
```

4.8.1 All Possible Regression

```r
ols_step_best_subset(model.wine)
```

```
             Best Subsets Regression
-------------------------------------------------
Model Index    Predictors
-------------------------------------------------
     1         flavor
     2         flavor oakiness
     3         aroma flavor oakiness
     4         clarity aroma flavor oakiness
     5         clarity aroma body flavor oakiness
-------------------------------------------------

                                                  Subsets Regression Summary
-----------------------------------------------------------------------------------------------------
                       Adj.        Pred
Model    R-Square    R-Square    R-Square     C(p)        AIC         SBIC         SBC         MSEP
-----------------------------------------------------------------------------------------------------
  1        0.6242      0.6137      0.5868    9.0436    130.0214     21.6859    134.9341     61.4102
  2        0.6611      0.6417      0.6058    6.8132    128.0901     20.1242    134.6404     57.0033
  3        0.7038      0.6776      0.6379    3.9278    124.9781     18.0702    133.1661     51.3383
  4        0.7147      0.6801      0.6102    4.6747    125.5480     19.2854    135.3736     50.9872
  5        0.7206      0.6769       0.587    6.0000    126.7552     21.0956    138.2183     51.5452
-----------------------------------------------------------------------------------------------------
AIC: Akaike Information Criteria
 SBIC: Sawa's Bayesian Information Criteria
 SBC: Schwarz Bayesian Criteria
 MSEP: Estimated error of prediction, assuming multivariate normality
 FPE: Final Prediction Error
 HSP: Hocking's Sp
 APC: Amemiya Prediction Criteria
```

4.8.2 Automated Stepwise Procedures

```r
## Backward Elimination (alpha_out = 0.1)
ols_step_backward_p(model.wine, p_val = 0.1)
```

```
                            Stepwise Summary
------------------------------------------------------------------------
Step    Variable         AIC        SBC       SBIC       R2       Adj. R2
------------------------------------------------------------------------
 0      Full Model     126.755    138.218    21.096    0.72060    0.67694
 1      body           125.548    135.374    19.285    0.71471    0.68013
 2      clarity        124.978    133.166    18.070    0.70377    0.67763
------------------------------------------------------------------------

Final Model Output
------------------

                        Model Summary
---------------------------------------------------------------
R                       0.839       RMSE                 1.098
R-Squared               0.704       MSE                  1.207
Adj. R-Squared          0.678       Coef. Var            9.338
Pred R-Squared          0.638       AIC                124.978
MAE                     0.868       SBC                133.166
---------------------------------------------------------------
 RMSE: Root Mean Square Error
 MSE: Mean Square Error
 MAE: Mean Absolute Error
 AIC: Akaike Information Criteria
 SBC: Schwarz Bayesian Criteria

                              ANOVA
-------------------------------------------------------------------
               Sum of
              Squares        DF    Mean Square      F          Sig.
-------------------------------------------------------------------
Regression    108.935         3         36.312    26.925    0.0000
Residual       45.853        34          1.349
Total         154.788        37
-------------------------------------------------------------------

                                 Parameter Estimates
```

```
------------------------------------------------------------------------------------------
      model        Beta    Std. Error    Std. Beta       t         Sig        lower     upper
------------------------------------------------------------------------------------------
(Intercept)       6.467         1.333                  4.852     0.000        3.759     9.176
      aroma       0.580         0.262        0.307     2.213     0.034        0.047     1.113
     flavor       1.200         0.275        0.603     4.364     0.000        0.641     1.758
   oakiness      -0.602         0.264       -0.217    -2.278     0.029       -1.140    -0.065
------------------------------------------------------------------------------------------
```

```r
## Forward Selection (alpha_in = 0.1)
ols_step_forward_p(model.wine, p_val = 0.1)
```

```
                             Stepwise Summary
-------------------------------------------------------------------------
Step    Variable        AIC        SBC        SBIC        R2       Adj. R2
-------------------------------------------------------------------------
 0      Base Model    165.209    168.484    55.141    0.00000    0.00000
 1      flavor        130.021    134.934    21.686    0.62417    0.61373
 2      oakiness      128.090    134.640    20.124    0.66111    0.64175
 3      aroma         124.978    133.166    18.070    0.70377    0.67763
-------------------------------------------------------------------------

Final Model Output
------------------

                         Model Summary
----------------------------------------------------------------
R                        0.839       RMSE                 1.098
R-Squared                0.704       MSE                  1.207
Adj. R-Squared           0.678       Coef. Var            9.338
Pred R-Squared           0.638       AIC                124.978
MAE                      0.868       SBC                133.166
----------------------------------------------------------------
 RMSE: Root Mean Square Error
 MSE: Mean Square Error
 MAE: Mean Absolute Error
 AIC: Akaike Information Criteria
 SBC: Schwarz Bayesian Criteria

                               ANOVA
--------------------------------------------------------------------
               Sum of
              Squares        DF     Mean Square      F         Sig.
```

```
-------------------------------------------------------------------
Regression     108.935         3         36.312    26.925    0.0000
Residual        45.853        34          1.349
Total          154.788        37
-------------------------------------------------------------------

                                  Parameter Estimates
----------------------------------------------------------------------------------------
      model      Beta    Std. Error    Std. Beta       t        Sig      lower     upper
----------------------------------------------------------------------------------------
(Intercept)     6.467         1.333                 4.852     0.000      3.759     9.176
     flavor     1.200         0.275        0.603    4.364     0.000      0.641     1.758
   oakiness    -0.602         0.264       -0.217   -2.278     0.029     -1.140    -0.065
      aroma     0.580         0.262        0.307    2.213     0.034      0.047     1.113
----------------------------------------------------------------------------------------
```

```r
## Stepwise Regression (alpha_in = 0.1, alpha_out = 0.1)
ols_step_both_p(model.wine, p_enter = 0.1, p_remove = 0.1)
```

```

                              Stepwise Summary
--------------------------------------------------------------------------
Step    Variable         AIC        SBC       SBIC       R2        Adj. R2
--------------------------------------------------------------------------
 0      Base Model     165.209    168.484    55.141    0.00000    0.00000
 1      flavor (+)     130.021    134.934    21.686    0.62417    0.61373
 2      oakiness (+)   128.090    134.640    20.124    0.66111    0.64175
 3      aroma (+)      124.978    133.166    18.070    0.70377    0.67763
--------------------------------------------------------------------------

Final Model Output
------------------

                         Model Summary
---------------------------------------------------------------
R                       0.839       RMSE                 1.098
R-Squared               0.704       MSE                  1.207
Adj. R-Squared          0.678       Coef. Var            9.338
Pred R-Squared          0.638       AIC                124.978
MAE                     0.868       SBC                133.166
---------------------------------------------------------------
 RMSE: Root Mean Square Error
 MSE: Mean Square Error
 MAE: Mean Absolute Error
 AIC: Akaike Information Criteria
 SBC: Schwarz Bayesian Criteria

                               ANOVA
--------------------------------------------------------------------
              Sum of
             Squares        DF    Mean Square      F          Sig.
--------------------------------------------------------------------
Regression    108.935        3         36.312     26.925     0.0000
Residual       45.853       34          1.349
Total         154.788       37
--------------------------------------------------------------------

                                  Parameter Estimates
-----------------------------------------------------------------------------------------
      model        Beta    Std. Error    Std. Beta      t        Sig      lower     upper
-----------------------------------------------------------------------------------------
(Intercept)       6.467         1.333                 4.852    0.000      3.759     9.176
     flavor       1.200         0.275        0.603    4.364    0.000      0.641     1.758
   oakiness      -0.602         0.264       -0.217   -2.278    0.029     -1.140    -0.065
      aroma       0.580         0.262        0.307    2.213    0.034      0.047     1.113
-----------------------------------------------------------------------------------------
```

4.9 Multicollinearity

4.9.1 A Simple Example

```r
y <- c(19, 20, 37, 39, 36, 38)
x1 <- c(4, 4, 7, 7, 7.1, 7.1)
x2 <- c(16, 16, 49, 49, 50.4, 50.4)
cor(data.frame(x1, x2))
```

```
          x1        x2
x1 1.0000000 0.9999713
x2 0.9999713 1.0000000
```

```r
fit_multi <- lm(y ~ x1 + x2)
summary(fit_multi)
```

```

Call:
```

```
lm(formula = y ~ x1 + x2)

Residuals:
   1    2    3    4    5    6 
-0.5  0.5 -1.0  1.0 -1.0  1.0 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -156.056    117.158  -1.332    0.275
x1            65.444     45.890   1.426    0.249
x2            -5.389      4.152  -1.298    0.285

Residual standard error: 1.225 on 3 degrees of freedom
Multiple R-squared:  0.9897,	Adjusted R-squared:  0.9829 
F-statistic: 144.3 on 2 and 3 DF,  p-value: 0.001043
```

```r
fit1_multi <- lm(y ~ x1)
summary(fit1_multi)
```

```

Call:
lm(formula = y ~ x1)

Residuals:
      1       2       3       4       5       6 
-0.5260  0.4740 -0.1925  1.8075 -1.7814  0.2186 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  -4.0293     2.3332  -1.727    0.159    
x1            5.8888     0.3762  15.654 9.73e-05 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 1.325 on 4 degrees of freedom
Multiple R-squared:  0.9839,	Adjusted R-squared:  0.9799 
F-statistic: 245.1 on 1 and 4 DF,  p-value: 9.725e-05
```

```r
ols_vif_tol(fit_multi)
```

```
  Variables    Tolerance      VIF
1        x1 5.738191e-05 17427.09
2        x2 5.738191e-05 17427.09
```

4.9.2 VIFs in the Wine Quality Data

```r
wine.x <- wine[, -ncol(wine)] # Assuming quality is the last column
cor(wine.x)
```

```
            clarity     aroma       body      flavor  oakiness
clarity   1.00000000 0.0619021 -0.3083783 -0.08515993 0.1832147
aroma     0.06190210 1.0000000  0.5489102  0.73656121 0.2016444
body     -0.30837826 0.5489102  1.0000000  0.64665917 0.1521059
flavor   -0.08515993 0.7365612  0.6466592  1.00000000 0.1797605
oakiness  0.18321471 0.2016444  0.1521059  0.17976051 1.0000000
```

```r
## VIF using olsrr (data frame output)
ols_vif_tol(model.wine)
```

```
  Variables Tolerance      VIF
1   clarity 0.7896462 1.266390
2     aroma 0.4199665 2.381143
3      body 0.4862649 2.056492
4    flavor 0.3728175 2.682277
5  oakiness 0.9118005 1.096731
```

4.9.3 VIFs in the Children Height Data

```r
## Data: Weight, height and age of children
wgt <- c(64, 71, 53, 67, 55, 58, 77, 57, 56, 51, 76, 68)
hgt <- c(57, 59, 49, 62, 51, 50, 55, 48, 42, 42, 61, 57)
age <- c(8, 10, 6, 11, 8, 7, 10, 9, 10, 6, 12, 9)

fit_age_hgt <- lm(wgt ~ hgt + age, data = child.data)
ols_vif_tol(fit_age_hgt)
```

```
  Variables Tolerance      VIF
1       hgt 0.6232021 1.604616
2       age 0.6232021 1.604616
```

5 Residual Diagnostics for Regression Modelling

5.1 Introduction

Note: this html contains materials for understanding residuals not the techniques that students need to master.

5.2 Introduction

In statistical modeling, identifying data points that don't fit—the **outliers**—is a critical step. The most reliable tool for this job is the **externally studentized residual**. Its power comes from a simple, intuitive idea: to judge a point fairly, you shouldn't use that point when building your model. This is the core principle of **Leave-One-Out Cross-Validation (LOOCV)**.

This article provides a complete walkthrough of this essential concept. We'll start with the basic linear model, introduce the necessary notation, explore the flaws of simpler residuals, and then formally define and prove the equivalence of the conceptual and computational formulas for studentized residuals. Finally, we'll make it all concrete with a simple example.

5.3 The Linear Model

Our discussion is based on the standard multiple linear regression model. In matrix form, the relationship between a response vector **Y** and a predictor matrix **X** is:

$$\mathbf{Y} = \mathbf{X}\beta + \epsilon$$

where:

- **Y** is an n x 1 vector of the observed outcomes.
- **X** is the n x p design matrix of predictor variables (where p is the number of coefficients, including the intercept).
- β is the p x 1 vector of unknown true coefficients we want to estimate.
- ϵ is an n x 1 vector of unobservable random errors, assumed to be independent and identically distributed with a mean of 0 and a variance of σ^2.

5.4 Residuals for OLS

5.4.1 Our Notations

To discuss models fit with all data versus those with one point removed, we need clear notation.

Full Data Model (Using all *n* observations)

- $\hat{\beta}$: The estimated coefficient vector.
- $\hat{y}_i$: The predicted value for observation *i* from this model.
- e_i: The **ordinary residual** ($e_i = y_i - \hat{y}_i$).
- $\hat{\sigma}$: The estimated standard deviation of the errors (Residual Standard Error).
- h_{ii}: The **leverage** of observation *i*, a measure of how much its x-values influence the model.

Leave-One-Out (LOOCV) Model

- $\hat{\beta}_{-i}$: The coefficient vector estimated after **removing** observation *i*.
- $\hat{y}_{i,-i}$: The predicted value for observation *i*, from the model fit **without** observation *i*.
- $e_{i,-i}$: The **deleted residual** ($e_{i,-i} = y_i - \hat{y}_{i,-i}$).
- $\hat{\sigma}_{-i}$: The standard deviation of the errors estimated from the model fit **without** observation *i*.

5.4.2 Non-studentized Residuals

Before getting to the correct solution, it's crucial to understand why simpler methods of standardizing residuals are flawed.

5.4.2.1 The Ordinary Residual (e_i): Too Small and x_i Dependent

The most basic residual, e_i, is problematic for two key reasons.

An outlier has an undue influence on the model, pulling the regression line towards itself. This makes its own predicted value, $\hat{y}_i$, artificially close to its actual value, y_i. As a result, its residual, e_i, is **deceptively small** and doesn't reflect the true magnitude of the error.

The variance of an ordinary residual is not constant; it depends on the point's leverage. The variance can be derived from the hat matrix $H = X(X^\top X)^{-1}X^\top$. Since

$$\hat{y} = HY,$$

we have

$$e = (I - H)\epsilon. \tag{5.1}$$

Thus,

$$\text{Var}(e) = (I - H)\,\sigma^2\,(I - H)^\top = (I - H)\sigma^2. \tag{5.2}$$

Therefore, for the ith residual,

$$\text{Var}(e_i) = \sigma^2(1 - h_{ii}). \tag{5.3}$$

Since leverage (h_{ii}) is always greater than 0, the variance of an ordinary residual is always **less than the true error variance,** σ^2. High-leverage points act as "anchors" for the line and have even smaller variance.

5.4.2.2 The LOOCV Residual ($e_{i,-i}$): Too large and x_i-Dependent Variance

The deleted residual, $e_{i,-i}$, solves the "too small" problem. Because the model isn't influenced by the point it's predicting, the residual is an honest measure of prediction error. However, its variance is still not constant. The variance of a deleted residual also depends on leverage, but in the opposite way.

$$\text{Var}(e_{i,-i}) = \frac{\sigma^2}{1 - h_{ii}} \tag{5.4}$$

From the key identity Equation 5.13,

$$e_{i,-i} = \frac{e_i}{1 - h_{ii}}. \tag{5.5}$$

Therefore,

$$\text{Var}(e_{i,-i}) = \frac{\text{Var}(e_i)}{(1 - h_{ii})^2} = \frac{\sigma^2(1 - h_{ii})}{(1 - h_{ii})^2} = \frac{\sigma^2}{1 - h_{ii}}. \tag{5.6}$$

Since $1 - h_{ii}$ is less than 1, the variance of a deleted residual is always **greater than the true error variance,** σ^2. This is because it has two sources of randomness: the error in the point itself (y_i) and the error in the prediction ($\hat{y}_{i,-i}$).

5.4.3 Studentized Residuals

5.4.3.1 Studentized LOOCV (Deleted) Residual

The correct solution is to take the LOOCV residual and divide it by its true standard error, which properly accounts for its larger, x-dependent variance. This is the **externally studentized residual**, t_i, defined as follows:

$$t_i = \frac{e_{i,-i}}{\text{SE}(e_{i,-i})} = \frac{e_{i,-i}}{\frac{\hat{\sigma}_{-i}}{\sqrt{1-h_{ii}}}} \tag{5.7}$$

This final value is a reliable diagnostic. Under the null hypothesis that the observation is not an outlier, it follows a **Student's t-distribution** with $n - p - 1$ degrees of freedom.

5.4.3.2 Studentized Full Data Residuals

Calculating the conceptual formula appears to require fitting *n* different regression models—a computationally expensive task. Fortunately, a mathematical identity allows us to calculate the exact same value using only the results from the single, full data model.

$$t_i = \frac{e_i}{\hat{\sigma}_{-i}\sqrt{1-h_{ii}}} \tag{5.8}$$

This is not an approximation; it is an **exact algebraic rearrangement** of the conceptual definition.

5.4.3.3 Equivalence of Equation 5.8 and Equation 5.7

5.4.3.3.1 Proof of Equivalence

Let's start with the conceptual definition of the studentized LOOCV residuals Equation 5.7 and show how it transforms into Equation 5.8.

- **Start with the conceptual LOOCV definition:**

$$t_i = \frac{e_{i,-i}}{\text{SE}(e_{i,-i})} = \frac{e_{i,-i}}{\frac{\hat{\sigma}_{-i}}{\sqrt{1-h_{ii}}}} \tag{5.9}$$

- **Substitute the key identity** into the numerator:

$$t_i = \frac{\frac{e_i}{1-h_{ii}}}{\frac{\hat{\sigma}_{-i}}{\sqrt{1-h_{ii}}}} \tag{5.10}$$

- **Simplify the complex fraction.** We can do this by multiplying the numerator by the reciprocal of the denominator:

$$t_i = \frac{e_i}{1-h_{ii}} \cdot \frac{\sqrt{1-h_{ii}}}{\hat{\sigma}_{-i}} \tag{5.11}$$

- **Cancel the terms.** Since $1-h_{ii} = (\sqrt{1-h_{ii}})^2$, one of the $\sqrt{1-h_{ii}}$ terms in the denominator cancels with the term in the numerator. This leaves us with the computational shortcut formula:

$$t_i = \frac{e_i}{\hat{\sigma}_{-i}\sqrt{1-h_{ii}}} \tag{5.12}$$

This proves that the two formulas are mathematically identical. The computational shortcut is simply a clever algebraic rearrangement of the more intuitive LOOCV definition, allowing for efficient and accurate calculation. □

Of course. Here is the modified `.qmd` file with the **standardized residual** (which you've labeled **STD-Full**) added to the table, the descriptions, and the plot.

The main changes include:

1. Adding the `STD-Full` column to the `residuals_df` data frame using R's `rstandard()` function.
2. Updating the list of calculated columns to include a description of **STD-Full**.
3. Modifying the plotting code to include **STD-Full** with its own distinct color and shape.

5.4.4 List of Residuals

In this article, we will compare the four residuals given as:

Table 5.1

Short Name	Full Name	Formula
NS-Full	Non-studentized Full-Data Residual	$\frac{e_i}{\hat{\sigma}}$
NS-LOO	Non-studentized LOOCV Residual	$\frac{e_{i,-i}}{\hat{\sigma}_{-i}}$
ST-LOO	Studentized LOOCV Residual	$\frac{e_{i,-i}}{\hat{\sigma}_{-i}/\sqrt{1-h_{ii}}}$
ST-Full	Studentized Full-Data Residual	$\frac{e_i}{\hat{\sigma}_{-i}\sqrt{1-h_{ii}}}$
STD-Full	Standardized (Internal Studentized) Residual	$\frac{e_i}{\hat{\sigma}\sqrt{1-h_{ii}}}$

5.4.5 Example of Various Residuals

5.4.5.1 The Linear Model

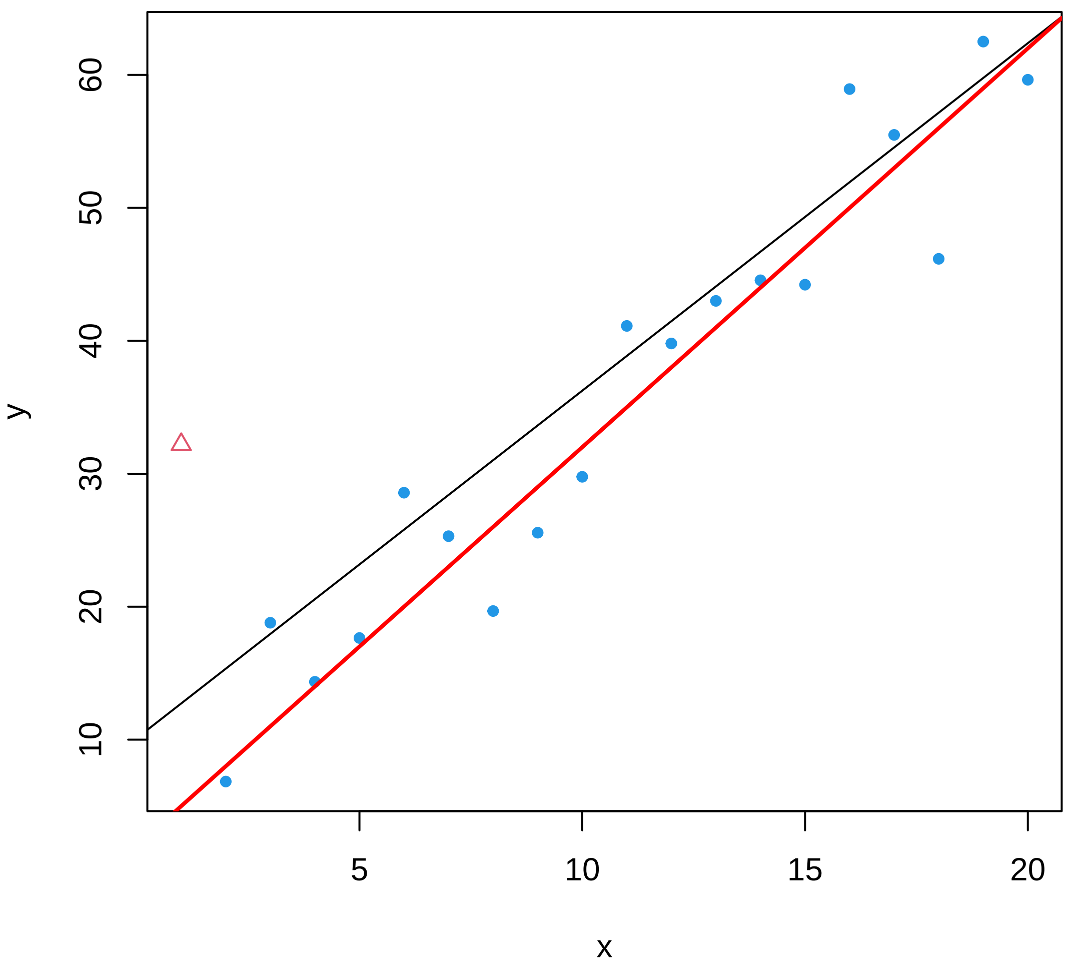
The simulation uses a **simple linear regression model** to describe the relationship between a single predictor variable, x_i, and a response variable, y_i. The underlying "true" model from which the data is generated is:

$$y_i = 2 + 3x_i + \epsilon_i$$

This means we have a true intercept of 2, a true slope of 3, and a random error term, ϵ_i, drawn from a normal distribution with a mean of 0 and a standard deviation of 5. One artificial outlier is added to this data to test the behavior of the different residual types. 5 unrelated predictors are added to the dataset.

```r
## Load libraries
library(dplyr)
library(knitr)

## -------------------------------
## 1) Data and full-model fit
## -------------------------------
set.seed(123)
n <- 20
x <- 1:n
```

```
y <- 2 + 3 * x + rnorm(n, mean = 0, sd = 5)
y[1] <- y[1] + 30
#y[11] <- y[11] - 30
o.index <- c(1)
flag.outlier <- rep(20, n)
flag.outlier[o.index] <- 2
full_data  <- data.frame(x = x, replicate(5, rnorm (n)), y = y)

plot(y~x, data=full_data, pch= flag.outlier, col=flag.outlier)
fit <- lm(y~., data=full_data)
abline (fit)
abline (a=2, b=3, col="red", lwd=2)
```



5.4.5.2 Description of Calculated Columns

The final table compiles several important quantities calculated during the simulation. Here's what each column represents:

- x_i: The predictor variable, which is simply the index of the observation from 1 to 20.
- h_i: The **leverage** of the i-th observation. It measures how influential a point's x-value is in determining the model's fit. A higher value indicates a more influential point.
- e_i: The **ordinary residual**, calculated as the difference between the actual value (y_i) and the predicted value ($\hat{y}_i$) from the model fit on all data.
- $\hat{\sigma}$: The **residual standard error** (or Root Mean Square Error) of the full model, representing the typical size of an ordinary residual.
- $e_{i,-i}$: The **deleted (or LOOCV) residual**. This is the difference between the actual value (y_i) and the value predicted for it by a model that was fit on all other data *except* point *i*.
- $\hat{e}_{i,-i}$: This column shows the deleted residual calculated using the efficient algebraic shortcut ($e_i/(1-h_{ii})$), verifying it's identical to the brute-force $e_{i,-i}$.
- $\hat{\sigma}_{-i}$: The **LOOCV residual standard error**, calculated from a model that was fit after removing observation *i*.
- $\tilde{\sigma}_{-i}$: The **LOOCV residual standard error**, calculated from the shortcut formula **?@eq-sigma_**-i.
- **NS-Full**: The **Non-studentized Full-Data Residual**, calculated as the ordinary residual divided by the full model's standard error ($e_i/\hat{\sigma}$).
- **NS-LOO**: The **Non-studentized LOOCV Residual**, calculated as the deleted residual divided by the corresponding LOOCV standard error ($e_{i,-i}/\hat{\sigma}_{-i}$).
- **STD-Full**: The **Standardized (or Internally Studentized) Residual**, calculated as the ordinary residual divided by its estimated standard error ($e_i/(\hat{\sigma}\sqrt{1-h_{ii}})$). This is provided by R's `rstandard()` function.
- **ST-LOO**: The **Studentized LOOCV Residual**, calculated using the conceptual formula by dividing the deleted residual by its true standard error.
- **ST-Full**: The **Studentized Full-Data Residual**, calculated using the efficient shortcut formula, which is provided by R's `rstudent()` function.

