

Elements of Nonparametric Statistics

Nicholas Henderson

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Preface

This book will serve as the main source of course notes for Biostatistics 685/Statistics 560, Winter 2020.

Chapter 1

Introduction

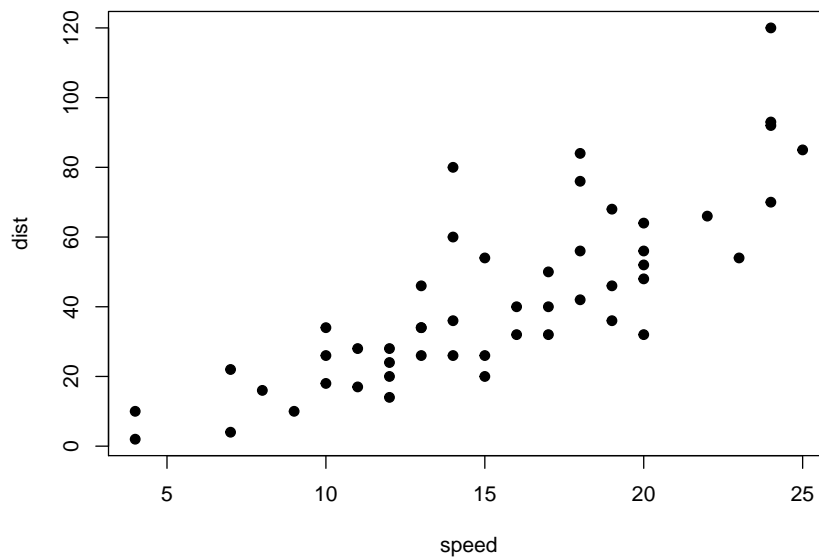


Figure 1.1: Hello World!

1.1 What is Nonparametric Statistics?

What is Parametric Statistics?

- Parametric models refer to probability distributions that can be fully described by a fixed number of parameters that do not change with the sample size.
- Typical examples include
 - Gaussian
 - Poisson
 - Exponential
 - Beta
- Could also refer to a regression setting where the mean function is described by a fixed number of parameters.

What is Nonparametric Statistics?

- It is difficult to give a concise, all-encompassing definition, but nonparametric statistics generally refers to statistical methods where there is not a clear parametric component.
- A more practical definition is that nonparametric statistics refers to flexible statistical procedures where very few assumptions are made regarding the distribution of the data or the form of a regression model.
- The uses of nonparametric methods in several common statistical contexts are described in Sections 1.3 - 1.7.

1.2 Outline of Course

This course is roughly divided into the following 5 categories.

1. Nonparametric Testing

- Rank-based Tests
- Permutation Tests

1. Estimation of Basic Nonparametric Quantities

- The Empirical Distribution Function
- Density Estimation

1. Nonparametric Confidence Intervals

- Bootstrap

1.3. EXAMPLE 1: NONPARAMETRIC VS. PARAMETRIC TWO-SAMPLE TESTING11

- Jackknife

1. Nonparametric Regression Part I (Smoothing Methods)

- Kernel Methods
- Splines
- Local Regression

1. Nonparametric Regression Part II (Machine Learning Methods)

- Decision Trees/CART
- Ensemble Methods

1.3 Example 1: Nonparametric vs. Parametric Two-Sample Testing

Suppose we have data from two groups. For example, outcomes from two different treatments.

- **Group 1 outcomes:** X_1, \dots, X_n an i.i.d (independent and identically distributed) sample from distribution function F_X . This means that

$$F_X(t) = P(X_i \leq t) \quad \text{for any } 1 \leq i \leq n$$

- **Group 2 outcomes:** Y_1, \dots, Y_m an i.i.d. sample from distribution function F_Y .

$$F_Y(t) = P(Y_i \leq t) \quad \text{for any } 1 \leq i \leq m$$

- To test the impact of a new treatment, we usually want to test whether or not F_X differs from F_Y in some way. This can be stated in hypothesis testing language as

$$\begin{aligned} H_0 &: F_X = F_Y \quad (\text{populations are the same}) \\ H_A &: F_X \neq F_Y \quad (\text{populations are different}) \end{aligned} \tag{1.1}$$

Parametric Tests

- Perhaps the most common parametric test for (1.1) is the **t-test**. The t-test assumes that

$$F_X = \text{Normal}(\mu_x, \sigma^2) \quad \text{and} \quad F_Y = \text{Normal}(\mu_y, \sigma^2) \tag{1.2}$$

- Under this parametric assumption, the hypothesis test (1.1) reduces to

$$H_0 : \mu_x = \mu_y \quad \text{vs.} \quad H_A : \mu_x \neq \mu_y \quad (1.3)$$

- The standard t-statistic (with a pooled estimate of σ^2) is the following

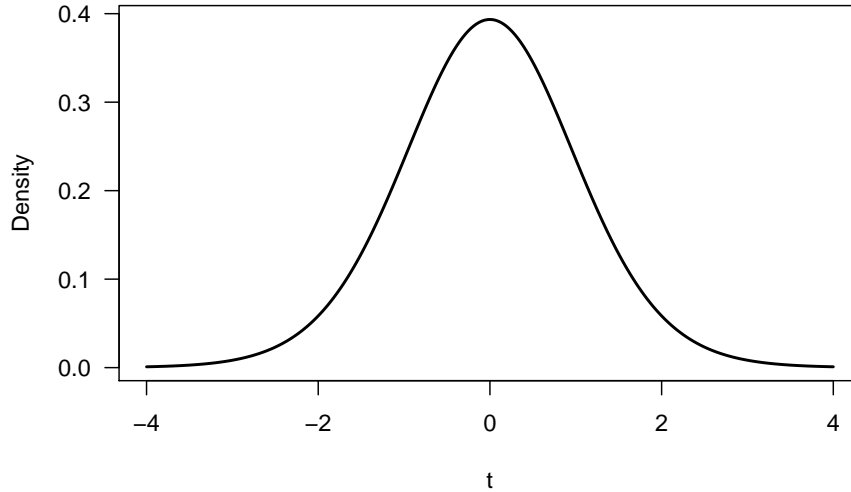
$$T = \frac{\bar{X} - \bar{Y}}{s_p \sqrt{\frac{1}{n} + \frac{1}{m}}}, \quad (1.4)$$

where $\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i$ and $\bar{Y} = \frac{1}{m} \sum_{i=1}^m Y_i$ are the group-specific sample means and s_p^2 is the pooled estimate of σ^2

$$s_p^2 = \frac{1}{m+n-2} \left\{ \sum_{i=1}^n (X_i - \bar{X})^2 + \sum_{i=1}^m (Y_i - \bar{Y})^2 \right\} \quad (1.5)$$

- The t-test is based on the **null distribution** of T - the distribution of T under the null hypothesis.
- Under the assumption of normality, the null distribution of T is a t distribution with $n + m - 2$ degrees of freedom.

Null Distribution of T when n = m = 10



- Notice that the null distribution of T depends on the parametric assumption that both $F_X = \text{Normal}(\mu_x, \sigma^2)$ and $F_Y = \text{Normal}(\mu_y, \sigma^2)$. Appealing to the Central Limit Theorem, one could argue that is a quite reasonable assumption.
- In addition to using the assumption that $F_X = \text{Normal}(\mu_x, \sigma^2)$ and $F_Y = \text{Normal}(\mu_y, \sigma^2)$, we used this parametric assumption (at least implicitly) in the formulation of the hypothesis test itself because we assumed that any difference between F_X and F_Y would be fully described by difference in μ_x and μ_y .
- So, in a sense, you are using the assumption of normality twice in the construction of the two-sample t-test.

Nonparametric Tests

- Two-sample nonparametric tests are meant to be “distribution-free”. This means the null distribution of the test statistic does not depend on any parametric assumptions about the two populations F_X and F_Y .
- Many such tests are based on **ranks**. The distribution of the ranks under the assumption that $F_X = F_Y$ do not depend on the form of F_X (assuming F_X is continuous).
- Also, the statements of hypotheses tests for nonparametric tests should not rely on any parametric assumptions about F_X and F_Y .
- For example, $H_A : F_X \neq F_Y$ or $H_A : F_X \geq F_Y$.

- Nonparametric tests usually tradeoff power for greater robustness.
- In general, if the parametric assumptions are correct, a nonparametric test will have less power than its parametric counterpart.
- If the parametric assumptions are not correct, parametric tests might have inappropriate type-I error control or lose power.

1.4 Example 2: Nonparametric Estimation

- Suppose we have n observations (X_1, \dots, X_n) which are assumed to be i.i.d. (independent and identically distributed). The distribution function of X_i is F_X .

- Suppose we are interested in estimating the entire distribution function F_X rather than specific features of the distribution of X_i such as the mean or standard deviation.
- In a **parametric** approach to estimating F_X , we would assume the distribution of X_i belongs to some parametric family of distributions. For example,

- $X_i \sim \text{Normal}(\mu, \sigma^2)$
- $X_i \sim \text{Exponential}(\lambda)$
- $X_i \sim \text{Beta}(\alpha, \beta)$

- If we assume that $X_i \sim \text{Normal}(\mu, \sigma^2)$, we only need to estimate 2 parameters to fully describe the distribution of X_i , and the number of parameters will not depend on the sample size.
- In a nonparametric approach to characterizing the distribution of X_i , we need to instead estimate the entire distribution function F_X or density function f_X .
- The distribution function F_X is usually estimated by the **empirical distribution function**

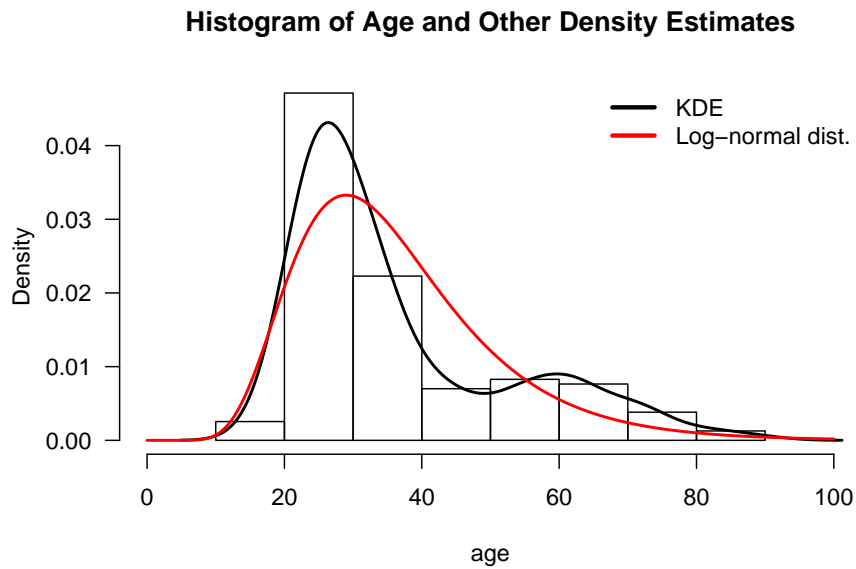
$$\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n I(X_i \leq t), \quad (1.6)$$

where $I()$ denotes the indicator function. That is, $I(X_i \leq t) = 1$ if $X_i \leq t$, and $I(X_i \leq t) = 0$ if $X_i > t$.

- The empirical distribution function is a discrete distribution function, and it can be thought of as an estimate having n "parameters".
- The density function of X_i is often estimated by a kernel density estimator (KDE). This is defined as

$$\hat{f}_n(t) = \frac{1}{nh_n} \sum_{i=1}^n K\left(\frac{t - X_i}{h_n}\right). \quad (1.7)$$

- $K()$ - the kernel function
- h_n - the bandwidth
- The KDE is a type of smoothing procedure.



1.5 Example 3: Confidence Intervals

- Inference for a wide range of statistical procedures is based on the following argument

$$\hat{\theta}_n \text{ has an approximate Normal}\left(\theta, \widehat{\text{Var}}(\hat{\theta}_n)\right) \text{ distribution} \quad (1.8)$$

- Above, $\hat{\theta}_n$ is an estimate of a parameter θ , and $\widehat{\text{Var}}(\hat{\theta}_n)$ is an estimate of the variance of $\hat{\theta}_n$.
- $se_n = \sqrt{\widehat{\text{Var}}(\hat{\theta}_n)}$ is usually referred to as the **standard error**.
- 95% confidence intervals are reported using the following formula

$$[\hat{\theta}_n - 1.96se_n, \hat{\theta}_n + 1.96se_n] \quad (1.9)$$

- Common examples of this include:

1. $\hat{\theta}_n = \bar{X}_n$.

In this case, appeals to the Central Limit Theorem would justify approximation (1.8). The variance of $\hat{\theta}_n$ would be σ^2 , and the standard error would typically be $se_n = \hat{\sigma}/\sqrt{n}$.

2. $\hat{\theta}_n = \text{Maximum Likelihood Estimate of } \theta$.

In this case, asymptotics would justify the approximate distribution $\hat{\theta}_n \sim \text{Normal}(\theta, \frac{1}{nI(\theta)})$, where $I(\theta)$ denotes the Fisher information. The standard error in this context is often $se_n = \{nI(\hat{\theta}_n)\}^{-1/2}$.

- Confidence intervals using (1.8) rely on a parametric approximation to the sampling distribution of the statistic $\hat{\theta}_n$.
- Moreover, even if one wanted to use something like (1.8), working out standard error formulas can be a great challenge in more complicated situations.

- The **bootstrap** is a simulation-based approach for computing standard errors and confidence intervals.

- The bootstrap does not rely on any particular parametric assumptions and can be applied in almost any context (though bootstrap confidence intervals can fail to work as desired in some situations).
- Through resampling from the original dataset, the bootstrap uses many possible alternative datasets to assess the variability in $\hat{\theta}_n$.

	OriginalDat	Dat1	Dat2	Dat3	Dat4
Obs. 1	0.20	0.20	0.80	0.20	0.30
Obs. 2	0.50	0.20	0.80	0.20	0.70
Obs. 3	0.30	0.30	0.50	0.80	0.20
Obs. 4	0.80	0.30	0.70	0.50	0.50
Obs. 5	0.70	0.70	0.20	0.30	0.20
theta.hat	0.50	0.34	0.60	0.40	0.38

-
- In the above example, we have 4 **bootstrap replications** for the statistic $\hat{\theta}$:

$$\hat{\theta}^{(1)} = 0.34 \quad (1.10)$$

$$\hat{\theta}^{(2)} = 0.60 \quad (1.11)$$

$$\hat{\theta}^{(3)} = 0.40 \quad (1.12)$$

$$\hat{\theta}^{(4)} = 0.38 \quad (1.13)$$

- In the above example, the bootstrap standard error for $\hat{\theta}_n$ would be the standard deviation of the bootstrap replications

$$\begin{aligned}
 se_{boot} &= \left(\frac{1}{3} \sum_{b=1}^4 \{ \hat{\theta}^{(b)} - \hat{\theta}^{(-)} \}^2 \right)^{1/2} \\
 &= \left((0.34 - 0.43)^2/3 + (0.60 - 0.43)^2/3 + (0.40 - 0.43)^2/3 + (0.38 - 0.43)^2/3 \right)^{1/2} \\
 &= 0.116 \quad (1.14)
 \end{aligned}$$

where $\hat{\theta}^{(-)} = 0.43$ is the average of the bootstrap replications.

- One would then report the confidence interval $[\hat{\theta} - 1.96 \times 0.116, \hat{\theta} + 1.96 \times 0.116]$. In practice, the number of bootstrap replications is typically much larger than 4.
- It is often better to construct confidence intervals using the percentiles from the bootstrap distribution of $\hat{\theta}$ rather than use a confidence interval of the form: $\hat{\theta} \pm 1.96 \times se_{boot}$.

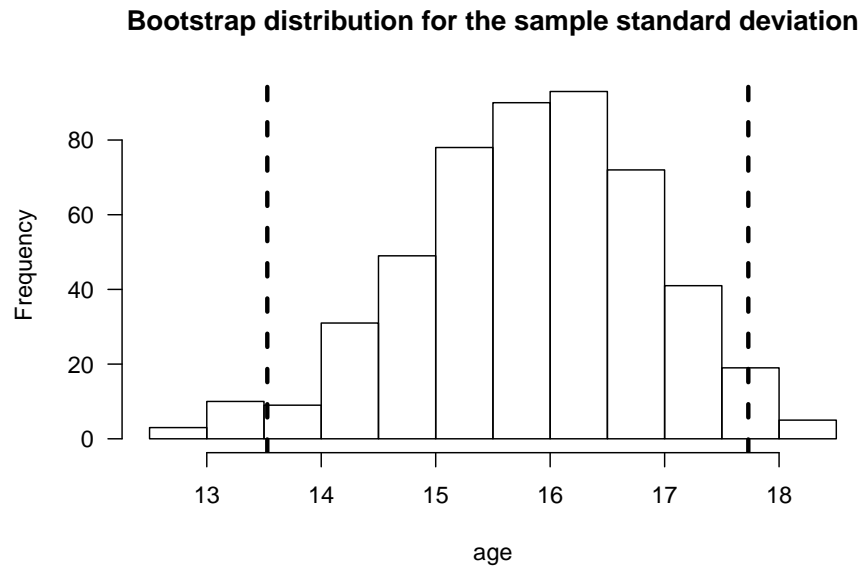


Figure 1.2: Bootstrap distribution of the sample standard deviation for the age variable from the kidney fitness data. Dashed vertical lines are placed at the 2.5 and 97.5 percentiles of the bootstrap distribution.

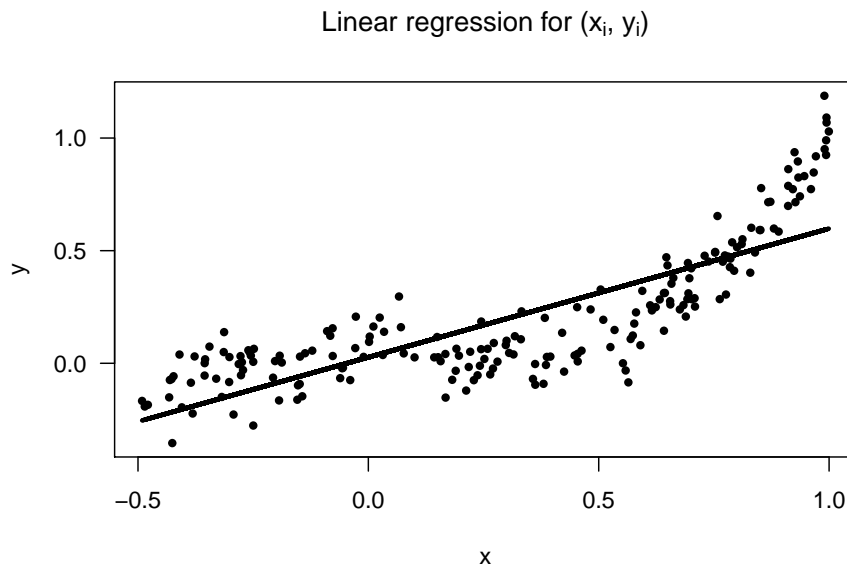
1.6 Example 4: Nonparametric Regression with a Single Covariate

- Regression is a common way of modeling the relationship between two different variables.
- Suppose we have n pairs of observations $(y_1, x_1), \dots, (y_n, x_n)$ where y_i and x_i are suspected to have some association.
- Linear regression would assume that these y_i and x_i are related by the following

$$y_i = \beta_0 + \beta_1 x_i + \varepsilon_i \quad (1.15)$$

with the assumption $\varepsilon_i \sim \text{Normal}(0, \sigma^2)$ often made.