```r
library(kableExtra)

full_model <- lm(y ~ ., data = full_data)
p <- length(coef(full_model))
leverage    <- hatvalues(full_model)
e_full      <- resid(full_model)
sigma_hat_val  <- summary(full_model)$sigma

rss_full <- sum(e_full^2)
df_loo <- n - p - 1
sigma_minus_i_shortcut <- sqrt((rss_full - (e_full^2 / (1 - leverage))) / df_loo)

## -------------------------------
## 2) LOOCV quantities (refit n times)
## --------------------------------
e_del_val <- numeric(n)
sigma_minus_i_val <- numeric(n)

for (i in 1:n) {
  loocv_model <- lm(y ~ ., data = full_data[-i, ])
  yhat_minus  <- predict(loocv_model, newdata = full_data[i, , drop = FALSE])
  e_del_val[i]    <- full_data$y[i] - yhat_minus
  sigma_minus_i_val[i] <- summary(loocv_model)$sigma
}

## --------------------------------
## 3) Assemble and round results
## --------------------------------
residuals_df <- data.frame(
  x = full_data$x,
  h = as.numeric(leverage),
  e_i = as.numeric(e_full),
  sigma_hat = as.numeric(sigma_hat_val),
  e_i_minus_i = as.numeric(e_del_val),
  e_i_minus_i_2 = e_full/(1-leverage),
  sigma_minus_i = as.numeric(sigma_minus_i_val),
  sigma_minus_i_shortcut = as.numeric(sigma_minus_i_shortcut),
  `NS-Full` = e_full / sigma_hat_val,
  `NS-LOO` = e_del_val / sigma_minus_i_val,
  `STD-Full` = rstandard(full_model), # <-- ADDED STANDARDIZED RESIDUAL
  `ST-LOO` = e_del_val / (sigma_minus_i_val / sqrt(1 - leverage)),
  `ST-Full` = rstudent(full_model)
) %>%
  mutate(across(where(is.numeric), ~ round(.x, 3)))


## 4) Create simple display names
display_names <- c("$x_i$", "$h_i$", "$e_i$", "$\\hat{\\sigma}$",
                   "$e_{i,-i}$", "$\\hat{e}_{i,-i}$",
                   "$\\hat{\\sigma}_{-i}$", "$\\tilde{\\sigma}_{-i}$",
                   "NS-Full", "NS-LOO", "STD-Full", "ST-LOO", "ST-Full") # <-- ADDED LABEL

## 5) Display the table
## Conditional check for output format
if (knitr::is_html_output()) {
  ## --- Code for HTML Output (using kableExtra) ---
  knitr::kable(
    residuals_df,
    caption = "Residual variants",
    col.names = display_names,
    align = "r",
    #format="html",
    escape = FALSE # Allows LaTeX and <br/> to render
  )
} else {
  ## --- Code for PDF/Other Output (using kableExtra) ---
  knitr::kable(
    residuals_df,
    caption = "Residual variants.",
    col.names = display_names,
    align = "r",
    format = "latex",
    booktabs = TRUE,
    escape = FALSE # Allows LaTeX and \\ to render
  ) %>%
    kable_styling(
      latex_options = "scale_down"
    )
}
```

```r
## Load libraries
library(dplyr)
library(tidyr)
library(ggplot2)
library(knitr)


## -------------------------------
## 3) Plotting Code with Updated Names
## -------------------------------

## Prepare data for plotting
plot_df <- residuals_df %>%
  ## Use the new, simple column names (R converts '-' to '.')
  select(
    x,
    NS.Full,
    NS.LOO,
    STD.Full, # <-- ADDED FOR PLOTTING
    ST.LOO,
    ST.Full
  ) %>%
```

Table 5.2: Residual variants.

x_i	h_i	e_i	$\widehat{\sigma}$	$e_{i,-i}$	$\widehat{e}_{i,-i}$	$\widehat{\sigma}_{-i}$	$\widetilde{\sigma}_{-i}$	NS-Full	NS-LOO	STD-Full	ST-LOO	ST-Full
1	0.247	17.638	7.57	23.434	23.434	5.257	5.257	2.330	4.457	2.686	3.867	3.867
2	0.241	-7.909	7.57	-10.418	-10.418	7.431	7.431	-1.045	-1.402	-1.199	-1.222	-1.222
3	0.364	-3.271	7.57	-5.147	-5.147	7.790	7.790	-0.432	-0.661	-0.542	-0.527	-0.527
4	0.555	1.553	7.57	3.490	3.490	7.851	7.851	0.205	0.445	0.308	0.297	0.297
5	0.257	-1.515	7.57	-2.038	-2.038	7.863	7.863	-0.200	-0.259	-0.232	-0.223	-0.223
6	0.400	-0.400	7.57	-0.666	-0.666	7.878	7.878	-0.053	-0.085	-0.068	-0.066	-0.066
7	0.253	0.247	7.57	0.331	0.331	7.879	7.879	0.033	0.042	0.038	0.036	0.036
8	0.303	-8.972	7.57	-12.871	-12.871	7.243	7.243	-1.185	-1.777	-1.419	-1.484	-1.484
9	0.347	-8.394	7.57	-12.852	-12.852	7.287	7.287	-1.109	-1.764	-1.372	-1.425	-1.425
10	0.573	-5.696	7.57	-13.342	-13.342	7.467	7.467	-0.752	-1.787	-1.152	-1.168	-1.168
11	0.117	7.175	7.57	8.127	8.127	7.565	7.565	0.948	1.074	1.009	1.009	1.009
12	0.441	0.998	7.57	1.786	1.786	7.870	7.870	0.132	0.227	0.176	0.170	0.170
13	0.359	1.298	7.57	2.026	2.026	7.865	7.865	0.171	0.258	0.214	0.206	0.206
14	0.395	0.698	7.57	1.153	1.153	7.875	7.875	0.092	0.146	0.119	0.114	0.114
15	0.228	-1.221	7.57	-1.583	-1.583	7.869	7.869	-0.161	-0.201	-0.184	-0.177	-0.177
16	0.402	7.998	7.57	13.365	13.365	7.292	7.292	1.057	1.833	1.366	1.418	1.418
17	0.433	3.996	7.57	7.048	7.048	7.729	7.729	0.528	0.912	0.701	0.687	0.687
18	0.414	-3.369	7.57	-5.746	-5.746	7.776	7.776	-0.445	-0.739	-0.581	-0.566	-0.566
19	0.258	3.073	7.57	4.141	4.141	7.812	7.812	0.406	0.530	0.471	0.457	0.457
20	0.414	-3.930	7.57	-6.707	-6.707	7.739	7.739	-0.519	-0.867	-0.678	-0.663	-0.663

```r
  pivot_longer(
    cols = -x,
    names_to = "residual_type",
    values_to = "residual_value"
  )

## Update the names in the mapping vectors
shape_map <- c(
  NS.Full  = 16,  # solid circle
  NS.LOO   = 1,   # hollow circle
  STD.Full = 2,   # hollow triangle <-- ADDED
  ST.LOO   = 6,   # asterisk
  ST.Full  = 10   # asterisk
)

labels_map <- c(
  NS.Full  = "NS-Full",
  NS.LOO   = "NS-LOO",
  STD.Full = "STD-Full", # <-- ADDED
  ST.LOO   = "ST-LOO",
  ST.Full  = "ST-Full"
)

color_map <- c(
  NS.Full  = "#1f77b4",  # blue
  NS.LOO   = "#ff7f0e", # orange
  STD.Full = "#9467bd",  # purple <-- ADDED
  ST.LOO   = "#2ca02c",  # green
  ST.Full  = "#d62728"   # red
)

## Generate the plot
ggplot(
  plot_df,
  aes(x = x, y = residual_value,
      shape = residual_type, color = residual_type, group = residual_type)
) +
  geom_hline(yintercept = 0, linetype = "dashed") +
  geom_point(size = 3, stroke = 1.2) + # Increased stroke for visibility
  scale_shape_manual(
    values = shape_map,
    breaks = names(labels_map),
    labels = unname(labels_map),
    name = "Residual Type"
  ) +
  scale_color_manual(
    values = color_map,
    breaks = names(labels_map),
    labels = unname(labels_map),
    name = "Residual Type"
  ) +
  labs(
    title = "Five Residual Variants vs x",
    x = "x_i",
    y = "Residual value"
  ) +
  theme_bw() +
  theme(
    legend.position = "right",
    legend.title = element_text(face = "bold")
  )
```

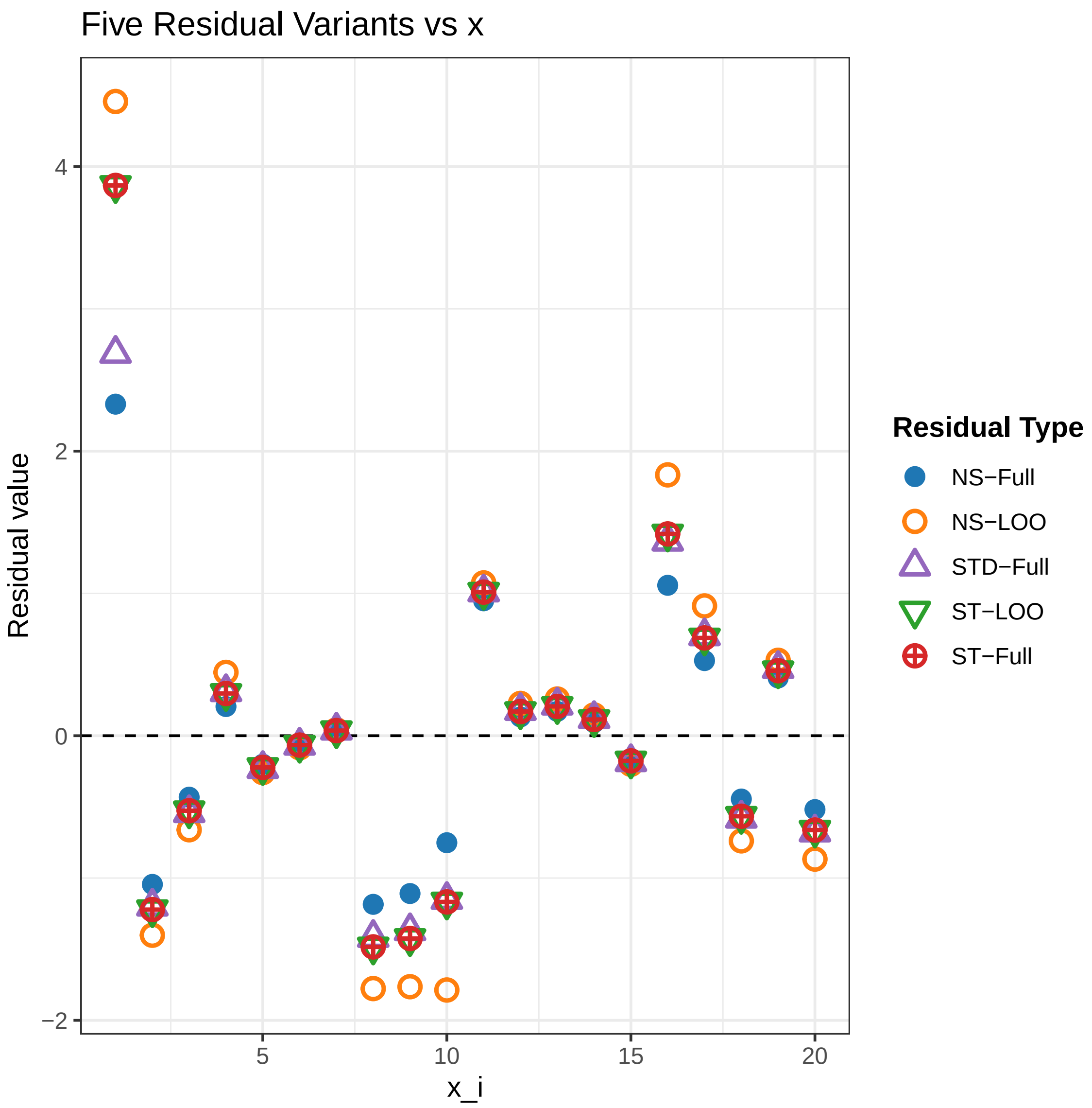


Figure 5.1: Five residual variants plotted against the predictor variable x.

From the above simulation results, we observe the following important facts:

- **Leverage and Influence:** The simulation confirms that leverage (h_{ii}) measures an observation's influence on the model's coefficients. It shows that points with higher leverage pull the regression line toward them, resulting in smaller, deceptively conservative full-data residuals (e_i).
- **Conservative Residuals:** The study highlights that the ordinary residual (e_i) is a "conservative" measure of error because its value for an outlier is systematically reduced by that same outlier's influence on the model.
- **Identity Verification:** The numerical results validated the key algebraic identity that connects the full-data residual (e_i) to the leave-one-out (deleted) residual ($e_{i,-i}$), as well as the identity for calculating the

LOOCV standard error ($\hat{\sigma}_{-i}$) from the full model's statistics. This demonstrates that all key LOOCV errors can be calculated efficiently from a single model fit.

- **Effective Studentization:** The final step of studentization, which uses leverage to properly scale the residuals, is shown to be crucial. It successfully transforms the residuals into a reliable diagnostic tool with a constant variance across all predictor values (x_i), causing them to behave much more like a standard normal or t-distribution.

5.5 Cook's Distance

5.5.1 Definition from the change in coefficients

Let $\hat{\beta}$ be the OLS estimate on all n cases and $\hat{\beta}_{(-i)}$ the estimate after deleting case i.
With p parameters (including intercept) and $\hat{\sigma}^2 = \text{MSE}$,

$$D_i = \frac{\big(\hat{\beta} - \hat{\beta}_{(-i)}\big)^\top (X^\top X)\,\big(\hat{\beta} - \hat{\beta}_{(-i)}\big)}{p\,\hat{\sigma}^2}\,.$$

This measures how far the whole coefficient vector moves (in the $X^\top X$ metric) when case i is removed, scaled **per parameter**.

5.5.1.1 Express D_i via the studentized LOOCV residual: t_i

Let h_{ii} be the leverage and define the LOOCV quantities $e_{i,-i}$ and $\hat{\sigma}_{-i}$ from the model refit **without** case i.
The externally studentized residual is

$$t_i = \frac{e_i}{\hat{\sigma}_{-i}\sqrt{1-h_{ii}}} = \frac{e_{i,-i}\sqrt{1-h_{ii}}}{\hat{\sigma}_{-i}}, \qquad \text{since} \quad e_{i,-i} = \frac{e_i}{1-h_{ii}}.$$

Then Cook's distance can be written as

$$D_i = \frac{n-p}{p}\,\frac{h_{ii}}{1-h_{ii}}\,\frac{t_i^2}{(n-p-1)+t_i^2}\,.$$

5.5.1.2 Exact null distribution

Under the classical linear model,

$$t_i^2 \sim F_{1,\,\nu}, \qquad \nu = n - p - 1.$$

Let

$$c_i = \frac{n-p}{p} \cdot \frac{h_{ii}}{1-h_{ii}}, \qquad W_i = \frac{t_i^2}{\nu + t_i^2}.$$

Because $t_i^2 \sim F_{1,\nu}$,

$$W_i \sim \text{Beta}\!\left(\tfrac{1}{2}, \tfrac{\nu}{2}\right), \qquad \frac{D_i}{c_i} = W_i \in [0,1]\,.$$

This yields exact, per–case p-values and critical values:

$$p_i = \Pr\!\left(W_i \ge \frac{D_i}{c_i}\right) = S_{\text{Beta}}\!\left(\frac{D_i}{c_i};\, \tfrac{1}{2},\, \tfrac{n-p-1}{2}\right),$$

$$d_{i,\alpha} = c_i\, q_{\text{Beta}}\!\left(1-\alpha;\, \tfrac{1}{2},\, \tfrac{n-p-1}{2}\right).$$

where S_{Beta} and q_{Beta} stand for the survival and quantile functions of Beta distribution.

5.5.1.3 The rough $4/n$ rule (average-leverage simplification)

Approximating a "typical" case by **average leverage** $h_{ii} \approx p/n$ gives

$$c_i = \frac{n-p}{p} \cdot \frac{p/n}{1-p/n} \approx 1.$$

The 95th percentile of W_i is

$$\text{qbeta}\!\left(0.95;\, \tfrac{1}{2},\, \tfrac{n-p-1}{2}\right) \;\approx\; \frac{F_{1,\nu,\,0.95}}{\nu + F_{1,\nu,\,0.95}} \;\approx\; \frac{3.84}{n-p-1} \;\approx\; \frac{4}{n} \quad (\text{when } p \ll n).$$

So $4/n$ is a **rule-of-thumb** 95% cutoff for an **average-leverage** point; the exact leverage–aware cutoff is $d_{i,\alpha}$ above (larger for high h_{ii}, smaller for low h_{ii}).

5.5.1.4 Comparing $4/n$ rules with the actual critical values

```r
library(dplyr)
library(tidyr)
library(gt)

## Exact 95% Cook's D cutoff under average leverage h_ii = p/n (so c_i = 1):
## d_{i,0.95} = qbeta(0.95; 1/2, (n - p - 1)/2), valid when nu = n - p - 1 > 0
cook_crit_avg <- function(n, p, alpha = 0.05) {
  nu <- n - p - 1
  if (nu <= 0) return(NA_real_)
  stats::qbeta(1 - alpha, shape1 = 0.5, shape2 = nu / 2)
}

## Grids (edit as needed)
n_vals <- c(20, 30, 50, 80)
p_vals <- c(2, 3, 5, 10)

df <- tidyr::crossing(n = n_vals, p = p_vals) %>%
  mutate(valid = p <= n - 2,
         nu    = n - p - 1L) %>%
  rowwise() %>%
  mutate(
    cook_crit_95 = if (valid) cook_crit_avg(n, p, 0.05) else NA_real_,
    `4/n`        = 4 / n,
    ratio        = cook_crit_95 / `4/n`,
    `p/n`        = p / n
  ) %>%
  ungroup() %>%
  filter(valid) %>%
  select(n, p, `p/n`, nu, cook_crit_95, `4/n`, ratio) %>%
  mutate(
    `p/n`         = round(`p/n`, 3),
    cook_crit_95  = round(cook_crit_95, 6),
    `4/n`         = round(`4/n`, 6),
    ratio         = round(ratio, 4)
  )

df |>
  gt() |>
  cols_label(
    n            = md("$n$"),
    p            = md("$p$"),
    `p/n`        = md("$p/n$"),
```

Table 5.3: Exact 95% Cook's D critical value (average leverage $h_{ii} = p/n \Rightarrow c_i = 1$) vs heuristic $4/n$.

n	p	p/n	$\nu = n - p - 1$	$d_{i,0.95}$	$4/n$	$d_{i,0.95}/(4/n)$
20	2	0.100	17	0.207508	0.200000	1.0375
20	3	0.150	16	0.219284	0.200000	1.0964
20	5	0.250	14	0.247316	0.200000	1.2366
20	10	0.500	9	0.362487	0.200000	1.8124
30	2	0.067	27	0.134893	0.133333	1.0117
30	3	0.100	26	0.139791	0.133333	1.0484
30	5	0.167	24	0.150733	0.133333	1.1305
30	10	0.333	19	0.187366	0.133333	1.4052
50	2	0.040	47	0.079282	0.080000	0.9910
50	3	0.060	46	0.080951	0.080000	1.0119
50	5	0.100	44	0.084510	0.080000	1.0564
50	10	0.200	39	0.094944	0.080000	1.1868
80	2	0.025	77	0.048973	0.050000	0.9795
80	3	0.038	76	0.049605	0.050000	0.9921
80	5	0.062	74	0.050920	0.050000	1.0184
80	10	0.125	69	0.054533	0.050000	1.0907

```r
    nu           = md("$\\nu = n - p - 1$"),
    cook_crit_95 = md("$d_{i,0.95}$"),
    `4/n`        = md("$4/n$"),
    ratio        = md("$d_{i,0.95} / (4/n)$")
  ) |>
  cols_align(
    align   = "right",
    columns = everything()
  )
```

5.5.2 Example for Cook's Distance:

```r
library(dplyr)
library(ggplot2)
library(knitr)

## --- 1) Data and full-model fit (your setup)

n <- 20
x <- 1:n
```

```
y <- 2 + 3 * x + rnorm(n, mean = 0, sd = 5)
y[1] <- y[1] + 30   # add an outlier at i = 1
y[11] <- y[11] + 30
full_data  <- data.frame(x = x, replicate(5, rnorm(n)), y = y)

fit <- lm(y ~ ., data = full_data)

## --- 2) Ingredients for Cook's D and thresholds
p      <- length(coef(fit))        # includes intercept
h      <- hatvalues(fit)           # leverage h_ii
D      <- cooks.distance(fit)      # Cook's D_i
nu     <- n - p - 1                # df for deleted-studentized residual
alpha  <- 0.05

## Per-case scaling factor: c_i = ((n-p)/p) * (h_ii/(1-h_ii))
c_i        <- ((n - p) / p) * (h / (1 - h))

## Exact per-case Beta 95% critical values:
## D_i / c_i ~ Beta(1/2, (n-p-1)/2)  =>  D_crit_i = c_i * qbeta(0.95, 1/2, (n-p-1)/2)
crit_beta_i <- c_i * qbeta(1 - alpha, shape1 = 0.5, shape2 = nu / 2)

## Average-leverage Beta 95% critical value:
## If h_ii = p/n (average leverage), then c_i = 1 exactly
crit_beta_avg <- qbeta(1 - alpha, shape1 = 0.5, shape2 = nu / 2)

## Heuristic 4/n line
crit_heur <- 4 / n

## --- 3) Assemble results table
df_cook <- tibble(
  i             = seq_len(n),
  h_ii          = as.numeric(h),
  D_i           = as.numeric(D),
  c_i           = as.numeric(c_i),
  crit_beta_i   = as.numeric(crit_beta_i),
  crit_beta_avg = crit_beta_avg,
  crit_heur     = crit_heur
)

## Print a compact table
knitr::kable(
  df_cook %>% mutate(across(where(is.numeric), ~ round(.x, 5))),
  caption = "Cook's D, leverage, and thresholds: per-case Beta 95%, average-leverage Beta 95%,
)
```

Table 5.4: Cook's D, leverage, and thresholds: per-case Beta 95%, average-leverage Beta 95%, and 4/n.

i	h_ii	D_i	c_i	crit_beta_i	crit_beta_avg	crit_heur
1	0.67204	1.62738	3.80555	1.07873	0.28346	0.2
2	0.31296	0.07715	0.84595	0.23979	0.28346	0.2
3	0.49722	0.08784	1.83660	0.52061	0.28346	0.2
4	0.61111	0.23875	2.91831	0.82724	0.28346	0.2
5	0.21633	0.02983	0.51265	0.14532	0.28346	0.2
6	0.14309	0.00469	0.31011	0.08790	0.28346	0.2
7	0.47629	0.07632	1.68900	0.47877	0.28346	0.2
8	0.41204	0.00004	1.30148	0.36892	0.28346	0.2
9	0.40499	0.29801	1.26407	0.35832	0.28346	0.2
10	0.17593	0.00026	0.39648	0.11239	0.28346	0.2
11	0.39917	0.73199	1.23380	0.34974	0.28346	0.2
12	0.10715	0.00088	0.22287	0.06318	0.28346	0.2
13	0.21158	0.01277	0.49837	0.14127	0.28346	0.2
14	0.30757	0.00026	0.82491	0.23383	0.28346	0.2
15	0.26786	0.04549	0.67944	0.19260	0.28346	0.2
16	0.71261	0.48354	4.60490	1.30532	0.28346	0.2
17	0.20630	0.01202	0.48271	0.13683	0.28346	0.2
18	0.27965	0.00082	0.72098	0.20437	0.28346	0.2
19	0.29482	0.03388	0.77642	0.22009	0.28346	0.2
20	0.29132	0.00775	0.76341	0.21640	0.28346	0.2

Cook's D by case with heuristic 4/n (red dotted), per-case Beta 95% critical values (blue dashed), and average-leverage Beta 95% line (purple dot-dash).

```r
## --- 4) Plot D_i with thresholds
thresh_df <- bind_rows(
  df_cook %>% transmute(i, value = crit_beta_i,   Type = "Beta 95% (per-case)"),
  tibble(i = seq_len(n), value = crit_beta_avg,   Type = "Beta 95% (avg leverage)"),
  tibble(i = seq_len(n), value = crit_heur,       Type = "4/n rule")
)

ggplot(df_cook, aes(x = i, y = D_i)) +
  geom_point(size = 2) +
  geom_line(data = thresh_df,
            aes(y = value, color = Type, linetype = Type),
            linewidth = 0.9) +
  scale_color_manual(values = c(
    "Beta 95% (per-case)"      = "#1f77b4",
    "Beta 95% (avg leverage)"  = "#7f3c8d",
    "4/n rule"                 = "#d62728"
  )) +
  scale_linetype_manual(values = c(
    "Beta 95% (per-case)"       = "dashed",
    "Beta 95% (avg leverage)"   = "dotdash",
    "4/n rule"                  = "dotted"
  )) +
  labs(x = "Observation i", y = "Cook's D_i") +
  theme_bw() +
  theme(legend.title = element_blank())
```

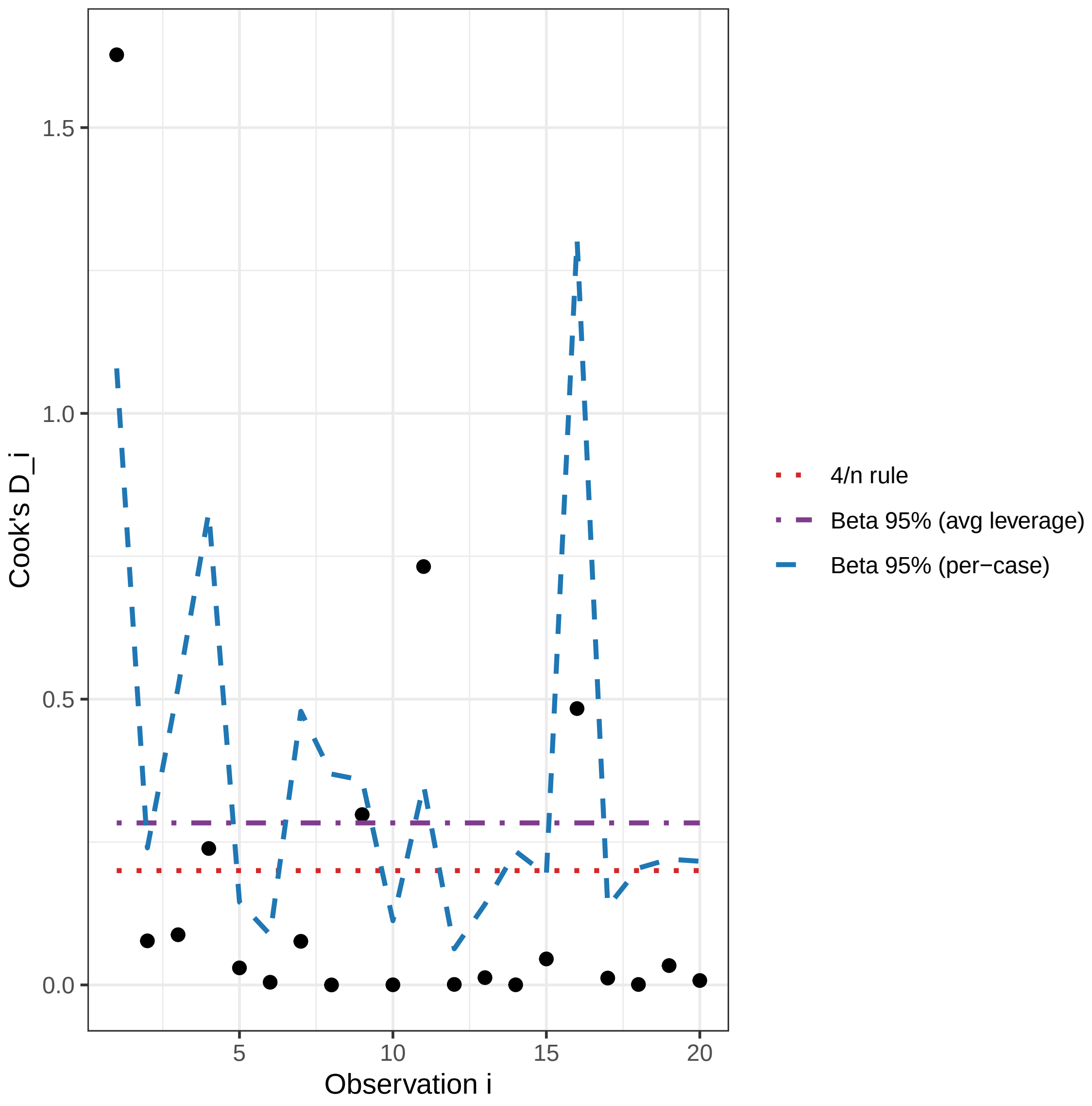


Figure 5.2: Cook's D by case with heuristic 4/n (red dotted), per-case Beta 95% critical values (blue dashed), and average-leverage Beta 95% line (purple dot-dash).

Appendix: Key Identities

The power of modern regression diagnostics comes from algebraic shortcuts that allow us to find the results of a leave-one-out process without the computational cost of refitting the model *n* times. The following two identities are fundamental to this efficiency.

Finding the LOOCV Residual ($e_{i,-i}$) from the Ordinary Residual (e_i)

This identity shows that we can find the "pure" leave-one-out residual using only the results from the single model fit on all data.

$$e_{i,-i} = \frac{e_i}{1-h_{ii}} \tag{5.13}$$

Finding the LOOCV Standard Error from the Full-Model Standard Error

Similarly, this formula provides an efficient shortcut to see how the model's overall error changes when a single point is removed.

$$\hat{\sigma}_{-i} = \sqrt{\frac{(n-p)\hat{\sigma}^2 - \frac{e_i^2}{1-h_{ii}}}{n-p-1}} \tag{5.14}$$

The derivation of this formula relies on first proving the relationship between the full model's Residual Sum of Squares (RSS) and the leave-one-out version (RSS_{-i}).

1. **Start with the definition** of the leave-one-out residual sum of squares:
$$RSS_{-i} = \sum_{k\neq i}(y_k - \mathbf{x}_k^T\hat{\beta}_{-i})^2$$

2. **Introduce the key identity** that relates the leave-one-out coefficient vector ($\hat{\beta}_{-i}$) to the full model's coefficient vector ($\hat{\beta}$):
$$\hat{\beta}_{-i} = \hat{\beta} - (X^TX)^{-1}\mathbf{x}_i\frac{e_i}{1-h_{ii}}$$

3. **Substitute this identity** into the expression for a generic leave-one-out residual, $e_{k,-i} = y_k - \mathbf{x}_k^T\hat{\beta}_{-i}$. After simplification, this yields:
$$e_{k,-i} = e_k + h_{ki}\frac{e_i}{1-h_{ii}}$$
where e_k is the ordinary residual and h_{ki} is the (k,i)-th element of the hat matrix.

4. **Substitute this back into the definition of** RSS_{-i}. After expanding the squared term and performing the summation (which involves considerable but standard matrix algebra), the expression simplifies to the elegant result:

$$RSS_{-i} = RSS - \frac{e_i^2}{1 - h_{ii}}$$

5. **Finally, derive the formula for** $\hat{\sigma}_{-i}$. We know that $\hat{\sigma}_{-i}^2 = \frac{RSS_{-i}}{n-p-1}$ and that $RSS = (n-p)\hat{\sigma}^2$. By substituting the result from Step 4, we arrive at the formula for the variance, and taking the square root gives us the standard error.

6 Logistic Regression

6.1 Odds as a Function of Probability

For an event with probability p, the odds is

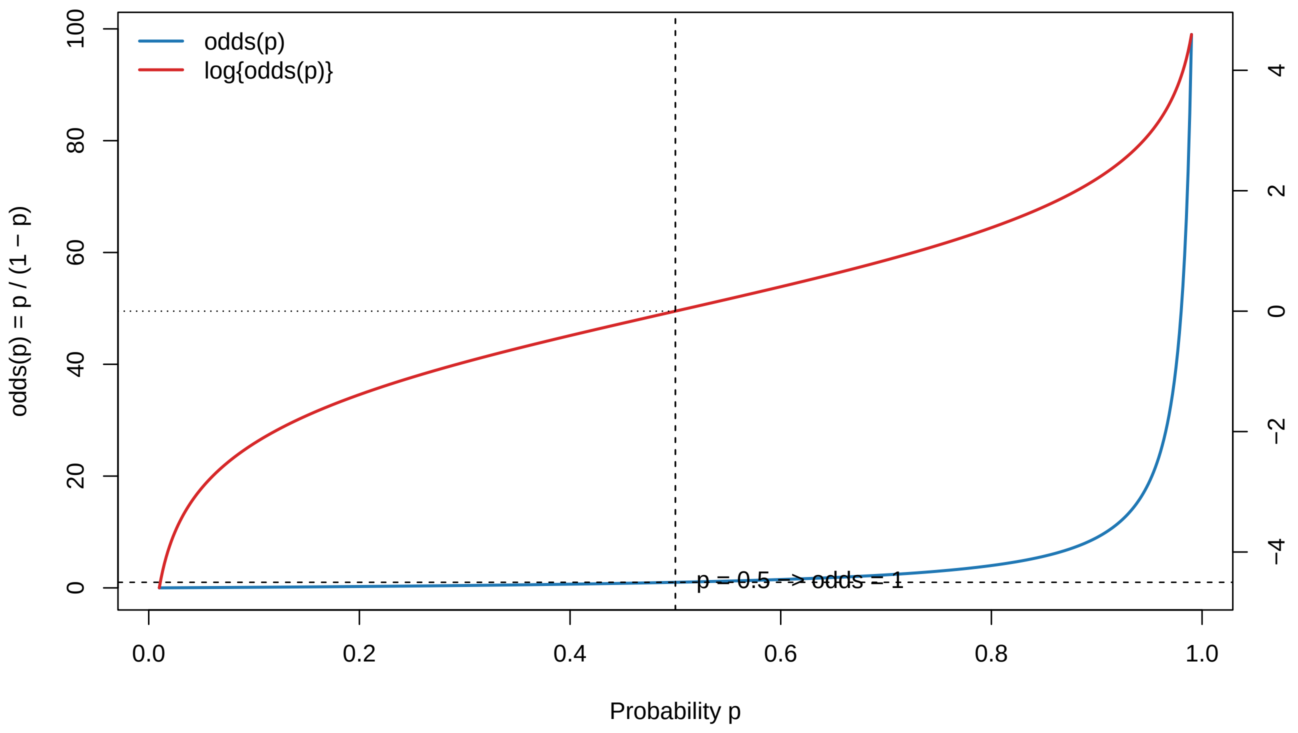
$$\text{odds}(p) = \frac{p}{1-p}$$

and the log-odds (logit) is

$$\text{logit}(p) = \log\left(\frac{p}{1-p}\right)$$

.