- In this model, there are only 3 parameters: $(\beta_0, \beta_1, \sigma^2)$, and the number of parameters stays fixed for all n .



-
- The nonparametric counterpart to linear regression is usually formulated in the following way

$$y_i = m(x_i) + \varepsilon_i \quad (1.16)$$

- Typically, one makes very few assumptions about the form of the mean function m , and it is not assumed m can be described by a finite number of parameters.
- There are a large number of nonparametric methods for estimating m .
- One popular method is the use of **smoothing splines**.
- With smoothing splines, one considers mean functions of the form

$$m(x) = \sum_{j=1}^n \beta_j g_j(x) \quad (1.17)$$

where $g_1, \dots, g_n(x)$ are a collection of spline basis functions.

- Because of the large number of parameters in (1.17), one should estimate the basis function weights β_j through penalized regression

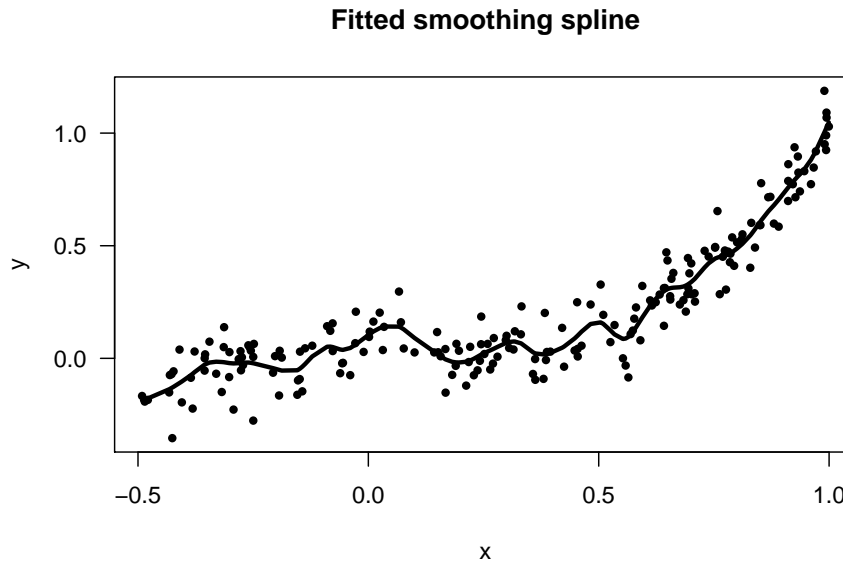
$$\text{minimize} \quad \sum_{i=1}^n \left(y_i - \sum_{j=1}^n \beta_j g_j(x_i) \right)^2 + \lambda \sum_{i=1}^n \sum_{j=1}^n \Omega_{ij} \beta_i \beta_j \quad (1.18)$$

where $\Omega_{ij} = \int g_i''(t) g_j''(t) dt$.

- Using coefficient estimates $\hat{\beta}_1, \dots, \hat{\beta}_n$ found from solving (1.17), the non-parametric estimate of the mean function is defined as

$$\hat{m}(x) = \sum_{j=1}^n \hat{\beta}_j g_j(x) \quad (1.19)$$

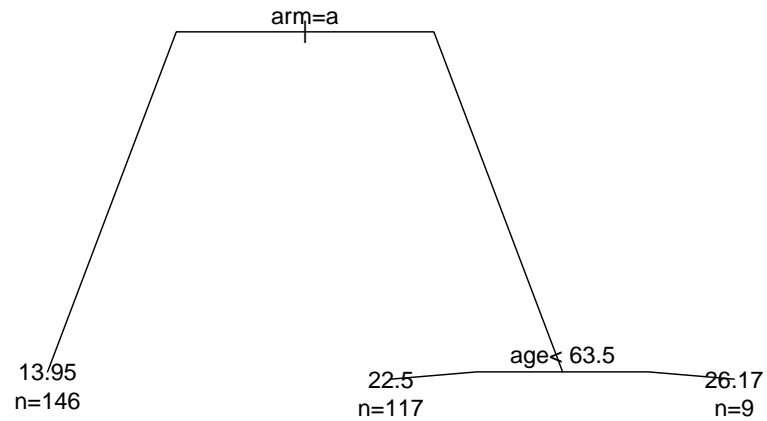
- While the estimation in (1.18) resembles parametric estimation for linear regression, notice that the number of parameters to be estimated will change with the sample size.
- Allowing the number of basis functions to grow with n is important. For a sufficiently large number of basis functions, one should be able to approximate the true mean function $m(x)$ arbitrarily closely.



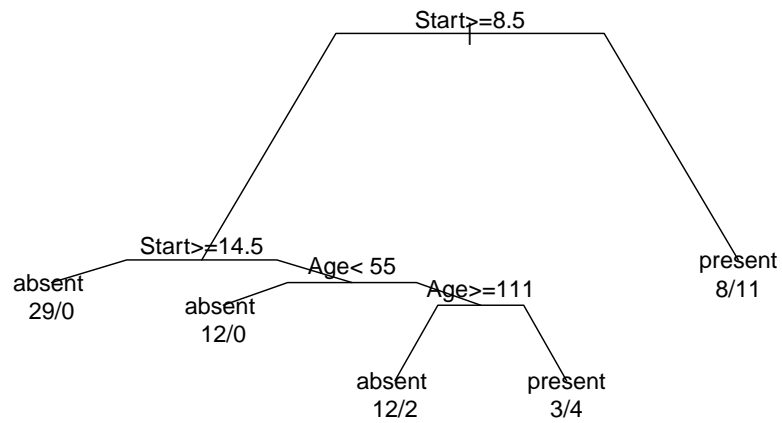
1.7 Example 5: Classification and Regression Trees (CART)

- Suppose we now have observations $(y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)$ where y_i is a continuous response and \mathbf{x}_i is a p -dimensional vector of covariates.
- Regression trees are a nonparametric approach for predicting y_i from \mathbf{x}_i .
- Here, the regression function is a **decision tree** rather than some fitted curve.
- With a decision tree, a final prediction from a covariate vector \mathbf{x}_i is obtained by answering a sequence of “yes or no” questions.
- When the responses y_i are binary, such trees are referred to as classification trees. Hence, the name: classification and regression trees (CART).

CART for Regression: Predicting an Oral Health Score



CART for Classification: Predicting Absence or Presence of Condition



-
- Classification and regression trees are constructed through **recursive partitioning**.

1.7. EXAMPLE 5: CLASSIFICATION AND REGRESSION TREES (CART)23

- Recursive partitioning is the process of deciding if and how to split a given node into two child nodes.
- Tree splits are usually chosen to minimize the “within-node” sum of squares.
- The size of the final is determined by a process of “pruning” the tree with cross-validation determining the best place to stop pruning.
- Regression trees are an example of a more algorithmic approach to constructing predictions (as opposed to probability modeling in more traditional statistical methods) with a strong emphasis on predictive performance as measured through cross-validation.

-
- While single regression trees have the advantage of being directly interpretable, their prediction performance is often not that great.
 - However, using collections of trees can be very effective for prediction and has been used in many popular learning methods. Examples include: random forests, boosting, and Bayesian additive regression trees (BART).
 - Methods such as these can perform well on much larger datasets. We will discuss additional methods if time allows.

Chapter 2

Working with R

You can download R by visiting <https://www.r-project.org/> and clicking on the **download R** link. Follow the instructions to complete installation. The most recent version is version 3.6.2.

It is not necessary to use this, but I find **RStudio** to be a very useful integrated development environment (IDE) for computing with **R**. **RStudio** may be downloaded and installed by visiting <https://rstudio.com/>

Part I

Nonparametric Testing

Chapter 3

Rank and Sign Statistics

3.1 Ranks

3.1.1 Definition

- Suppose we have n observations $\mathbf{X} = (X_1, \dots, X_n)$. The **rank** R_i of the i^{th} observation is defined as

$$R_i = R_i(\mathbf{X}) = \sum_{j=1}^n I(X_i \geq X_j) \quad (3.1)$$

where

$$I(X_i \geq X_j) = \begin{cases} 1 & \text{if } X_i \geq X_j \\ 0 & \text{if } X_i < X_j \end{cases} \quad (3.2)$$

- The largest observation has a rank of n .
- The smallest observation has a rank of 1 (if there are no ties).
- I am using the notation $R_i(\mathbf{X})$ to emphasize that the rank of the i^{th} observations depends on the entire vector of observations rather than only on the value of X_i .
- You can compute ranks in **R** using the **rank** function:

```
x <- c(3, 7, 1, 12, 6)  ## 5 observations
rank(x)
```

```
## [1] 2 4 1 5 3
```

3.1.2 Handling Ties

- In the definition of ranks shown in (3.1), tied observations receive their maximum possible rank.
- For example, suppose that $(X_1, X_2, X_3, X_4) = (0, 1, 1, 2)$. In this case, one could argue whether both observations 2 and 3 should be ranked 2^{nd} or 3^{rd} while observations 1 and 4 should unambiguously receive ranks of 1 and 4 respectively.
- Under definition (3.1), both observations 2 and 3 receive a rank of 3.
- In **R**, handling ties in a way that is consistent with definition (3.1) is done using the **ties.method** = “**max**” argument

```
x <- c(0, 1, 1, 2)
rank(x, ties.method="max")
```

```
## [1] 1 3 3 4
```

- The default in **R** is to replace the ranks of tied observations with their “average” rank

```
x <- c(0, 1, 1, 2)
rank(x)
```

```
## [1] 1.0 2.5 2.5 4.0
```

- As another example of the “average” definition of ranks, consider the following example:

```
y <- c(2, 9, 7, 7, 3, 2, 1)
rank(y, ties.method="max")
```

```
## [1] 3 7 6 6 4 3 1
```

```
rank(y)
```

```
## [1] 2.5 7.0 5.5 5.5 4.0 2.5 1.0
```

- When defining ranks using the “average” or “midrank” approach to handling ties, we replace tied ranks with the average of the two “adjacent” ranks.
- For example, if we have a vector of ranks (R_1, R_2, R_3, R_4) where $R_2 = R_3 = 3$ and $R_1 = 4$ and $R_4 = 1$, then the vector of modified ranks using the “average” approach to handling ties would be

$$(R'_1, R'_2, R'_3, R'_4) = \left(4, \frac{4+1}{2}, \frac{4+1}{2}, 1\right) \quad (3.3)$$

- The “average” approach is the most common way of handling ties when computing the Wilcoxon rank sum statistic.

3.1.3 Properties of Ranks

Suppose (X_1, \dots, X_n) is random sample from a continuous distribution F (so that the probability of ties is zero). Then, the following properties hold for the associated ranks R_1, \dots, R_n .

- Each R_i follows a discrete uniform distribution

$$P(R_i = j) = 1/n, \quad \text{for any } j = 1, \dots, n. \quad (3.4)$$

- The expectation of R_i is

$$E(R_i) = \sum_{j=1}^n jP(R_i = j) = \frac{1}{n} \sum_{j=1}^n j = \frac{(n+1)}{2} \quad (3.5)$$

- The variance of R_i is

$$\text{Var}(R_i) = E(R_i^2) - E(R_i)^2 = \frac{1}{n} \sum_{j=1}^n j^2 - \left(\frac{n+1}{2}\right)^2 = \frac{n^2-1}{12} \quad (3.6)$$

- The random variables R_1, \dots, R_n are **not** independent (why?). However, the vector $\mathbf{R}_n = (R_1, \dots, R_n)$ is uniformly distributed on the set of $n!$ permutations of $(1, 2, \dots, n)$.

Exercise 3.1: Suppose X_1, X_2, X_3 are i.i.d. observations from a continuous distribution function F_X . Compute the covariance matrix of the vector of ranks $(R_1(\mathbf{X}), R_2(\mathbf{X}), R_3(\mathbf{X}))$.

Exercise 3.2: Again, suppose that X_1, X_2, X_3, X_4 are i.i.d. observations from a continuous distribution function F_X . Let $T = R_1(\mathbf{X}) + R_2(\mathbf{X})$. Compute $P(T = j)$ for $j = 3, 4, 5, 6, 7$.

3.2 The Wilcoxon Rank Sum (WRS) Test: A Two-Sample Test

3.2.1 Goal of the Test

- The Wilcoxon Rank Sum (WRS) test (sometimes referred to as the Wilcoxon-Mann-Whitney test) is a popular, rank-based two-sample test.
- The one-sided WRS test is used to test whether or not observations from one group tend to be larger (or smaller) than observations from the other group.
- Suppose we have observations from two groups: $X_1, \dots, X_n \sim F_X$ and $Y_1, \dots, Y_m \sim F_Y$.
- Roughly speaking, the one-sided WRS tests the following hypothesis

$$\begin{aligned} H_0 : & \quad F_X = F_Y \quad \text{versus} \\ H_A : & \quad \text{Observations from } F_X \text{ tend to be larger than observations from } F_Y \end{aligned} \quad (3.7)$$

- What is meant by “tend to be larger” in the alternative hypothesis?
- Two common ways of stating the alternative hypothesis for the WRS include
 1. The stochastic dominance alternative

$$\begin{aligned} H_0 : & \quad F_X = F_Y \quad \text{versus} \\ H_A : & \quad F_X \text{ is stochastically larger than } F_Y \end{aligned} \quad (3.8)$$

2. The “shift” alternative

$$\begin{aligned} H_0 : & \quad F_X = F_Y \quad \text{versus} \\ H_A : & \quad F_X(t) = F_Y(t - \Delta), \Delta > 0. \end{aligned} \quad (3.9)$$

- A distribution function F_X is said to be stochastically larger than F_Y if $F_X(t) \leq F_Y(t)$ for all t with $F_X(t) < F_Y(t)$ for at least one value of t .
- Note that the “shift alternative” implies stochastic dominance.
- Why do we need to specify an alternative?

- It is often stated that the WRS test is a test of equal medians.

3.2. THE WILCOXON RANK SUM (WRS) TEST: A TWO-SAMPLE TEST 33

- This is true under the assumption that the relevant alternative is of the form $F_X(t) = F_Y(t - \Delta)$.
- However, one could have a scenario where the two groups have equal medians, but the WRS test has a very high probability of rejecting H_0 .
- In addition, in many applications, it is difficult to justify that the “shift alternative” is a reasonable assumption.
- An alternative is to view the WRS test as performing the following hypothesis test:

$$\begin{aligned} H_0 : & \quad P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) = 1/2 \quad \text{versus} \\ H_A : & \quad P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) > 1/2 \end{aligned} \quad (3.10)$$

See Divine et al. (2018) for more discussion around this formulation of the WRS test.

- The hypothesis test (3.10) makes fewer assumptions about how F_X and F_Y are related and is, in many cases, more interpretable.
- For example, in medical applications, it is often more natural to answer the question: what is the probability that the outcome under treatment 1 is better than the outcome under treatment 2.
- The justification of hypothesis test (3.10) comes through the close connection between the WRS test statistic W and the Mann-Whitney statistic M . Specifically, $W = M + n(n+1)/2$. (Although, often M is defined as $M = mn + n(n+1)/2 - W$).
- The Mann-Whitney statistic divided by mn is an estimate of the probability:

$$P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) = 1/2.$$

- The reason for stating H_0 in (3.10) as

$$H_0 : P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) = 1/2$$

is to cover the case of either a continuous or discrete distribution.

- When both X_i and Y_j are samples from a continuous distribution we will have $P(X_i = Y_j) = 0$, and we should then think of the null hypothesis as $H_0 : P(X_i > Y_j)$.
- For the case when both X_i and Y_j have a discrete distribution, consider an example where X_i and Y_j have the same discrete distribution with probabilities $P(X_i = 0) = p_0$, $P(X_i = 1) = p_1$, and $P(X_i = 2) = 1 - p_0 - p_2$.

- With this common discrete distribution on $\{0, 1, 2\}$, we can see that $P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) = 1/2$ because

$$\begin{aligned}
 P(X_i > Y_j) + \frac{1}{2}P(X_i = Y_j) &= P(X_i = 1, Y_j = 0) + P(X_i = 2, Y_j = 0) + P(X_i = 2, Y_j = 1) \\
 &+ \frac{1}{2} \left[P(X_i = 0, Y_j = 0) + P(X_i = 1, Y_j = 1) + P(X_i = 2, Y_j = 2) \right] \\
 &= p_1 p_0 + (1 - p_1 - p_0) p_0 + (1 - p_1 - p_0) p_1 \\
 &+ p_0^2 + p_1^2 + \frac{1}{2} - p_0 - p_1 + p_0 p_1 \\
 &= 1/2
 \end{aligned}$$

3.2.2 Definition of the WRS Test Statistic

- The WRS test statistic is based on computing the sum of ranks (ranks based on the pooled sample) in one group.
- The motivation for the WRS test statistic is the following: if observations from group 1 tend to be larger than those from group 2, the average rank from group 1 should exceed the average rank from group 2.
- A sufficiently large value of the average rank from group 1 will allow us to reject H_0 in favor of H_A .

- We will define the pooled data vector \mathbf{Z} as

$$\mathbf{Z} = (X_1, \dots, X_n, Y_1, \dots, Y_m)$$

This is a vector with length $n + m$.

- The Wilcoxon rank-sum test statistic W for testing hypotheses of the form (3.8) is then defined as

$$W = \sum_{i=1}^n R_i(\mathbf{Z}) \quad (3.11)$$

- In other words, the WRS test statistic is the sum of the ranks for those observations coming from group 1 (i.e., the group with the X_i as observations).
- If the group 1 observations tend to, in fact, be larger than the group 2 observations, then we should expect the sum of the ranks in this group to be larger than the sum of the ranks from group 2.

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- Under H_0 , we can treat both X_i and Y_i as being observations coming from a common distribution function F .
- Hence, the expectation of $R_i(\mathbf{Z})$ under the null hypothesis is

$$E_{H_0}\{R_i(\mathbf{Z})\} = \frac{n + m + 1}{2}$$

and thus the expectation of W under H_0

$$E_{H_0}(W) = \sum_{i=1}^n E_{H_0}\{R_i(\mathbf{Z})\} = \frac{n(n + m + 1)}{2}$$

- It can be shown that the variance of W under the null hypothesis is

$$\text{Var}_{H_0}(W) = \frac{mn(m + n + 1)}{12}$$

3.2.3 Computing p-values for the WRS Test

Exact Distribution

- The p-value for the WRS test is found by computing the probability

$$\text{p-value} = P_{H_0}(W \geq w_{obs}) \quad (3.12)$$

where w_{obs} is the observed WRS test statistic that we get from our data.

- Computing p-values for the WRS test requires us to work with the **null distribution** of W . That is, the distribution of W under the assumption that $F_X = F_Y$.
- The exact null distribution is found by using the fact that each possible ordering of the ranks has the same probability. That is,

$$P\{R_1(\mathbf{Z}) = r_1, \dots, R_{n+m}(\mathbf{Z}) = r_{n+m}\} = \frac{1}{(n + m)!}, \quad (3.13)$$

where (r_1, \dots, r_{n+m}) is any permutation of the set $\{1, 2, \dots, n + m\}$. Note that the null distribution only depends on n and m .