```r
## Plot odds(p) with a right-hand axis for log(odds(p)),
## using different line colors for the two curves.
## Defaults: p in [0.01, 0.99].
## Args:
##   p_min, p_max : endpoints for p-grid (0<p_min<p_max<1)
##   n            : number of grid points
##   annotate     : add reference lines/labels if TRUE
##   odds_col     : color for odds(p)
##   logit_col    : color for log(odds(p))
##   lwd1, lwd2   : line widths for the two curves


plot_odds <- function(p_min = 0.01, p_max = 0.99, n = 400,
                      annotate = TRUE,
                      odds_col = "steelblue",
                      logit_col = "firebrick",
                      lwd1 = 2, lwd2 = 2) {
  stopifnot(p_min > 0, p_max < 1, p_min < p_max, n >= 10)
  p <- seq(p_min, p_max, length.out = n)
  odds <- p / (1 - p)
  logit <- log(odds)

  ## Left y-axis: odds(p)
  plot(p, odds, type = "l", lwd = lwd1, col = odds_col,
       xlab = "Probability p",
       ylab = "odds(p) = p / (1 - p)")
  if (annotate) {
    abline(h = 1, v = 0.5, lty = 2)
    text(0.52, 1.05, "p = 0.5 → odds = 1", adj = 0)
  }

  ## Right y-axis: logit(p) = log(odds)
  op <- par(new = TRUE)
  on.exit(par(op), add = TRUE)
  plot(p, logit, type = "l", lwd = lwd2, col = logit_col,
       axes = FALSE, xlab = "", ylab = "")
  axis(4)
  mtext("log{odds(p)} = log{p/(1 - p)}", side = 4, line = 3)

  if (annotate) {
    abline(v = 0.5, lty = 2)
    # logit(0.5) = 0 reference (horizontal) on the right-axis scale
    usr <- par("usr")
    segments(x0 = usr[1], y0 = 0, x1 = 0.5, y1 = 0, lty = 3)
  }

  legend("topleft",
         legend = c("odds(p)", "log{odds(p)}"),
         col = c(odds_col, logit_col),
         lwd = c(lwd1, lwd2), bty = "n")

  invisible(list(p = p, odds = odds, logit = logit))
}

## Example usage:
## plot_odds()  # defaults: steelblue for odds, firebrick for log-odds (right axis)
plot_odds(odds_col = "#1f77b4", logit_col = "#d62728", n = 600)
```



6.2 Logistic Regression

Let $Y_i \in \{0,1\}$ denote a binary outcome, and let $\mathbf{x}_i = (x_{i1}, \dots, x_{ip})^\top$ be the vector of predictors **excluding** the intercept.
Let $\beta = (\beta_1, \dots, \beta_p)^\top$ denote the slope coefficients, and β_0 the intercept.
The logistic regression model specifies

$$p_i \;=\; P(Y_i = 1 \mid \mathbf{x}_i),$$

with

$$\log\left(\frac{p_i}{1-p_i}\right) \;=\; \beta_0 + \mathbf{x}_i^\top \beta \;=\; \beta_0 + \sum_{j=1}^{p} \beta_j x_{ij}.$$

Equivalently, the fitted probability is

$$p_i(\mathbf{x}_i;\beta) \;=\; \frac{\exp(\beta_0 + \mathbf{x}_i^\top \beta)}{1+\exp(\beta_0 + \mathbf{x}_i^\top \beta)} \;=\; \frac{1}{1+\exp(-(\beta_0 + \mathbf{x}_i^\top \beta))}.$$

This formulation expresses the **log-odds** of success as a linear function of predictors, ensuring that fitted probabilities remain in the range $(0,1)$.
The **odds** satisfy

$$\frac{p_i}{1-p_i} \;=\; \exp(\beta_0 + \mathbf{x}_i^\top \beta),$$

so a one-unit increase in x_{ij} (holding other predictors fixed) multiplies the odds of success by $\exp(\beta_j)$.

6.3 A Dataset Simulated from Logistic Regression

We simulate data from a logistic model where the **logit** is a linear function of x:

$$\operatorname{logit} p(x) = \log\left(\frac{p(x)}{1-p(x)}\right) = \beta_0 + \beta_1 x,$$

so that

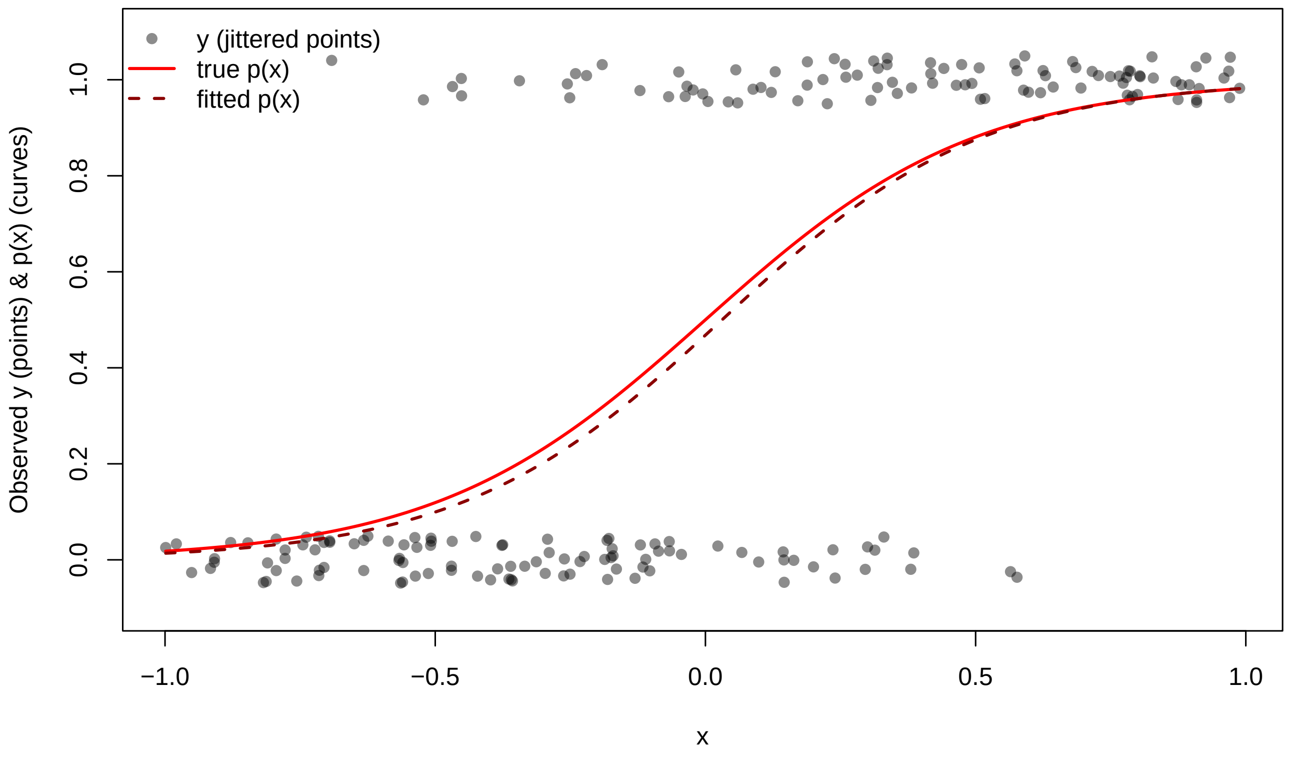
$$p(x) = \operatorname{logit}^{-1}(\beta_0 + \beta_1 x) = \frac{1}{1+\exp\{-(\beta_0+\beta_1 x)\}}.$$

We then display the observed y_i (binary outcomes) and the true probability curve $p(x)$ in red.

```r
set.seed(123)

## -- Truth (edit as desired) --
n     <- 200
beta0 <- 0
beta1 <-  4

## -- Simulate --
x   <- runif(n, -1, 1)             # predictor
eta <- beta0 + beta1 * x
p   <- plogis(eta)                 # true p(x)
y   <- rbinom(n, size = 1, prob = p) # outcomes

sim.data <- data.frame(x = x, y = y, p = p)
```

6.3.1 Fit a logistic model to the simulated data

```r
## -- Optional: fit a model to the simulated data --
sim.fit <- glm(y ~ x, data = sim.data, family = binomial())
p_fit <- predict(sim.fit, newdata = data.frame(x = x), type = "response")

## -- Plot: points for y_i (jittered), red line for true p(x) --
## Define jitter amount
jit <- 0.05
## jitter to separate 0/1 visually
yj <- jitter(sim.data$y, amount = jit)

plot(sim.data$x, yj,
     pch = 16, col = rgb(0, 0, 0, 0.45),
     xlab = "x",
     ylab = "Observed y (points) & p(x) (curves)",
     ylim = c(-0.1, 1.1))

## True probability curve (red)
xg <- seq(min(x), max(x), length.out = 500)
lines(xg, plogis(beta0 + beta1 * xg), col = "red", lwd = 2)

## Optional: add fitted probability curve (dashed dark red)
lines(xg, predict(sim.fit, newdata = data.frame(x = xg), type = "response"),
      col = "darkred", lwd = 2, lty = 2)

legend("topleft",
       legend = c("y (jittered points)", "true p(x)", "fitted p(x)"),
       pch    = c(16, NA, NA),
       lty    = c(NA, 1, 2),
       col    = c(rgb(0,0,0,0.45), "red", "darkred"),
       lwd    = c(NA, 2, 2),
       bty    = "n")
```



6.4 Example: Coronary Heart Disease Data

6.4.1 Load a dataset

This dataset is about a follow-up study to determine the development of coronary heart disease (CHD) over 9 years of follow-up of 609 white males from Evans County, Georgia.

Variable meanings (as provided):

- `chd`: 1 if a person has the disease, 0 otherwise.
- `smk`: 1 if smoker, 0 if not.
- `cat`: 1 if catecholamine level is high, 0 if low.
- `sbp`: systolic blood pressure (continuous).
- `age`: age in years (continuous).
- `chl`: cholesterol level (continuous).
- `ecg`: 1 if electrocardiogram is abnormal, 0 if normal.
- `hpt`: 1 if high blood pressure, 0 if normal.

```r
## Adjust the path if needed. The default is your original V: drive path.
data_path <- "evans.dat"

## Read data (expects a header row)
CHD.data <- read.table(data_path, header = TRUE)
if (knitr::is_html_output()){
  CHD.data
} else{
  CHD.data[1:20,]
}
```

```
    id chd age cat chl dbp ecg sbp smk hpt
1   21   0  56   0 270  80   0 138   0   0
2   31   0  43   0 159  74   0 128   1   0
3   51   1  56   1 201 112   1 164   1   1
4   71   0  64   1 179 100   0 200   1   1
5   74   0  49   0 243  82   0 145   1   0
6   91   0  46   0 252  88   0 142   1   0
7  111   1  52   0 179  80   1 128   1   0
8  131   0  63   0 217  92   0 135   0   0
9  141   0  42   0 176  76   0 114   1   0
10 191   0  55   0 250 114   1 182   0   1
11 201   0  74   0 293 100   0 166   0   1
12 241   0  53   0 179  90   0 158   0   0
13 251   0  58   0 201  86   0 142   1   0
14 261   0  56   0 206  85   0 120   1   0
15 271   0  69   0 225  84   0 168   0   1
```

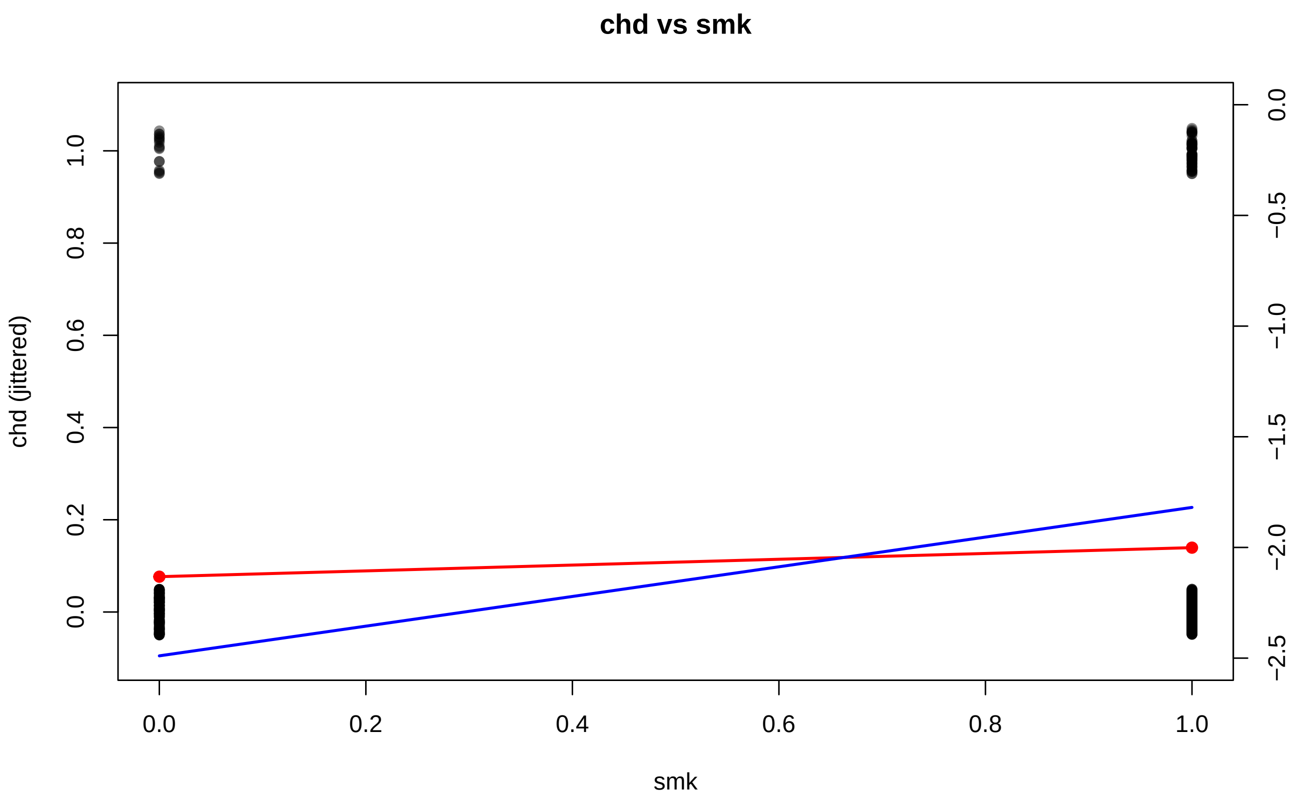
```
16 283   1  51   1 259 102   1 135   0   1
17 291   0  43   0 193  78   0 118   1   0
18 311   0  64   1 185 100   1 180   0   1
19 312   0  44   0 150 108   0 160   0   1
20 331   0  42   0 211  86   1 122   0   0
```

6.4.2 Fit Logistic Regression Model for a Single Variable

```r
vars <- c("smk", "sbp", "age", "chl")
#jit  <- 0.01  # global jitter amount for y

## par(mfrow = c(2, 2), mar = c(4, 4, 2, 4) + 0.1)  # extra right margin for axis(4)

for (v in vars) {
  ## Univariate logistic regression using ORIGINAL variable name in the formula
  fit <- glm(
    formula = reformulate(v, response = "chd"),
    data    = CHD.data,
    family  = binomial()
  )
  print(summary(fit))

  ## Base scatter of chd with small jitter (left axis: probability scale)
  plot(
    CHD.data[[v]],
    jitter(CHD.data$chd, amount = jit),
    pch  = 16, col = rgb(0, 0, 0, 0.45),
    xlab = v, ylab = "chd (jittered)",
    main = paste("chd vs", v),
    ylim = c(-0.1, 1.1)
  )

  ## Fitted  (x) in red (left axis)
  if (length(unique(CHD.data[[v]])) == 2) {
    # binary predictor
    xcat <- sort(unique(CHD.data[[v]]))
    nd   <- setNames(data.frame(xcat), v)
    pcat <- predict(fit, newdata = nd, type = "response")
    points(xcat, pcat, pch = 19, col = "red")
    lines(xcat, pcat, col = "red", lwd = 2)

    # Right-axis: logit{ (x)} with fixed y-limits
    logit_p <- log(pcat / (1 - pcat))
    par(new = TRUE)
    plot(
      xcat, logit_p, type = "l", lwd = 2, col = "blue",
      axes = FALSE, xlab = "", ylab = "",
      xlim = range(CHD.data[[v]]), ylim = c(-2.5, 0)
    )
    axis(4)
    mtext("logit(p(x))", side = 4, line = 3)
    par(new = FALSE)

  } else {
    # continuous predictor
    xg <- seq(min(CHD.data[[v]]), max(CHD.data[[v]]), length.out = 400)
    nd <- setNames(data.frame(xg), v)
    pg <- predict(fit, newdata = nd, type = "response")
    lines(xg, pg, col = "red", lwd = 2)

    # Right-axis: logit{ (x)} with fixed y-limits
    logit_pg <- log(pg / (1 - pg))
    par(new = TRUE)
    plot(
      xg, logit_pg, type = "l", lwd = 2, col = "blue",
      axes = FALSE, xlab = "", ylab = "",
      xlim = range(xg), ylim = c(-2.5, 0)
    )
    axis(4)
    mtext("logit(p(x))", side = 4, line = 3)
    par(new = FALSE)
  }
}
```

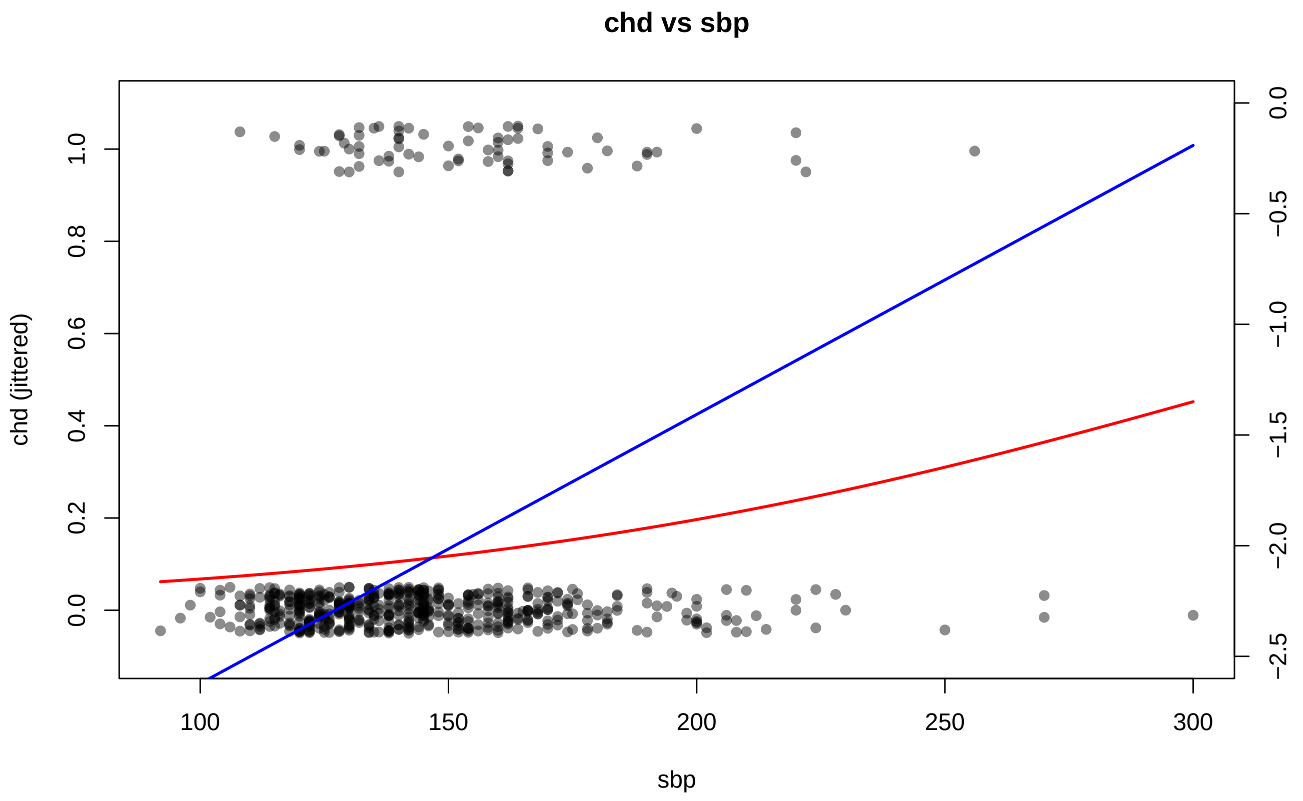
```
Call:
glm(formula = reformulate(v, response = "chd"), family = binomial(),
    data = CHD.data)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  -2.4898     0.2524  -9.865   <2e-16 ***
smk           0.6706     0.2919   2.297   0.0216 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)
```

```
    Null deviance: 438.56  on 608  degrees of freedom
Residual deviance: 432.81  on 607  degrees of freedom
AIC: 436.81

Number of Fisher Scoring iterations: 5
```



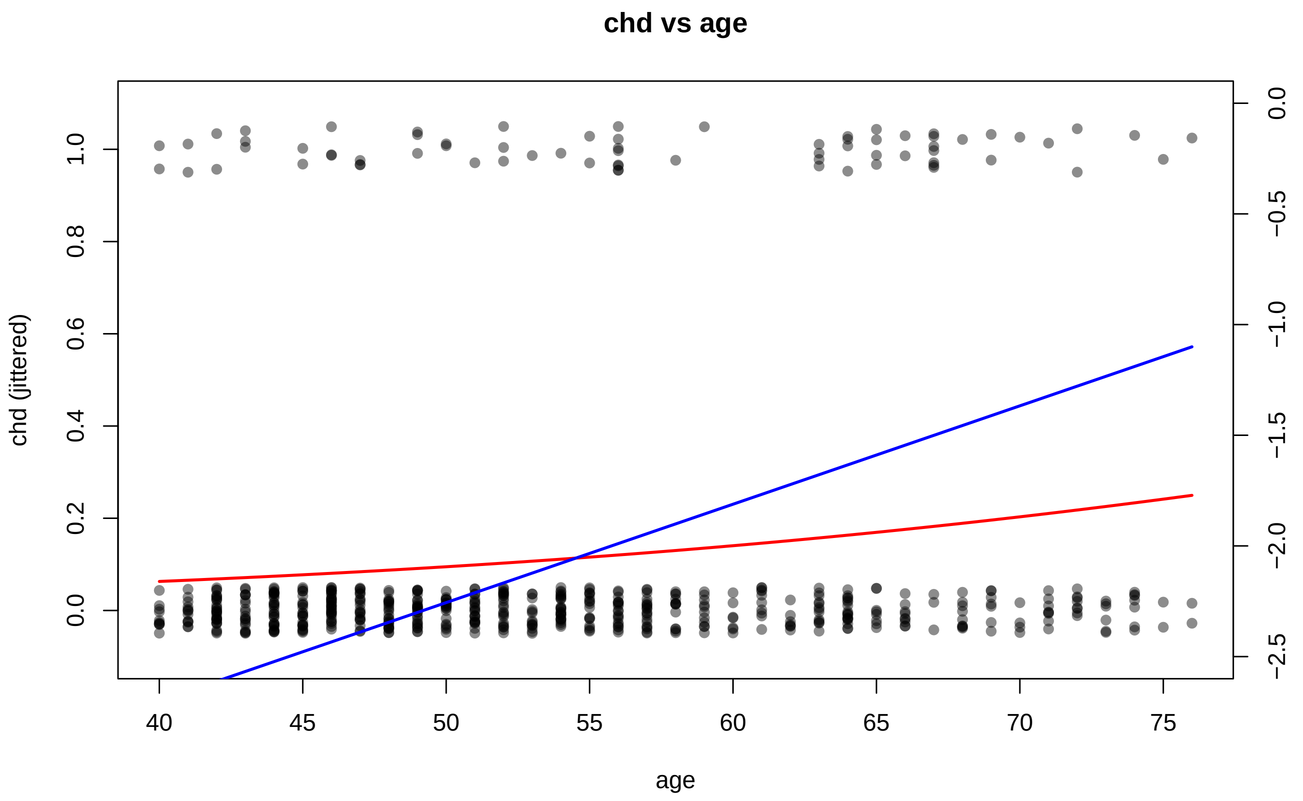
```
Call:
glm(formula = reformulate(v, response = "chd"), family = binomial(),
    data = CHD.data)

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.837912   0.629805  -6.094  1.1e-09 ***
sbp          0.012154   0.004036   3.011   0.0026 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 438.56  on 608  degrees of freedom
```