- Also, there are $\binom{n+m}{n}$ possible ways to assign distinct ranks to group 1.
- Consider an example with $n = m = 2$. In this case, there are $\binom{4}{2} = 6$ distinct ways to assign 2 ranks to group 1. What is the null distribution of the WRS test statistic? Try to verify that

$$\begin{aligned} P_{H_0}(W = 7) &= 1/6 \\ P_{H_0}(W = 6) &= 1/6 \\ P_{H_0}(W = 5) &= 1/3 \\ P_{H_0}(W = 4) &= 1/6 \\ P_{H_0}(W = 3) &= 1/6. \end{aligned}$$

Large-Sample Approximate Distribution

- Looking at (3.11), we can see that the WRS test statistic is a sum of nearly independent random variables (at least nearly independent for large n and m).
- Thus, we can expect that an appropriately centered and scaled version of W should be approximately Normally distributed (recall the Central Limit Theorem).
- The standardized version \tilde{W} of the WRS is defined as

$$\tilde{W} = \frac{W - E_{H_0}(W)}{\sqrt{\text{Var}_{H_0}(W)}} = \frac{W - n(n+m+1)/2}{\sqrt{mn(n+m+1)/12}} \quad (3.14)$$

- Under H_0 , \tilde{W} converges in distribution to a $\text{Normal}(0, 1)$ random variable.
- A p-value using this large-sample approximation would then be computed in the following way

$$\begin{aligned} \text{p-value} &= P_{H_0}(W \geq w_{\text{obs}}) = P\left(\frac{W - n(n+m+1)/2}{\sqrt{mn(n+m+1)/12}} \geq \frac{w_{\text{obs}} - n(n+m+1)/2}{\sqrt{mn(n+m+1)/12}}\right) \\ &= P_{H_0}\left(\tilde{W} \geq \frac{w_{\text{obs}} - n(n+m+1)/2}{\sqrt{mn(n+m+1)/12}}\right) = 1 - \Phi\left(\frac{w_{\text{obs}} - n(n+m+1)/2}{\sqrt{mn(n+m+1)/12}}\right), \end{aligned}$$

where $\Phi(t)$ denotes the cumulative distribution function of a standard Normal random variable.

- Often, in practice, a continuity correction is applied when using this large-sample approximation. For example, we would compute the probability $P_{H_0}(W \geq w_{\text{obs}} - 0.5)$ with the Normal approximation rather than $P_{H_0}(W \geq w_{\text{obs}})$ directly.
-

- Many statistical software packages (including **R**) will not compute p-values using the exact distribution in the presence of ties.
- The **coin** package in **R** does allow you to perform a permutation test in the presence of ties.

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- A “two-sided” Wilcoxon rank sum test can also be performed. The two-sided hypothesis tests could either be stated as

$$\begin{aligned} H_0 : & \quad F_X = F_Y \quad \text{versus} \\ H_A : & \quad F_X \text{ is stochastically larger or smaller than } F_Y \end{aligned}$$

or

$$\begin{aligned} H_0 : & \quad F_X = F_Y \quad \text{versus} \\ H_A : & \quad F_X(t) = F_Y(t - \Delta), \Delta \neq 0. \end{aligned}$$

or

$$\begin{aligned} H_0 : & \quad P(X_i > Y_i) + \frac{1}{2}P(X_i = Y_i) = 1/2 \quad \text{versus} \\ H_A : & \quad P(X_i > Y_i) + \frac{1}{2}P(X_i = Y_i) \neq 1/2 \end{aligned}$$

Exercise 3.3. Using the exact distribution, what is the smallest possible one-sided p-value associated with the WRS test for a fixed value of n and m (assuming the probability of ties is zero)?

3.2.4 Computing the WRS test in R

- To illustrate performing the WRS test in **R**, we can use the **wine** dataset from the **rattle.data** package. This dataset is also available from the UCI Machine Learning Repository.

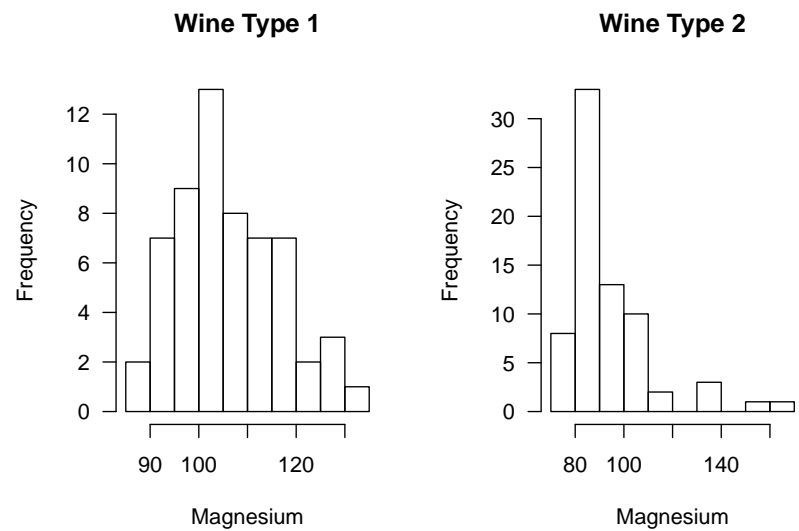
```
library(rattle.data)
head(wine)
```

##	Type	Alcohol	Malic	Ash	Alcalinity	Magnesium	Phenols	Flavanoids	Nonflavanoids
## 1	1	14.23	1.71	2.43	15.6	127	2.80	3.06	0.28
## 2	1	13.20	1.78	2.14	11.2	100	2.65	2.76	0.26
## 3	1	13.16	2.36	2.67	18.6	101	2.80	3.24	0.30
## 4	1	14.37	1.95	2.50	16.8	113	3.85	3.49	0.24
## 5	1	13.24	2.59	2.87	21.0	118	2.80	2.69	0.39
## 6	1	14.20	1.76	2.45	15.2	112	3.27	3.39	0.34
##	Proanthocyanins Color Hue Dilution Proline								
## 1		2.29	5.64	1.04	3.92	1065			
## 2		1.28	4.38	1.05	3.40	1050			
## 3		2.81	5.68	1.03	3.17	1185			
## 4		2.18	7.80	0.86	3.45	1480			
## 5		1.82	4.32	1.04	2.93	735			
## 6		1.97	6.75	1.05	2.85	1450			

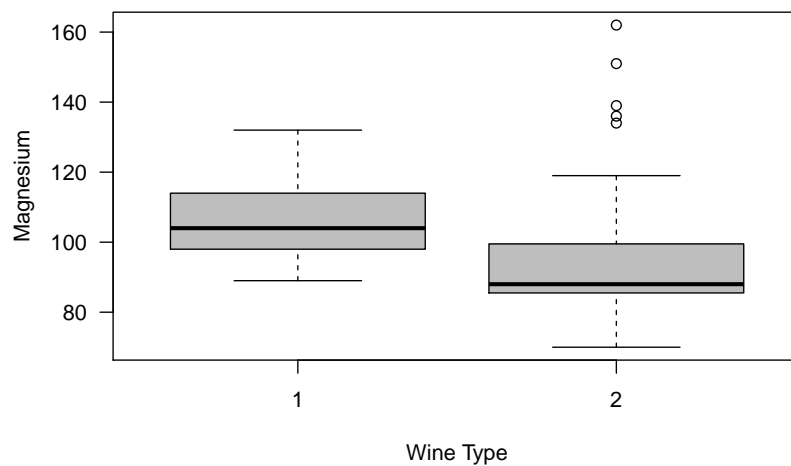
- This dataset contains three types of wine. We will only consider the first two.

```
wine2 <- subset(wine, Type==1 | Type==2)
wine2$Type <- factor(wine2$Type)
```

- Let us consider the difference in the level of magnesium across the two



types of wine.



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- Suppose we are interested in testing whether or not magnesium levels in Type 1 wine are generally larger than magnesium levels in Type 2 wine. This can be done with the following code

```
wilcox.test(x=wine2$Magnesium[wine2$Type==1], y=wine2$Magnesium[wine2$Type==2],
            alternative="greater")
```

```
##
## Wilcoxon rank sum test with continuity correction
##
## data: wine2$Magnesium[wine2$Type == 1] and wine2$Magnesium[wine2$Type == 2]
## W = 3381.5, p-value = 8.71e-10
## alternative hypothesis: true location shift is greater than 0
```

- You could also use the following code to perform this test (just be careful about the ordering of the levels of **Type**)

```
wilcox.test(Magnesium ~ Type, data=wine2, alternative="greater")
```

```
##
## Wilcoxon rank sum test with continuity correction
##
## data: Magnesium by Type
## W = 3381.5, p-value = 8.71e-10
## alternative hypothesis: true location shift is greater than 0
```

- What is the value of the WRS test statistic? We can code this directly with the following steps:

```
W <- wilcox.test(x=wine2$Magnesium[wine2$Type==1], y=wine2$Magnesium[wine2$Type==2])
```

```
n <- sum(wine2$Type==1)
m <- sum(wine2$Type==2)
zz <- rank(wine2$Magnesium) ## vector of pooled ranks
sum(zz[wine2$Type==1]) ## The WRS test statistic
```

```
## [1] 5151.5
```

- The statistic returned by the **wilcox.test** function is actually equal to $W - n(n+1)/2$ not W

```
sum(zz[wine2$Type==1]) - n*(n + 1)/2
```

```
## [1] 3381.5
```

```
W$statistic
```

```
##      W
## 3381.5
```

- $\{W - n(n + 1)/2\}$ is equal to the Mann-Whitney statistic. Thus, $W\$statistic/(mn)$ is an estimate of the probability $P(X_i > Y_j) + P(X_i = Y_j)/2$.

```
W$statistic/(m*n)
```

```
##      W
## 0.8072332
```

- Let's check how the Mann-Whitney statistic matches a simulation-based estimate of this probability

```
ind1 <- which(wine2$Type==1)
ind2 <- which(wine2$Type==2)
xgreater <- rep(0, 100)
for(k in 1:100) {
  xi <- sample(ind1, size=1)
  yi <- sample(ind2, size=1)
  xgreater[k] <- ifelse(wine2$Magnesium[xi] > wine2$Magnesium[yi], 1, 0) +
    ifelse(wine2$Magnesium[xi] == wine2$Magnesium[yi], 1/2, 0)
}
mean(xgreater) ## estimate of this probability
```

```
## [1] 0.78
```

- This simulation-based estimate of $P(X_i > Y_j) + P(X_i = Y_j)/2$ is quite close to the value of the Mann-Whitney statistic divided by mn .

3.2.5 Additional Notes for the WRS test

3.2.5.1 Comparing Ordinal Data

- The WRS test is often suggested when comparing categorical data which are **ordinal**.

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- For example, we might have 4 categories:
 - Poor
 - Fair
 - Good
 - Excellent
- In this case, there is a natural ordering of the categories but any numerical values assigned to these categories would be arbitrary.
- In such cases, we might be interested in testing whether or not outcomes tend to be better in one group than the other rather than simply comparing whether or not the distribution is different between the two groups.
- A WRS test is useful here since we can still compute ranks without having to choose arbitrary numbers for each category.
- Thinking of the “probability greater than alternative (3.10)” or “stochastically larger than alternative (3.8)” interpretation of the WRS test is probably more reasonable than the “shift alternative (3.9)” interpretation.
- Note that there will probably be many ties when comparing ordinal data.

3.2.5.2 The Hodges-Lehmann Estimator

- The Hodges-Lehmann Estimator $\hat{\Delta}$ is an estimator of Δ in the location-shift model

$$F_X(t) = F_Y(t - \Delta)$$

- The Hodges-Lehmann is defined as the median difference among all possible (group 1, group 2) pairs. Specifically,

$$\hat{\Delta} = \text{median}\{(X_i - Y_j); i = 1, \dots, n; j = 1, \dots, m\}$$

- We won’t discuss the Hodges-Lehmann estimator in detail in this course, but in many statistical software packages, the Hodges-Lehmann is often reported when computing the WRS test.
- In **R**, the Hodges-Lehmann estimator can be obtained by using the **conf.int=TRUE** argument in the **wilcox.test** function

```
WC <- wilcox.test(x=wine2$Magnesium[wine2$Type==1], y=wine2$Magnesium[wine2$Type==2],
                 conf.int=TRUE)
WC$estimate      ## The Hodges-Lehmann estimate

## difference in location
##                14.00005
```

3.3 One Sample Tests

3.3.1 The Sign Test

3.3.1.1 Motivation and Definition

- The **sign test** can be thought of as a test of whether or not the median of a distribution is greater than zero (or greater than some other fixed value θ_0).
- Frequently, the sign test is applied in the following context:
 - Suppose we have observations D_1, \dots, D_n which arise from the model

$$D_i = \theta + \varepsilon_i, \quad (3.15)$$

where ε_i are iid random variables each with distribution function F_ϵ that is assumed to have a median of zero. Moreover, we will assume the density function $f_\epsilon(t)$ of ε_i is symmetric around zero.

- The distribution function of D_i is then

$$F_D(t) = P(D_i \leq t) = P(\varepsilon_i \leq t - \theta) = F_\epsilon(t - \theta) \quad (3.16)$$

- Likewise, the density function $f_D(t)$ of D_i is given by

$$f_D(t) = f_\epsilon(t - \theta) \quad (3.17)$$

- In this context, θ is usually referred to as a **location parameter**.
- The goal here is to test $H_0 : \theta = \theta_0$ vs. $H_A : \theta > \theta_0$. (Often, $\theta_0 = 0$).

- This sort of test usually comes up in the context of **paired data**. Common examples include
 - patients compared “pre and post treatment”
 - students before and after the introduction of a new teaching method
 - comparison of “matched” individuals who are similar (e.g., same age, sex, education, etc.)
 - comparing consistency of measurements made on the same objects
- In such cases, we have observations X_i and Y_i for $i = 1, \dots, n$ where it is not necessarily reasonable to think of X_i and Y_i as independent.

	Baseline_Measure	Post_Treatment_Measure
Patient 1	Y1	X1
Patient 2	Y2	X2
Patient 3	Y3	X3
Patient 4	Y4	X4

- We can define $D_i = X_i - Y_i$ as the difference in the i^{th} pair.
- With this setup, a natural question is whether or not the differences D_i tend to be greater than zero or not.

- The **sign** statistic S_n is defined as

$$S_n = \sum_{i=1}^n I(D_i > 0) \quad (3.18)$$

- If the null hypothesis $H_0 : \theta = 0$ is true, then we should expect that roughly half of the observations will be positive.
- This suggests that we will reject H_0 if $S_n \geq c$, where c is a number that is greater than $n/2$.

3.3.1.2 Null Distribution and p-values for the Sign Test

- Notice that the sign statistic defined in (3.18) is the sum of independent Bernoulli random variable.
- That is, we can think of $Z_i = I(D_i > 0)$ as a random variable with success probability $p(\theta)$ where the formula for $p(\theta)$ is

$$p(\theta) = P(Z_i = 1) = P(D_i > 0) = 1 - F_D(0) = 1 - F_\epsilon(-\theta)$$

- This implies that S_n is a binomial random variable with n trials and success probability $p(\theta)$. That is,

$$S_n \sim \text{Binomial}(n, p(\theta)) \quad (3.19)$$

- Because $p(0) = 1/2$, $S_n \sim \text{Binomial}(n, 1/2)$ under H_0 .
- Notice that the “null distribution” of the sign statistic is “distribution free” in the sense that the null distribution of S_n does not depend on the distribution of D_i .

- The p-value for the one-sided sign test can be computed by

$$\text{p-value} = P_{H_0}(S_n \geq s_{obs}) = \sum_{j=s_{obs}}^n P_{H_0}(S_n = j) = \sum_{j=s_{obs}}^n \binom{n}{j} \frac{1}{2^n},$$

where s_{obs} is the observed value of the sign statistic.

```
### How to compute the p-value for the sign test using R
xx <- rnorm(100)
sign.stat <- sum(xx > 0) ## This is the value of the sign statistic
1 - pbinom(sign.stat - 1, size=100, prob=1/2) ## p-value for sign test
```

```
## [1] 0.04431304
```

- The reason that this is the right expression using **R** is that for any positive integer w

$$P_{H_0}(S_n \geq w) = 1 - P_{H_0}(S_n < w) = 1 - P_{H_0}(S_n \leq w - 1) \quad (3.20)$$

and the **R** function **pbinom(t, n, prob)** computes $P(X \leq t)$ where X is a binomial random variable with n trials and success probability **prob**.

- You can also perform the one-sided sign test by using the **binom.test** function in **R**.

```
btest <- binom.test(sign.stat, n=100, p=0.5, alternative="greater")
btest$p.value
```

```
## [1] 0.04431304
```

3.3.1.3 Two-sided Sign Test

- Notice that the number of negative values of D_i can be expressed as

$$\sum_{i=1}^n I(D_i < 0) = n - S_n \quad (3.21)$$

if there are no observations that equal zero exactly. Large value of $n - S_n$ would be used in favor of another possible one-sided alternative $H_A : \theta < 0$.

- If we now want to test the two-sided alternative

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

you would need to compute the probability under the null hypothesis of observing a “more extreme” observation than the one that was actually observed.

- Extreme is defined by thinking about the fact that we would have rejected H_0 if either S_n or $n - S_n$ were very large.
- For example, if $n = 12$, then the expected value of the sign statistic would be 6. If $s_{obs} = 10$, then the collection of “more extreme” events would be ≤ 2 or ≥ 10 .
- The two-sided p-value is determined by looking at the tail probabilities on both sides

$$\text{p-value} = \begin{cases} P_{H_0}(S_n \geq s_{obs}) + P_{H_0}(S_n \leq n - s_{obs}) & \text{if } s_{obs} \geq n/2 \\ P_{H_0}(S_n \leq s_{obs}) + P_{H_0}(S_n \geq n - s_{obs}) & \text{if } s_{obs} < n/2 \end{cases}$$

- It actually works out that

$$\text{p-value} = \begin{cases} 2P_{H_0}(S_n \geq s_{obs}) & \text{if } s_{obs} \geq n/2 \\ 2P_{H_0}(S_n \leq s_{obs}) & \text{if } s_{obs} < n/2 \end{cases}$$

- Also, you can note that this p-value would be the same that you would get from performing the test $H_0 : p = 1/2$ vs. $H_A : p \neq 1/2$ when it is assumed that $S_n \sim \text{Binomial}(n, p)$.
- Another note: It is often suggested that one should drop observations which are exactly zero when performing the sign test.

3.3.2 The Wilcoxon Signed Rank Test

- The Wilcoxon signed rank test can be applied under the same scenario that we used the sign test.
- One criticism of the sign test is that it ignores the magnitude of the observations.
- For example, the sign test statistic S treats observations $D_i = 0.2$ and $D_i = 3$ the same.
- The **Wilcoxon signed rank statistic** T_n weights the signs of D_i by the rank of its absolute value.
- Specifically, the Wilcoxon signed rank statistic is defined as

$$T_n = \sum_{i=1}^n \text{sign}(D_i) R_i(|\mathbf{D}|)$$

where the sign function is defined as

$$\text{sign}(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{if } x < 0 \end{cases}$$

- Here, $R_i(|\mathbf{D}|)$ is the rank of the i^{th} element from the vector $|\mathbf{D}| = (|D_1|, |D_2|, \dots, |D_n|)$.
- Intuitively, the Wilcoxon signed rank statistic is measuring whether or not large values of $|D_i|$ tend to be associated with positive vs. negative values of D_i .

Exercise 3.4. Suppose we had data $(-2, 1, -1/2, 3/2, 3)$. What would be the value of the Wilcoxon signed rank statistic?

Exercise 3.5. Under the assumptions of model (3.15), what is the density function of $|D_i|$ and $-|D_i|$?

Exercise 3.6. Under the assumptions of model (3.15) and assuming that $\theta = 0$, show that the expectation of the Wilcoxon signed-rank statistic is 0.

3.3.2.1 Asymptotic Distribution

- As mentioned in the above exercise, the expectation of T_n under H_0 is zero.
- It can be shown that the variance under the null hypothesis is

$$\text{Var}_{H_0}(T_n) = \frac{n(2n+1)(n+1)}{6}$$

- Similar, to the large-sample approximation we used for the WRS test, we have the following asymptotic result for the Wilcoxon signed-rank test

$$\frac{T_n}{\sqrt{\text{Var}_{H_0}(T_n)}} \rightarrow \text{Normal}(0, 1) \quad \text{as } n \rightarrow \infty$$

- Because the variance of T is dominated by the term $n^3/3$ for very large n , we could also say that under H_0 that

$$\frac{T_n}{\sqrt{n^3/3}} \rightarrow \text{Normal}(0, 1) \quad \text{as } n \rightarrow \infty \quad (3.22)$$

In other words, we can say that T_n has an approximately $\text{Normal}(0, n^3/3)$ for large n .

3.3.2.2 Exact Distribution

- The exact distribution of the Wilcoxon signed rank statistic T_n is somewhat more complicated than the exact distribution of the WRS test statistic. Nevertheless, there exists functions in **R** for working with this exact distribution.

3.3.3 Using R to Perform the Sign and Wilcoxon Tests

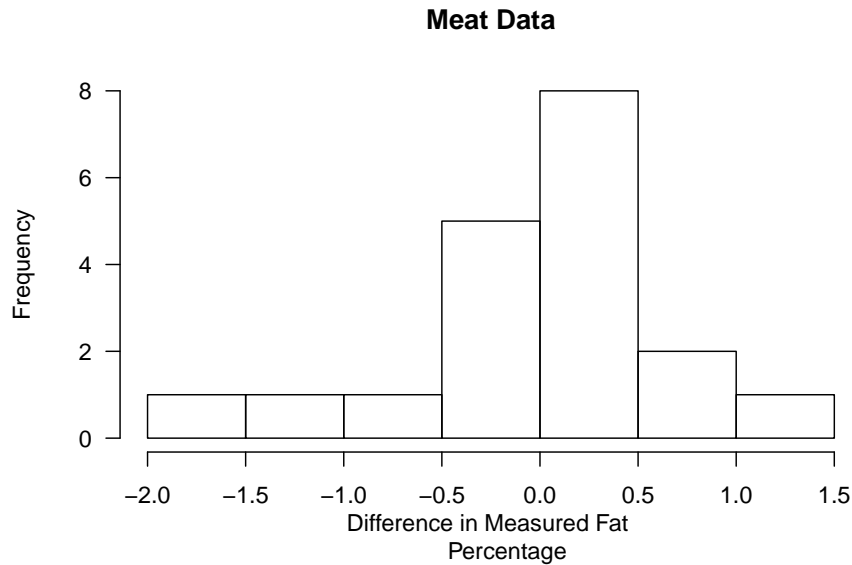
- Let's first look at the **Meat** data from the **PairedData R** package.
- This data set contains 20 observations with each observation corresponding to a single piece of meat. For each observation, we have two measures of fat percentage that were obtained different measuring techniques.

```
library(PairedData, quietly=TRUE, warn.conflicts=FALSE) ## loading PairedData package
data(Meat) ## loading Meat data
head(Meat)
```

```
##   AOAC Babcock      MeatType
## 1 22.0    22.3      Wiener
## 2 22.1    21.8      Wiener
## 3 22.1    22.4      Wiener
## 4 22.2    22.5      Wiener
## 5 24.6    24.9 ChoppedHam
## 6 25.3    25.6 ChooppedPork
```

- Define the differences D_i as the **Babcock** measurements minus the **AOAC** measures. We will drop the single observation that equals zero.

```
DD <- Meat[,2] - Meat[,1]
DD <- DD[DD!=0]
hist(DD, main="Meat Data", xlab="Difference in Measured Fat
      Percentage", las=1)
```



```
summary(DD)
```

```
##      Min.   1st Qu.   Median     Mean  3rd Qu.    Max.
## -1.60000 -0.25000  0.30000  0.04211  0.40000  1.10000
```

The Sign Test in R

- Let's first test the hypothesis $H_0 : \theta = 0$ vs. $H_A : \theta \neq 0$ using the two-sided sign test. This can be done using the **binom.test** function

```
binom.test(sum(DD > 0), n = length(DD), p=0.5)$p.value
```

```
## [1] 0.6476059
```

Wilcoxon Signed Rank Test in R

- You can actually use the function **wilcox.test** to perform the Wilcoxon signed rank test in addition to the Wilcoxon rank sum test. To perform the Wilcoxon signed rank test in **R**, you just need to enter data for the **x** argument and leave the **y** argument empty.


```
wilcox.test(x=DD)
```

```
## Warning in wilcox.test.default(x = DD): cannot compute exact p-value with ties
```

```
##
## Wilcoxon signed rank test with continuity correction
##
## data: DD
## V = 118.5, p-value = 0.3534
## alternative hypothesis: true location is not equal to 0
```

- You will note that the p-value for the Wilcoxon signed rank test is lower than that of the sign test. In general, the Wilcoxon signed rank test is somewhat more “sensitive” than the sign test meaning that it will have a greater tendency to reject H_0 for small deviations from H_0 .
- We can explore this sensitivity comparison with a small simulation study. We will consider a scenario where $D_i = 0.4 + \varepsilon_i$ with ε_i having a t distribution with 3 degrees of freedom.

```
set.seed(1327)
n.reps <- 500 ## number of simulation replications
samp.size <- 50 ## the sample size
wilcox.reject <- rep(0, n.reps)
sign.reject <- rep(0, n.reps)
for(k in 1:n.reps) {
  dsim <- .4 + rt(samp.size, df=3)
  wilcox.reject[k] <- ifelse(wilcox.test(x=dsim)$p.value < 0.05, 1, 0)
  sign.reject[k] <- ifelse(binom.test(sum(dsim > 0),
                                     n=samp.size, p=0.5)$p.value < 0.05, 1, 0)
}
mean(wilcox.reject) ## proportion of times Wilcoxon signed rank rejected H0
```

```
## [1] 0.614
```

```
mean(sign.reject) ## proportion of times Wilcoxon signed rank rejected H0
```

```
## [1] 0.488
```

3.4 Power and Comparisons with Parametric Tests

3.4.1 The Power Function of a Test

- The **power** of a test is the probability that a test rejects the null hypothesis when the alternative hypothesis is true.
- The alternative hypothesis H_A is usually characterized by a large range of values of the parameter of interest. For example, $H_A : \theta > 0$ or $H_A : \theta \neq 0$.
- For this reason, it is better to think of power as a function that varies across the range of the alternative hypothesis.
- To be more precise, we will define the power function as a function of some parameter θ where the null hypothesis corresponds to $\theta = \theta_0$ and the alternative hypothesis represents a range of alternative values of θ .
- The power function $\gamma_n(\cdot)$ of a testing procedure is defined as

$$\gamma_n(\delta) = P_{\theta=\delta}\{\text{reject } H_0\} \quad \text{for } \delta \in H_A.$$

- The notation $P_{\theta=\delta}\{\text{reject } H_0\}$ means that we are computing this probability under the assumption that the parameter of interest θ equals δ .

The Approximate Power Function of the Sign Test

- Let us consider the sign test for testing $H_0 : \theta = 0$ vs. $\theta > 0$.
- The sign test is based on the value of the sign statistic S_n .
- Recalling (3.19), we know that $S_n \sim \text{Binomial}(n, p(\theta))$. Hence,

$$\sqrt{n}\left(\frac{S_n}{n} - p(\theta)\right) \longrightarrow \text{Normal}\left(0, p(\theta)(1 - p(\theta))\right) \quad \text{as } n \longrightarrow \infty \quad (3.23)$$

- The sign test will reject H_0 when $S_n \geq c_{\alpha,n}$ where the constant $c_{\alpha,n}$ is chosen so that $P_{H_0}(S_n \geq c_{\alpha,n}) = \alpha$. Using the large-sample approximation (3.23), you can show that

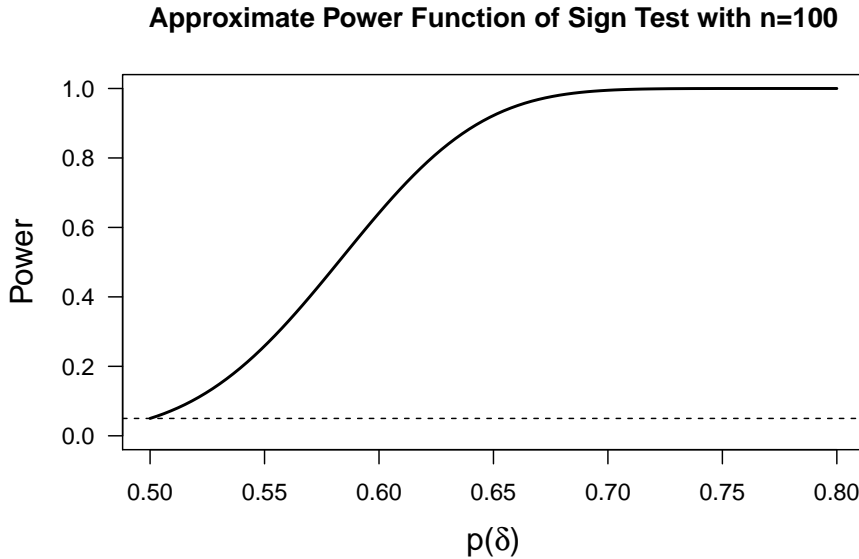
$$c_{\alpha,n} = \frac{n + \sqrt{n}z_{1-\alpha}}{2}, \quad (3.24)$$

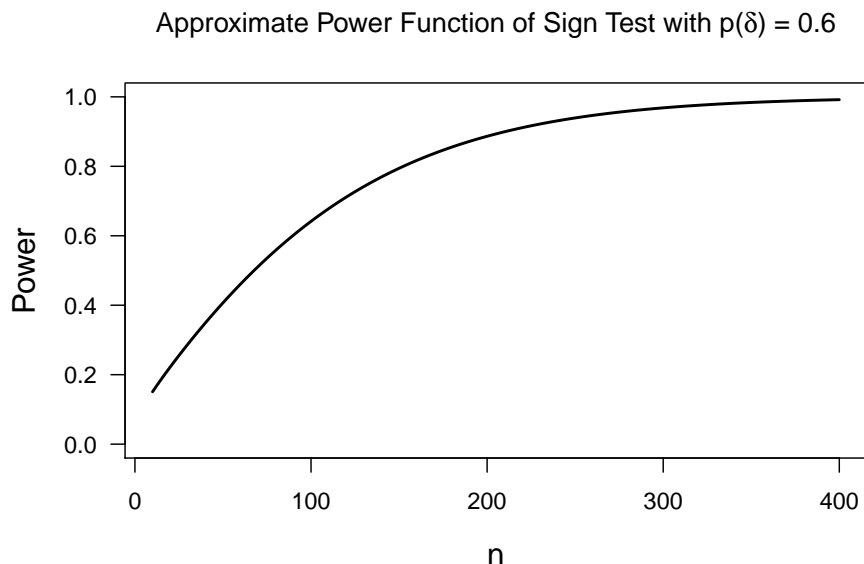
where $z_{1-\alpha}$ denotes the upper $1 - \alpha$ quantile of the standard normal distribution. In other words, $\Phi(z_{1-\alpha}) = 1 - \alpha$.

- Also, when using large-sample approximation (3.23), the power of this test to detect a value of $\theta = \delta$ is given by

$$\begin{aligned}
 \gamma_n(\delta) &= P_{\theta=\delta}\{S_n \geq c_{\alpha,n}\} = P_{\theta=\delta}\left\{\frac{\sqrt{n}(S_n/n - p(\delta))}{\sqrt{p(\delta)(1-p(\delta))}} \geq \frac{\sqrt{n}(c_{\alpha,n}/n - p(\delta))}{\sqrt{p(\delta)(1-p(\delta))}}\right\} \\
 &= 1 - \Phi\left(\frac{\sqrt{n}(c_{\alpha,n}/n - p(\delta))}{\sqrt{p(\delta)(1-p(\delta))}}\right) \\
 &= 1 - \Phi\left(\frac{z_{1-\alpha}}{2\sqrt{p(\delta)(1-p(\delta))}} - \frac{\sqrt{n}(p(\delta) - 1/2)}{\sqrt{p(\delta)(1-p(\delta))}}\right) \quad (3.25)
 \end{aligned}$$

- Notice that the power of the test depends more directly on the term $p(\delta) = P_{\theta=\delta}(D_i > 0)$. Recall from Section 3.3.1 that $p(\delta) = 1 - F_\epsilon(-\delta)$, where F_ϵ is the distribution function of ϵ_i in the model $D_i = \theta + \epsilon_i$.
- So, in any power or sample size calculation, it would be more sensible to think about plausible values for $p(\delta)$ rather than δ itself. Plus, $p(\delta)$ has the direct interpretation $p(\delta) = P_{\theta=\delta}(D_i > 0)$.





Exercise 3.7: Derive the formula for $c_{\alpha,n}$ shown in (3.24).

3.4.2 Power Comparisons and Asymptotic Relative Efficiency

- Notice that for the sign statistic power function shown in (3.25), we have that

$$\lim_{n \rightarrow \infty} \gamma_n(\delta) = \begin{cases} \alpha & \text{if } \delta = 0 \\ 1 & \text{if } \delta > 0 \end{cases} \quad (3.26)$$

- The above type of limit for the power function is will be true for most “reasonable” tests.
 - Indeed, a test whose power function satisfies (3.26) is typically called a **consistent** tests.
-

- If nearly all reasonable tests are consistent, then how can we compare tests with respect to their power?

- One approach is to use simulations to compare power for several plausible alternatives. While this can be useful for a specific application, it limits our ability to make more general statements about power comparisons.
- Another approach might be to determine for which values of (δ, n) one test has greater power than another. However, this could be tough to interpret (no test will be uniformly more powerful for all distributions) or even difficult to compute.
- One way to think about power is to think about the **relative efficiency** of two testing procedures. The efficiency of a test in this context is the sample size required to achieve a certain level of power.

- To find the asymptotic relative efficiency, we first need to derive the asymptotic power function.
- For our hypothesis $H_0 : \theta = \theta_0$ vs. $H_A : \theta > \theta_0$, this is defined as

$$\tilde{\gamma}(\delta) = \lim_{n \rightarrow \infty} \gamma_n(\theta_0 + \delta/\sqrt{n})$$

- Considering the sequence of “local alternatives” $\theta_n = \theta_0 + \delta/\sqrt{n}$, we avoid the problem of the power always converging to 1.
- It can be shown that

$$\tilde{\gamma}(\delta) = 1 - \Phi\left(z_{1-\alpha} - \delta \frac{\mu'(\theta_0)}{\sigma(\theta_0)}\right) \quad (3.27)$$

as long as we can find functions $\mu(\cdot)$ and $\sigma(\cdot)$ such that

$$\frac{\sqrt{n}(V_n - \mu(\theta_n))}{\sigma(\theta_n)} \longrightarrow \text{Normal}(0, 1) \quad (3.28)$$

where the test of $H_0 : \theta = \theta_0$ vs. $H_A : \theta > \theta_0$ is based on the test statistic V_n with rejection of H_0 occurring whenever $V_n \geq c_{\alpha, n}$. Statement (3.28) assumes that the distribution of V_n is governed by θ_n for each n .

- The ratio $e(\theta_0) = \mu'(\theta_0)/\sigma(\theta_0)$ is the **asymptotic efficiency** of the test.
- When comparing two tests with efficiency $e_1(\theta_0)$ and $e_2(\theta_0)$, the asymptotic relative efficiency of test 1 vs. test 2 is defined as

$$ARE_{12}(\theta_0) = \left(\frac{e_1(\theta_0)}{e_2(\theta_0)}\right)^2 \quad (3.29)$$

Interpretation of Asymptotic Efficiency of Tests

- Roughly speaking, the asymptotic relative efficiency $ARE_{12}(\theta_0)$ approximately equals n_2/n_1 where n_1 is the sample size needed for test 1 to achieve power β and n_2 is the sample size needed for test 2 to achieve power β . This is true for an arbitrary β .
- To further justify this interpretation notice that, for large n , we should have

$$c_{\alpha,n} \approx \mu(\theta_0) + \frac{\sigma(\theta_0)z_{1-\alpha}}{\sqrt{n}} \quad (3.30)$$

(This approximation for $c_{\alpha,n}$ comes from the asymptotic statement in (3.28))

- Now, consider the power for detecting $H_A : \theta = \theta_A$ (where we will assume that θ_A is “close” to θ_0). Using (3.28), the approximate power in this setting is

$$\begin{aligned} P_{\theta_A}(V_n \geq c_{\alpha,n}) &= P_{\theta_A}\left(\frac{\sqrt{n}(V_n - \mu(\theta_A))}{\sigma(\theta_A)} \geq \frac{\sqrt{n}(c_{\alpha,n} - \mu(\theta_A))}{\sigma(\theta_A)}\right) \\ &\approx 1 - \Phi\left(\frac{\sqrt{n}(c_{\alpha,n} - \mu(\theta_A))}{\sigma(\theta_A)}\right) \\ &= 1 - \Phi\left(\frac{\sqrt{n}(\mu(\theta_0) - \mu(\theta_A))}{\sigma(\theta_A)} + \frac{z_{1-\alpha}\sigma(\theta_0)}{\sigma(\theta_A)}\right) \end{aligned} \quad (3.31)$$

- Hence, if we want to achieve a power level of β for the alternative $H_A : \theta = \theta_A$, we need the corresponding sample size $n_\beta(\theta_A)$ to satisfy

$$\frac{\sqrt{n_\beta(\theta_A)}(\mu(\theta_0) - \mu(\theta_A))}{\sigma(\theta_A)} + \frac{z_{1-\alpha}\sigma(\theta_0)}{\sigma(\theta_A)} = z_{1-\beta} \quad (3.32)$$

which reduces to

$$n_\beta(\theta_A) = \left(\frac{z_{1-\beta}\sigma(\theta_A) - z_{1-\alpha}\sigma(\theta_0)}{\mu(\theta_0) - \mu(\theta_A)}\right)^2 \approx \left(\frac{[z_{1-\beta} - z_{1-\alpha}]\sigma(\theta_0)}{(\theta_A - \theta_0)\mu'(\theta_0)}\right)^2 \quad (3.33)$$

- So, if we were comparing two testing procedures and we computed the approximate sample sizes $n_\beta^1(\theta_A)$ and $n_\beta^2(\theta_A)$ needed to reach β power for the alternative $H_A : \theta = \theta_A$, the sample size ratio (using approximation (3.33)) would be

$$\frac{n_\beta^2(\theta_A)}{n_\beta^1(\theta_A)} = \left(\frac{\mu'_1(\theta_0)\sigma_2(\theta_0)}{\mu'_2(\theta_0)\sigma_1(\theta_0)}\right)^2 = ARE_{12}(\theta_0) \quad (3.34)$$

- Notice that $ARE_{12}(\theta_0) > 1$ indicates that the test 1 is better than test 2 because the sample size required for test 1 would be less than the sample size required for test 2.
- It is also worth noting that our justification for the interpretation of $ARE_{12}(\theta_0)$ was not very rigorous or precise, but it is possible to make a more rigorous statement. See, for example, Chapter 13 of Lehmann and Romano (2006) for a more rigorous treatment of relative efficiency.
- In Lehmann and Romano (2006), they have a result that states (under appropriate assumptions) that

$$\lim_{\theta \downarrow \theta_0} \frac{N_2(\theta)}{N_1(\theta)} = ARE_{12}(\theta_0) \quad (3.35)$$

where $N_1(\theta)$ and $N_2(\theta)$ are the sample sizes required to have power β against alternative θ .