```
Residual deviance: 430.06  on 607  degrees of freedom
AIC: 434.06

Number of Fisher Scoring iterations: 4
```

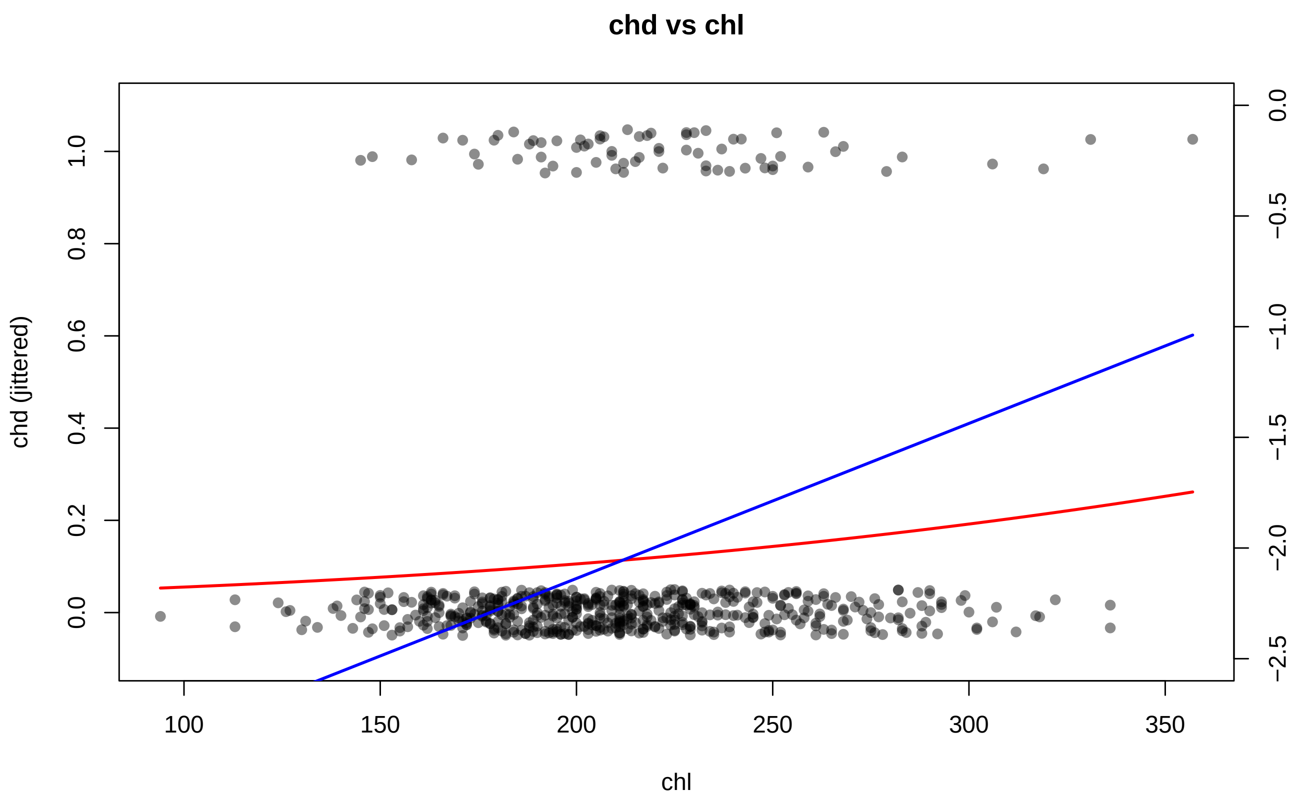


```
Call:
glm(formula = reformulate(v, response = "chd"), family = binomial(),
    data = CHD.data)

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept) -4.47833    0.75610  -5.923 3.16e-09 ***
age          0.04445    0.01315   3.381 0.000723 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 438.56  on 608  degrees of freedom
Residual deviance: 427.22  on 607  degrees of freedom
AIC: 431.22
```

```
Number of Fisher Scoring iterations: 5
```



```
Call:
glm(formula = reformulate(v, response = "chd"), family = binomial(),
    data = CHD.data)

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.538260   0.686879  -5.151 2.59e-07 ***
chl          0.007004   0.003064   2.286   0.0223 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 438.56  on 608  degrees of freedom
Residual deviance: 433.42  on 607  degrees of freedom
AIC: 437.42

Number of Fisher Scoring iterations: 4
```



6.4.3 Fit Logistic Regression Model with all variables

We fit a logistic regression with a logit link:

```r
fit1_chd <- glm(
  chd ~ smk + cat + sbp + age + chl + ecg + hpt,
  data = CHD.data,
  family = binomial(link = "logit")
)
summary(fit1_chd)
```

```
Call:
glm(formula = chd ~ smk + cat + sbp + age + chl + ecg + hpt,
    family = binomial(link = "logit"), data = CHD.data)

Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -6.048892   1.345165  -4.497  6.9e-06 ***
smk          0.855951   0.306505   2.793  0.00523 **
cat          0.732763   0.376129   1.948  0.05139 .
```

```
sbp         -0.006995   0.006976  -1.003  0.31600
age          0.033956   0.015344   2.213  0.02690 *
chl          0.008970   0.003274   2.740  0.00615 **
ecg          0.417776   0.295553   1.414  0.15750
hpt          0.655498   0.359976   1.821  0.06861 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 438.56  on 608  degrees of freedom
Residual deviance: 399.35  on 601  degrees of freedom
AIC: 415.35

Number of Fisher Scoring iterations: 5
```

Notes for interpretation:

- Positive coefficients increase the log-odds of CHD; negative coefficients decrease it.
- For indicator variables (e.g., `smk`), `exp(beta)` is the adjusted odds ratio comparing the group with value 1 versus 0, holding others fixed.
- For continuous predictors (e.g., `sbp`, `age`), `exp(beta)` is the multiplicative change in the odds for a one□unit increase. For a *d*-unit increase, the OR is `exp(d * beta)`.

6.5 Inference for Coefficients: Confidence Intervals and Covariance Matrix

We extract profile□likelihood CIs and the covariance matrix to confirm standard errors.

```r
ci_95 <- confint(fit1_chd, level = 0.95)     # profile-likelihood CI
vcov_mat <- vcov(fit1_chd)                     # covariance matrix of coefficients
se_vec   <- sqrt(diag(vcov_mat))           # standard errors

ci_95
```

```
                   2.5 %       97.5 %
(Intercept) -8.718003347 -3.427904298
smk          0.275699158  1.483333169
cat         -0.006873216  1.471885644
sbp         -0.021166144  0.006266328
age          0.003687290  0.064005215
chl          0.002533226  0.015404292
ecg         -0.171584621  0.990632546
```

```
hpt         -0.050184520  1.364993401
```

```
vcov_mat
```

```
             (Intercept)           smk           cat           sbp
(Intercept)  1.809468553 -1.014526e-01  0.1391440386 -4.908229e-03
smk         -0.101452600  9.394560e-02 -0.0032961000 -1.653230e-04
cat          0.139144039 -3.296100e-03  0.1414730484 -9.299960e-04
sbp         -0.004908229 -1.653230e-04 -0.0009299960  4.866901e-05
age         -0.011142995  7.738971e-04 -0.0017879998 -1.311191e-05
chl         -0.002111134  3.161443e-05  0.0003146354 -1.821907e-06
ecg          0.003442546  9.255483e-03 -0.0204455233 -2.982539e-04
hpt          0.139817180  6.954592e-03 -0.0044220690 -1.486400e-03
                     age           chl           ecg           hpt
(Intercept) -1.114300e-02 -2.111134e-03  3.442546e-03  1.398172e-01
smk          7.738971e-04  3.161443e-05  9.255483e-03  6.954592e-03
cat         -1.788000e-03  3.146354e-04 -2.044552e-02 -4.422069e-03
sbp         -1.311191e-05 -1.821907e-06 -2.982539e-04 -1.486400e-03
age          2.354442e-04 -1.480501e-06 -4.972374e-05  4.044434e-04
chl         -1.480501e-06  1.071766e-05  5.040548e-05 -6.046197e-05
ecg         -4.972374e-05  5.040548e-05  8.735130e-02  9.506863e-04
hpt          4.044434e-04 -6.046197e-05  9.506863e-04  1.295828e-01
```

```
se_vec  # should match the SE column in summary(fit1_chd)
```

```
(Intercept)         smk         cat         sbp         age         chl
1.345164879 0.306505459 0.376129032 0.006976318 0.015344190 0.003273784
        ecg         hpt
0.295552531 0.359976081
```

6.6 Inference for Odds Ratios

6.6.1 Interpretation of Odds Ratios in Logistic Regression

A multiple logistic regression model expresses the log-odds (logit) of an event as a linear function of predictors:

$$\log\left(\frac{p}{1-p}\right) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k.$$

Here,

- $p = \Pr(Y = 1 \mid x_1, x_2, \ldots, x_k)$ is the probability of the event,
- β_0 is the intercept, and
- each β_j represents the **change in the log-odds** of the event per one-unit increase in x_j, *holding all other variables constant*.

Exponentiating both sides gives the model in odds form:

$$\frac{p}{1-p} = \exp(\beta_0) \times \exp(\beta_1 x_1) \times \exp(\beta_2 x_2) \times \cdots \times \exp(\beta_k x_k).$$

An R function for OR at two Profiles

The or_from_predict R function is a utility designed to calculate the Odds Ratio (OR) and its 95% confidence interval (CI) between two specific covariate profiles (new1 and new0) for a given logistic regression model (fit). The calculation is performed on the link (logit) scale. For a logistic model $\text{logit}(p) = \eta = \mathbf{X}\beta$, the log-Odds Ratio (logOR) is the difference between the linear predictors (η_1, η_0) for the two profiles:

$$\widehat{\text{logOR}} = \eta_1 - \eta_0 = (\mathbf{x}_1^T - \mathbf{x}_0^T)\beta = \mathbf{c}^T\beta \tag{6.1}$$

Here, $\mathbf{c} = \mathbf{x}_1 - \mathbf{x}_0$ is the linear contrast vector derived from the model matrices of the two profiles. The function estimates the variance of this contrast as $\text{Var}(\widehat{\text{logOR}}) = \mathbf{c}^T\mathbf{V}\mathbf{c}$, where $\mathbf{V}$ is the model's variance-covariance matrix (vcov(fit)). The standard error $SE = \sqrt{\mathbf{c}^T\mathbf{V}\mathbf{c}}$ is used to compute the $100(1-\alpha)\%$ confidence interval for the logOR:

$$\widehat{\text{logOR}} \pm z_{1-\alpha/2} \times SE.$$

These values (estimate and CI bounds) are then exponentiated to produce the final $\widehat{\text{OR}} = \exp(\widehat{\text{logOR}})$ and its 95% CI. The function also prints two helpful summaries to the console: a data frame showing only the variables that differ between the new0 and new1 profiles, and a 2x3 table presenting the estimates and CIs for both the OR and the logOR.

The R function to find ORs

```r
## Compute OR and 95% CI via predict() on the LINK scale
## OR = exp( eta(new1) - eta(new0) ), where eta(.) = logit{ (.)}
## Compute OR via predict() contrast on the LINK scale, also:
## (ii) print a 2-row data.frame of only variables that differ between new0 and new1
## (iii) print a 2x3 table (rows: OR, logOR; cols: Estimate, CI_low, CI_up)
or_from_predict <- function(fit, new1, new0, level = 0.95, digits = 4, tol = 1e-12) {
  stopifnot(is.data.frame(new1), is.data.frame(new0))

  ## --- REFACTORED SECTION START ---
  ## ---- (ii) Two-row data.frame with only changed variables ----

  ## Helper function to find differing variables between two profiles
  ## This is defined *inside* or_from_predict for encapsulation
  get_changed_vars <- function(d0, d1, tolerance) {
    common <- intersect(names(d0), names(d1))
    diffv  <- vapply(common, function(nm) {
      x0 <- d0[[nm]]; x1 <- d1[[nm]]
      if (is.numeric(x0) && is.numeric(x1)) {
        !isTRUE(all.equal(as.numeric(x0), as.numeric(x1), tolerance = tolerance))
      } else {
        !identical(x0, x1)
      }
    }, logical(1))

    keep <- common[diffv]
    if (length(keep) == 0L) {
      out <- data.frame(`_no_changes_` = "no differences")
      rownames(out) <- c("new0", "new1")
      return(out)
    }
    out <- rbind(d0[keep], d1[keep])
    rownames(out) <- c("new0", "new1")
    out
  }

  ## Call the helper function
  changes_df <- get_changed_vars(new0, new1, tol)
  ## --- REFACTORED SECTION END ---


  ## ---- Linear contrast for log-OR and its variance ----

  ## (i) Calculate logOR estimate using predict(type="link")
  ## eta(.) = logit{p(.)}
  eta1 <- predict(fit, newdata = new1, type = "link")
  eta0 <- predict(fit, newdata = new0, type = "link")
  logOR_hat <- as.numeric(eta1 - eta0) # logOR = eta1 - eta0

  ## (ii) Calculate standard error using the contrast vector 'cvec'
  X1 <- model.matrix(delete.response(terms(fit)), data = new1)
  X0 <- model.matrix(delete.response(terms(fit)), data = new0)
  cvec      <- as.numeric(X1 - X0)
  V         <- vcov(fit)
  se_logOR  <- sqrt(as.numeric(t(cvec) %*% V %*% cvec))

  alpha  <- 1 - level
  z      <- qnorm(1 - alpha / 2)
  ci_log <- c(logOR_hat - z * se_logOR, logOR_hat + z * se_logOR)
  ## ---- 2x3 table: rows OR and logOR; columns Estimate, CI_low, CI_up ----
  res_tab <- data.frame(
    Estimate = c(exp(logOR_hat),          logOR_hat),
    CI_low   = c(exp(ci_log[1L]),         ci_log[1L]),
    CI_up    = c(exp(ci_log[2L]),         ci_log[2L]),
    row.names = c("OR", "logOR")
  )

  ## ---- Print requested items ----
  cat("\nVariables that differ between new0 and new1:\n")
  print(changes_df)
  cat("\nOdds Ratio summary:\n")
  print(round(res_tab, digits = digits)) # Added rounding for neatness

  ## ---- Return (invisibly) ----
  invisible(list(
    OR         = exp(logOR_hat),
    CI_OR      = exp(ci_log),
    logOR      = logOR_hat,
    CI_logOR   = ci_log,
    se_logOR   = se_logOR,
    changes    = changes_df,
    table      = res_tab
  ))
}

## --- Example usage ---
## Suppose 'fit1_chd' is your fitted model and 'CHD.data' is your data
## base_prof <- as.data.frame(lapply(CHD.data, function(col) if (is.numeric(col)) mean(col) else
## new0 <- base_prof; new0$smk <- 0
## new1 <- base_prof; new1$smk <- 1
## or_from_predict(fit1_chd, new1 = new1, new0 = new0)


mean_profile <- function(data, vars_binary_as = c(0,1)) {
  ## Build a single-row data.frame of typical values:
  out <- lapply(data, function(col) {
    if (is.numeric(col)) {
      # If strictly 0/1, keep mean (works fine for GLM prediction),
      # or switch to mode if you prefer.
      if (all(col %in% c(0,1))) mean(col) else mean(col, na.rm = TRUE)
    } else {
      # Fallback to first level for factors/characters
      if (is.factor(col)) levels(col)[1] else unique(col)[1]
    }
  })
  as.data.frame(out)
}
```

6.6.2 Examples of Finding ORs and Their CIs for the CHD Dataset

6.6.2.1 OR Smoking (smk) (1 vs 0)

```
### 1) Smoking OR: smk = 1 vs 0 (other vars at their means)
## Example profiles at sample means (adjust as you like)
base_prof <- mean_profile(CHD.data)
new0 <- base_prof; new0$smk <- 0
new1 <- base_prof; new1$smk <- 1

res_smk <- or_from_predict(fit1_chd, new1 = new1, new0 = new0)
```

```
Variables that differ between new0 and new1:
     smk
new0   0
new1   1

Odds Ratio summary:
      Estimate CI_low  CI_up
OR      2.3536 1.2907 4.2917
logOR   0.8560 0.2552 1.4567
```

How to read this:

- `OR_smk > 1` suggests higher odds of CHD among smokers (adjusted for other variables). If the 95% CI excludes 1, the association is statistically significant at the 5% level.

6.6.2.2 OR for Systolic Blood Pressure (sbp): from 120 to 160

We compute the adjusted OR for a 40□unit increase in sbp (from 120 to 160):

```
### 2) SBP OR: 160 vs 120 (other vars at their means)
new0 <- base_prof; new0$sbp <- 120
new1 <- base_prof; new1$sbp <- 160

res_sbp <- or_from_predict(fit1_chd, new1 = new1, new0 = new0)
```

```
Variables that differ between new0 and new1:
     sbp
new0 120
new1 160

Odds Ratio summary:
      Estimate  CI_low  CI_up
OR      0.7559  0.4375 1.3062
logOR  -0.2798 -0.8267 0.2671
```

6.6.2.3 OR for Combined Effects of Two Variables: Smoking with an Age Difference

Suppose we compare two groups that differ in **smoking status** and **age**:

- **Group A:** `smk = 1`, `age = 50` (all other covariates equal)
- **Group B:** `smk = 0`, `age = 30`

The log□odds contrast is ($A = \beta_{smk} + (50 - 20)\beta_{age}$), so the OR is (exp$(A)$).

```r
new0 <- base_prof; new0$age <- 30; new0$smk <- 0
new1 <- base_prof; new1$age <- 50; new1$smk <- 1

res_ageAsmk <- or_from_predict(fit1_chd, new1 = new1, new0 = new0)
```

```
Variables that differ between new0 and new1:
     age smk
new0  30   0
new1  50   1

Odds Ratio summary:
      Estimate CI_low   CI_up
OR      4.6417 1.8546 11.6168
logOR   1.5351 0.6177  2.4525
```

6.7 Assessing Statistical Significance with Wilks' Theorem (Analogue of F-test for OLS)

In the context of logistic regression, Wilks' theorem provides the basis for the Likelihood Ratio Test (LRT) used to assess the significance of predictor variables. The theorem states that when comparing a full model (M_1) to a nested null model (M_0), the test statistic, Λ, asymptotically follows a chi-squared (χ^2) distribution under the null hypothesis (i.e., that the simpler model M_0 is correct).

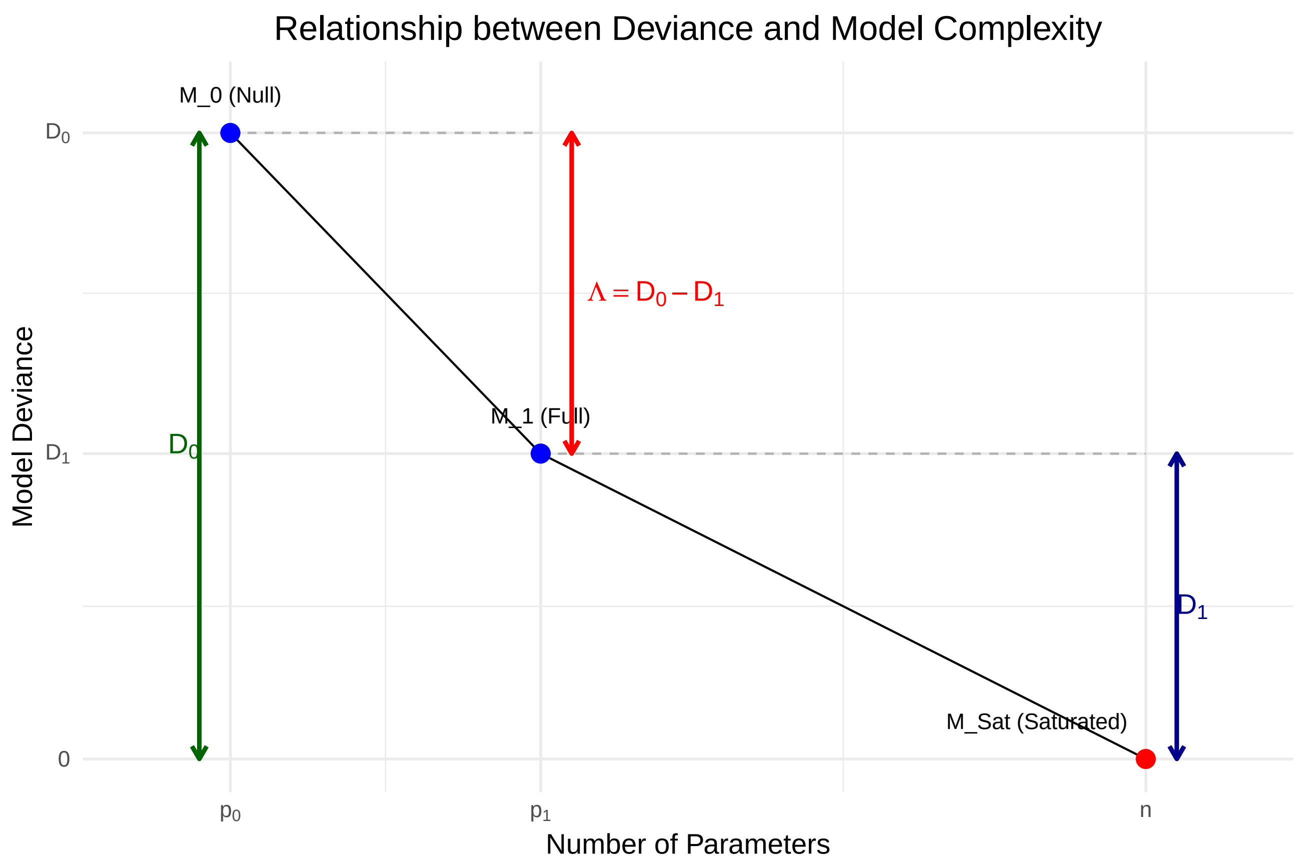
The statistic Λ is calculated as the difference in the maximized log-likelihoods:

$$\Lambda = -2(\log L_0 - \log L_1) \tag{6.2}$$

where log L_0 and log L_1 are the log-likelihoods of the null and full models, respectively. In logistic regression, this is equivalent to the difference in the deviances: $\Lambda = \text{Deviance}_0 - \text{Deviance}_1$. This test statistic Λ represents the reduction in deviance (a measure of badness-of-fit) achieved by adding the extra predictors to the model.

The following R code chunk generates a conceptual plot of this relationship:

```r
#| label: plot-lrt-concept
#| echo: false
#| fig-cap: "Conceptual plot of Deviance versus Number of Parameters, illustrating the Likelih

library(ggplot2)

## 1. Create conceptual data for the plot
## These are just for illustration
n_obs <- 60 # Number of observations
p0 <- 1     # Parameters in null model (intercept)
p1 <- 21    # Parameters in full model (e.g., intercept + 7 predictors)
psat <- n_obs # Parameters in saturated model (1 per observation)

D0 <- 41 # Null deviance
D1 <- 20 # Full model deviance (residual deviance of M1)
D_sat <- 0 # Saturated model deviance

## Data frame for the three points
plot_data <- data.frame(
  model = c("M_0 (Null)", "M_1 (Full)", "M_Sat (Saturated)"),
  params = c(p0, p1, psat),
  deviance = c(D0, D1, D_sat),
  ## Add custom justification and nudges for labels
  hjust_val = c(0.5, 0.5, 1.1), # Right-align the last label
  nudge_x_val = c(0, 0, 0)
)

## 2. Create the ggplot
ggplot(plot_data, aes(x = params, y = deviance)) +
  ## Draw dashed guide lines for D0 and D1
  geom_segment(aes(x = p0, y = D0, xend = p1, yend = D0), linetype = "dashed", color = "grey70
  geom_segment(aes(x = p1, y = D1, xend = psat, yend = D1), linetype = "dashed", color = "grey

  ## Connect the points with lines
  geom_line(color = "black", linetype = "solid", linewidth = 0.5) +
  ## Draw the main points
  geom_point(size = 4, aes(color = model)) +

  ## --- MODIFIED LABEL PLACEMENT ---
  ## Label the points using custom nudge/justification
  geom_text(
    aes(label = model, hjust = hjust_val, nudge_x = nudge_x_val),
    nudge_y = 2.5,  # Use a much smaller vertical nudge
    size = 4
  ) +

  ## --- ADDED BACK D0 and D1 ANNOTATIONS ---
  ## D0 (Null Deviance)
  geom_segment(
    aes(x = p0 - 2, y = D0, xend = p0 - 2, yend = D_sat), # Nudged left
    arrow = arrow(ends = "both", length = unit(0.1, "inches")),
    color = "darkgreen",
    linewidth = 1
  ) +
  annotate(
    "text",
    x = p0 - 3, y = D0 / 2, # Nudged left
    label = "D[0]", parse = TRUE,
    color = "darkgreen", hjust = 0.5, size = 5
  ) +

  ## D1 (Residual Deviance of Full Model)
  geom_segment(
    aes(x = psat + 2, y = D1, xend = psat + 2, yend = D_sat), # Nudged right
    arrow = arrow(ends = "both", length = unit(0.1, "inches")),
    color = "darkblue",
    linewidth = 1
  ) +
  annotate(
    "text",
    x = psat + 3, y = D1 / 2, # Nudged right
    label = "D[1]", parse = TRUE,
    color = "darkblue", hjust = 0.5, size = 5
  ) +

  ## LRT statistic Λ = D0 - D1
  geom_segment(
    aes(x = p1 + 2, y = D0, xend = p1 + 2, yend = D1), # Nudged right
    arrow = arrow(ends = "both", length = unit(0.1, "inches")),
    color = "red",
    linewidth = 1
  ) +
  annotate(
    "text",
    x = p1 + 3, y = D1 + (D0 - D1) / 2, # Nudged right
    label = "Lambda == D[0] - D[1]",
    parse = TRUE,
    color = "red", hjust = 0, size = 5
  ) +

  ## Customize axes to show the symbolic labels
  scale_x_continuous(
    breaks = c(p0, p1, psat),
    labels = c(expression(p[0]), expression(p[1]), expression(n)),
    expand = expansion(mult = 0.1) # Add some padding
  ) +
  scale_y_continuous(
    breaks = c(D_sat, D1, D0),
    labels = c(expression(0), expression(D[1]), expression(D[0]))
  ) +

  ## Labels and Title
  labs(
    title = "Relationship between Deviance and Model Complexity",
    x = "Number of Parameters",
    y = "Model Deviance"
  ) +

  ## Clean theme
  theme_minimal(base_size = 14) +
  theme(
    plot.title = element_text(hjust = 0.5),
    legend.position = "none" # Remove legend, as points are labeled
  ) +
  scale_color_manual(values = c("M_0 (Null)" = "blue", "M_1 (Full)" = "blue", "M_Sat (Saturate
```



As the diagram illustrates, the null model (M_0) has fewer parameters (p_0) and a higher deviance (D_0, or worse fit), while the full model (M_1) has more parameters (p_1) and a lower deviance (D_1). The Likelihood Ratio Test statistic D is the magnitude of this drop in deviance.

For assessing the overall significance of a regression model (`fit1_chd`), this involves comparing it to its corresponding intercept-only (null) model. The degrees of freedom for the χ^2 test is the difference in the number of parameters, $df = p_1 - p_0$, which equals the number of predictors in the full model.

Here is an R code chunk demonstrating how to compute this p-value directly from a `glm` fit object, assuming it is named `fit1_chd`.

```r
## Calculate the Likelihood Ratio Test statistic (D) and degrees of freedom (df)
## by comparing the model's deviance to the null (intercept-only) deviance,
## both of which are stored in the 'fit1_chd' object.
summary(fit1_chd)
```

```
Call:
glm(formula = chd ~ smk + cat + sbp + age + chl + ecg + hpt,
    family = binomial(link = "logit"), data = CHD.data)
```

```
Coefficients:
             Estimate Std. Error z value Pr(>|z|)
(Intercept) -6.048892   1.345165  -4.497  6.9e-06 ***
smk          0.855951   0.306505   2.793  0.00523 **
cat          0.732763   0.376129   1.948  0.05139 .
sbp         -0.006995   0.006976  -1.003  0.31600
age          0.033956   0.015344   2.213  0.02690 *
chl          0.008970   0.003274   2.740  0.00615 **
ecg          0.417776   0.295553   1.414  0.15750
hpt          0.655498   0.359976   1.821  0.06861 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 438.56  on 608  degrees of freedom
Residual deviance: 399.35  on 601  degrees of freedom
AIC: 415.35

Number of Fisher Scoring iterations: 5
```

```r
lrt_statistic <- fit1_chd$null.deviance - fit1_chd$deviance
lrt_df <- fit1_chd$df.null - fit1_chd$df.residual

## Compute the p-value from the chi-squared distribution
## We use lower.tail = FALSE to get P(ChiSq > D)
p_value <- pchisq(lrt_statistic, lrt_df, lower.tail = FALSE)

## Create and print the result in an ANOVA-like table
## Row 1: Null model
## Row 2: Full model (fit1_chd), showing the test against the null
lrt_table <- data.frame(
  "Resid. Df" = c(fit1_chd$df.null, fit1_chd$df.residual),
  "Resid. Dev" = c(round(fit1_chd$null.deviance, 4), round(fit1_chd$deviance, 4)),
  "Test Df" = c(NA, lrt_df),
  "Test Statistic (D)" = c(NA, round(lrt_statistic, 4)),
  "p-value" = c(NA, format.pval(p_value, digits = 4)),
  row.names = c("Null Model", "Full Model (fit1_chd)"),
  check.names = FALSE # Prevent R from changing 'p-value' to 'p.value'
)

cat("Likelihood Ratio Test for Model Significance:\n")
```

```
Likelihood Ratio Test for Model Significance:
```

```r
lrt_table
```

```
                       Resid. Df Resid. Dev Test Df Test Statistic (D)   p-value
Null Model                   608   438.5583      NA                 NA      <NA>
Full Model (fit1_chd)        601   399.3539       7            39.2044 1.787e-06
```

Using built-in anova() function

```r
fit0_chd <- glm (chd~1, data = CHD.data, family = binomial())
anova(fit0_chd, fit1_chd)
```

```
Analysis of Deviance Table

Model 1: chd ~ 1
Model 2: chd ~ smk + cat + sbp + age + chl + ecg + hpt
  Resid. Df Resid. Dev Df Deviance  Pr(>Chi)
1       608     438.56
2       601     399.35  7   39.204 1.787e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
anova(fit1_chd, test="LRT")
```

```
Analysis of Deviance Table

Model: binomial, link: logit

Response: chd

Terms added sequentially (first to last)

     Df Deviance Resid. Df Resid. Dev  Pr(>Chi)
NULL                   608     438.56
smk   1   5.7453       607     432.81 0.0165324 *
cat   1  14.3716       606     418.44 0.0001501 ***
sbp   1   0.7574       605     417.68 0.3841353
age   1   5.2821       604     412.40 0.0215455 *
chl   1   7.8619       603     404.54 0.0050489 **
ecg   1   1.8701       602     402.67 0.1714609
hpt   1   3.3159       601     399.35 0.0686113 .
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

6.8 Assessing Predictive Effect-Size (Anologue to R^2_{adj})

While the LRT assesses overall model significance (in-sample fit), it's also crucial to evaluate how well the model predicts new, unseen data (out-of-sample performance). A common method is to split the data into a training set (e.g., 2/3 of the data) and a test set (e.g., 1/3). The model is fit using only the training data and then used to make predictions for the test data. We can then compare these predictions to the actual outcomes in the test set.

6.8.1 Understanding the Confusion Matrix and Metrics

To evaluate a model's predictive performance, we classify its probabilistic predictions using a threshold (typically 0.5) and compare them to the true outcomes in a **Confusion Matrix**:

	Predicted: 0	**Predicted: 1**
Actual: 0	True Negative (TN)	False Positive (FP)
Actual: 1	False Negative (FN)	True Positive (TP)

From this matrix, we derive several key performance metrics:

- **Misclassification Error Rate (ER):** The proportion of all predictions that were incorrect.

$$\text{Error Rate} = \frac{FP + FN}{TP + TN + FP + FN}$$

- **Precision (Positive Predictive Value):** Answers: "Of all the times the model predicted positive, how often was it correct?" This is crucial when the cost of a **False Positive** is high.

$$\text{Precision} = \frac{TP}{TP + FP}$$

- **Recall (Sensitivity or True Positive Rate):** Answers: "Of all the actual positive cases, how many did the model find?" This is crucial when the cost of a **False Negative** is high.

$$\text{Recall (TPR)} = \frac{TP}{TP + FN}$$

- **ROC Curve and AUC:** An **ROC (Receiver Operating Characteristic) Curve** is a graph that shows a model's diagnostic ability across *all possible classification thresholds*. It plots the **True Positive Rate (Recall)** on the y-axis against the **False Positive Rate** (FPR = $\frac{FP}{FP+TN}$) on the x-axis.
  - **Interpretation:** The curve shows the trade-off between sensitivity (finding all the positives) and specificity (not mislabeling negatives). A random "no-skill" classifier is represented by a diagonal line from (0,0) to (1,1). A perfect classifier would hug the **top-left corner** (TPR = 1, FPR = 0).

  - **AUC (Area Under the Curve):** The AUC summarizes the entire curve into a single number from 0 to 1. An AUC of 0.5 corresponds to a random guess, while an AUC of 1.0 represents a perfect model.

- **Precision-Recall (PR) Curve:** A **PR Curve** plots **Precision** (y-axis) against **Recall** (x-axis) at all possible thresholds.
  - **Interpretation:** This curve shows the trade-off between how *reliable* a positive prediction is (Precision) and how *complete* the model is at finding all positives (Recall).
  - **When to Use:** The PR curve is particularly informative when the dataset is **imbalanced** (i.e., one class, like "fraud" or "disease," is much rarer than the other). Unlike the ROC curve, the PR curve's baseline (the "no-skill" line) is a horizontal line at the proportion of positive cases, which makes it easier to see if the model is performing significantly better than chance in a low-positive-rate scenario. A perfect classifier would hug the **top-right corner** (Precision = 1, Recall = 1).

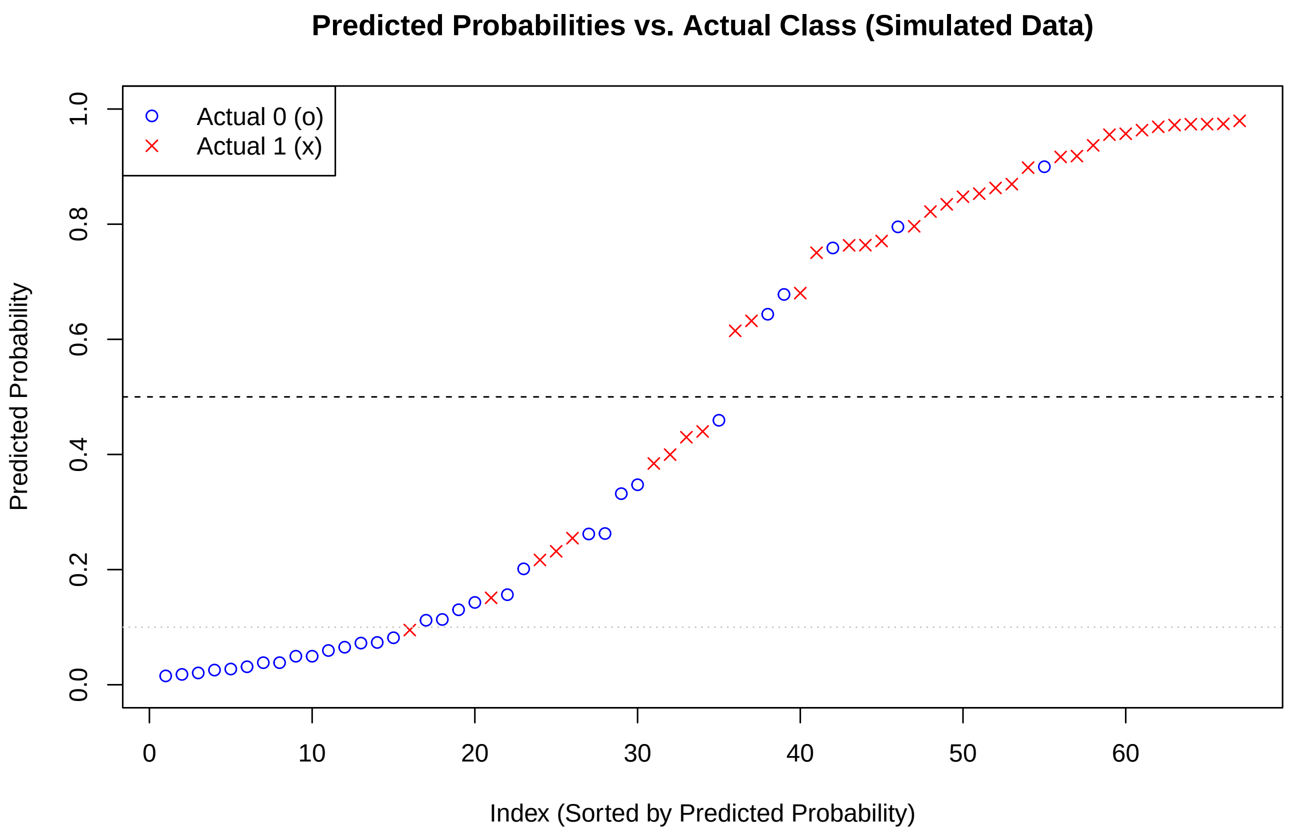
6.8.2 Illustration with the Simulated Dataset

This section applies the train/test split and model evaluation workflow to the `sim.data` created in the previous step.

```r
## Load the pROC library for AUC calculation
## install.packages("pROC") # Uncomment to install if needed
library(pROC)

## --- 1. Split the data ---
## We use 'sim.data' which has 200 rows
set.seed(123) # for reproducibility
n_sim <- nrow(sim.data)
train_size_sim <- floor(2/3 * n_sim)
train_indices_sim <- sample(1:n_sim, size = train_size_sim)
train_data_sim <- sim.data[train_indices_sim, ]
test_data_sim  <- sim.data[-train_indices_sim, ]

## --- 2. Refit the model on the training data ---
## We fit the model y ~ x on the training data
fit_train_sim <- glm(
  y ~ x,
  data = train_data_sim,
  family = binomial(link = "logit")
)

## --- 3. Make predictions on the test data ---
## Note: The true probabilities 'p' are also in test_data_sim
## We predict from the *fitted* model
pred_probs_sim <- predict(fit_train_sim, newdata = test_data_sim, type = "response")
```

Plotting the Predictive Probabilities with True Labels

```r
## --- 5. Plot sorted predicted probabilities ---

## Create a data frame for plotting
plot_data_sim <- data.frame(
  Prob = pred_probs_sim,
  Actual = as.factor(test_data_sim$y),
  TrueProb = test_data_sim$p # Include true probs for comparison
)

## Sort by predicted probability
plot_data_sim <- plot_data_sim[order(plot_data_sim$Prob), ]
plot_data_sim$Rank <- 1:nrow(plot_data_sim)

## Create the plot
plot(
  plot_data_sim$Rank,
  plot_data_sim$Prob,
  pch = ifelse(plot_data_sim$Actual == 0, 1, 4),
  col = ifelse(plot_data_sim$Actual == 0, "blue", "red"),
  xlab = "Index (Sorted by Predicted Probability)",
  ylab = "Predicted Probability",
  main = "Predicted Probabilities vs. Actual Class (Simulated Data)",
  ylim = c(0, 1)
)
abline(h = 0.5, lty = 2, col = "black")
abline(h = 0.1, lty = 3, col = "grey")

## Add the true probability curve (sorted by predicted prob)
## This shows how well the fitted model's predictions align with the true probs
#lines(plot_data_sim$Rank, plot_data_sim$TrueProb[order(plot_data_sim$Prob)], col = "darkgreen


## Add a legend
legend(
  "topleft",
  legend = c("Actual 0 (o)", "Actual 1 (x)"),
  pch = c(1, 4),
  lty = c(NA, NA),
  lwd = c(NA, NA),
  col = c("blue", "red")
)
```



Confusion Matrix with threshold=0.5

```
## --- 4. Assess accuracy ---

## 4a. Misclassification Error Rate (using 0.5 threshold)
threshold <- 0.5
pred_class_sim <- ifelse(pred_probs_sim > threshold, 1, 0)
conf_matrix_sim <- table(Actual = test_data_sim$y, Predicted = pred_class_sim)

## --- MODIFIED LINES START ---
cat("Confusion Matrix (Counts, threshold = 0.5):\n")
```

```
Confusion Matrix (Counts, threshold = 0.5):
```

```
print(conf_matrix_sim)
```

```
      Predicted
Actual  0  1
     0 26  5
     1  9 27
```

```r
cat("\nRow Proportions (Given Actual, % Predicted -- Relates to TPR/FPR):\n")
```

```
Row Proportions (Given Actual, % Predicted -- Relates to TPR/FPR):
```

```r
## margin = 1 calculates proportions across rows
print(round(prop.table(conf_matrix_sim, margin = 1), 3))
```

```
      Predicted
Actual     0     1
     0 0.839 0.161
     1 0.250 0.750
```

```r
cat("\nColumn Proportions (Given Predicted, % Actual -- Relates to Precision):\n")
```

```
Column Proportions (Given Predicted, % Actual -- Relates to Precision):
```

```r
## margin = 2 calculates proportions across columns
print(round(prop.table(conf_matrix_sim, margin = 2), 3))
```

```
      Predicted
Actual     0     1
     0 0.743 0.156
     1 0.257 0.844
```

```r
## --- MODIFIED LINES END ---


## Check if matrix has 2x2 dimensions, otherwise metrics will fail
if (all(dim(conf_matrix_sim) == c(2, 2))) {
  TN <- conf_matrix_sim[1, 1]
  FP <- conf_matrix_sim[1, 2]
  FN <- conf_matrix_sim[2, 1]
  TP <- conf_matrix_sim[2, 2]

  ## Calculate metrics
  error_rate <- (FP + FN) / (TP + TN + FP + FN)
  TPR_Recall <- TP / (TP + FN) # True Positive Rate (Recall / Sensitivity)
  FPR <- FP / (FP + TN)       # False Positive Rate (1 - Specificity)
  Precision <- TP / (TP + FP)  # Positive Predictive Value
  cat(paste("\nMisclassification Error Rate:", round(error_rate, 4), "\n"))
  cat(paste("True Positive Rate (Recall):", round(TPR_Recall, 4), "\n"))
  cat(paste("False Positive Rate:", round(FPR, 4), "\n"))
  cat(paste("Precision:", round(Precision, 4), "\n"))
} else {
  cat("\nCannot calculate full metrics: model predicted only one class.\n")
}
```

```
Misclassification Error Rate: 0.209
True Positive Rate (Recall): 0.75
False Positive Rate: 0.1613
Precision: 0.8438
```

Confusion Matrix with threshold=0.1

```
threshold <- 0.1
pred_class_sim <- ifelse(pred_probs_sim > threshold, 1, 0)
conf_matrix_sim <- table(Actual = test_data_sim$y, Predicted = pred_class_sim)

## --- MODIFIED LINES START ---
cat("Confusion Matrix (Counts, threshold = 0.1):\n")
```

```
Confusion Matrix (Counts, threshold = 0.1):
```

```
print(conf_matrix_sim)
```

```
      Predicted
Actual  0  1
     0 15 16
     1  1 35
```

```
cat("\nRow Proportions (Given Actual, % Predicted -- Relates to TPR/FPR):\n")
```

```
Row Proportions (Given Actual, % Predicted -- Relates to TPR/FPR):
```

```
## margin = 1 calculates proportions across rows
print(round(prop.table(conf_matrix_sim, margin = 1), 3))
```

```
      Predicted
Actual     0     1
     0 0.484 0.516
     1 0.028 0.972
```

```
cat("\nColumn Proportions (Given Predicted, % Actual -- Relates to Precision):\n")
```

```

Column Proportions (Given Predicted, % Actual -- Relates to Precision):
```

```
## margin = 2 calculates proportions across columns
print(round(prop.table(conf_matrix_sim, margin = 2), 3))
```

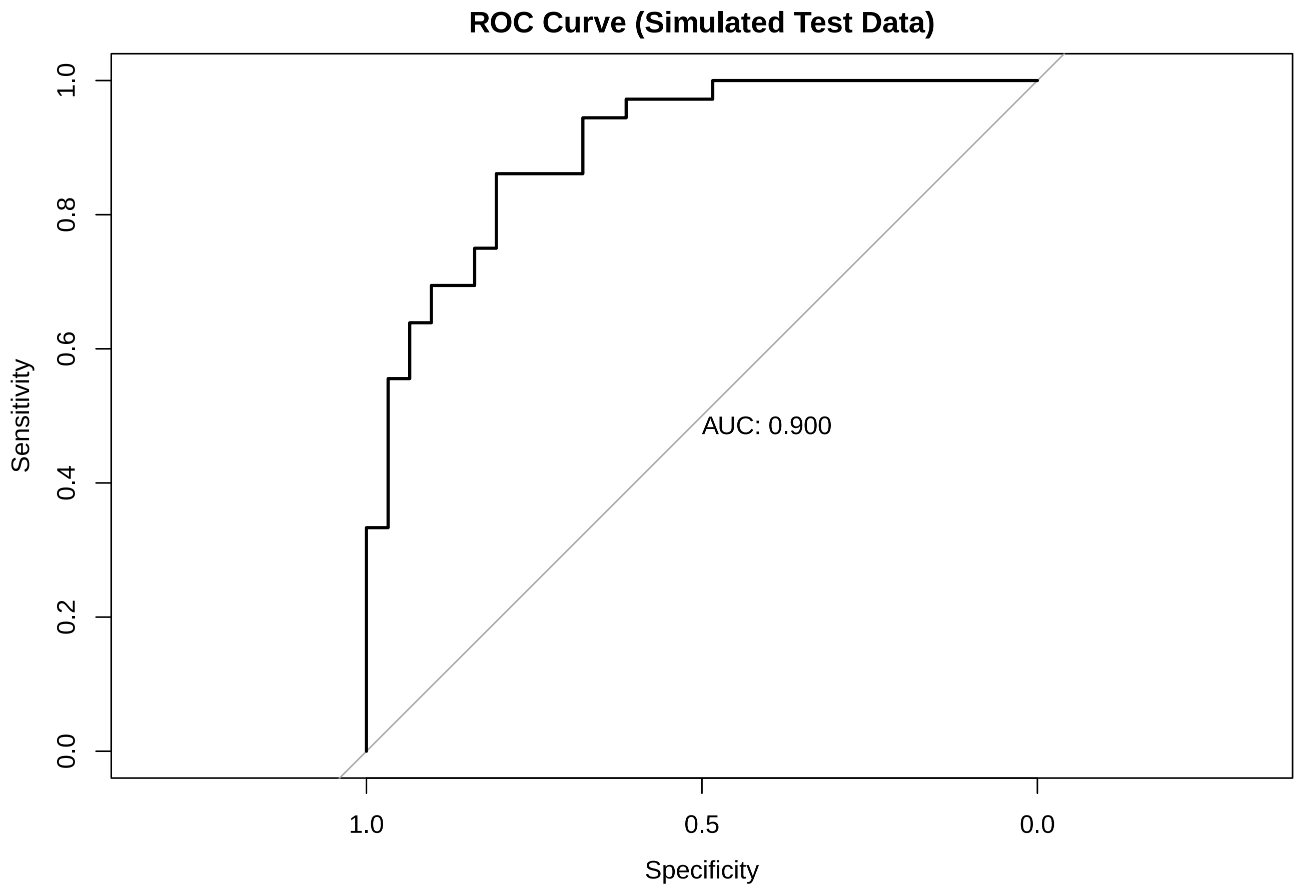
```
      Predicted
Actual     0     1
     0 0.938 0.314
     1 0.062 0.686
```

```
## --- MODIFIED LINES END ---


## Check if matrix has 2x2 dimensions
if (all(dim(conf_matrix_sim) == c(2, 2))) {
  TN <- conf_matrix_sim[1, 1]
  FP <- conf_matrix_sim[1, 2]
  FN <- conf_matrix_sim[2, 1]
  TP <- conf_matrix_sim[2, 2]

  ## Calculate metrics
  error_rate <- (FP + FN) / (TP + TN + FP + FN)
  TPR_Recall <- TP / (TP + FN) # True Positive Rate (Recall / Sensitivity)
  FPR <- FP / (FP + TN)      # False Positive Rate (1 - Specificity)
  Precision <- TP / (TP + FP)  # Positive Predictive Value

  cat(paste("\nMisclassification Error Rate:", round(error_rate, 4), "\n"))
  cat(paste("True Positive Rate (Recall):", round(TPR_Recall, 4), "\n"))
  cat(paste("False Positive Rate:", round(FPR, 4), "\n"))
  cat(paste("Precision:", round(Precision, 4), "\n"))
} else {
  cat("\nCannot calculate full metrics: model predicted only one class.\n")
}
```

```
Misclassification Error Rate: 0.2537
True Positive Rate (Recall): 0.9722
False Positive Rate: 0.5161
Precision: 0.6863
```

ROC curve and Area Under the ROC (AUC)

```
## 4b. Area Under the Curve (AUC)
roc_curve_sim <- roc(test_data_sim$y, pred_probs_sim, quiet = TRUE)

## Plot the ROC curve
plot(roc_curve_sim, main = "ROC Curve (Simulated Test Data)", print.auc = TRUE)
```



```
auc_value_sim <- auc(roc_curve_sim)
cat(paste("Area Under the Curve (AUC):", round(auc_value_sim, 4), "\n\n"))
```

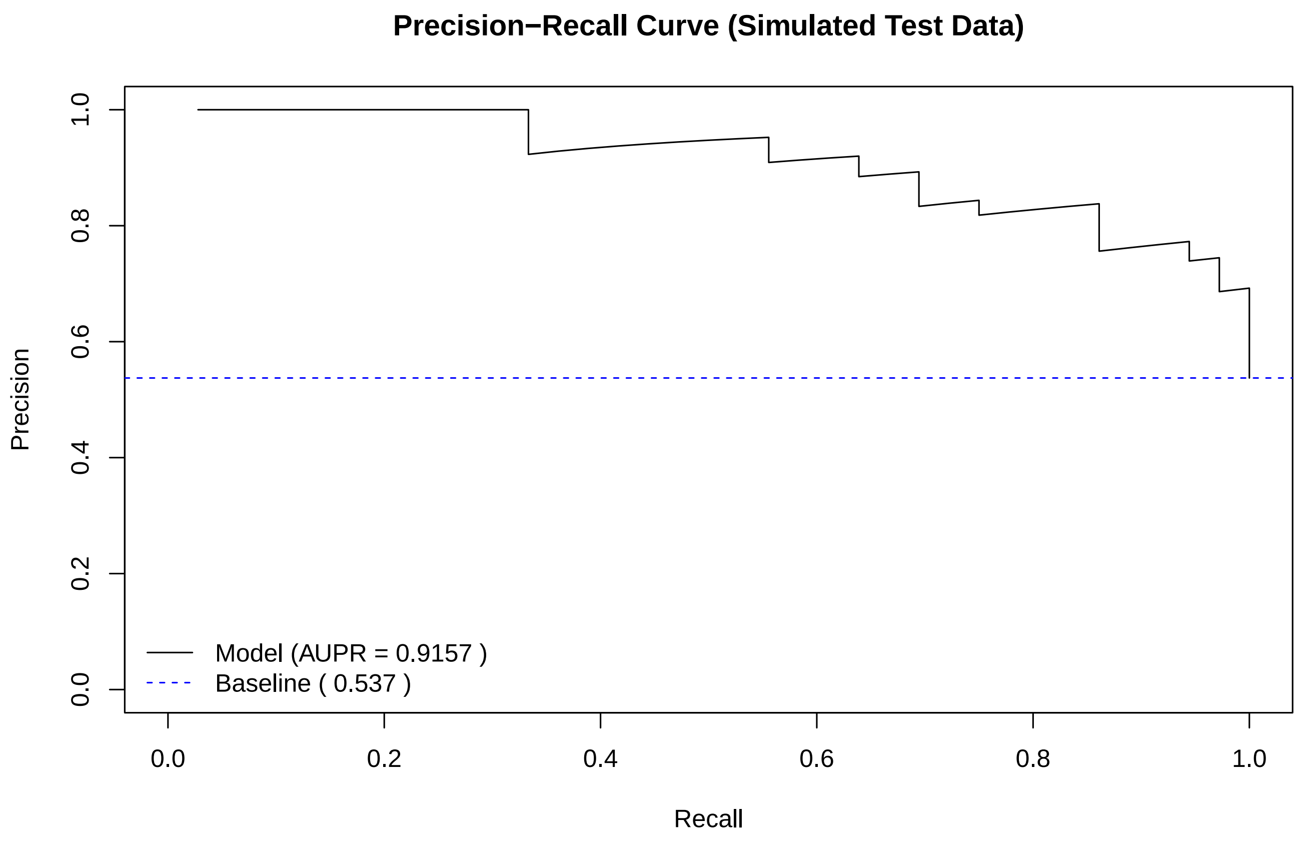
```
Area Under the Curve (AUC): 0.8996
```

PR curve and Area Under PR Curve (AUPR)

```r
## Load the ROCR library
## install.packages("ROCR") # Uncomment to install if needed
library(ROCR)

## --- 1. Create a 'prediction' object ---
## 'prediction' takes all predictions and all true labels
pred_obj <- prediction(pred_probs_sim, test_data_sim$y)

## --- 2. Create a 'performance' object for PR ---
## "prec" is for precision, "rec" is for recall
perf_pr <- performance(pred_obj, measure = "prec", x.measure = "rec")

## --- 3. Calculate Area Under the PR Curve (AUPR) ---
perf_auc <- performance(pred_obj, measure = "aucpr") # "aucpr" = Area Under PR Curve
aupr_value <- perf_auc@y.values[[1]]
cat(paste("Area Under PR Curve (AUPR):", round(aupr_value, 4), "\n"))
```

```
Area Under PR Curve (AUPR): 0.9157
```

```r
## --- 4. Plot the performance object ---
plot(perf_pr,
     main = "Precision-Recall Curve (Simulated Test Data)",
     xlim = c(0, 1),
     ylim = c(0, 1),
     col = "black")

## --- 5. Calculate and add the 'no-skill' baseline ---
baseline_precision_sim <- sum(test_data_sim$y == 1) / length(test_data_sim$y)
abline(h = baseline_precision_sim, col = "blue", lty = 2)

## --- 6. Add a legend with AUPR ---
legend("bottomleft",
       legend = c(
           paste("Model (AUPR =", round(aupr_value, 4), ")"),  # <-- MODIFIED LINE
           paste("Baseline (", round(baseline_precision_sim, 3), ")")
       ),
       col = c("black", "blue"),
       lty = c(1, 2),
       bty = "n") # bty="n" removes the box
```

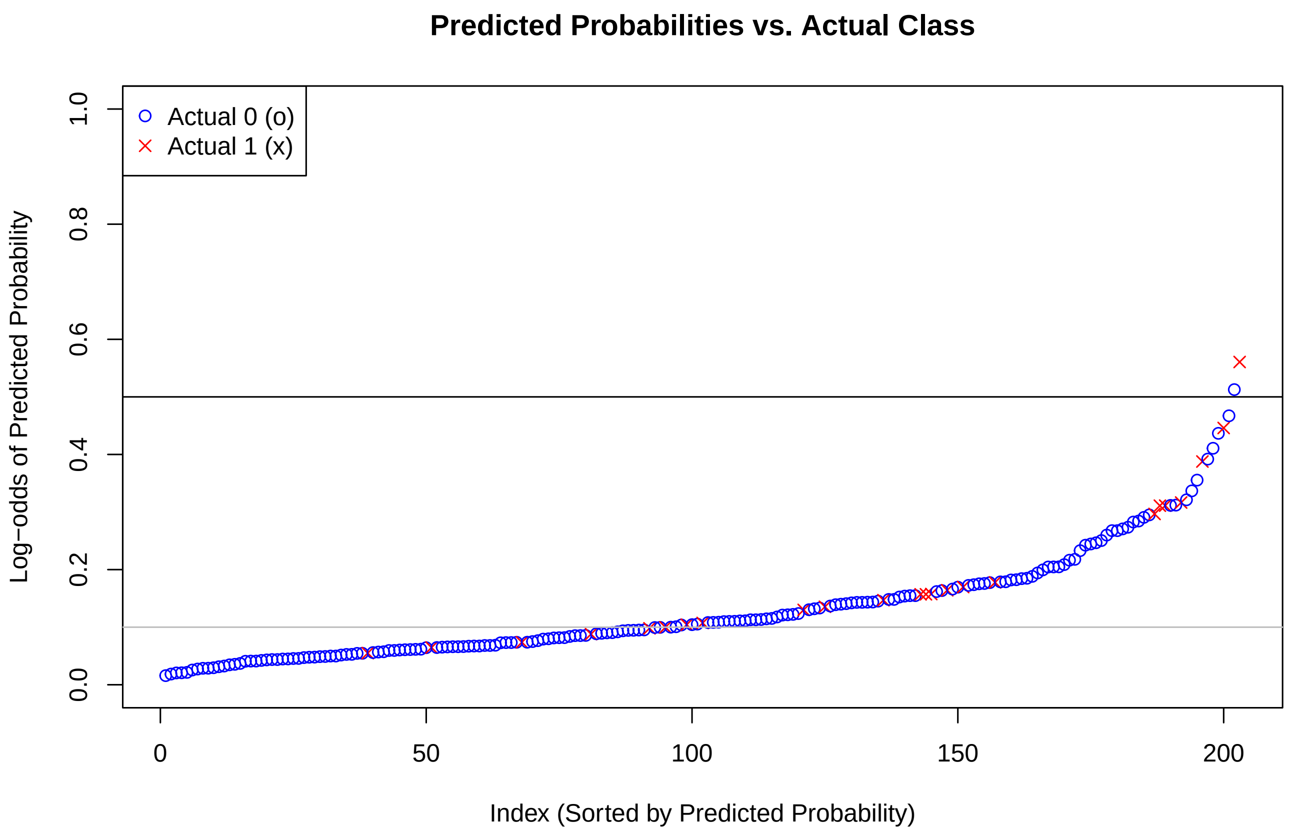


6.8.3 Application to the CHD Dataset

```r
## Load the pROC library for AUC calculation
## install.packages("pROC") # Uncomment to install if needed
library(pROC)

## --- 1. Split the data ---
set.seed(123) # for reproducibility
n <- nrow(CHD.data)
train_size <- floor(2/3 * n)
train_indices <- sample(1:n, size = train_size)
train_data <- CHD.data[train_indices, ]
test_data  <- CHD.data[-train_indices, ]

## --- 2. Refit the model on the training data ---
fit_train <- glm(
  chd ~ smk + cat + sbp + age + chl + ecg + hpt,
  data = train_data,
  family = binomial(link = "logit")
)

## --- 3. Make predictions on the test data ---
pred_probs <- predict(fit_train, newdata = test_data, type = "response")
```