3.4.3 Efficiency Examples

The Sign Test

- Let us return to the example of the sign statistic S_n and its use in testing the hypothesis $H_0 : \theta = 0$ vs. $H_A : \theta > 0$.
- Notice that the sign test rejects $H_0 : \theta = 0$ for $V_n > c_{\alpha,n}$ where $V_n = S_n/n$ and S_n is the sign statistic.
- When V_n is defined this way (3.28) is satisfied when $\mu(\theta) = p(\theta)$ and $\sigma(\theta) = \sqrt{p(\theta)(1-p(\theta))}$ where $p(\theta) = 1 - F_\epsilon(-\theta)$.
- Thus, the efficiency of the sign test for testing $H_0 : \theta = 0$ vs. $H_A : \theta > 0$ is

$$\frac{\mu'(0)}{\sigma(0)} = \frac{p'(0)}{\sqrt{p(0)(1-p(0))}} = 2f_\epsilon(0)$$

where $f_\epsilon(t) = F'_\epsilon(t)$.

The One-Sample t-test

- Assume that we have data D_1, \dots, D_n generated under the same assumption as in our discussion of the sign test and the Wilcoxon signed-rank test. That is,

$$D_i = \theta + \varepsilon_i,$$

where ε_i are assumed to have median 0 with ε_i having p.d.f. f_ε

- The one-sample t-test will reject $H_0 : \theta = 0$ whenever $V_n > c_{\alpha,n}$, where V_n is defined to be

$$V_n = \frac{\bar{D}}{\hat{\sigma}}$$

- Note that (3.28) will apply if we choose

$$\begin{aligned} \mu(\theta) &= E_\theta(D_i) = \theta \\ \sigma(\theta) &= \sqrt{\text{Var}_\theta(D_i)} = \sqrt{\text{Var}(\varepsilon_i)} = \sigma_\varepsilon \end{aligned}$$

- These choices of $\mu(\theta)$ and $\sigma(\theta)$ work because

$$\begin{aligned} \frac{\sqrt{n}(V_n - \mu(\theta_n))}{\sigma(\theta_n)} &= \frac{\sqrt{n}(\bar{D} - \theta_n)}{\sigma_\varepsilon} + \sqrt{n}\theta_n \left(\frac{1}{\hat{\sigma}} - \frac{1}{\sigma_\varepsilon} \right) \\ &= \frac{\sqrt{n}(\bar{D} - \theta_n)}{\sigma_\varepsilon} + \delta \left(\frac{1}{\hat{\sigma}} - \frac{1}{\sigma_\varepsilon} \right) \\ &\rightarrow \text{Normal}(0, 1) \end{aligned}$$

- So, the efficiency of the one-sample t-test is given by

$$\frac{\mu'(0)}{\sigma(0)} = \frac{1}{\sigma_\varepsilon}$$

The Wilcoxon Rank Sum Test

- Using the close relation between the WRS test statistic and the Mann-Whitney statistic, the WRS test can be represented as rejecting H_0 when $V_N \geq c_{\alpha,N}$ where V_N is

$$V_N = \frac{1}{mn} \sum_{i=1}^n \sum_{j=1}^m I(X_i \geq Y_j)$$

and $N = n + m$.

- The power of the WRS test is usually analyzed in the context of the “shift alternative”. Namely, we are assuming that $F_X(t) = F_Y(t - \theta)$ and test $H_0 : \theta = 0$ vs. $H_A : \theta > 0$.

- The natural choice for $\mu(\theta)$ is the expectation of V_N when θ is the true shift parameter.
- So, let $\mu(\theta) = P_\theta(X_i \geq Y_j)$. This can be written in terms of F_Y and f_Y :

$$\begin{aligned}\mu(\theta) &= \int_{-\infty}^{\infty} P_\theta(X_i \geq Y_j | Y_j = t) f_Y(t) dt = \int_{-\infty}^{\infty} P_\theta(X_i \geq t) f_Y(t) dt \\ &= \int_{-\infty}^{\infty} \{1 - F_X(t)\} f_Y(t) dt = 1 - \int_{-\infty}^{\infty} F_Y(t - \theta) f_Y(t) dt \quad (3.36)\end{aligned}$$

- You can show that (3.28) holds (see e.g., Chapter 14 of Van der Vaart (2000)) if you choose $\sigma^2(\theta)$ to be

$$\sigma^2(\theta) = \frac{1}{1-\lambda} \text{Var}\{F_Y(X_i)\} + \frac{1}{\lambda} \text{Var}\{F_Y(Y_i - \theta)\} \quad (3.37)$$

Here, $n/(m+n) \rightarrow \lambda$.

- Thus, the efficiency of testing $H_0 : \theta = 0$ for the WRS test is

$$e(0) = \frac{\mu'(0)}{\sigma(0)} = \frac{\int_{-\infty}^{\infty} f^2(t) dt}{\sigma(0)} \quad (3.38)$$

3.4.4 Efficiency Comparisons for Several Distributions

Sign Test vs. One-Sample t-test

- Comparisons of the Efficiency of the sign and one-sample t-test only require us to find $f_\epsilon(0)$ and σ_ϵ^2 for different assumptions about the residual density f_ϵ .
- For the Logistic(0,1) distribution, $f_\epsilon(0) = 1/4$ and the standard deviation is $\pi/\sqrt{3}$. Hence, the asymptotic relative efficiency of the sign test vs. the one-sample t-test is $(\pi/2\sqrt{3})^2 = \pi^2/12$.
- The relative efficiencies for the sign vs. t-test for other distributions are shown below

Distribution	Efficiency	(3.39)
--------------	------------	--------

Normal(0, 1)	$2/\pi$	(3.40)
--------------	---------	--------

Logistic(0, 1)	$\pi^2/12$	(3.41)
----------------	------------	--------

Laplace(0, 1)	2	(3.42)
---------------	---	--------

Uniform(-1, 1)	1/3	(3.43)
----------------	-----	--------

t-dist $_\nu$	$[4(\nu/(\nu-2))\Gamma^2\{(\nu+1)/2\}]/[\Gamma^2(\nu/2)\nu\pi]$	(3.44)
---------------	---	--------

WRS Test vs. Two-Sample t-test

- The relative efficiencies for the WRS test vs. the two-sample t-test for several distributions are shown below.

Distribution	Efficiency	(3.45)
Normal(0, 1)	$3/\pi$	(3.46)
Logistic(0, 1)	$\pi^2/9$	(3.47)
Laplace(0, 1)	$3/2$	(3.48)
Uniform(−1, 1)	1	(3.49)
t-dist ₃	1.24	(3.50)
t-dist ₅	1.90	(3.51)
		(3.52)

3.4.5 A Power “Contest”

- To compare power for specific sample sizes, effect sizes, and distributional assumptions, a simulation study can be more helpful than statements about asymptotic relative efficiency.
- Below shows the results of a simulation study in **R** which compares power for the one-sample testing problem.
- This simulation study compares the sign test, Wilcoxon signed rank test, and the one-sample t-test.
- It is assumed that $n = 200$ and that responses D_i are generated from the following model:

$$D_i = 0.2 + \varepsilon_i$$

- Three choices for the distribution of ε_i were considered:
 - $\varepsilon_i \sim \text{Logistic}(0, 1)$
 - $\varepsilon_i \sim \text{Normal}(0, 1)$
 - $\varepsilon_i \sim \text{Uniform}(-3/2, 3/2)$
- The **R** code and simulation results are shown below.

```
set.seed(148930)
theta <- 0.2
n <- 200
nreps <- 500
```

```

RejectSign <- RejectWilcoxonSign <- RejectT <- matrix(NA, nrow=nreps, ncol=4)
for(k in 1:nreps) {
  xx <- theta + rlogis(n)
  yy <- theta + rnorm(n)
  zz <- theta + runif(n, min=-3/2, max=3/2)
  ww <- theta + (rexp(n, rate=1) - rexp(n, rate=1))/sqrt(2)

  RejectSign[k,1] <- ifelse(binom.test(x=sum(xx > 0), n=n, p=0.5)$p.value < 0.05, 1, 0)
  RejectWilcoxonSign[k,1] <- ifelse(wilcox.test(xx)$p.value < 0.05, 1, 0)
  RejectT[k,1] <- ifelse(t.test(xx)$p.value < 0.05, 1, 0)

  RejectSign[k,2] <- ifelse(binom.test(x=sum(yy > 0), n=n, p=0.5)$p.value < 0.05, 1, 0)
  RejectWilcoxonSign[k,2] <- ifelse(wilcox.test(yy)$p.value < 0.05, 1, 0)
  RejectT[k,2] <- ifelse(t.test(yy)$p.value < 0.05, 1, 0)

  RejectSign[k,3] <- ifelse(binom.test(x=sum(zz > 0), n=n, p=0.5)$p.value < 0.05, 1, 0)
  RejectWilcoxonSign[k,3] <- ifelse(wilcox.test(zz)$p.value < 0.05, 1, 0)
  RejectT[k,3] <- ifelse(t.test(zz)$p.value < 0.05, 1, 0)

  RejectSign[k,4] <- ifelse(binom.test(x=sum(ww > 0), n=n, p=0.5)$p.value < 0.05, 1, 0)
  RejectWilcoxonSign[k,4] <- ifelse(wilcox.test(ww)$p.value < 0.05, 1, 0)
  RejectT[k,4] <- ifelse(t.test(ww)$p.value < 0.05, 1, 0)
}

power.results <- data.frame(Distribution=c("Logistic", "Normal", "Uniform", "Laplace"),
  SignTest=colMeans(RejectSign), WilcoxonSign=colMeans(RejectWilcoxonSign),
  tTest=colMeans(RejectT))

```

Distribution	SignTest	WilcoxonSign	tTest
Logistic	0.25	0.37	0.34
Normal	0.59	0.77	0.81
Uniform	0.44	0.87	0.90
Laplace	0.93	0.92	0.81

Table 3.1: Estimated power for three one-sample tests and three distributions. 500 simulation replications were used.

3.5 Linear Rank Statistics in General

3.5.1 Definition

- The Wilcoxon rank sum statistic is an example of a statistic that belongs to a more general class of rank statistics.

- This is the class of **linear rank statistics**.
- Suppose we have observations $\mathbf{Z} = (Z_1, \dots, Z_N)$. A linear rank statistic is a statistic T_N that can be expressed as

$$T_N = \sum_{i=1}^N c_{iN} a_N(R_i(\mathbf{Z})) \quad (3.53)$$

- The terms c_{1N}, \dots, c_{NN} are usually called **coefficients**. These are fixed numbers and are not random variables.
- The terms $a_N(R_i(\mathbf{Z}))$ are commonly referred to as **scores**.
- Typically, the scores are generated from a given function ψ in the following way

$$a_N(i) = \psi\left(\frac{i}{N+1}\right)$$

Example: WRS statistic

- For the Wilcoxon rank sum test, we separated the data $\mathbf{Z} = (Z_1, \dots, Z_N)$ into two groups.
- The first n observations were from group 1 while the last m observations were from group 2.
- The WRS statistic was then defined as

$$W = \sum_{i=1}^n R_i(\mathbf{Z})$$

- In this case, the WRS statistic can be expressed in the form (3.53) if we choose the coefficients to be the following

$$c_{iN} = \begin{cases} 1 & \text{if } i \leq n \\ 0 & \text{if } i > n \end{cases}$$

and we choose the scores to be

$$a_N(i) = i$$

3.5.2 Properties of Linear Rank Statistics

- The expected value of the linear rank statistic (if the distribution of the Z_i is continuous) is

$$E(T_N) = N\bar{c}_N\bar{a}_N, \quad (3.54)$$

where $\bar{c}_N = \frac{1}{N} \sum_{j=1}^N c_{jN}$ and $\bar{a}_N = \frac{1}{N} \sum_{j=1}^N a_N(j)$

- The formula (3.54) for the expectation only uses the fact that $R_i(\mathbf{Z})$ has a discrete uniform distribution. So,

$$E\{a_N(R_i(\mathbf{Z}))\} = \sum_{j=1}^N a_N(j)P\{R_i(\mathbf{Z}) = j\} = \sum_{j=1}^N \frac{a_N(j)}{N} = \bar{a}_N$$

Using this, we can then see that

$$E(T_N) = \sum_{j=1}^N c_{jN}E\{a_N(R_i(\mathbf{Z}))\} = \sum_{j=1}^N c_{jN}\bar{a}_N = N\bar{c}_N\bar{a}_N$$

- A similar argument can show that the variance of T_N is

$$\text{Var}(T_N) = \frac{N^2}{n-1} \sigma_a^2 \sigma_c^2,$$

where $\sigma_c^2 = \frac{1}{N} \sum_{j=1}^N (c_{jN} - \bar{c}_N)^2$ and $\sigma_a^2 = \frac{1}{N} \sum_{j=1}^N (a_N(j) - \bar{a}_N)^2$

- To perform hypothesis testing when using a general linear rank statistics, working with the exact distribution or performing permutation tests can often be computationally demanding.
- Using a large-sample approximation is often easier.
- As long as a few conditions for the coefficients and scores are satisfied, one can state the following

$$\frac{T_N - E(T_N)}{\sqrt{\text{Var}(T_N)}} \rightarrow \text{Normal}(0, 1),$$

where, as we showed, both $E(T_N)$ and $\text{Var}(T_N)$ both have closed-form expressions for an arbitrary linear rank statistic.

3.5.3 Other Examples of Linear Rank Statistics

3.5.3.1 The van der Waerden statistic and the normal scores test

- Van der Waerden's rank statistic is used for two-sample problems where the first n observations come from group 1 while the last m observations come from group 2.
- Van der Waerden's rank statistic VW_N is defined as

$$VW_N = \sum_{j=1}^n \Phi^{-1} \left(\frac{\mathbf{R}_j(\mathbf{Z})}{N+1} \right)$$

- The function Φ^{-1} denotes the inverse of the cumulative distribution function of a standard Normal random variable.
- The statistic VW_N is a linear rank statistic with coefficients

$$c_{iN} = \begin{cases} 1 & \text{if } i \leq n \\ 0 & \text{if } i > n \end{cases}$$

and scores determined by

$$a_N(i) = \Phi^{-1} \left(\frac{i}{N+1} \right)$$

- A test based on van der Waerden's statistic is often referred to as the **normal scores test**.
- The normal scores test is often suggested as an attractive test when the underlying data has an approximately normal distribution.
- If you plot a histogram of the van der Waerden scores $a_N(i)$ it should look roughly like a Gaussian distribution (if there are not too many ties).

3.5.3.2 The median test

- The median test is also a two-sample rank test.
- While the Wilcoxon rank sum test looks at the average rank within group 1, the median test instead looks at how many of the ranks from group 1 are less than the median rank (which should equal $(N+1)/2$).
- The test statistic M_N for the median test is defined as

$$M_N = \sum_{i=1}^n I \left(R_i(\mathbf{Z}) \leq \frac{N+1}{2} \right)$$

because $(N+1)/2$ will be the median rank.

- This is a linear rank statistic with coefficients

$$c_{iN} = \begin{cases} 1 & \text{if } i \leq n \\ 0 & \text{if } i > n \end{cases}$$

and scores

$$a_N(i) = \begin{cases} 1 & \text{if } i \leq (N+1)/2 \\ 0 & \text{if } i > (N+1)/2 \end{cases}$$

- The median test could be used to test whether or not observations from group 1 tend to be smaller than those from group 2.

3.5.4 Choosing the scores $a_N(i)$

- The rank tests we have discussed so far are nonparametric in the sense that their null distribution does not depend on any particular parametric assumptions about the distributions from which the observations arise.
- For power calculations, we often think of some parameter or “effect size” modifying the base distribution in some way.
- For example, we often think of the shift alternative $F_X(t) = F_Y(t - \theta)$ in the two-sample problem.

- In parametric statistics, when testing $H_0 : \theta = 0$ the most powerful test of $H_0 : \theta = \theta_0$ vs. $H_A : \theta = \theta_A$ is based on rejecting H_0 whenever the likelihood ratio is large enough:

$$\text{Reject } H_0 \text{ if: } \frac{p_{\theta_A}(\mathbf{z})}{p_{\theta_0}(\mathbf{z})} \geq c_{\alpha,n} \quad (3.55)$$

This is the Neyman-Pearson Lemma.

- The same property is true if we are considering tests based on ranks. The most powerful test for testing $H_0 : \theta = \theta_0$ vs. $H_A : \theta = \theta_A$ is based on

$$\text{Reject } H_0 \text{ if: } \frac{P_{\theta_A}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z}))}{P_{\theta_0}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z}))} \geq c_{\alpha,n} \quad (3.56)$$

- The main difference between (3.55) and (3.56) is that the distribution $P_{\theta_A}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z}))$ is unknown unless we are willing to make certain distributional assumptions.

- Nevertheless, we can approximate this probability if θ_A is a location parameter “close” to θ_0

$$P_{\theta_A}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z})) \approx P_{\theta_0}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z})) + \frac{\theta_A}{N!} \sum_{i=1}^N c_{iN} E \left\{ \frac{\partial \log f(Z_{(i)})}{\partial Z} \right\}$$

where $Z_{(i)}$ denotes the i^{th} order statistic. See, for example, Chapter 13 of Van der Vaart (2000) for more details on the derivation of this approximation.

- So, large values of the linear rank statistic $T_N = \sum_{i=1}^N c_{iN} a_N(i)$ will approximately correspond to large values of $P_{\theta_A}(R_1(\mathbf{Z}), \dots, R_N(\mathbf{Z}))$ if we choose the scores to be

$$a_N(i) = E \left\{ \frac{\partial \log f(Z_{(i)})}{\partial Z} \right\}$$

- Linear rank statistics with scores generated this way are usually called **locally most powerful** rank tests.

- The best choice of the scores will depend on what we assume about the density f .
- For example, if we assume that $f(z)$ is Normal(0, 1), then

$$\frac{\partial \log f(z)}{\partial z} = -z$$

- The approximate expectation of the order statistics from a Normal(0, 1) distribution are

$$E\{Z_{(i)}\} \approx \Phi^{-1} \left(\frac{i}{N+1} \right)$$

This implies that the van der Waerden’s scores are approximately optimal if we assume the distribution of the Z_i is Normal.

- This can also be worked out for other choices of $f(z)$.
- If $f(z)$ is a Logistic distribution, the optimal scores correspond to the Wilcoxon rank sum test statistic.
- If $f(z)$ is Laplace (meaning that $f(z) = \frac{1}{2}e^{-|z|}$), then the optimal scores correspond to the median test.