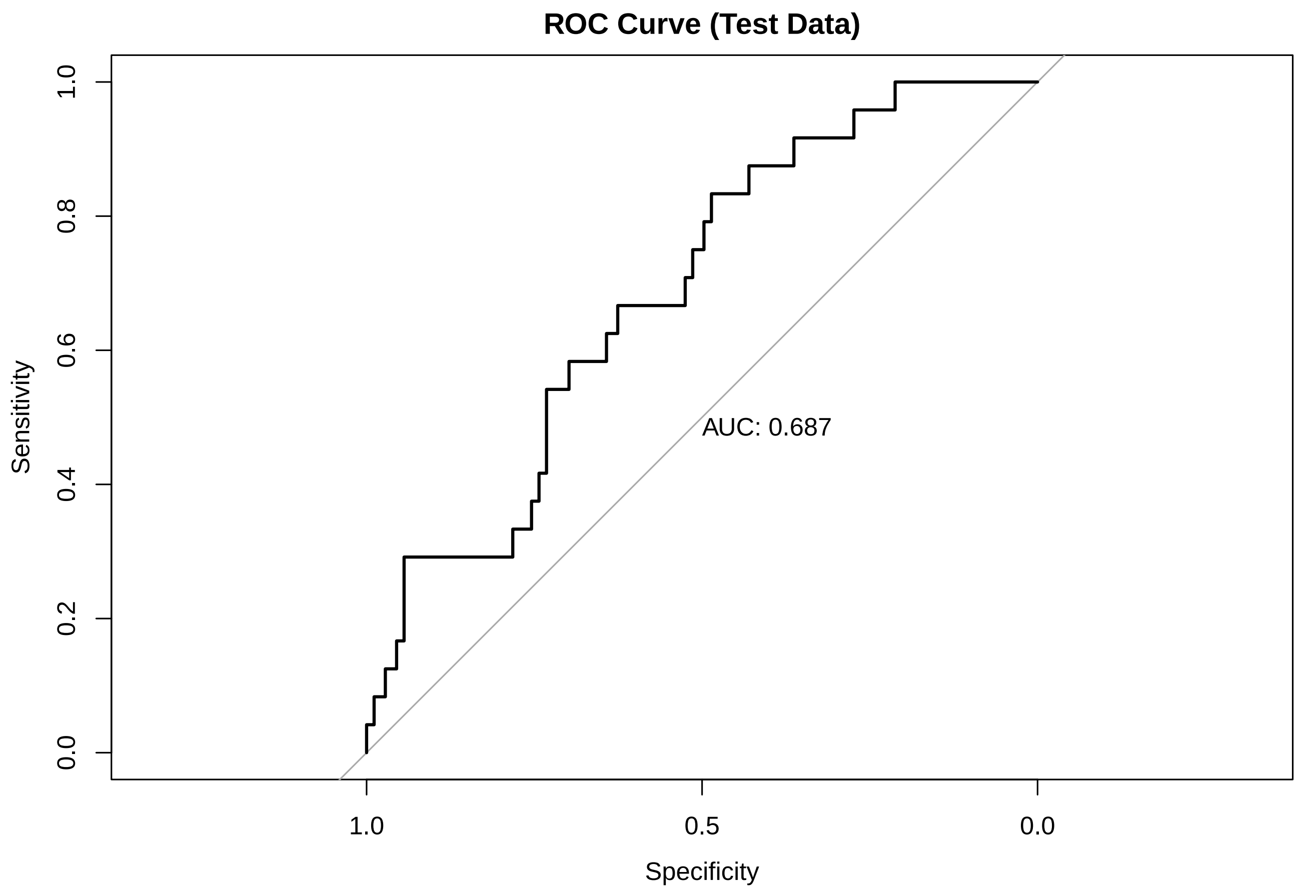
Plot Predictive Probabilities

```r
## --- 5. Plot sorted predicted probabilities ---

## Create a data frame for plotting
plot_data <- data.frame(
  Prob = pred_probs,
  Actual = as.factor(test_data$chd)
)

## Sort by predicted probability
plot_data <- plot_data[order(plot_data$Prob), ]
plot_data$Rank <- 1:nrow(plot_data)

## Create the plot
## We use 'pch' (plot character) to set different symbols
## 'pch = 1' is 'o' (default)
## 'pch = 4' is 'x'
plot(
  plot_data$Rank,
  plot_data$Prob,
  pch = ifelse(plot_data$Actual == 0, 1, 4),
  col = ifelse(plot_data$Actual == 0, "blue", "red"),
  xlab = "Index (Sorted by Predicted Probability)",
  ylab = "Log-odds of Predicted Probability",
  main = "Predicted Probabilities vs. Actual Class",
  ylim = c(0,1)
)
abline(h=0.5)
abline(h=0.1, col="grey")

## Add a legend
legend(
  "topleft",
  legend = c("Actual 0 (o)", "Actual 1 (x)"),
  pch = c(1, 4),
  col = c("blue", "red")
)
```



ROC curve and Area Under the ROC (AUC)

```
## 4b. Area Under the Curve (AUC)
roc_curve <- roc(test_data$chd, pred_probs, quiet = TRUE)

## Plot the ROC curve
plot(roc_curve, main = "ROC Curve (Test Data)", print.auc = TRUE)
```



```
auc_value <- auc(roc_curve)
cat(paste("Area Under the Curve (AUC):", round(auc_value, 4), "\n\n"))
```

```
Area Under the Curve (AUC): 0.6872
```

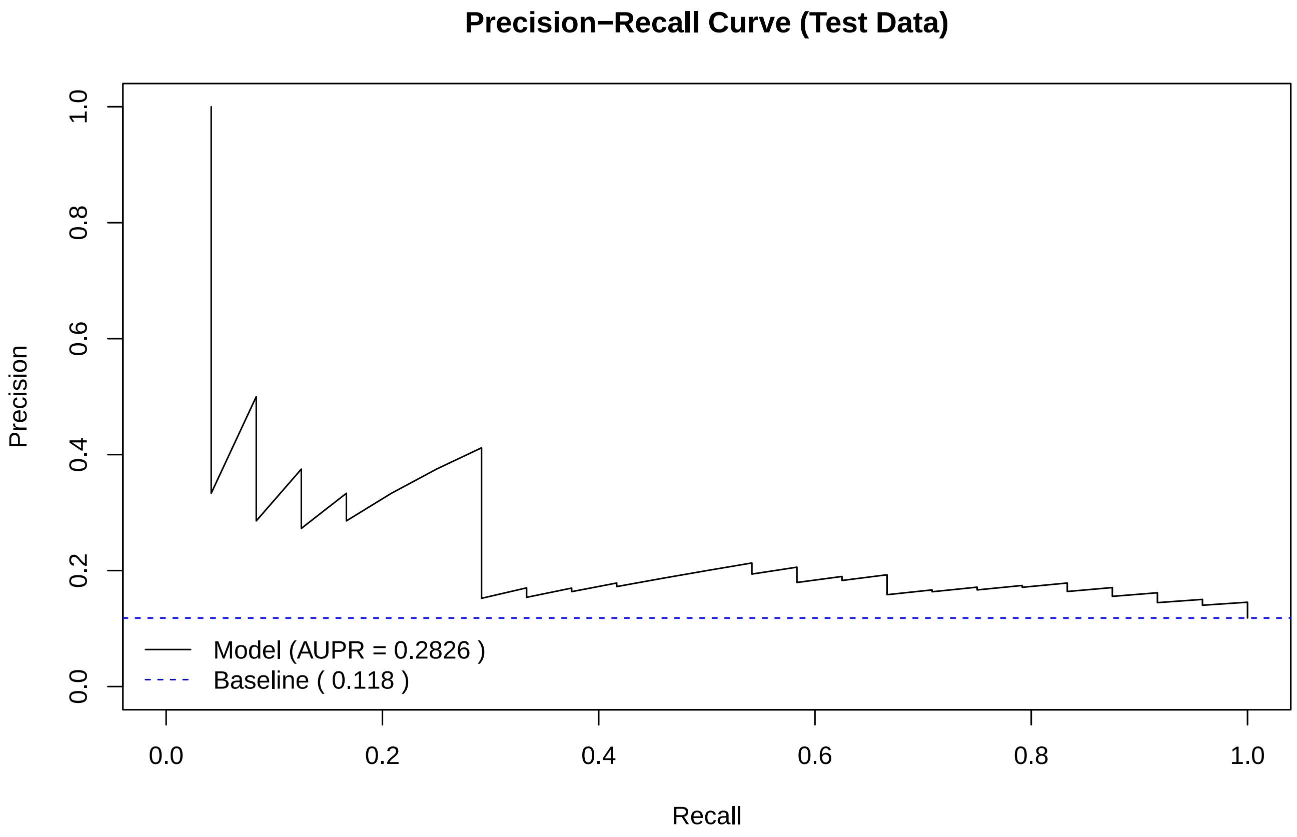
PR curve and Area Under PR Curve (AUPR)

```
## Load the ROCR library
## install.packages("ROCR") # Uncomment to install if needed
library(ROCR)

## --- 1. Create a 'prediction' object ---
## 'prediction' takes all predictions and all true labels
## We use 'pred_probs' and 'test_data$chd' from the CHD data split
pred_obj <- prediction(pred_probs, test_data$chd)

## --- 2. Create a 'performance' object for PR ---
## "prec" is for precision, "rec" is for recall
```

```r
perf_pr <- performance(pred_obj, measure = "prec", x.measure = "rec")

## --- 3. Calculate Area Under the PR Curve (AUPR) ---
perf_auc <- performance(pred_obj, measure = "aucpr") # "aucpr" = Area Under PR Curve
aupr_value <- perf_auc@y.values[[1]]
cat(paste("Area Under PR Curve (AUPR):", round(aupr_value, 4), "\n"))
```

```
Area Under PR Curve (AUPR): 0.2826
```

```r
## --- 4. Plot the performance object ---
plot(perf_pr,
     main = "Precision-Recall Curve (Test Data)",
     xlim = c(0, 1),
     ylim = c(0, 1),
     col = "black")

## --- 5. Calculate and add the 'no-skill' baseline ---
baseline_precision <- sum(test_data$chd == 1) / length(test_data$chd)
abline(h = baseline_precision, col = "blue", lty = 2)

## --- 6. Add a legend with AUPR ---
legend("bottomleft",
       legend = c(
           paste("Model (AUPR =", round(aupr_value, 4), ")"),  # <-- MODIFIED LINE
           paste("Baseline (", round(baseline_precision, 3), ")")
       ),
       col = c("black", "blue"),
       lty = c(1, 2),
       bty = "n") # bty="n" removes the box
```


Precision−Recall Curve (Test Data)
Precision
Recall
0.0
0.2
0.4
0.6
0.8
1.0
Model (AUPR = 0.2826)
Baseline (0.118)

7 Randomized Complete Block Design

7.1 Completely Randomized Design

7.1.1 Design on R

```
treatments <- LETTERS[1:4]
rep.treatments <- rep(treatments, each = 5)
rep.treatments
```

```
 [1] "A" "A" "A" "A" "A" "B" "B" "B" "B" "B" "C" "C" "C" "C" "C" "D" "D" "D" "D"
[20] "D"
```

```
sample (rep.treatments)
```

```
 [1] "A" "C" "C" "B" "D" "B" "B" "D" "D" "A" "B" "D" "C" "A" "A" "B" "A" "C" "C"
[20] "D"
```

```
data.frame(run.ID = 1:20, treatment = sample (rep.treatments))
```

```
   run.ID treatment
1       1         D
2       2         C
3       3         A
4       4         B
5       5         C
6       6         B
7       7         C
8       8         C
9       9         D
10     10         B
11     11         C
12     12         A
13     13         B
14     14         D
```

```
15      15          A
16      16          A
17      17          A
18      18          D
19      19          D
20      20          B
```

7.1.2 Plasma Etching Experiment

This section analyzes data from a **Completely Randomized Design (CRD)**. In a CRD, experimental units (in this case, the silicon wafers being etched) are assigned to treatments (the RF Power levels) completely at random. The primary goal is to determine if changing the RF Power level has a statistically significant effect on the mean etch rate.

7.1.2.1 Data and Visualization

We begin by loading the data into a single, tidy `data.frame`. The response variable, `rate`, contains all the etch rate observations. The predictor variable, `power`, is a **factor**, which is R's way of representing a categorical variable. This tells R to treat the different power levels as distinct groups.

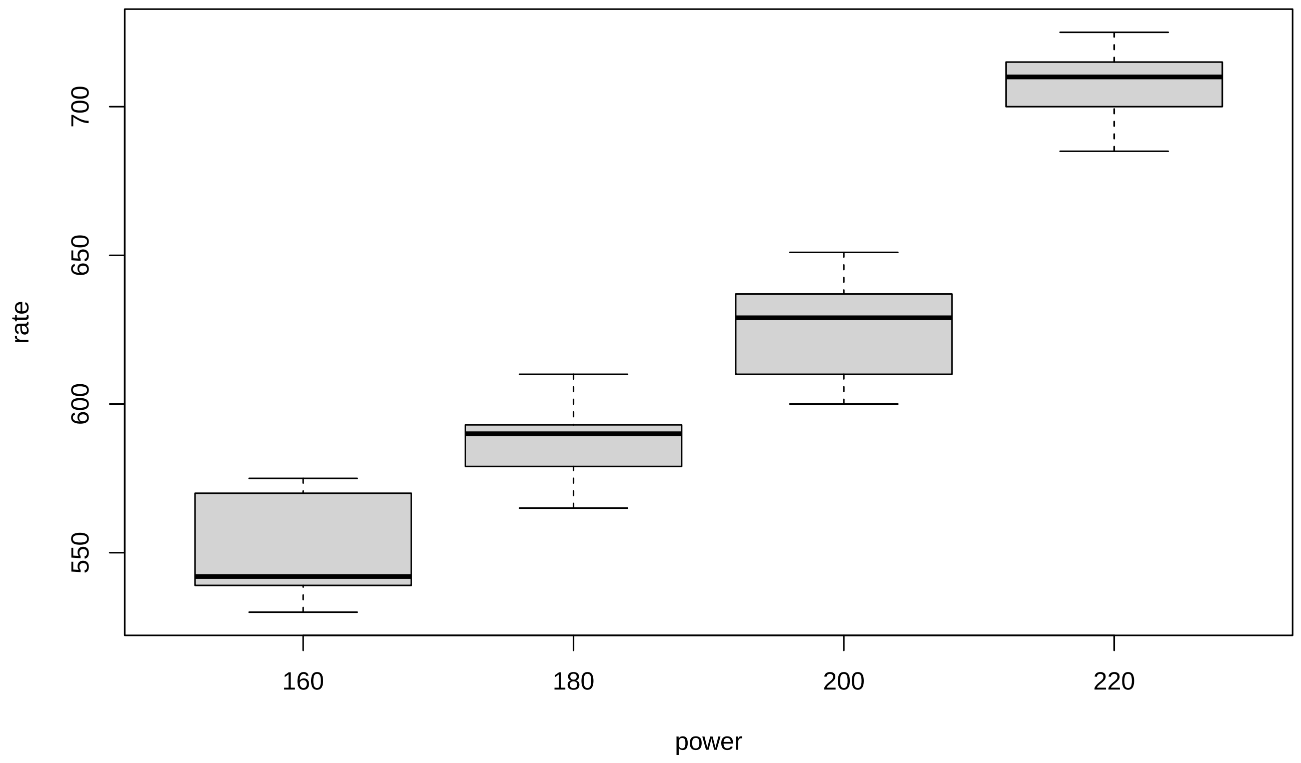
```r
## Define the data vectors
rate <- c(575, 542, 530, 539, 570, 565, 593, 590, 579, 610,
          600, 651, 610, 637, 629, 725, 700, 715, 685, 710)
power_levels <- c(160, 180, 200, 220)

## Create the data frame
etching_df <- data.frame(
  rate = rate,
  power = factor(rep(power_levels, each = 5))
)

## Display the first few rows
etching_df
```

```
   rate power
1   575   160
2   542   160
3   530   160
4   539   160
5   570   160
6   565   180
7   593   180
8   590   180
```

```
9    579    180
10   610    180
11   600    200
12   651    200
13   610    200
14   637    200
15   629    200
16   725    220
17   700    220
18   715    220
19   685    220
20   710    220
```

Grouped Boxplots

```r
boxplot(rate~power, data=etching_df)
```



Using ggplot to visualize grouped data

```r
library(ggplot2)
library(dplyr) # Using dplyr for easier data manipulation

## Calculate group means and their start/end indices
```

```r
mean_rates <- etching_df %>%
  mutate(obs_index = row_number()) %>%
  group_by(power) %>%
  summarise(
    mean_rate = mean(rate),
    x_start = min(obs_index) - 0.5,
    x_end = max(obs_index) + 0.5
  )

ggplot(etching_df, aes(x = 1:nrow(etching_df), y = rate, color = power)) +
  geom_hline(
    yintercept = mean(etching_df$rate),
    linetype = "solid",
    color = "black",
    size = 1
  ) +
  # ----------------------------------------
  geom_point(size = 3, alpha = 0.7) + # Plot individual data points
  geom_segment(
    data = mean_rates,
    aes(x = x_start, xend = x_end, y = mean_rate, yend = mean_rate),
    linetype = "dashed",
    size = 1.2
  ) + # Add line segments for group means
  labs(
    title = "Etch Rate Observations by RF Power Level",
    x = "Observation Index",
    y = "Etch Rate",
    color = "RF Power (W)"
  ) +
  scale_color_brewer(palette = "Set1") +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5))
```

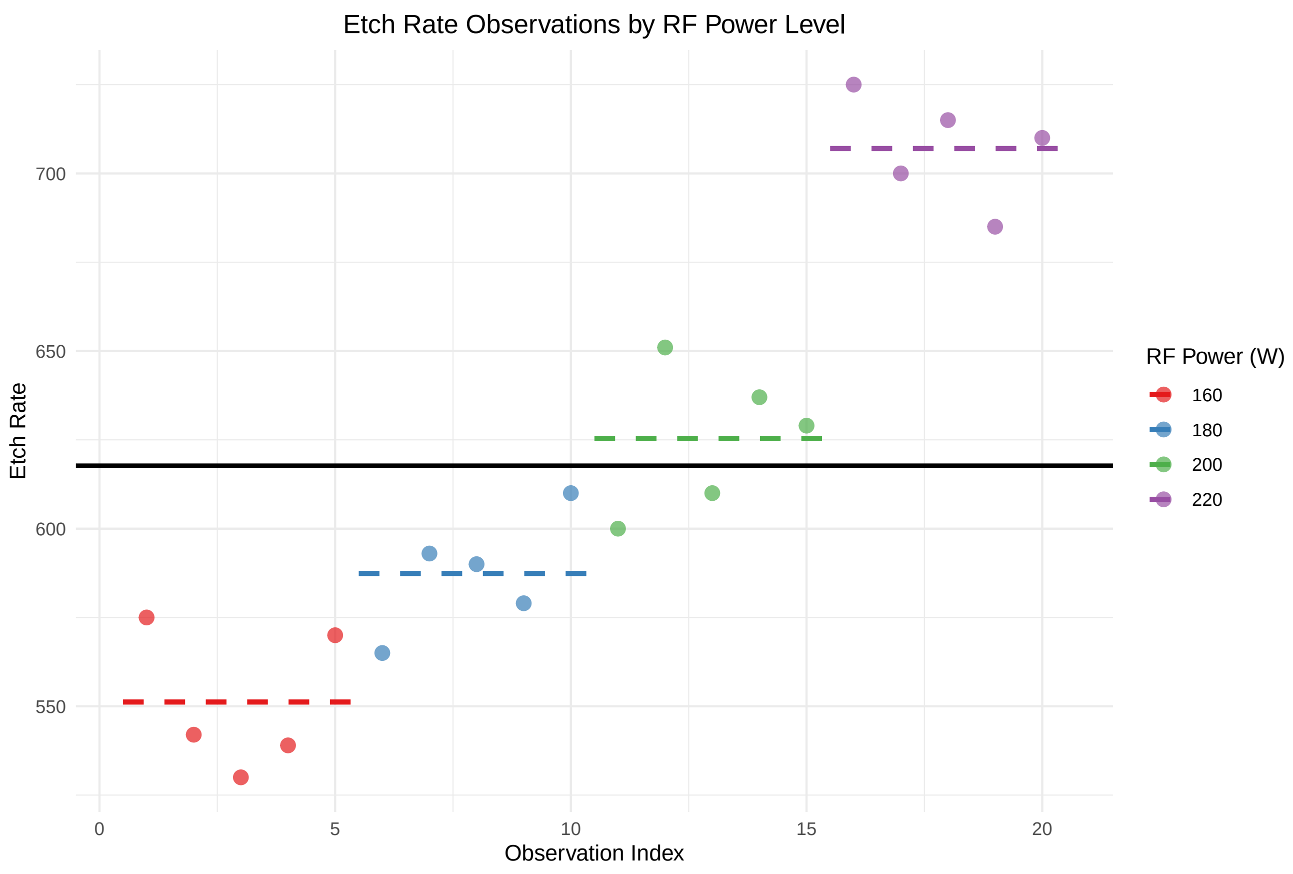


Figure 7.1: Index Plot of Etch Rate with Group-Specific Mean Lines

7.1.2.2 Cell Mean Models (zero-intercept)

```
fit_nointercpt <- lm(rate ~ 0+power, data = etching_df)
model.matrix(fit_nointercpt)
```

```
   power160 power180 power200 power220
1         1        0        0        0
2         1        0        0        0
3         1        0        0        0
4         1        0        0        0
5         1        0        0        0
6         0        1        0        0
7         0        1        0        0
8         0        1        0        0
9         0        1        0        0
10        0        1        0        0
```

```
11        0        0        1        0
12        0        0        1        0
13        0        0        1        0
14        0        0        1        0
15        0        0        1        0
16        0        0        0        1
17        0        0        0        1
18        0        0        0        1
19        0        0        0        1
20        0        0        0        1
attr(,"assign")
[1] 1 1 1 1
attr(,"contrasts")
attr(,"contrasts")$power
[1] "contr.treatment"
```

```
summary(fit_nointercpt)
```

```

Call:
lm(formula = rate ~ 0 + power, data = etching_df)

Residuals:
   Min     1Q Median     3Q    Max 
 -25.4  -13.0    2.8   13.2   25.6 

Coefficients:
         Estimate Std. Error t value Pr(>|t|)    
power160  551.200      8.169   67.47   <2e-16 ***
power180  587.400      8.169   71.90   <2e-16 ***
power200  625.400      8.169   76.55   <2e-16 ***
power220  707.000      8.169   86.54   <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom
Multiple R-squared:  0.9993,    Adjusted R-squared:  0.9991 
F-statistic:  5768 on 4 and 16 DF,  p-value: < 2.2e-16
```

```
confint(fit_nointercpt)
```

```
            2.5 %   97.5 %
power160 533.8815 568.5185
```

```
power180 570.0815 604.7185
power200 608.0815 642.7185
power220 689.6815 724.3185
```

```r
anova(fit_nointercpt)
```

```
Analysis of Variance Table

Response: rate
          Df  Sum Sq Mean Sq F value    Pr(>F)
power      4 7699172 1924793    5768 < 2.2e-16 ***
Residuals 16    5339     334
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

This ANOVA result is typically unwanted. If we want to see the causal effect of power, we need to compare to intercept-only model:

```r
fit_intercept <- lm(rate ~ 1, data = etching_df)
anova(fit_intercept, fit_nointercpt)
```

```
Analysis of Variance Table

Model 1: rate ~ 1
Model 2: rate ~ 0 + power
  Res.Df   RSS Df Sum of Sq      F    Pr(>F)
1     19 72210
2     16  5339  3     66871 66.797 2.883e-09 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

7.1.2.3 Centralized Effect Model (Sum-to-Zero Constraint)

We fit a linear model using the `lm()` function to perform an **Analysis of Variance (ANOVA)**. The model is specified as `rate ~ power`, and we now include the `data = etching_df` argument.

To get interpretable estimates for the treatment effects (τ_i), we use a **sum-to-zero constraint** (`contr.sum`), which forces the sum of the treatment effects to be zero ($\sum \tau_i = 0$).

```r
fit <- lm(rate ~ power, data = etching_df, contrasts = list(power = contr.sum))
```

Model Matrix:

```r
model.matrix(fit)
```

```
   (Intercept) power1 power2 power3
1            1      1      0      0
2            1      1      0      0
3            1      1      0      0
4            1      1      0      0
5            1      1      0      0
6            1      0      1      0
7            1      0      1      0
8            1      0      1      0
9            1      0      1      0
10           1      0      1      0
11           1      0      0      1
12           1      0      0      1
13           1      0      0      1
14           1      0      0      1
15           1      0      0      1
16           1     -1     -1     -1
17           1     -1     -1     -1
18           1     -1     -1     -1
19           1     -1     -1     -1
20           1     -1     -1     -1
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$power
    [,1] [,2] [,3]
160    1    0    0
180    0    1    0
200    0    0    1
220   -1   -1   -1
```

Summary of lm fitting results:

```r
summary.fit <- summary(fit)
summary.fit
```

```
Call:
lm(formula = rate ~ power, data = etching_df, contrasts = list(power = contr.sum))

Residuals:
   Min     1Q Median     3Q    Max 
 -25.4  -13.0    2.8   13.2   25.6 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  617.750      4.085 151.234  < 2e-16 ***
power1       -66.550      7.075  -9.406 6.39e-08 ***
power2       -30.350      7.075  -4.290 0.000563 ***
power3         7.650      7.075   1.081 0.295602    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom
Multiple R-squared:  0.9261,    Adjusted R-squared:  0.9122 
F-statistic:  66.8 on 3 and 16 DF,  p-value: 2.883e-09
```

Confidence Interval for Centralized Effects:

The output of the model provides estimates for the overall mean ($\hat{\mu}$) and the treatment effects for the first k-1 levels ($\hat{\tau}_1, \hat{\tau}_2, \hat{\tau}_3$).

- $\hat{\mu}$ (the Intercept) is the estimate of the grand mean etch rate across all power levels.
- $\hat{\tau}_i$ is the estimated effect of the i-th power level, representing how much that level's mean deviates from the grand mean.

Using the sum-to-zero constraint, we can manually calculate the effect for the final level, $\hat{\tau}_4$.

```r
# Define a named vector of all linear combinations
#
# NOTE: Replace 'power1', 'power2', 'power3' with the
# actual names from your coef(fit) output.
#
# The names on the left (e.g., "Level_1_Effect") are
# for you; they will label the output rows.
library(biostat3)
k_all_levels <- c(
  "Effect for Level 1" = "power1",
  "Effect for Level 2" = "power2",
  "Effect for Level 3" = "power3",
  "Effect for Level 4" = "-power1 - power2 - power3"
)
# Run lincom on the whole vector
lincom(fit, k_all_levels)
```

```
                      Estimate 2.5 %     97.5 %    Df Sum of Sq
```

```
Effect for Level 1 -66.55   -80.41666 -52.68334 1  29526.02
Effect for Level 2 -30.35   -44.21666 -16.48334 1  6140.817
Effect for Level 3 7.65     -6.216659 21.51666  1  390.15
Effect for Level 4 89.25    75.38334  103.1167  1  53103.75
```

```
##### Estimate of Treatment Means
```

We can verify the above results by looking at the point estimate of centralized effect by direct calculation. The construction of CI is more complicated, hence, omitted.

```
## Extract coefficients
est <- coef(fit)
tau4.hat <- -sum(est[-1])
taui.hat <- c(est[-1], tau4.hat)
print(taui.hat)
```

```
power1 power2 power3
-66.55 -30.35   7.65  89.25
```

7.1.2.3.1 ANOVA

The ANOVA table partitions the total variation into variation **between** treatment groups (`power`) and variation **within** treatment groups (random error). The **p-value** (Pr(>F)) indicates if the treatment has a significant effect.

```
anova(fit)
```

```
Analysis of Variance Table

Response: rate
          Df Sum Sq Mean Sq F value    Pr(>F)
power      3  66871 22290.2  66.797 2.883e-09 ***
Residuals 16   5339   333.7
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

7.1.2.4 Baseline Model (Default for R)

Fitting the model without specifying contrasts uses R's default ("treatment" contrast), which sets $\tau_1 = 0$. The fundamental results (ANOVA, treatment means) remain unchanged.