3.6 Additional Reading

- Additional reading which covers the material discussed in this chapter includes:
 - Chapters 3-4 from Hollander et al. (2013)

Chapter 4

Rank Tests for Multiple Groups

- We can roughly think of the tests discussed in Chapter 3 as being related to the well-known parametric tests shown in the table below.

Parametric Test	Nonparametric Tests
One-Sample t-test	Wilcoxon Signed Rank/Sign Test
Two-Sample t-test	Wilcoxon Rank Sum/Normal Scores/Median Test

- The **Kruskal-Wallis** test can be thought of as the nonparametric analogue of one-way analysis of variance (ANOVA).
- For $K \geq 3$ groups, one-way ANOVA considers the analysis of observations arising from the following model

$$Y_{kj} = \mu_k + \varepsilon_{kj}, \quad j = 1, \dots, n_k; k = 1, \dots, K \quad (4.1)$$

where it is often assumed that $\varepsilon_{kj} \sim \text{Normal}(0, \sigma^2)$.

- Usually, the one-way ANOVA hypothesis of interest is something like

$$H_0 : \mu_1 = \mu_2 = \dots = \mu_K \quad (4.2)$$

which is often referred to as the homogeneity hypothesis.

- A test of the hypothesis (4.2) is based on decomposing the observed vari-

ation in the responses Y_{kj} :

$$\begin{aligned} \underbrace{\sum_{k=1}^K \sum_{j=1}^{n_k} (Y_{kj} - \bar{Y}_{..})^2}_{SST} &= \sum_{k=1}^K \sum_{j=1}^{n_k} (\bar{Y}_{k.} - \bar{Y}_{..})^2 + \sum_{k=1}^K \sum_{j=1}^{n_k} (Y_{kj} - \bar{Y}_{k.})^2 \\ &= \underbrace{\sum_{k=1}^K n_k (\bar{Y}_{k.} - \bar{Y}_{..})^2}_{SSA} + \underbrace{\sum_{k=1}^K \sum_{j=1}^{n_k} (Y_{kj} - \bar{Y}_{k.})^2}_{SSE} \end{aligned} \quad (4.3)$$

where $\bar{Y}_{k.} = \frac{1}{n_k} \sum_{j=1}^{n_k} Y_{kj}$ and $\bar{Y}_{..} = \frac{1}{K} \sum_{k=1}^K \bar{Y}_{k.}$.

- Large values of $SSA = \sum_{k=1}^K n_k (\bar{Y}_{k.} - \bar{Y}_{..})^2$ provide evidence against the null hypothesis (4.2). The alternative hypothesis here is that there is at least one pair of means μ_h, μ_l such that $\mu_h \neq \mu_l$.

4.1 The Kruskal-Wallis Test

4.1.1 Definition

- Instead of assuming (4.1) for the responses Y_{kj} , a nonparametric way of thinking about this problem is to instead only assume that

$$Y_{kj} \sim F_k \quad (4.4)$$

That is, $Y_{k1}, Y_{k2}, \dots, Y_{kn_k}$ is an i.i.d. sample from F_k for each k .

- A nonparametric version of the one-way ANOVA homogeneity hypothesis is

$$H_0 : F_1 = F_2 = \dots = F_K \quad (4.5)$$

- The “shift alternative” in this case can be stated as

$$H_A : F_k(t) = F(t - \Delta_k), \quad \text{for } k = 1, \dots, K \quad \text{and not all } \Delta_k \text{ equal} \quad (4.6)$$

- The **Kruskal-Wallis test statistic** KW_N is similar to the SSA term (defined in (4.3)) in the one-way ANOVA setting.
- Rather than comparing the group-specific means $\bar{Y}_{k.}$ with the overall mean $\bar{Y}_{..}$, the Kruskal-Wallis test statistic compares the group-specific rank means $\bar{R}_{k.}$ with their overall expectation under the null hypothesis.

- The Kruskal-Wallis test statistic is defined as

$$KW_N = \frac{12}{N(N-1)} \sum_{k=1}^K n_k \left(\bar{R}_{k.} - \frac{N+1}{2} \right)^2, \quad \text{where } N = \sum_{k=1}^K n_k \quad (4.7)$$

- In (4.7), $\bar{R}_{k.}$ is the average rank of those in the k^{th} group

$$\bar{R}_{k.} = \frac{1}{n_k} \sum_{j=1}^{n_k} R_{kj}(\mathbf{Z}), \quad (4.8)$$

where \mathbf{Z} denotes the pooled-data vector and $R_{kj}(\mathbf{Z})$ denotes the rank of Y_{kj} in the “pooled-data ranking”.

- What is the expectation of $\bar{R}_{k.}$ under the null hypothesis (4.5)?
- Again, if the null hypothesis is true, we can treat all of our responses Y_{kj} as just an i.i.d. sample of size N from a common distribution function F .
- Hence, as we showed in (3.5) from Chapter 3, $E\{R_{kj}(\mathbf{Z})\} = (N+1)/2$ under the assumption that the data are an i.i.d. sample from a common distribution function.
- So, the intuition behind the definition of KW_N is that the differences $\bar{R}_{k.} - \frac{N+1}{2}$ should be small whenever the homogeneity hypothesis (4.5) is true.

- When $K = 2$, the following relationship between the Kruskal-Wallis statistic KW_N and the Wilcoxon rank sum test statistic W from Chapter 3 holds.

$$KW_N = \frac{12}{mn(N+1)} \left(W - \frac{n(N+1)}{2} \right)^2. \quad (4.9)$$

- Hence, the p-value from a Kruskal-Wallis test and a (two-sided) WRS test should be the same when $K = 2$.
- However, you cannot directly perform a one-sided test using the Kruskal-Wallis test.

- **Exercise 4.1** If $K = 2$, show that equation (4.9) holds.

Group	Y	Rank
Group 1	1.00	8
Group 1	-1.20	2
Group 1	-1.50	1
Group 2	0.00	5
Group 2	-0.10	4
Group 2	1.10	9
Group 3	0.90	7
Group 3	-0.40	3
Group 3	0.60	6

An Example

- Consider the data shown in the table. In this case, $N = 9$, $\bar{R}_{1.} = 11/3$, $\bar{R}_{2.} = 6$, and $\bar{R}_{3.} = 16/3$. The Kruskal-Wallis statistic is

$$KW_N = \frac{1}{2} \left\{ 3(11/3 - 5)^2 + 3(6 - 5)^2 + 3(16/3 - 5)^2 \right\} = 13/9$$

4.1.2 Asymptotic Distribution and Connection to One-Way ANOVA

- The Kruskal-Wallis statistic KW_N has an asymptotic chi-square distribution with $K - 1$ degrees of freedom under the null hypothesis (4.5).
- This follows from the fact that $(\bar{R}_{k.} - (N+1)/2)$ is approximately normally distributed for large n_k .
- R** uses the large-sample approximation when computing the p-value for the Kruskal-Wallis test.

-
- The Kruskal-Wallis test can also be thought of as the test you would obtain if you applied the one-way ANOVA setup to the ranks of Y_{kj} .
 - The one-way ANOVA test is based on the value of SSA where, as in (4.3), SSA is defined as

$$SSA = \sum_{k=1}^K n_k (\bar{Y}_{k.} - \bar{Y}_{..})^2$$

- You then reject H_0 , when $SSA/SSE = SSA/(SST - SSA)$ is sufficiently large.

- Notice that if we computed SSA using the ranks $R_{kj}(\mathbf{Z})$ rather than the observations Y_{kj} , we would get:

$$\begin{aligned}
 SSA_r &= \sum_{k=1}^K n_k (\bar{R}_{k.} - \bar{R}_{..})^2 \\
 &= \sum_{k=1}^K n_k (\bar{R}_{k.} - \frac{N+1}{2})^2 \\
 &= \frac{N(N-1)}{12} KW_N
 \end{aligned} \tag{4.10}$$

- If you were applying ANOVA to the ranks of Y_{kj} , SST_r would be the following fixed constant:

$$SST_r = \frac{N(N+1)(N-1)}{12}$$

- So, any test of the homogeneity hypothesis would be based on just the value of SSA_r which, as we showed in (4.10), is just a constant times the Kruskal-Wallis statistic.

4.2 Performing the Kruskal-Wallis Test in R

- We will look at performing Kruskal-Wallis tests in **R** by using the “InsectSprays” dataset.

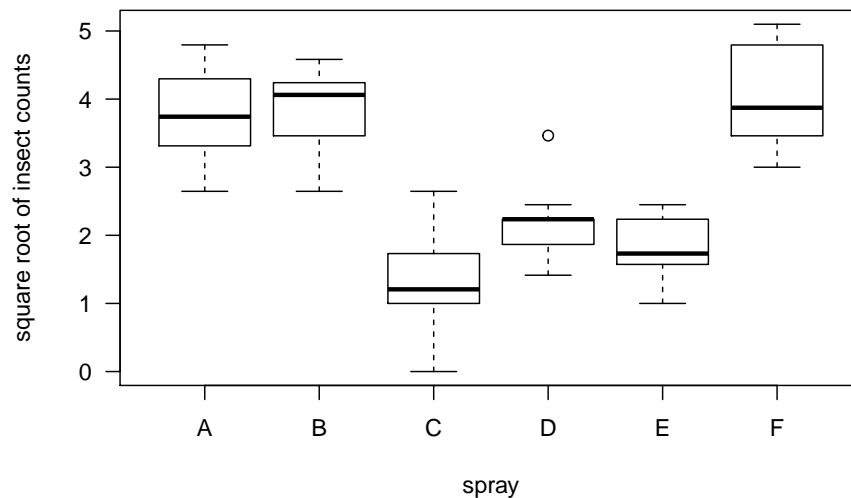
```
head(InsectSprays)
```

```
##    count spray
## 1     10    A
## 2      7    A
## 3     20    A
## 4     14    A
## 5     14    A
## 6     12    A
```

- This dataset has 72 observations.
- The variable **count** is the number of insects measured in some agricultural unit.
- The variable **spray** was the type of spray used on that unit.

- You could certainly argue that a standard ANOVA is not appropriate in this situation because the responses are counts, and for count data, the variance is usually a function of the mean.
- A generalized linear model with a log link function might be more appropriate.
- Applying a square-root transformation to count data is also a commonly suggested approach. (The square-root transformation is the “variance-stabilizing transformation” for Poisson-distributed data).

```
boxplot(sqrt(count) ~ spray, data=InsectSprays, las=1,
        ylab="square root of insect counts")
```



-
- Let us perform a test of homogeneity using both the one-way ANOVA approach and a Kruskal-Wallis test

```
anova(lm(sqrt(count) ~ spray, data=InsectSprays))
```

```
## Analysis of Variance Table
##
```



```
## Response: sqrt(count)
##           Df Sum Sq Mean Sq F value    Pr(>F)
## spray      5 88.438 17.6876  44.799 < 2.2e-16 ***
## Residuals 66 26.058  0.3948
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
a <- kruskal.test(sqrt(count) ~ spray, data=InsectSprays)
a$p.value
```

```
## [1] 1.510844e-10
```

- Notice that applying the square root transformation does not affect the value of the Kruskal-Wallis statistic or the Kruskal-Wallis p-value.

```
kruskal.test(count ~ spray, data=InsectSprays)
```

```
##
## Kruskal-Wallis rank sum test
##
## data:  count by spray
## Kruskal-Wallis chi-squared = 54.691, df = 5, p-value = 1.511e-10
```

- This invariance to data transformation is not true for the standard one-way ANOVA.

```
anova(lm(count ~ spray, data=InsectSprays))
```

```
## Analysis of Variance Table
##
## Response: count
##           Df Sum Sq Mean Sq F value    Pr(>F)
## spray      5 2668.8  533.77  34.702 < 2.2e-16 ***
## Residuals 66 1015.2   15.38
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

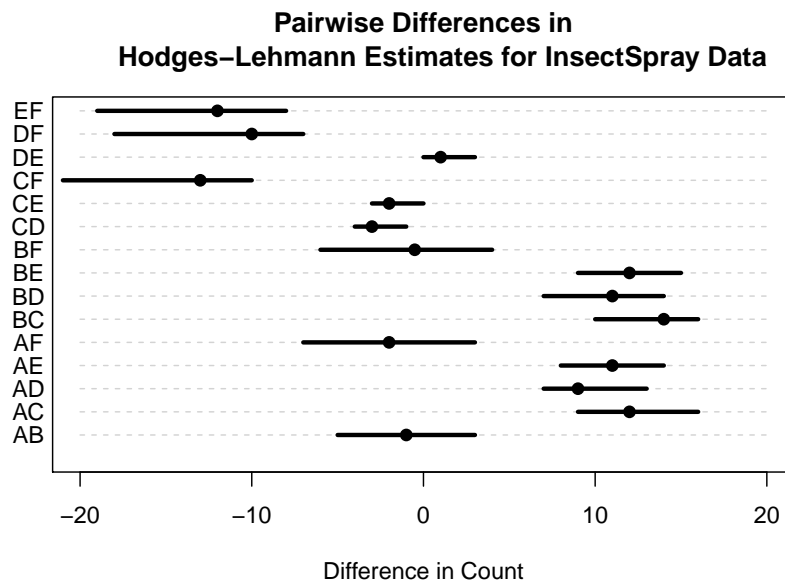
4.3 Comparison of Specific Groups

- A Kruskal-Wallis test performs a test of the overall homogeneity hypothesis

$$H_0 : F_1 = F_2 = \dots = F_K \quad (4.11)$$

- However, a rejection of the homogeneity hypothesis does not indicate which group differences are primarily the source of this rejection nor does it provide any measure of the “magnitude” of the differences between each of the groups.
- Dunn’s test is the suggested way to compute pairwise tests of stochastic dominance.
- Performing a series of pairwise Wilcoxon rank sum test can lead to violations of transitivity. For example, group A is “better” than B which is better than C, but group C is better than A.
- In **R**, Dunn’s test can be performed using the **dunn.test** package.

- In traditional one-way ANOVA one often reports pairwise differences in the means and their associated confidence intervals.
- In the context of a Kruskal-Wallis test, one could report pairwise differences in the Hodges-Lehmann estimate though other comparisons may also be of interest.
- One nice approach is to use the proportional odds model interpretation of the Kruskal-Wallis test and then report the difference in the estimated proportional odds coefficients. See Section 7.6 of <http://hbiostat.org/doc/bbr.pdf> for more details on the proportional odds model.



4.4 An Additional Example

- We will use the “cane” dataset from the **boot** package.

```
library(boot)
data(cane)
head(cane)
```

```
##      n  r  x var block
## 1  87 76 19   1     A
## 2 119  8 14   2     A
## 3  94 74  9   3     A
## 4  95 11 12   4     A
## 5 134  0 12   5     A
## 6  92  0  3   6     A
```

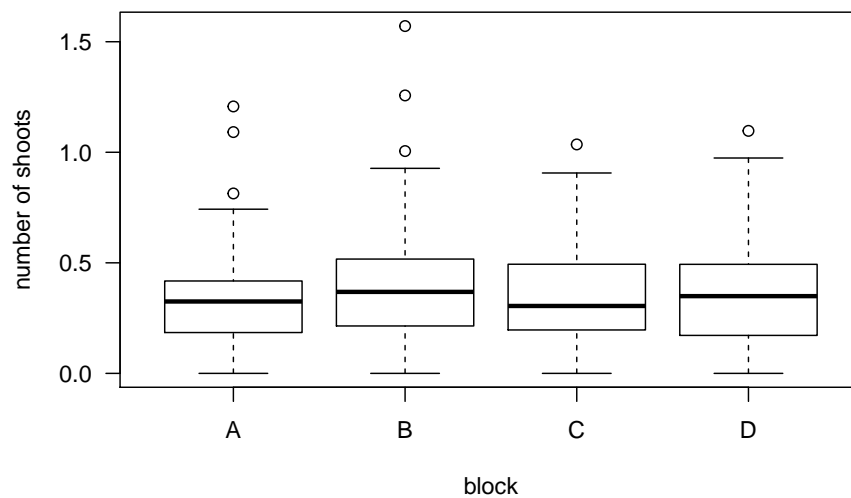
- These data come from a study trying to determine the susceptibility of different types of sugar cane to a particular type of disease.
- The variable **n** contains the total number of shoots in each plot.
- The variable **r** contains the total number of diseased shoots.

- We can create a new variable **prop** that measures the proportion of shoots that are diseased.

```
cane$prop <- cane$r/cane$n
```

- You could certainly argue that a logistic regression model is a better approach here, but we will analyze the transformed proportions using the arcsine square root transformation.

```
cane$prop.trans <- asin(sqrt(cane$prop))
boxplot(prop.trans ~ block, data=cane, las=1, ylab="number of shoots")
```



```
kruskal.test(prop ~ block, data=cane)
```

```
##
## Kruskal-Wallis rank sum test
##
## data: prop by block
## Kruskal-Wallis chi-squared = 1.1355, df = 3, p-value = 0.7685
```

4.5 Additional Reading

- Additional reading which covers the material discussed in this chapter includes:
 - Chapters 6 from Hollander et al. (2013)

Chapter 5

Permutation Tests

- Permutation tests are a useful tool that allows you to avoid depending on specific parametric assumptions.
- Permutation tests are also useful in more complex modern applications where it can be difficult to work out the theoretical null distribution of the desired test statistic.

5.1 Notation

- A **permutation** π of a set S is a function $\pi : S \rightarrow S$ is a function that is both one-to-one and onto.
- We will usually think of S as the set of observation indices in which case $S = \{1, \dots, N\}$ for sample size N .
- Each permutation π of $S = \{1, \dots, N\}$ defines a particular ordering of the elements of S . For this reason, a permutation is often expressed as the following ordered list

$$\pi = (\pi(1), \pi(2), \dots, \pi(N))$$

- In other words, we can think of a permutation of S as a particular ordering of the elements of S .
- For example, if $S = \{1, 2, 3\}$, and π_1 is a permutation of S defined as $\pi_1(1) = 3$, $\pi_1(2) = 1$, $\pi_1(3) = 2$, then this permutation expressed as an ordered list would be

$$\pi_1 = (3, 1, 2)$$

- There are 5 other possible permutations of S :

$$\pi_2 = (1, 2, 3)$$

$$\pi_3 = (2, 1, 3)$$

$$\pi_4 = (1, 3, 2)$$

$$\pi_5 = (3, 2, 1)$$

$$\pi_6 = (2, 3, 1)$$

- If S has N distinct elements, there are $N!$ possible permutations of S .
- We will let \mathcal{S}_N denote the set of all permutations of the set $\{1, \dots, N\}$.

5.2 Permutation Tests for the Two-Sample Problem

- Permutation tests for two-sample problems are motivated by the following reasoning:
 - If there is no real difference between the two groups, there is nothing “special” about the difference in means between the two groups.
 - The observed difference in the mean between the two groups should not be notably different than mean differences from randomly formed groups.
 - Forming “random” groups can be done by using many permutations of the original data.

5.2.1 Example 1

- Suppose we have observations from two groups $X_1, \dots, X_n \sim F_X$ and $Y_1, \dots, Y_m \sim F_Y$.
- Let $\mathbf{Z} = (Z_1, \dots, Z_N)$ denote the pooled data

$$(Z_1, \dots, Z_N) = (X_1, \dots, X_n, Y_1, \dots, Y_m) \quad (5.1)$$

- For a permutation π of $\{1, \dots, N\}$, we will let \mathbf{Z}_π denote the corresponding permuted dataset

$$\mathbf{Z}_\pi = (Z_{\pi(1)}, Z_{\pi(2)}, \dots, Z_{\pi(N)}) \quad (5.2)$$

- For example, the columns in Table 5.1 are just permutations of the original data \mathbf{Z} .

	OriginalData	Perm1	Perm2	Perm3	Perm4	Perm5
z1	0.60	-0.60	0.60	-0.90	0.70	0.60
z2	-0.80	-1.40	-0.60	0.70	-0.40	-0.60
z3	-0.60	0.70	0.20	0.60	-1.40	-0.80
z4	-0.90	0.20	-0.40	0.20	0.20	0.30
z5	0.30	-0.40	-1.30	-0.40	-0.90	-0.40
z6	-1.30	-1.30	-1.40	-0.60	-0.80	0.70
z7	0.20	0.30	0.70	-1.40	0.30	-0.90
z8	0.70	0.60	0.30	-1.30	0.60	0.20
z9	-1.40	-0.90	-0.80	0.30	-0.60	-1.40
z10	-0.40	-0.80	-0.90	-0.80	-1.30	-1.30
mean difference	0.16	0.12	0.12	0.80	0.00	0.36

Table 5.1: Example of Permuting a Vector of Responses. This example assumes $n=m=5$.

- Suppose we want to base a test on the difference in the means between the two groups

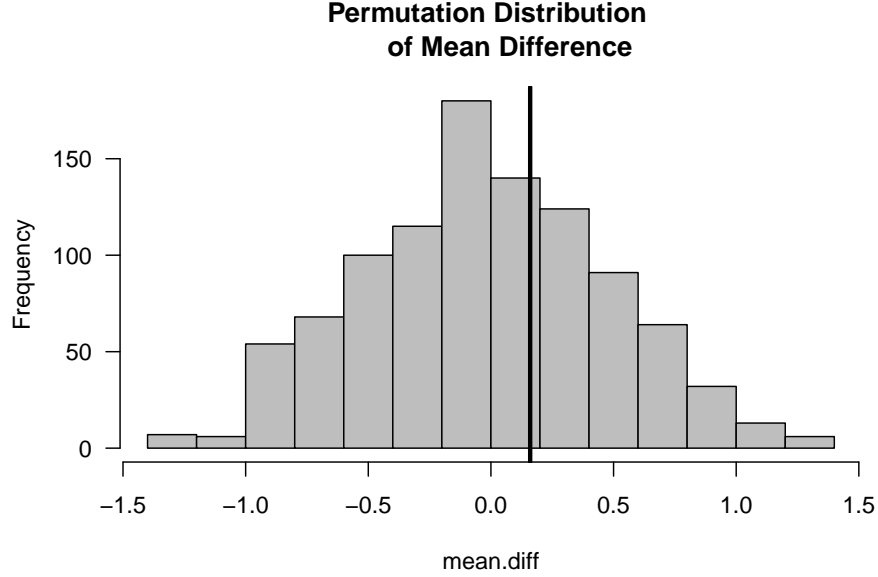
$$T_N(\mathbf{Z}) = \bar{X} - \bar{Y} = \frac{1}{n} \sum_{i=1}^n Z_i - \frac{1}{m} \sum_{i=n+1}^N Z_i \quad (5.3)$$

- We will let t_{obs} denote the observed value of the mean difference. That is, $t_{obs} = T_N(\mathbf{Z}_{obs})$, where \mathbf{Z}_{obs} is the vector of the observed data.
- Under the null hypothesis that $F_X = F_Y$, the observed mean difference should not be “abnormal” when compared with the mean differences from many other permutations of the data.

```

z <- c(0.6, -0.8, -0.6, -0.9, 0.3, -1.3, 0.2, 0.7, -1.4, -0.4) ## data
observed.diff <- mean(z[1:5]) - mean(z[6:10]) ## observed mean difference
nperms <- 1000
mean.diff <- rep(NA, nperms)
for(k in 1:nperms) {
  ss <- sample(1:10, size=10) ## draw a random permutation
  z.perm <- z[ss] ## form the permuted dataset
  mean.diff[k] <- mean(z.perm[1:5]) - mean(z.perm[6:10]) ## compute mean difference
                                                         ## for permuted dataset
}
hist(mean.diff, las=1, col="grey", main="Permutation Distribution
of Mean Difference")
abline(v=observed.diff, lwd=3)

```



5.2.2 Permutation Test p-values

- The one-sided p-value for the permutation test is

$$\begin{aligned} \text{p-value} &= \frac{\text{number of permutations such that } T_N \geq t_{obs}}{N!} \\ &= \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} I(T_N(\mathbf{Z}_\pi) \geq t_{obs}) \end{aligned}$$

- The two-sided p-value for the two-sample problem would be

$$\text{p-value} = \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} I(|T_N(\mathbf{Z}_\pi)| \geq |t_{obs}|)$$

- As we did when producing the above histogram, the permutation-test p-value is often computed by using a large number of random permutations rather than computing the test statistic for every possible permutation.
- The Monte Carlo permutation-test p-value is defined as

$$\text{p-value}_{mc} = \frac{1}{S+1} \left[1 + \sum_{s=1}^S I(T_N(\mathbf{Z}_{\pi_s}) \geq t_{obs}) \right] \quad (5.4)$$

where π_1, \dots, π_S are randomly drawn permutations

- The two-sided (Monte Carlo) p-value for the example shown in Table 5.1 is

```
pval.mc <- (1 + sum(abs(mean.diff) >= abs(observed.diff)))/(nperms + 1)
round(pval.mc, 2)
```

```
## [1] 0.76
```

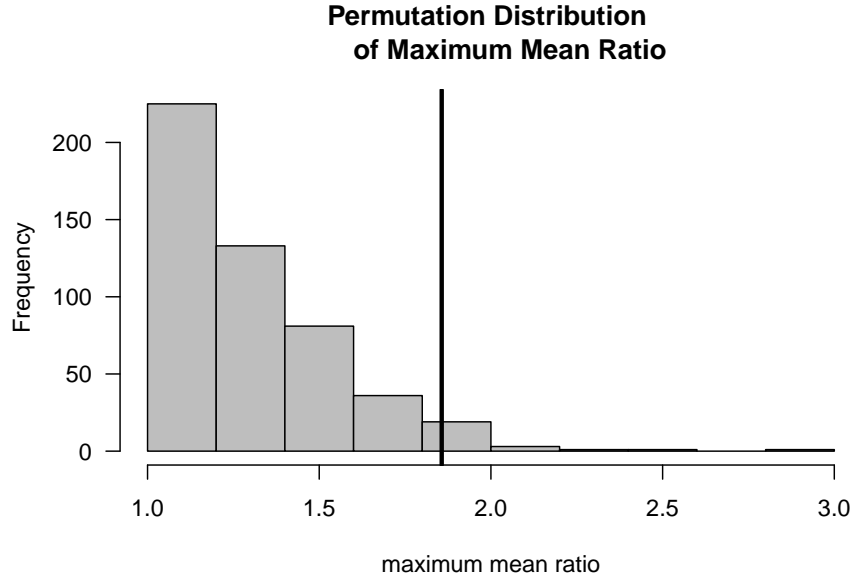
5.2.3 Example 2: Ratios of Means

- With permutation tests, you are not limited to difference in means. You can choose the statistic $T_N(\mathbf{Z})$ to measure other contrasts of interest.
- For example, with nonnegative data you might be interested in the ratio of means between the two groups

$$T_N(\mathbf{Z}) = \max \left\{ \bar{X}/\bar{Y}, \bar{Y}/\bar{X} \right\} \quad (5.5)$$

- Let us see how this works for a simulated example with $n = m = 20$ where we assume that $X_1, \dots, X_n \sim \text{Exponential}(1)$ and $Y_1, \dots, Y_m \sim \text{Exponential}(1/2)$.

```
set.seed(5127)
xx <- rexp(20, rate=1)
yy <- rexp(20, rate=0.5)
zz <- c(xx, yy) ## this is the original data
t.obs <- max(mean(zz[1:20])/mean(zz[21:40]), mean(zz[21:40])/mean(zz[1:20]))
nperms <- 500
mean.ratio <- rep(0, nperms)
for(k in 1:nperms) {
  ss <- sample(1:40, size=40)
  zz.perm <- zz[ss]
  mean.ratio[k] <- max(mean(zz.perm[1:20])/mean(zz.perm[21:40]),
                      mean(zz.perm[21:40])/mean(zz.perm[1:20]))
}
hist(mean.ratio, las=1, col="grey", main="Permutation Distribution
of Maximum Mean Ratio", xlab="maximum mean ratio")
abline(v=t.obs, lwd=3)
```



- The two-side (Monte Carlo) permutation test p-value is:

```
pval.mc <- (1 + sum(mean.ratio >= t.obs))/(nperms + 1)
round(pval.mc, 2)
```

```
## [1] 0.04
```

5.2.4 Example 3: Differences in Quantiles

- Permutation tests are especially useful in problems where working out the null distribution is difficult, or when certain approximations of the null distributions are hard to justify.
- An example of this occurs if you want to compare medians, or more generally, compare quantiles between two groups.
- The difference-in-quantiles statistic would be defined as

$$T_N(\mathbf{Z}) = Q_p(Z_1, \dots, Z_n) - Q_p(Z_{n+1}, \dots, Z_N)$$

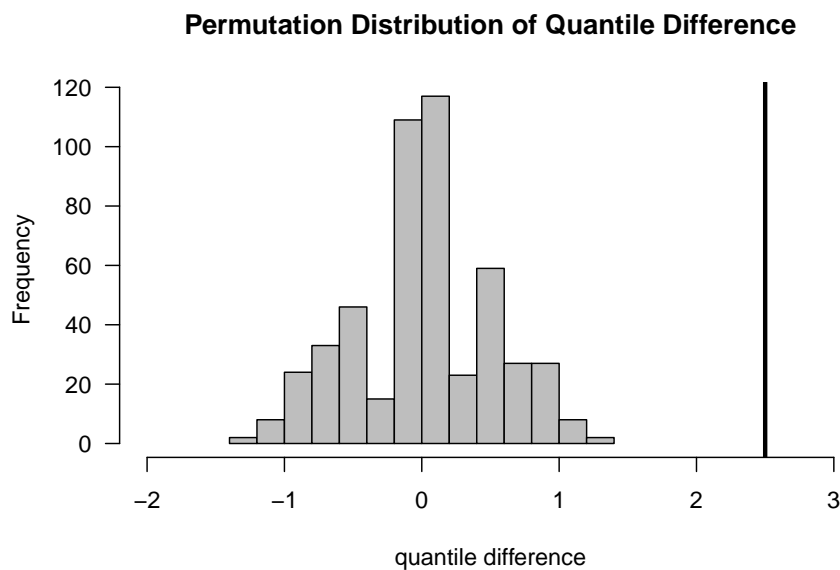
where $Q_p(X_1, \dots, X_H)$ denotes the p^{th} quantile from the data X_1, \dots, X_H .

- The difference in quantiles could be computed with the following **R** code:

```
z <- rnorm(10)
quantile(z[1:5], probs=.3) - quantile(z[6:10], probs=.3)
```

```
##          30%
## 0.2671133
```

- Note that setting **probs=.5** in the **quantile** function will return the median.



- **Exercise 5.1** Suppose we have the following data from two groups $(X_1, X_2, X_3) = (-1, 0, 1)$ and $(Y_1, Y_2, Y_3) = (4, -2, 2)$. Compute the (two-sided) permutation p-value for the following two statistics:

- $T_N(\mathbf{Z}) = \text{median}(X_1, X_2, X_3) - \text{median}(Y_1, Y_2, Y_3)$.
- $T_N(\mathbf{Z}) = \bar{X} - \bar{Y}$.

- **Exercise 5.2.** Suppose we have data from two groups such that $X_1, \dots, X_n \sim \text{Normal}(0, 1)$ and $Y_1, \dots, Y_m \sim \text{Normal}(1, 1)$. Using $n = m = 50$ and 500 simulation replications, compute 500 significance thresholds from the one-sided permutation test which uses the statistic $T_N(\mathbf{Z}) = \bar{X} - \bar{Y}$. How does this compare with the t-statistic threshold of approximately $1.64 * \sqrt{2/50}$?

- **Exercise 5.3.** Suppose we have data from two groups such that $X_1, \dots, X_n \sim \text{Normal}(0, 1)$ and $Y_1, \dots, Y_m \sim \text{Normal}(1, 1)$. Using $n = m = 50$ and 500 simulation replications, compute the power of the permutation test which uses the statistic $T_N(\mathbf{Z}) = \bar{X} - \bar{Y}$ to detect this true alternative. How, does the power compare with the (two-sided) two-sample t-statistic and the (two-sided) Wilcoxon rank sum test?

5.3 The Permutation Test as a Conditional Test

- A permutation test is an example of a **conditional test**.
- Typically, the p-value is defined as

$$\text{p-value} = P(T \geq t_{obs} | H_0) \quad (5.6)$$

for some test statistic T .

- In other words, the p-value is the probability that a random variable which follows the null distribution exceeds t_{obs} .
- In many problems however, the null hypothesis H_0 is not determined by a single parameter but contains many parameters.
- For example, the null hypothesis in a t-test is really $H_0 : \mu_x = \mu_y$ and $\sigma > 0$. That is, the null hypothesis is true for many different values of σ .

- When H_0 contains many parameter values, one approach for computing a p-value is to choose the test statistic T so that its distribution is the same for every point in H_0 .
- A more general approach is to instead compute a **conditional p-value**
- A conditional p-value is defined as

$$\text{p-value} = P(T \geq t_{obs} | S = s, H_0)$$

where S is a sufficient statistic for the unknown terms in H_0 .

- A classic example of this is Fisher's exact test.

- A permutation test computes a conditional p-value where the sufficient statistic is the vector of order statistics $(Z_{(1)}, Z_{(2)}, \dots, Z_{(N)})$.
- Recall that the order statistics are defined as

$$\begin{aligned} Z_{(1)} &= \text{smallest observation} \\ Z_{(2)} &= \text{second smallest observation} \\ &\vdots \\ Z_{(N)} &= \text{largest observation} \end{aligned}$$

- What is the conditional distribution of the observed data conditional on the observed order statistics?
- It is:

$$\begin{aligned} f_{Z_1, \dots, Z_N | Z_{(1)}, \dots, Z_{(N)}}(z_{\pi(1)}, \dots, z_{\pi(N)} | z_1, \dots, z_N) &= \frac{f_{Z_1, \dots, Z_N}(z_{\pi(1)}, \dots, z_{\pi(N)})}{f_{Z_{(1)}, \dots, Z_{(N)}}(z_1, \dots, z_N)} \\ &= \frac{f_{Z_i}(z_{\pi(1)}) \cdots f_{Z_i}(z_{\pi(N)})}{N! f_{Z_i}(z_1) \cdots f_{Z_i}(z_N)} \\ &= \frac{1}{N!} \end{aligned}$$

(See Chapter 5 of Casella and Berger (2002) for a detailed description of the distribution of order statistics)

- In other words, if we know the value of: $Z_{(1)} = z_1, \dots, Z_{(N)} = z_N$, then any event of the form $\{Z_1 = z_{\pi(1)}, \dots, Z_N = z_{\pi(N)}\}$ has an equal probability of occurring for any permutation chosen.
- This equal probability of $1/N!$ is only true under H_0 where we can regard the data as coming from a common distribution.

- If we are conditioning on $Z_{(1)} = z_1, \dots, Z_{(N)} = z_N$, then the probability that $T_N(Z_1, \dots, Z_N) \geq t$ is just the number of permutations of (z_1, \dots, z_N) where the test statistic is greater than t divided by $N!$.
- In other words

$$P\{T_N(Z_1, \dots, Z_N) \geq t | Z_{(1)} = z_1, \dots, Z_{(N)} = z_N\} \quad (5.7)$$

$$= \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} I(T_N(z_{\pi(1)}, \dots, z_{\pi(N)}) \geq t) \quad (5.8)$$

- Let us now consider a concrete example.
- Suppose we have a two-sample problem with four observations. The first two observations come from the first group while the last two observations come from the second group.
- The order statistics that we will condition on are:

$$Z_{(1)} = z_1 = -3 \quad (5.9)$$

$$Z_{(2)} = z_2 = -1 \quad (5.10)$$

$$Z_{(3)} = z_3 = 2 \quad (5.11)$$

$$Z_{(4)} = z_4 = 5 \quad (5.12)$$

- If T_4 is the mean difference

$$T_4(Z_1, Z_2, Z_3, Z_4) = \frac{Z_1 + Z_2 - Z_3 - Z_4}{2} \quad (5.13)$$

what is the probability

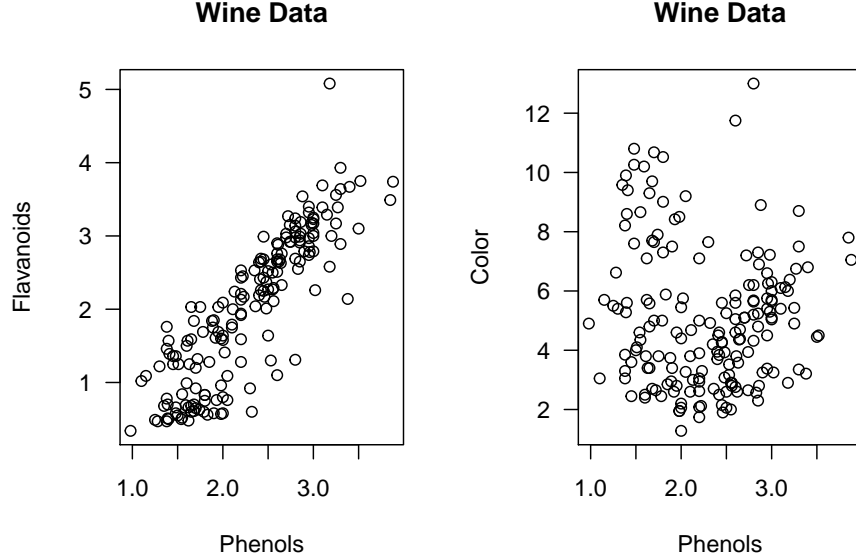
$$P\left\{T_4(Z_1, Z_2, Z_3, Z_4) \geq 2.5 \mid Z_{(1)} = z_1, Z_{(2)} = z_2, Z_{(3)} = z_3, Z_{(4)} = z_4\right\} \quad (5.14)$$

- From the below table, we see that the number of times $T_4 \geq 2.5$ occurs is 8. Hence,

$$\begin{aligned} & P\left\{T_4(Z_1, Z_2, Z_3, Z_4) \geq 2.5 \mid Z_{(1)} = z_1, Z_{(2)} = z_2, Z_{(3)} = z_3, Z_{(4)} = z_4\right\} \\ &= 8/24 = 1/3. \end{aligned}$$

a1	a2	a3	a4	P(Z1 = a1, Z2=a2, Z3=a3, Z4=a4 order stat)	T(a1, a2, a3, a4)	T(a1, a2, a3, a4) >= 2.5
-3	-1	2	5	1/24	-5.50	0
-3	-1	5	2	1/24	-5.50	0
-3	2	-1	5	1/24	-2.50	0
-3	2	5	-1	1/24	-2.50	0
-3	5	-1	2	1/24	0.50	0
-3	5	2	-1	1/24	0.50	0
-1	-3	2	5	1/24	-5.50	0
-1	-3	5	2	1/24	-5.50	0
-1	2	-3	5	1/24	-0.50	0
-1	2	5	-3	1/24	-0.50	0
-1	5	-3	2	1/24	2.50	1
-1	5	2	-3	1/24	2.50	1
2	-3	-1	5	1/24	-2.50	0
2	-3	5	-1	1/24	-2.50	0
2	-1	-3	5	1/24	-0.50	0
2	-1	5	-3	1/24	-0.50	0
2	5	-3	-1	1/24	5.50	1
2	5	-1	-3	1/24	5.50	1
5	-3	-1	2	1/24	0.50	0
5	-3	2	-1	1/24	0.50	0
5	-1	-3	2	1/24	2.50	1
5	-1	2	-3	1/24	2.50	1
5	2	-3	-1	1/24	5.50	1
5	2	-1	-3	1/24	5.50	1

5.4 A Permutation Test for Correlation



- Suppose we have N pairs of observations $(U_1, V_1), \dots, (U_N, V_N)$
- The correlation between these pairs is defined as

$$\rho_{UV} = \frac{\text{Cov}(U_i, V_i)}{\sigma_U \sigma_V} \quad (5.15)$$

- The test statistic of interest here is the sample correlation

$$T_N(\mathbf{U}, \mathbf{V}) = \frac{\sum_{i=1}^N (U_i - \bar{U})(V_i - \bar{V})}{\sqrt{\sum_{i=1}^N (U_i - \bar{U})^2 \sum_{i=1}^N (V_i - \bar{V})^2}} \quad (5.16)$$

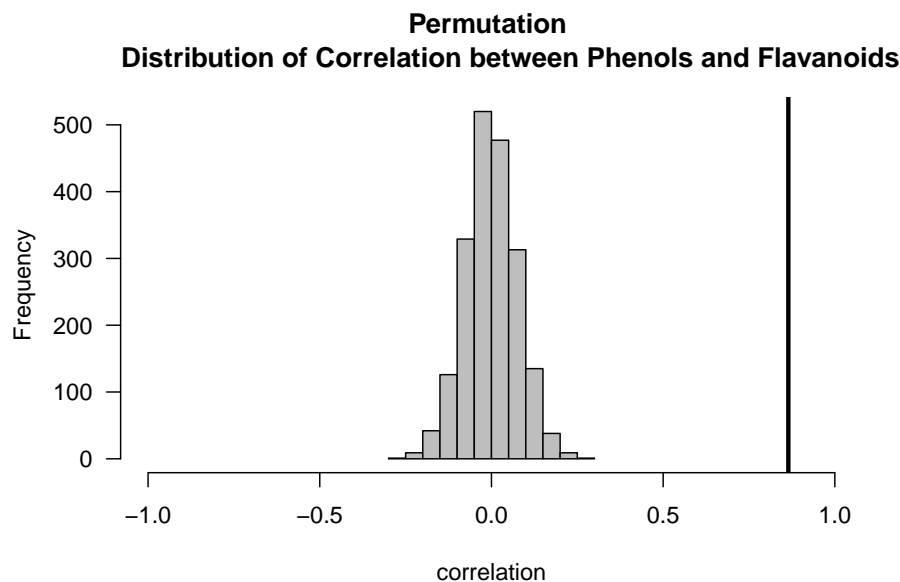
- To find the the permutation distribution, we only need to look at $T_N(\mathbf{U}_\pi, \mathbf{V})$ for different permutations π .
 - In other words, we are computing correlation among pairs of the form $(U_{\pi(1)}, V_1), \dots, (U_{\pi(N)}, V_N)$.
 - We only need to look at \mathbf{U}_π because this achieves the objective of randomly “switching observation pairs”.
-

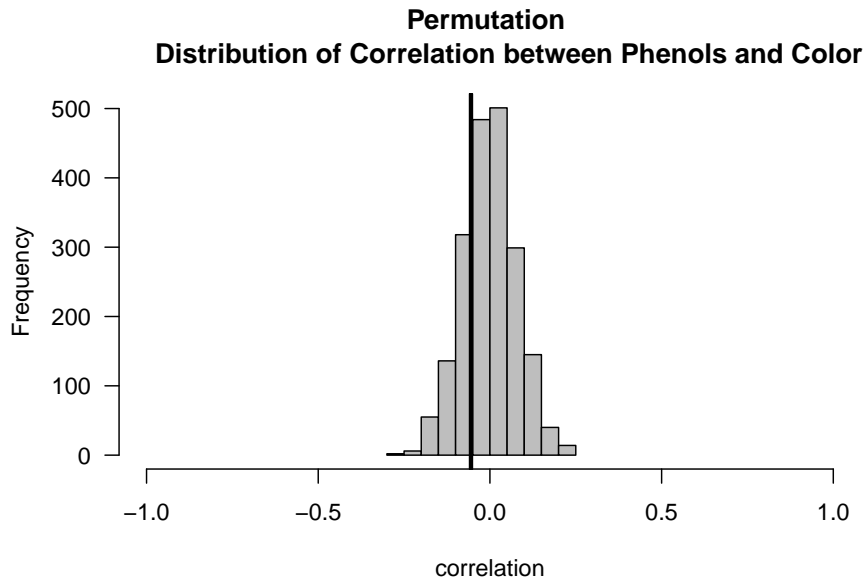
- The two-sided p-value for the permutation test of $H_0 : \rho_{UV} = 0$ vs. $H_A : \rho_{UV} \neq 0$ is

$$\text{p-value} = \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} I(|T_N(\mathbf{U}_\pi, \mathbf{V})| \geq |t_{obs}|)$$