```
fit1 <- lm(rate ~ power, data = etching_df)
model.matrix(fit1)
```

```
   (Intercept) power180 power200 power220
1            1        0        0        0
2            1        0        0        0
3            1        0        0        0
4            1        0        0        0
5            1        0        0        0
6            1        1        0        0
7            1        1        0        0
8            1        1        0        0
9            1        1        0        0
10           1        1        0        0
11           1        0        1        0
12           1        0        1        0
13           1        0        1        0
14           1        0        1        0
15           1        0        1        0
16           1        0        0        1
17           1        0        0        1
18           1        0        0        1
19           1        0        0        1
20           1        0        0        1
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$power
[1] "contr.treatment"
```

```
summary(fit1)
```

```

Call:
lm(formula = rate ~ power, data = etching_df)

Residuals:
   Min     1Q Median     3Q    Max 
 -25.4  -13.0    2.8   13.2   25.6 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  551.200      8.169  67.471  < 2e-16 ***
```

```
power180      36.200     11.553   3.133  0.00642 **
power200      74.200     11.553   6.422 8.44e-06 ***
power220     155.800     11.553  13.485 3.73e-10 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom
Multiple R-squared:  0.9261,    Adjusted R-squared:  0.9122
F-statistic:  66.8 on 3 and 16 DF,  p-value: 2.883e-09
```

Using 200 as the baseline

If we want to treat power200 as the baseline, we do this:

```
# modifying the levels of power
etching_df$power <- factor(etching_df$power, levels=c("200","160", "180", "220"))
```

```
fit1_200 <- lm(rate ~ power, data = etching_df)
model.matrix(fit1_200)
```

```
   (Intercept) power160 power180 power220
1            1        1        0        0
2            1        1        0        0
3            1        1        0        0
4            1        1        0        0
5            1        1        0        0
6            1        0        1        0
7            1        0        1        0
8            1        0        1        0
9            1        0        1        0
10           1        0        1        0
11           1        0        0        0
12           1        0        0        0
13           1        0        0        0
14           1        0        0        0
15           1        0        0        0
16           1        0        0        1
17           1        0        0        1
18           1        0        0        1
19           1        0        0        1
20           1        0        0        1
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$power
[1] "contr.treatment"
```

```
summary(fit1_200)
```

```
Call:
lm(formula = rate ~ power, data = etching_df)

Residuals:
   Min     1Q Median     3Q    Max 
 -25.4  -13.0    2.8   13.2   25.6 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  625.400      8.169  76.553  < 2e-16 ***
power160     -74.200     11.553  -6.422 8.44e-06 ***
power180     -38.000     11.553  -3.289  0.00462 ** 
power220      81.600     11.553   7.063 2.68e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom
Multiple R-squared:  0.9261,	Adjusted R-squared:  0.9122 
F-statistic:  66.8 on 3 and 16 DF,  p-value: 2.883e-09
```

ANOVA

```
anova(fit1_200)
```

```
Analysis of Variance Table

Response: rate
          Df Sum Sq Mean Sq F value    Pr(>F)    
power      3  66871 22290.2  66.797 2.883e-09 ***
Residuals 16   5339   333.7                      
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Using 220 as the baseline

If we want to treat power220 as the baseline, we do this:

```r
etching_df$power <- factor(etching_df$power, levels=c("220","160", "180","200" ))
```

```r
fit1_220 <- lm(rate ~ power, data = etching_df)
model.matrix(fit1_220)
```

```
   (Intercept) power160 power180 power200
1            1        1        0        0
2            1        1        0        0
3            1        1        0        0
4            1        1        0        0
5            1        1        0        0
6            1        0        1        0
7            1        0        1        0
8            1        0        1        0
9            1        0        1        0
10           1        0        1        0
11           1        0        0        1
12           1        0        0        1
13           1        0        0        1
14           1        0        0        1
15           1        0        0        1
16           1        0        0        0
17           1        0        0        0
18           1        0        0        0
19           1        0        0        0
20           1        0        0        0
attr(,"assign")
[1] 0 1 1 1
attr(,"contrasts")
attr(,"contrasts")$power
[1] "contr.treatment"
```

```r
summary(fit1_220)
```

```


Call:
lm(formula = rate ~ power, data = etching_df)

Residuals:
   Min     1Q Median     3Q    Max 
 -25.4  -13.0    2.8   13.2   25.6 

Coefficients:
```

```
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  707.000      8.169  86.542  < 2e-16 ***
power160    -155.800     11.553 -13.485 3.73e-10 ***
power180    -119.600     11.553 -10.352 1.69e-08 ***
power200     -81.600     11.553  -7.063 2.68e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 18.27 on 16 degrees of freedom
Multiple R-squared:  0.9261,    Adjusted R-squared:  0.9122
F-statistic:  66.8 on 3 and 16 DF,  p-value: 2.883e-09
```

ANOVA

```
anova(fit1_220)
```

```
Analysis of Variance Table

Response: rate
          Df Sum Sq Mean Sq F value    Pr(>F)
power      3  66871 22290.2  66.797 2.883e-09 ***
Residuals 16   5339   333.7
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

7.1.2.5 Pairwise Comparisons

Since our ANOVA result was significant, we perform **post-hoc tests** to determine exactly which pairs of power levels have different means.

7.1.2.5.1 Fisher's LSD Test

The **Fisher's Least Significant Difference (LSD)** test does not control the family-wise error rate but is more powerful.

```
with(etching_df, pairwise.t.test(rate, power, p.adj = "none"))
```

```

    Pairwise comparisons using t tests with pooled SD

data:  rate and power
```

```
    220     160     180
160 3.7e-10 -       -
180 1.7e-08 0.0064  -
200 2.7e-06 8.4e-06 0.0046

P value adjustment method: none
```

7.1.2.5.2 Tukey's HSD Test

Tukey's Honest Significant Difference (HSD) controls the **family-wise error rate**, adjusting p-values to account for multiple comparisons.

```r
fit.aov <- aov(rate ~ power, data = etching_df)
TukeyHSD(fit.aov)
```

```
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = rate ~ power, data = etching_df)

$power
          diff         lwr        upr     p adj
160-220 -155.8 -188.854376 -122.74562 0.0000000
180-220 -119.6 -152.654376  -86.54562 0.0000001
200-220  -81.6 -114.654376  -48.54562 0.0000146
180-160   36.2    3.145624   69.25438 0.0294279
200-160   74.2   41.145624  107.25438 0.0000455
200-180   38.0    4.945624   71.05438 0.0215995
```

7.1.2.6 Checking Model Assumptions

The validity of our ANOVA results depends on three key assumptions about the model's residuals. We use diagnostic plots to check them.

```r
r <- rstudent(fit)
fitted <- fitted.values(fit)
```

7.1.2.6.1 Normality of Residuals

A **Normal Q-Q plot** is used to check if the residuals are normally distributed. The points should fall closely along the straight diagonal line.

```r
qqnorm(r)
qqline(r)
```

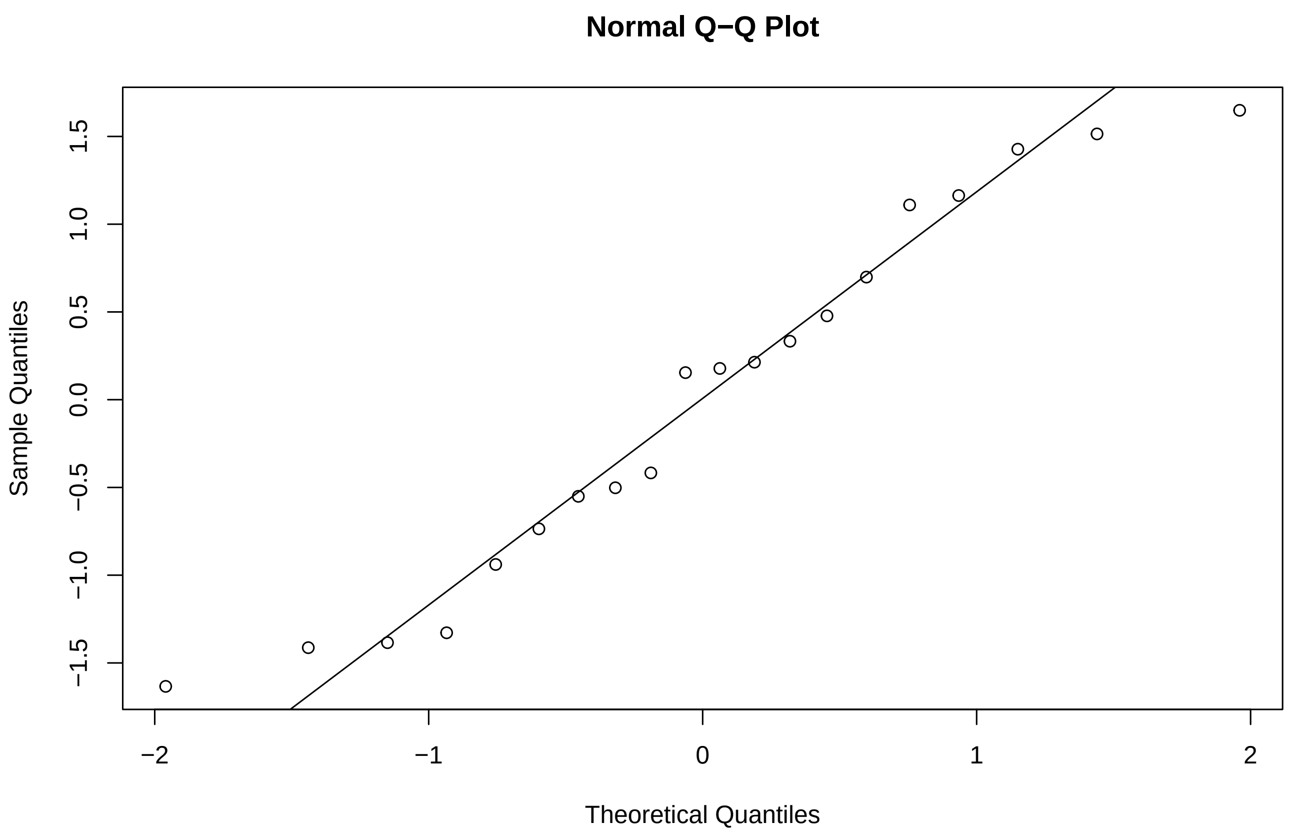


Figure 7.2: Normal Q-Q plot of standardized residuals.

7.1.2.6.2 Independence of Residuals

A plot of **residuals versus run order** helps check for independence. We look for random scatter around the zero line.

```r
plot(r, ylab = "Standardized residuals", xlab = "Run order",
     main = "Plot of residuals vs. run order")
abline(h = 0)
```

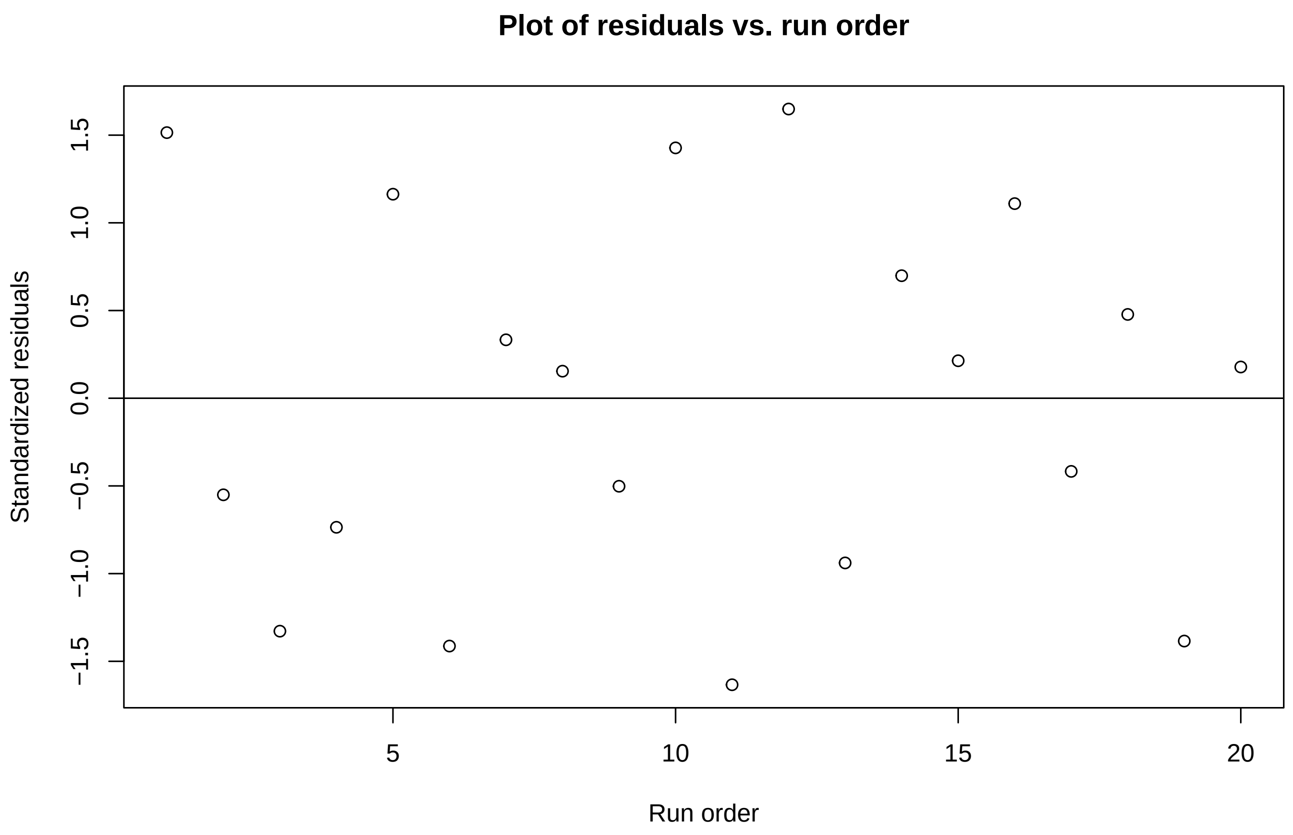


Figure 7.3: Standardized residuals vs. run order.

7.1.2.6.3 Constant Variance (Homoscedasticity)

A plot of **residuals versus fitted values** helps check for constant variance. The spread of residuals should be roughly constant across all fitted values.

```r
plot(fitted, r, ylab = "Standardized residuals",
     xlab = "Fitted values", main = "Plot of residuals vs. fitted values")
abline(h = 0)
```

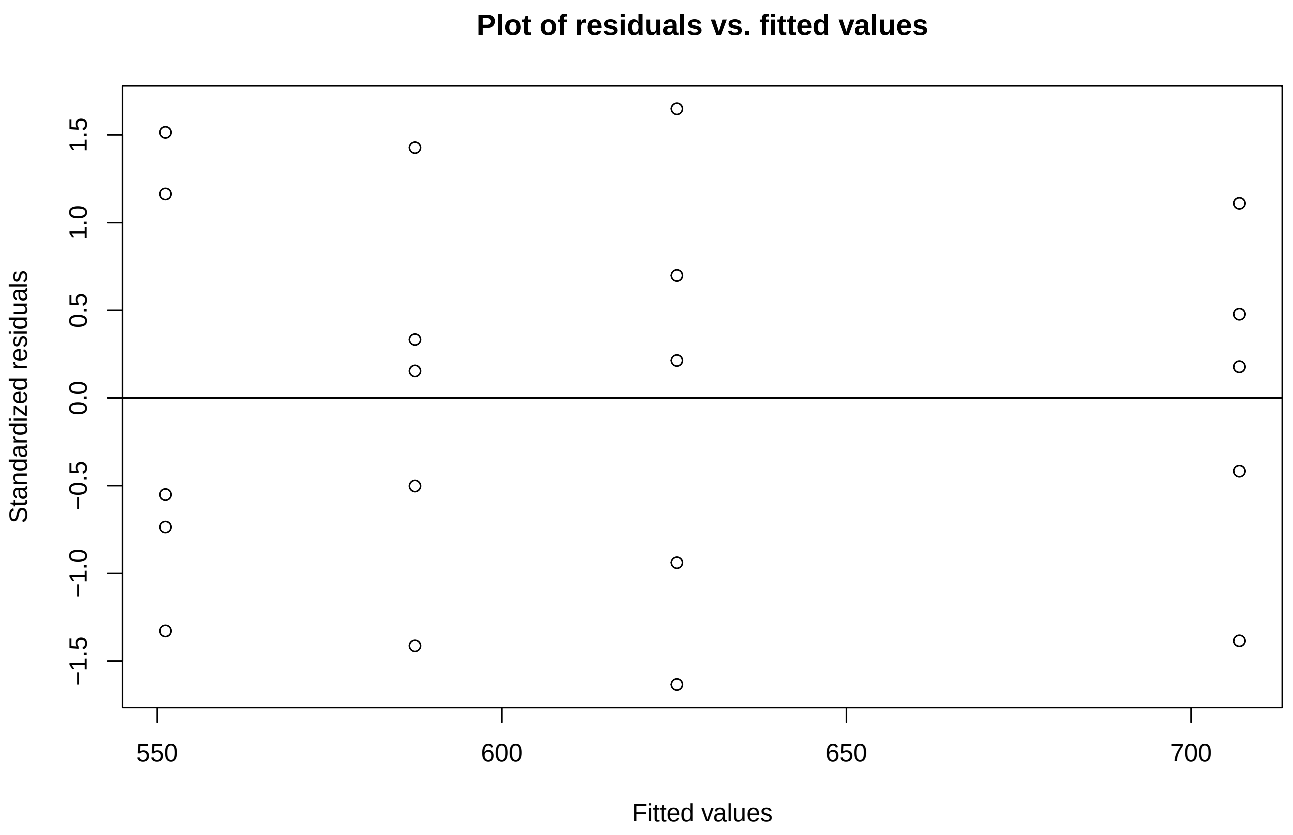


Figure 7.4: Standardized residuals vs. fitted values.

7.2 Unbalanced Designs with Unequal Sample Sizes

The ANOVA framework also handles **unbalanced designs**. We again start by creating a data frame.

```
## Create the data frame
bricks_df <- data.frame(
  density = c(21.8, 21.9, 21.7, 21.6, 21.7,
              21.7, 21.4, 21.5, 21.4,
              21.9, 21.8, 21.8, 21.6, 21.5,
              21.9, 21.7, 21.8, 21.4),
  temperature = factor(c(rep(100, 5), rep(125, 4), rep(150, 5), rep(175, 4)))
)

bricks_df
```

```
   density temperature
1     21.8         100
2     21.9         100
```

```
3     21.7          100
4     21.6          100
5     21.7          100
6     21.7          125
7     21.4          125
8     21.5          125
9     21.4          125
10    21.9          150
11    21.8          150
12    21.8          150
13    21.6          150
14    21.5          150
15    21.9          175
16    21.7          175
17    21.8          175
18    21.4          175
```

```r
## Fit the model and get the ANOVA table
fit2 <- lm(density ~ temperature, data = bricks_df)
summary(fit2)
```

```
Call:
lm(formula = density ~ temperature, data = bricks_df)

Residuals:
   Min     1Q Median     3Q    Max 
-0.300 -0.100  0.000  0.095  0.200 

Coefficients:
               Estimate Std. Error t value Pr(>|t|)    
(Intercept)    21.74000    0.07171 303.150   <2e-16 ***
temperature125 -0.24000    0.10757  -2.231   0.0425 *  
temperature150 -0.02000    0.10142  -0.197   0.8465    
temperature175 -0.04000    0.10757  -0.372   0.7156    
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1604 on 14 degrees of freedom
Multiple R-squared:  0.3025,	Adjusted R-squared:  0.153 
F-statistic: 2.024 on 3 and 14 DF,  p-value: 0.1569
```

```r
anova(fit2)
```

```
Analysis of Variance Table

Response: density
            Df  Sum Sq  Mean Sq F value Pr(>F)
temperature  3 0.15611 0.052037  2.0237 0.1569
Residuals   14 0.36000 0.025714
```

In this case, the large p-value (0.133) indicates that there is no statistically significant evidence that firing temperature affects brick density.

7.3 Randomized Complete Block Design

7.3.1 Vascular Graft Experiment

This section analyzes a **Randomized Complete Block Design (RCBD)**, used to control for a known source of variability (here, "batches of resin," treated as **blocks**).

7.3.1.1 Data and Visulization

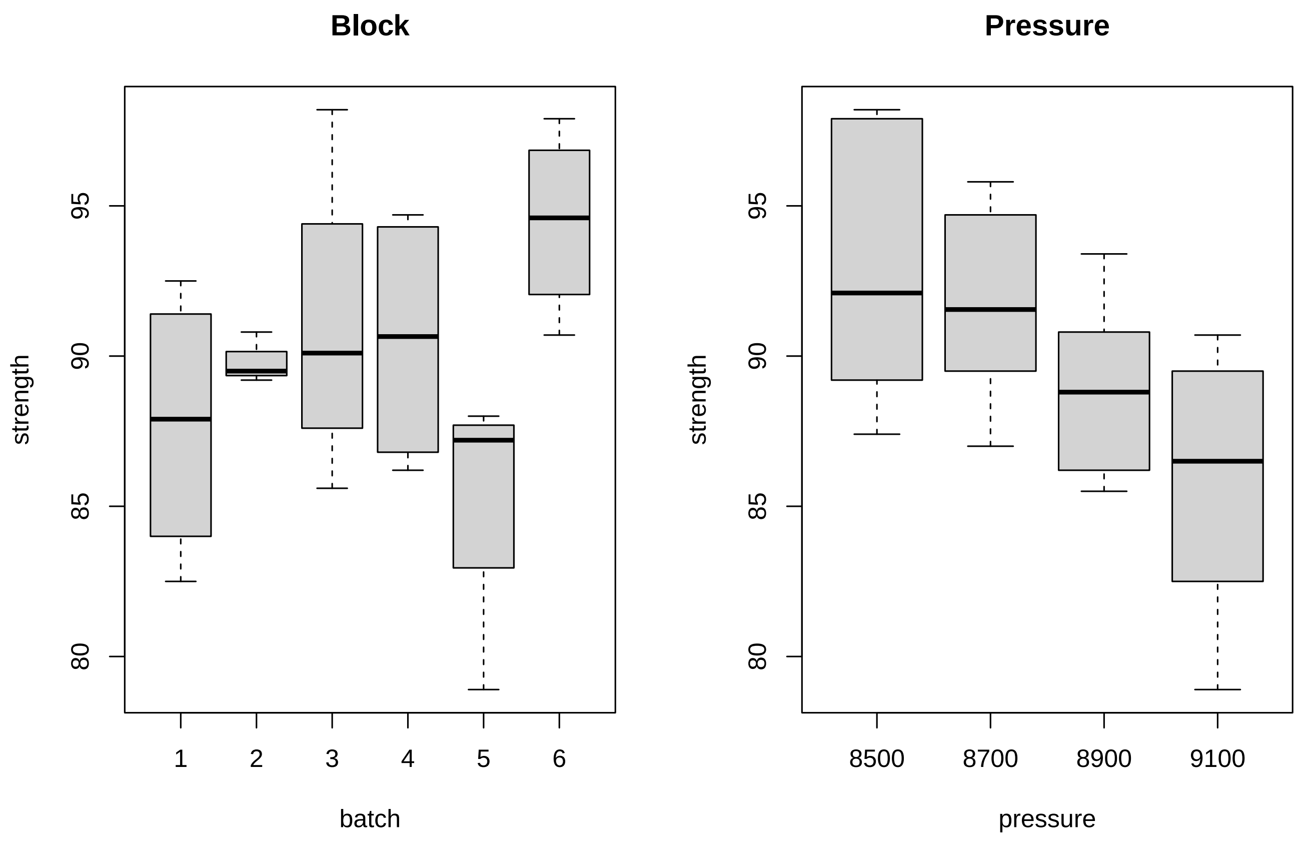
We structure the data in a `data.frame` to identify the response, treatment (`pressure`), and block (`batch`) for each observation.

```r
## Define data vectors
strength <- c(90.3, 89.2, 98.2, 93.9, 87.4, 97.9,
              92.5, 89.5, 90.6, 94.7, 87.0, 95.8,
              85.5, 90.8, 89.6, 86.2, 88.0, 93.4,
              82.5, 89.5, 85.6, 87.4, 78.9, 90.7)
pressure_levels <- rep(c(8500, 8700, 8900, 9100), each = 6)
batch_levels <- rep(1:6, 4)

## Create the data frame
graft_df <- data.frame(
  strength = strength,
  pressure = factor(pressure_levels),
  batch = factor(batch_levels)
)


graft_df
```

```
   strength pressure batch
1      90.3     8500     1
2      89.2     8500     2
3      98.2     8500     3
4      93.9     8500     4
5      87.4     8500     5
6      97.9     8500     6
7      92.5     8700     1
8      89.5     8700     2
9      90.6     8700     3
10     94.7     8700     4
11     87.0     8700     5
12     95.8     8700     6
13     85.5     8900     1
14     90.8     8900     2
15     89.6     8900     3
16     86.2     8900     4
17     88.0     8900     5
18     93.4     8900     6
19     82.5     9100     1
20     89.5     9100     2
21     85.6     9100     3
22     87.4     9100     4
23     78.9     9100     5
24     90.7     9100     6
```

Visualize the Block and Treatment Effects

```
par (mfrow = c(1,2))
#boxplot
plot(strength ~ batch, data=graft_df , main = "Block")
plot(strength ~ pressure, data=graft_df , main = "Pressure")
```



Interaction Plots

```r
ggplot(graft_df, aes(x = pressure, y = strength, group = batch, color = batch)) +
  stat_summary(fun = mean, geom = "line", size = 1) +
  stat_summary(fun = mean, geom = "point", size = 3) +
  labs(
    title = "Interaction Plot: Batch and Pressure",
    x = "Pressue",
    y = "Strength",
    color = "Batch"
  ) +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5))
```

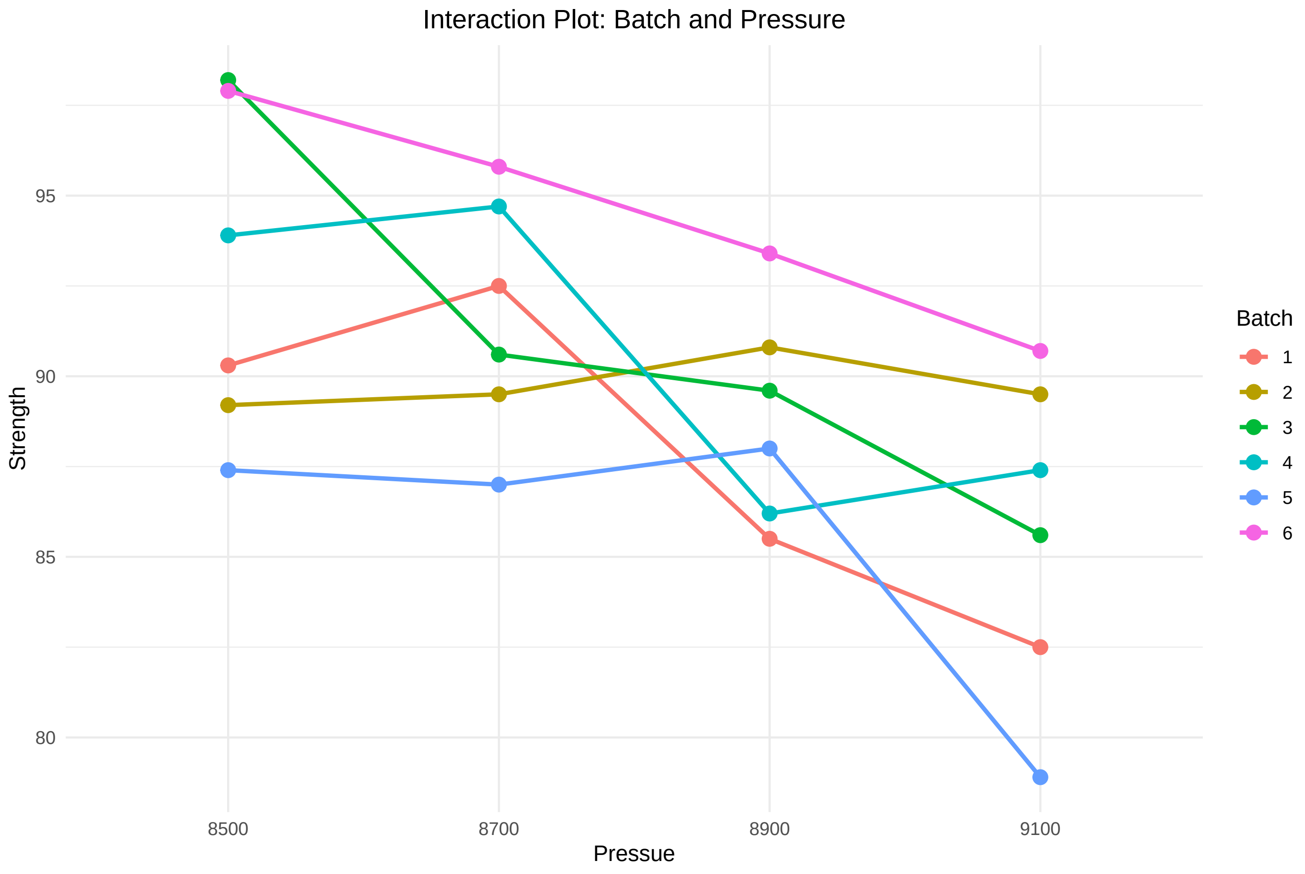


Figure 7.5: Interaction between Material Type and Temperature.

7.3.1.2 Model Fitting and ANOVA

The model `strength ~ pressure + batch` partitions the total variance into treatment, block, and error components. Our primary interest is in the significance of the `pressure` factor.

```r
rcbd.fit1 <- aov(strength ~ pressure + batch, data = graft_df)
anova(rcbd.fit1)
```

```
Analysis of Variance Table

Response: strength
          Df Sum Sq Mean Sq F value   Pr(>F)
pressure   3 178.17  59.390  8.1071 0.001916 **
batch      5 192.25  38.450  5.2487 0.005532 **
Residuals 15 109.89   7.326
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The small p-value for `pressure` (0.0019) provides strong evidence that extrusion pressure significantly affects graft strength after accounting for batch differences.

7.3.1.3 Model Adequacy Checks

The assumptions for an RCBD are the same as for a CRD. We perform the same diagnostic checks.

```r
rcbd.r1 <- rstudent(rcbd.fit1)
rcbd.fitted1 <- fitted.values(rcbd.fit1)

qqnorm(rcbd.r1, main = "Normal Q-Q Plot")
qqline(rcbd.r1)
plot(rcbd.fitted1, rcbd.r1, ylab = "Standardized residuals",
     xlab = "Fitted values", main = "Residuals vs. Fitted")
abline(h = 0)
plot(graft_df$pressure, rcbd.r1, ylab = "Standardized residuals",
     xlab = "Extrusion pressure", main = "Residuals vs. Treatment")
abline(h = 0)
plot(graft_df$batch, rcbd.r1, ylab = "Standardized residuals",
     xlab = "Batches of raw material", main = "Residuals vs. Block")
abline(h = 0)
```

7.3.1.4 Pairwise Comparisons

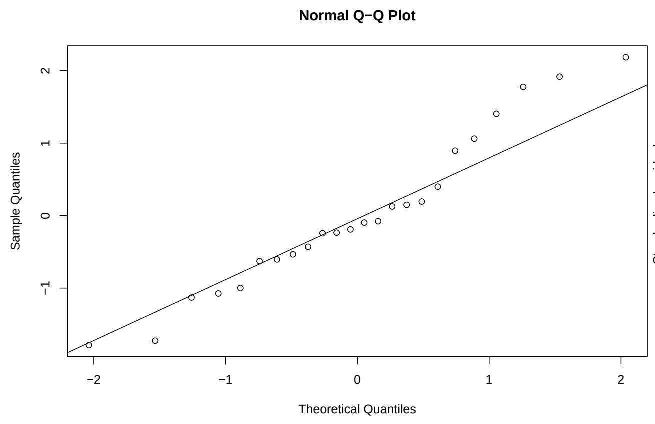
Again, since the treatment factor (`pressure`) is significant, we perform post-hoc tests.

7.3.1.4.1 Tukey's HSD Test

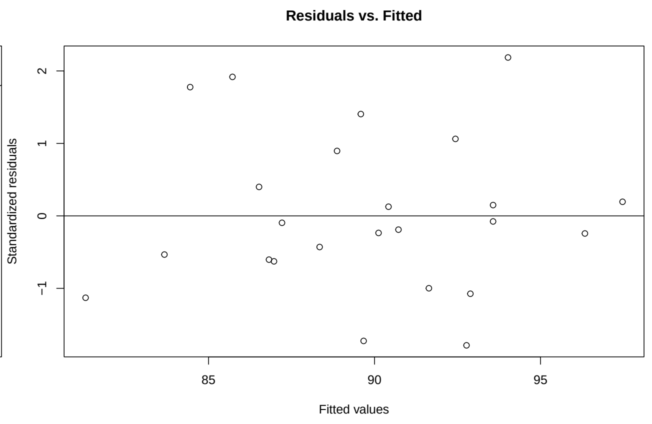
Tukey's HSD compares all pairs of treatment levels while controlling the family-wise error rate.

```r
TukeyHSD(rcbd.fit1, which = "pressure")
```

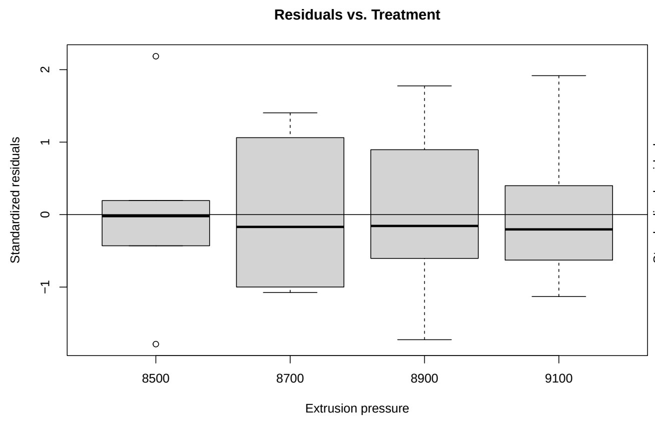
```
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = strength ~ pressure + batch, data = graft_df)

$pressure
               diff        lwr       upr     p adj
8700-8500 -1.133333  -5.637161  3.370495 0.8854831
8900-8500 -3.900000  -8.403828  0.603828 0.1013084
9100-8500 -7.050000 -11.553828 -2.546172 0.0020883
```



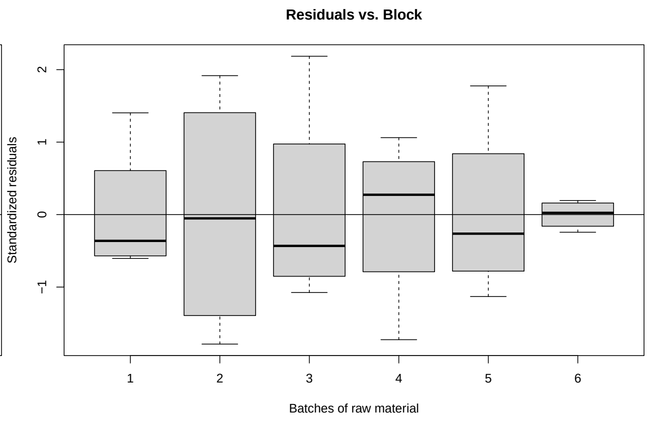
(a) Normal Q-Q Plot



(a) Residuals vs. Fitted Values



(a) Residuals vs. Treatment (Pressure)



(a) Residuals vs. Block (Batch)

```
8900-8700 -2.766667  -7.270495  1.737161 0.3245644
9100-8700 -5.916667 -10.420495 -1.412839 0.0086667
9100-8900 -3.150000  -7.653828  1.353828 0.2257674
```

7.3.1.4.2 Fisher's LSD Test

The `LSD.test()` function from the `agricolae` package correctly handles the error structure of an RCBD.

```
## install.packages("agricolae")
library(agricolae)

out <- LSD.test(rcbd.fit1, trt = "pressure", p.adj = "none", group = FALSE)
print(out$comparison)
```

```
            difference pvalue signif.        LCL       UCL
8500 - 8700   1.133333 0.4795         -2.1974047  4.464071
8500 - 8900   3.900000 0.0247       *  0.5692620  7.230738
8500 - 9100   7.050000 0.0004     ***  3.7192620 10.380738
8700 - 8900   2.766667 0.0970       . -0.5640714  6.097405
8700 - 9100   5.916667 0.0018      **  2.5859286  9.247405
8900 - 9100   3.150000 0.0621       . -0.1807380  6.480738
```

8 Two-Factor Factorial Design

8.1 Battery Design Experiment

This analysis explores data from a **two-factor factorial experiment** designed to assess the lifespan of a battery. The experiment investigates two factors: **material type** (with 3 levels) and **operating temperature** (with 3 levels: 15°C, 70°C, and 125°C). The primary goal is to understand not only how each factor individually affects battery life but, more importantly, whether the effect of temperature depends on the material type used. This combined effect is known as an **interaction**.

8.2 Data Setup and Preparation

First, we organize the raw data into a structured `data.frame`. This is a best practice in R that makes the data easier to manage and the code more readable. We create columns for the response variable `life` and the two factors, `material` and `temperature`, ensuring they are treated as categorical variables (factors) for the analysis.

```r
## Response variable: battery life
life <- c(130,155,74,180,  34,40,80,75,   20,70,82,58,
          150,188,159,126, 136,122,106,115, 25,70,58,45,
          138,110,168,160, 174,120,150,139, 96,104,82,60)

## Create the data frame
battery_df <- data.frame(
  life = life,
  material = factor(rep(1:3, each = 12)),
  temperature = factor(rep(rep(c(15, 70, 125), each = 4), 3))
)

## Preview the data
battery_df
```

```
   life material temperature
1   130        1          15
2   155        1          15
3    74        1          15
```

```
4   180          1          15
5    34          1          70
6    40          1          70
7    80          1          70
8    75          1          70
9    20          1         125
10   70          1         125
11   82          1         125
12   58          1         125
13  150          2          15
14  188          2          15
15  159          2          15
16  126          2          15
17  136          2          70
18  122          2          70
19  106          2          70
20  115          2          70
21   25          2         125
22   70          2         125
23   58          2         125
24   45          2         125
25  138          3          15
26  110          3          15
27  168          3          15
28  160          3          15
29  174          3          70
30  120          3          70
31  150          3          70
32  139          3          70
33   96          3         125
34  104          3         125
35   82          3         125
36   60          3         125
```

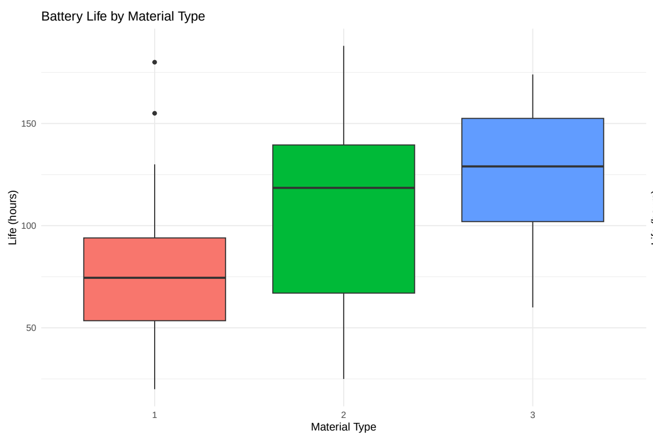
8.3 Exploratory Data Analysis and Visualization

Before fitting a formal model, we visualize the data to get an intuition for the relationships between the factors and the response.

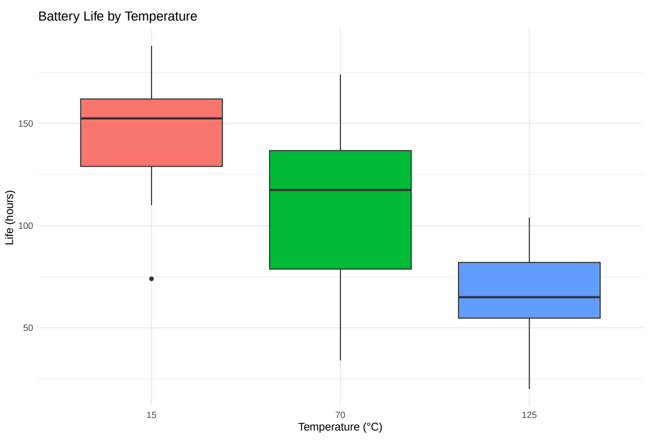
8.4 Boxplots of Main Effects

Boxplots are excellent for examining the distribution of battery life for each level of our factors independently. This gives us a preliminary look at the **main effects**—the individual impact of material type and temperature.

```r
library(ggplot2)

## Boxplot for Material Type
ggplot(battery_df, aes(x = material, y = life, fill = material)) +
  geom_boxplot() +
  labs(title = "Battery Life by Material Type", x = "Material Type", y = "Life (hours)") +
  theme_minimal() +
  theme(legend.position = "none")
## Boxplot for Temperature
ggplot(battery_df, aes(x = temperature, y = life, fill = temperature)) +
  geom_boxplot() +
  labs(title = "Battery Life by Temperature", x = "Temperature (°C)", y = "Life (hours)") +
  theme_minimal() +
  theme(legend.position = "none")
```



(a) Distribution of Battery Life by Material and Temperature.



(a) Distribution of Battery Life by Material and Temperature.

8.5 Interaction Plot

The most crucial plot for a factorial experiment is the **interaction plot**. It displays the mean battery life for each combination of material and temperature. If the lines are parallel, it suggests there is no interaction. If the lines are not parallel (i.e., they cross or diverge), it indicates that the effect of temperature on battery life is different for each material type, signaling a likely interaction.

```r
ggplot(battery_df, aes(x = temperature, y = life, group = material, color = material)) +
  stat_summary(fun = mean, geom = "line", size = 1) +
  stat_summary(fun = mean, geom = "point", size = 3) +
  labs(
    title = "Interaction Plot: Material Type and Temperature",
    x = "Temperature (°C)",
    y = "Average Battery Life (hours)",
    color = "Material Type"
  ) +
  theme_minimal() +
  theme(plot.title = element_text(hjust = 0.5))
```

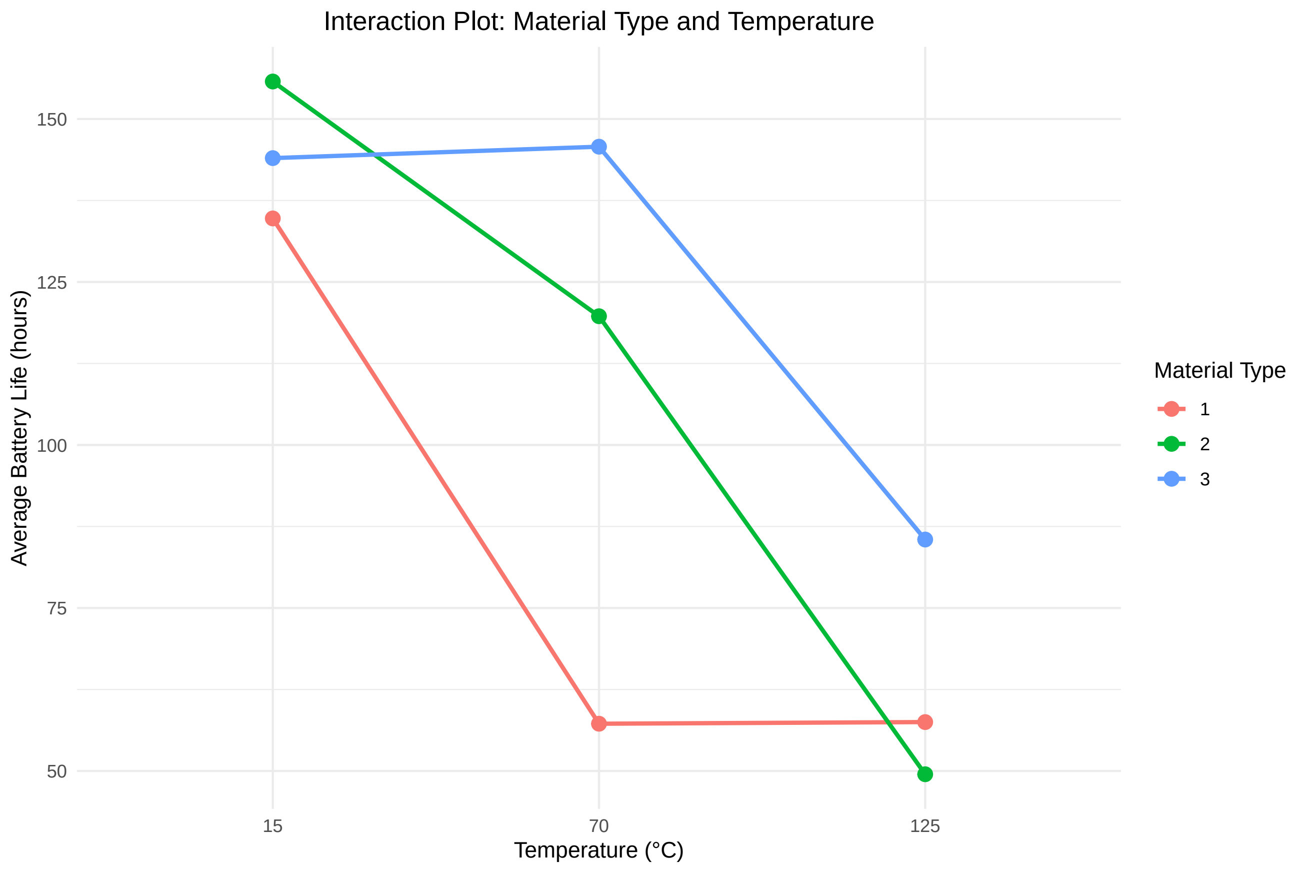


Figure 8.3: Interaction between Material Type and Temperature.

The non-parallel lines in the plot strongly suggest that a significant interaction effect is present. Specifically, the performance of Material 3 drops less dramatically with increasing temperature compared to Materials 1 and 2.

8.6 Model Fitting and Analysis of Variance (ANOVA)

We now fit a linear model to formally test the significance of the main effects and the interaction term. The model `life ~ material * temperature` is shorthand for `life ~ material + temperature + material:temperature`. We use a sum-to-zero contrast (`contr.sum`) for balanced interpretation of the effects. The **ANOVA table** will tell us if the variation caused by our factors is statistically significant compared to the random variation in the data.

```
## Fit the full factorial model
battery_fit <- lm(life ~ material * temperature,
                  data = battery_df,
                  contrasts = list(material = contr.sum, temperature = contr.sum))

summary(battery_fit)
```

```
Call:
lm(formula = life ~ material * temperature, data = battery_df,
    contrasts = list(material = contr.sum, temperature = contr.sum))

Residuals:
    Min      1Q  Median      3Q     Max
-60.750 -14.625   1.375  17.938  45.250

Coefficients:
                       Estimate Std. Error t value Pr(>|t|)
(Intercept)             105.528      4.331  24.367  < 2e-16 ***
material1               -22.361      6.125  -3.651  0.00111 **
material2                 2.806      6.125   0.458  0.65057
temperature1             39.306      6.125   6.418  7.1e-07 ***
temperature2              2.056      6.125   0.336  0.73975
material1:temperature1   12.278      8.662   1.417  0.16778
material2:temperature1    8.111      8.662   0.936  0.35735
material1:temperature2  -27.972      8.662  -3.229  0.00325 **
material2:temperature2    9.361      8.662   1.081  0.28936
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 25.98 on 27 degrees of freedom
Multiple R-squared:  0.7652,    Adjusted R-squared:  0.6956
F-statistic:    11 on 8 and 27 DF,  p-value: 9.426e-07
```

```r
## Generate the ANOVA table
anova(battery_fit)
```

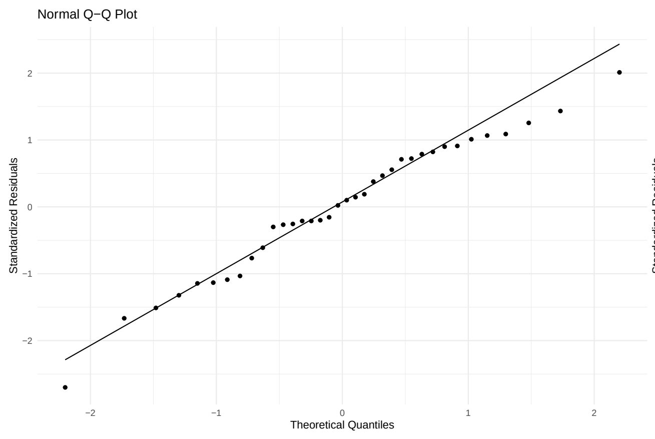
```
Analysis of Variance Table

Response: life
                     Df Sum Sq Mean Sq F value    Pr(>F)    
material              2  10684  5341.9  7.9114  0.001976 ** 
temperature           2  39119 19559.4 28.9677 1.909e-07 ***
material:temperature  4   9614  2403.4  3.5595  0.018611 *  
Residuals            27  18231   675.2                      
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The ANOVA table shows very small p-values (`Pr(>F)`) for `material`, `temperature`, and, most importantly, the `material:temperature` interaction. This confirms our visual inspection: all effects are statistically significant. **Because the interaction is significant, our interpretation should focus on the interaction itself rather than the main effects in isolation.**

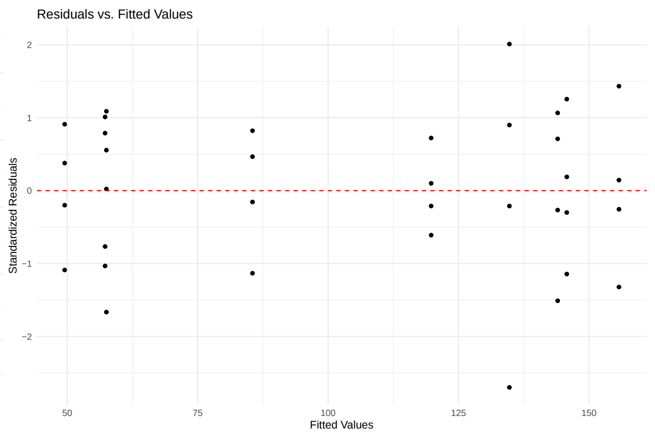
8.7 Model Adequacy Checks

The validity of our ANOVA results depends on the model's residuals meeting certain assumptions (normality, constant variance, independence). We check these with diagnostic plots.

```r
## Extract standardized residuals and fitted values
battery_fit_diag <- data.frame(
  residuals = rstandard(battery_fit),
  fitted = fitted.values(battery_fit)
)

## Normal Q-Q Plot
p1 <- ggplot(battery_fit_diag, aes(sample = residuals)) +
  stat_qq() +
  stat_qq_line() +
  labs(title = "Normal Q-Q Plot", x = "Theoretical Quantiles", y = "Standardized Residuals") +
  theme_minimal()

## Residuals vs. Fitted Plot
p2 <- ggplot(battery_fit_diag, aes(x = fitted, y = residuals)) +
  geom_point() +
  geom_hline(yintercept = 0, linetype = "dashed", color = "red") +
  labs(title = "Residuals vs. Fitted Values", x = "Fitted Values", y = "Standardized Residuals
  theme_minimal()

p1
p2
```



(a) Diagnostic plots for the battery life model.



(a) Diagnostic plots for the battery life model.

The Normal Q-Q plot shows the points falling roughly along the line, suggesting the normality assumption is met. The Residuals vs. Fitted plot shows a random scatter of points around the zero line, indicating that the variance is reasonably constant. The model assumptions appear to be satisfied.

8.8 Post-Hoc Analysis: Pairwise Comparisons

Since the interaction is significant, we must compare the means of the nine specific treatment combinations (3 materials × 3 temperatures). Simply comparing the average effect of Material 1 vs. Material 2 would be misleading, as that difference depends on the temperature.

8.9 Tukey's HSD Test

Tukey's Honest Significant Difference (HSD) test is a post-hoc test that compares all possible pairs of means while controlling the family-wise error rate. We apply it to an `aov` model object. The output for the `material:temperature` interaction shows which specific combinations are significantly different from one another.

```r
## Fit the model using aov() for Tukey's test
battery_aov <- aov(life ~ material * temperature, data = battery_df)
```

```r
## Perform Tukey's HSD test
TukeyHSD(battery_aov)
```

```
  Tukey multiple comparisons of means
    95% family-wise confidence level

Fit: aov(formula = life ~ material * temperature, data = battery_df)

$material
        diff        lwr      upr     p adj
2-1 25.16667 -1.135677 51.46901 0.0627571
3-1 41.91667 15.614323 68.21901 0.0014162
3-2 16.75000 -9.552344 43.05234 0.2717815

$temperature
            diff        lwr       upr     p adj
70-15  -37.25000  -63.55234 -10.94766 0.0043788
125-15 -80.66667 -106.96901 -54.36432 0.0000001
125-70 -43.41667  -69.71901 -17.11432 0.0009787

$`material:temperature`
               diff         lwr        upr     p adj
2:15-1:15     21.00  -40.823184  82.823184 0.9616404
3:15-1:15      9.25  -52.573184  71.073184 0.9998527
1:70-1:15    -77.50 -139.323184 -15.676816 0.0065212
2:70-1:15    -15.00  -76.823184  46.823184 0.9953182
3:70-1:15     11.00  -50.823184  72.823184 0.9994703
1:125-1:15   -77.25 -139.073184 -15.426816 0.0067471
2:125-1:15   -85.25 -147.073184 -23.426816 0.0022351
3:125-1:15   -49.25 -111.073184  12.573184 0.2016535
3:15-2:15    -11.75  -73.573184  50.073184 0.9991463
1:70-2:15    -98.50 -160.323184 -36.676816 0.0003449
2:70-2:15    -36.00  -97.823184  25.823184 0.5819453
3:70-2:15    -10.00  -71.823184  51.823184 0.9997369
1:125-2:15   -98.25 -160.073184 -36.426816 0.0003574
2:125-2:15  -106.25 -168.073184 -44.426816 0.0001152
3:125-2:15   -70.25 -132.073184  -8.426816 0.0172076
1:70-3:15    -86.75 -148.573184 -24.926816 0.0018119
2:70-3:15    -24.25  -86.073184  37.573184 0.9165175
3:70-3:15      1.75  -60.073184  63.573184 1.0000000
1:125-3:15   -86.50 -148.323184 -24.676816 0.0018765
2:125-3:15   -94.50 -156.323184 -32.676816 0.0006078
3:125-3:15   -58.50 -120.323184   3.323184 0.0742711
2:70-1:70     62.50    0.676816 124.323184 0.0460388
```

```
3:70-1:70     88.50   26.676816 150.323184 0.0014173
1:125-1:70     0.25  -61.573184  62.073184 1.0000000
2:125-1:70    -7.75  -69.573184  54.073184 0.9999614
3:125-1:70    28.25  -33.573184  90.073184 0.8281938
3:70-2:70     26.00  -35.823184  87.823184 0.8822881
1:125-2:70   -62.25 -124.073184  -0.426816 0.0474675
2:125-2:70   -70.25 -132.073184  -8.426816 0.0172076
3:125-2:70   -34.25  -96.073184  27.573184 0.6420441
1:125-3:70   -88.25 -150.073184 -26.426816 0.0014679
2:125-3:70   -96.25 -158.073184 -34.426816 0.0004744
3:125-3:70   -60.25 -122.073184   1.573184 0.0604247
2:125-1:125   -8.00  -69.823184  53.823184 0.9999508
3:125-1:125   28.00  -33.823184  89.823184 0.8347331
3:125-2:125   36.00  -25.823184  97.823184 0.5819453
```

8.10 Fisher's LSD Method

The **Fisher's Least Significant Difference (LSD)** method is another option for pairwise comparisons. To test the interaction means, we must specify both factors in the `trt` argument.

```r
library(agricolae)

## Perform LSD test on the interaction term
lsd_results <- LSD.test(battery_aov, trt = c("material", "temperature"),
                        p.adj = "none", group = FALSE)

## Print the comparison table
print(lsd_results$comparison)
```

```
              difference pvalue signif.         LCL        UCL
1:125 - 1:15      -77.25 0.0003     *** -114.950479 -39.549521
1:125 - 1:70        0.25 0.9892          -37.450479  37.950479
1:125 - 2:125       8.00 0.6667          -29.700479  45.700479
1:125 - 2:15      -98.25 0.0000     *** -135.950479 -60.549521
1:125 - 2:70      -62.25 0.0022      **  -99.950479 -24.549521
1:125 - 3:125     -28.00 0.1392          -65.700479   9.700479
1:125 - 3:15      -86.50 0.0001     *** -124.200479 -48.799521
1:125 - 3:70      -88.25 0.0001     *** -125.950479 -50.549521
1:15 - 1:70        77.50 0.0002     ***   39.799521 115.200479
1:15 - 2:125       85.25 0.0001     ***   47.549521 122.950479
1:15 - 2:15       -21.00 0.2631          -58.700479  16.700479
1:15 - 2:70        15.00 0.4214          -22.700479  52.700479
1:15 - 3:125       49.25 0.0124       *   11.549521  86.950479
```

```
1:15 - 3:15         -9.25 0.6187          -46.950479  28.450479
1:15 - 3:70        -11.00 0.5544          -48.700479  26.700479
1:70 - 2:125         7.75 0.6765          -29.950479  45.450479
1:70 - 2:15        -98.50 0.0000     *** -136.200479 -60.799521
1:70 - 2:70        -62.50 0.0021      ** -100.200479 -24.799521
1:70 - 3:125       -28.25 0.1358          -65.950479   9.450479
1:70 - 3:15        -86.75 0.0001     *** -124.450479 -49.049521
1:70 - 3:70        -88.50 0.0000     *** -126.200479 -50.799521
2:125 - 2:15      -106.25 0.0000     *** -143.950479 -68.549521
2:125 - 2:70       -70.25 0.0007     *** -107.950479 -32.549521
2:125 - 3:125      -36.00 0.0605       .  -73.700479   1.700479
2:125 - 3:15       -94.50 0.0000     *** -132.200479 -56.799521
2:125 - 3:70       -96.25 0.0000     *** -133.950479 -58.549521
2:15 - 2:70         36.00 0.0605       .   -1.700479  73.700479
2:15 - 3:125        70.25 0.0007     ***   32.549521 107.950479
2:15 - 3:15         11.75 0.5279          -25.950479  49.450479
2:15 - 3:70         10.00 0.5907          -27.700479  47.700479
2:70 - 3:125        34.25 0.0732       .   -3.450479  71.950479
2:70 - 3:15        -24.25 0.1980          -61.950479  13.450479
2:70 - 3:70        -26.00 0.1685          -63.700479  11.700479
3:125 - 3:15       -58.50 0.0036      **  -96.200479 -20.799521
3:125 - 3:70       -60.25 0.0029      **  -97.950479 -22.549521
3:15 - 3:70         -1.75 0.9248          -39.450479  35.950479
```

The results from both Tukey's HSD and Fisher's LSD provide detailed p-values for comparing pairs of treatment combinations, allowing us to make specific conclusions, such as "at 125°C, Material 3 has a significantly longer life than Materials 1 and 2."