```
library(rattle.data)
## Computing the permutation distribution for correlation
## between flavanoids and phenols

n.obs <- nrow(wine) ## number of observations
t.obs.pf <- cor(wine$Phenols, wine$Flavanoids) ## observed correlation
nperms <- 2000
cor.perm.pf <- rep(0, nperms)
for(k in 1:nperms) {
  ss <- sample(1:n.obs, size=n.obs)
  uu.perm <- wine$Phenols[ss]
  cor.perm.pf[k] <- cor(uu.perm, wine$Flavanoids)
}
hist(cor.perm.pf, xlim=c(-1, 1), las=1, col="grey", main="Permutation
Distribution of Correlation between Phenols and Flavanoids",
      xlab="correlation")
abline(v=t.obs.pf, lwd=3)
```





- Now let us compute the p-values for both the Phenols/Flavanoids and Phenols/Color association tests.

```
# p-value for correlation between Phenols/Flavanoids
pval.mc <- (1 + sum(abs(cor.perm.pf) >= abs(t.obs.pf)))/(nperms + 1)
round(pval.mc, 4)
```

```
## [1] 5e-04
```

```
# p-value for correlation between Phenols/Color
pval.mc <- (1 + sum(abs(cor.perm.pc) >= abs(t.obs.pc)))/(nperms + 1)
round(pval.mc, 4)
```

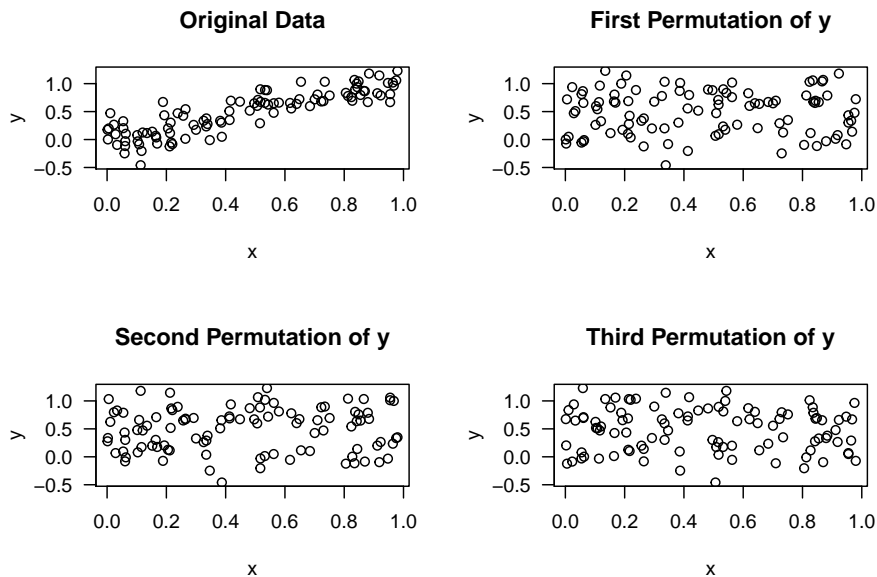
```
## [1] 0.4648
```

5.5 A Permutation Test for Variable Importance in Regression and Machine Learning

- The idea of permutation testing can also be applied in the context of regression.

5.5. A PERMUTATION TEST FOR VARIABLE IMPORTANCE IN REGRESSION AND MACHINE LEARNING

- In regression, we have a series of responses y_1, \dots, y_N , and we have a series of associated covariates vectors \mathbf{x}_i .
- For regression, we are going to perform permutations on the vector of responses $\mathbf{y} = (y_1, \dots, y_N)$ and compute some measure for each permutation.
- For example, we might compute some measure of variable importance for each permutation.
- The idea here is that when permuting \mathbf{y} , the association between \mathbf{y} and any “important covariates” should be lost.
- We want to see what the typical values of our variable importance measures will be when we break any association between \mathbf{y} and a covariate.



-
- The approach of permuting the response vector can be useful in the context of difficult-to-interpret variable importance measures or variable importance measures which are known to have certain biases.
 - This idea has been suggested as an alternative way of measuring variable importance for random forests (see e.g., Altmann et al. (2010) or Nembrini (2019))
 - With these approaches, we permute the response vector \mathbf{y} many times.

- A permutation p-value for the importance of a particular variable will be the proportion of permutations where that variable's importance score exceeded the importance score from the original data. (In this case, a smaller p-value would mean the variable was more important).
- Specifically, the permutation p-value for the importance of variable h would be given by

$$\text{p-value}_h = \frac{1}{N!} \sum_{\pi \in \mathcal{S}_N} I\left(s_h(\mathbf{y}_\pi, \mathbf{X}) \geq s_h(\mathbf{y}, \mathbf{X})\right) \quad (5.17)$$

where \mathbf{y} denotes the vector of responses and \mathbf{X} denotes the design matrix.

- Here, $s_h(\mathbf{y}, \mathbf{X})$ denotes the variable importance score for variable h when using response vector \mathbf{y} and design matrix \mathbf{X} .
- Note that the formula (5.17) could be applied in the context of any method that generates a variable importance score from \mathbf{y} and \mathbf{X} .

- Let us see an example of that if we look at a random forest model for predicting wine type from the **wine** data.
- First, we will load the data and fit a random forest model.

```
library(rattle.data)
library(randomForest)
```

```
## randomForest 4.6-14
```

```
## Type rfNews() to see new features/changes/bug fixes.
```

```
wine2 <- subset(wine, Type==1 | Type==2)
wine2$Type <- factor(wine2$Type)
X <- model.matrix(Type ~ . -1, data=wine2)
yy <- wine2$Type
n <- length(yy)
nvars <- ncol(X)

## Variable importance scores using original data
originalRF <- randomForest(X, y=yy)
var.imp <- originalRF$importance
var.imp
```

5.5. A PERMUTATION TEST FOR VARIABLE IMPORTANCE IN REGRESSION AND MACHINE LEARNING9

##	MeanDecreaseGini
## Alcohol	16.4477773
## Malic	1.6547628
## Ash	0.9512346
## Alcalinity	1.8280983
## Magnesium	4.2799222
## Phenols	2.4436762
## Flavanoids	6.2584880
## Nonflavanoids	0.5184224
## Proanthocyanins	0.6201685
## Color	10.0968269
## Hue	0.5552606
## Dilution	1.0398252
## Proline	17.3324599

- Now, let us compare these original variable importance scores with the importance scores obtained across 10,000 permuted datasets.

```
nperm <- 10000
VarImpMat <- matrix(0, nrow=nperm, ncol=ncol(X))
for(k in 1:nperm) {
  ytmp <- yy[sample(1:n,size=n)]
  rf.fit <- randomForest(X, y=ytmp)
  VarImpMat[k,] <- rf.fit$importance
  ## VarImpMat[k,h] contains the importance score of
  ## variable h in permutation k
}

perm.pval <- rep(0, nvars)
for(h in 1:nvars) {
  perm.pval[h] <- (1 + sum(VarImpMat[,h] >= var.imp[h]))/(nperm + 1)
}
```

	Permutation p-val
Alcohol	0.000
Malic	1.000
Ash	1.000
Alcalinity	1.000
Magnesium	0.923
Phenols	1.000
Flavanoids	0.080
Nonflavanoids	1.000
Proanthocyanins	1.000
Color	0.000
Hue	1.000
Dilution	1.000
Proline	0.000

Chapter 6

U-Statistics

6.1 Definition

- Suppose we have i.i.d. observations X_1, \dots, X_n .
- U-statistics are a family of statistics used to estimate quantities that can be written as

$$\theta = E\left\{h(X_1, \dots, X_r)\right\} \quad (6.1)$$

- The U-statistic U which estimates (6.1) is given by the following formula:

$$U = \frac{1}{\binom{n}{r}} \sum_{c \in \mathcal{C}_{n,r}} h(X_{c_1}, \dots, X_{c_r}) \quad (6.2)$$

- The function h is usually called the **kernel** of the U-statistic. We will assume the kernel is symmetric.
- The integer r is called the **order** of the U-statistic. Typically, $r = 1$, $r = 2$, or $r = 3$ at most.
- In (6.2), $\mathcal{C}_{n,r}$ denotes the set of all $\binom{n}{r}$ combinations of size r from the set $\{1, \dots, n\}$.
- For example, if $n = 3$ and $r = 2$ then

$$\mathcal{C}_{n,r} = \{(1, 2), (1, 3), (2, 3)\}$$

- For many common U-statistics $r = 2$ in which case (6.2) can be written as

$$U = \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=i+1}^n h(X_i, X_j) \quad (6.3)$$

6.2 Examples

- A wide range of well-known statistics can be represented as U-statistics.

6.2.1 Example 1: The Sample Mean

- The sample mean is actually an example of a U-statistic with $r = 1$.
- Choosing $h(x) = x$ means that the corresponding U-statistic is

$$U_m = \frac{1}{n} \sum_{i=1}^n X_i$$

- Taking the expectation of $h(X_1)$ gives the parameter that U_m is estimating

$$E\{h(X_1)\} = E\{X_1\} = \mu$$

6.2.2 Example 2: The Sample Variance

- The sample variance is actually another example of a U-statistic. In this case, $r = 2$.
- To show why this is the case, choose the kernel $h(x_1, x_2)$ to be

$$h(x_1, x_2) = \frac{1}{2}(x_1 - x_2)^2$$

- The expectation of this kernel is $\sigma^2 = E\{h(X_1, X_2)\}$ because

$$\begin{aligned} E\{h(X_1, X_2)\} &= \frac{1}{2} \left[E(X_1^2) - 2E(X_1)E(X_2) + E(X_2^2) \right] \\ &= \frac{1}{2} \left[\sigma^2 + \mu^2 - 2\mu^2 + \sigma^2 + \mu^2 \right] \\ &= \sigma^2 \end{aligned} \tag{6.4}$$

- Also, by using formula (6.2), this choice of kernel generates the sample

variance at its U-statistic:

$$\begin{aligned}
 U_{var} &= \frac{1}{\binom{n}{2}} \sum_{c \in \mathcal{C}_{n,2}} h(X_{c_1}, X_{c_2}) = \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=i+1}^n \frac{1}{2} (X_i - X_j)^2 \\
 &= \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=1}^n \frac{1}{4} (X_i - X_j)^2 \\
 &= \frac{1}{2n(n-1)} \sum_{i=1}^n \sum_{j=1}^n \{(X_i - \bar{X})^2 - 2(X_i - \bar{X})(X_j - \bar{X}) + (X_j - \bar{X})^2\} \\
 &= \frac{1}{2n(n-1)} \sum_{i=1}^n n(X_i - \bar{X})^2 + \frac{1}{2n(n-1)} \sum_{j=1}^n n(X_j - \bar{X})^2 \\
 &= \frac{1}{n-1} \sum_{i=1}^n (X_i - \bar{X})^2
 \end{aligned}$$

- Typically, the variance has the interpretation of $\sigma^2 = E\{(X_i - \mu)^2\}$. That is, σ^2 measures the expected squared deviation of X_i from its mean.
- Given the form of the U-statistic (6.4), we can also interpret the variance in the following way: if we select two observations X_i and X_j at random, the expected squared distance between X_i and X_j will be $2\sigma^2$.
- You can see this through the following computer experiment.

```

n <- 50000
xx <- rlogis(n, location=2, scale=0.75)
diff.sq <- rep(0, 5000)
for(k in 1:5000) {
  idx <- sample(1:n, size=2)
  diff.sq[k] <- (xx[idx[1]] - xx[idx[2]])^2
}
round(var(xx), 3)

```

```
## [1] 1.857
```

```
round(mean(diff.sq)/2, 3)
```

```
## [1] 1.83
```

6.2.3 Example 3: Gini's Mean Difference

- Gini's mean difference statistic is defined as

$$U_G = \frac{1}{\binom{n}{2}} \sum_{i=1}^n \sum_{j=i+1}^n |X_i - X_j|$$

- This is a U-statistic with $r = 2$ and kernel

$$h(X_1, X_2) = |X_1 - X_2|$$

- The parameter that we are estimating with Gini's mean difference statistic is:

$$\theta_G = E\{|X_1 - X_2|\}$$

- Gini's mean difference parameter θ_G can be interpreted in the following way: If we draw two observations at random from our population, θ_G represents the expected absolute difference between these two observations.
- The Gini coefficient θ_{Gc} is a popular measure of inequality. It is related to the mean difference parameter via

$$\theta_{Gc} = \frac{\theta_G}{2\mu},$$

where $\mu = E(X_i)$.

- **Exercise 6.1.** Compute the Gini coefficient θ_{Gc} when it is assumed that
 - $X_i \sim \text{Normal}(\mu, \sigma^2)$, for $\mu > 0$.
 - $X_i \sim \text{Exponential}(\lambda)$, (**Hint:** The difference between two independent Exponential random variables has a Laplace distribution).

6.2.4 Example 4: Wilcoxon Signed Rank Statistic

- The Wilcoxon signed rank test statistic is related to the following U statistic

$$U_{WS} = \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=i+1}^n I(X_i + X_j \geq 0)$$

- U_{WS} is a U-statistic of order 2 with kernel

$$h(x, y) = I(x + y \geq 0)$$

- Hence, U_{WS} can be interpreted as an estimate of the following parameter

$$\theta_{WS} = P(X_i + X_j \geq 0) = P(X_i \geq -X_j)$$

- If the distribution of X_i is symmetric around 0, θ_{WS} will be equal to 1/2.

- Recall that the Wilcoxon signed rank test is designed to detect distributions which are not symmetric around 0.
- The Wilcoxon signed rank statistic T_n that we defined in Chapter 3 had the following formula

$$T_n = \sum_{i=1}^n \text{sign}(X_i) R_i(|\mathbf{X}|)$$

- Additional algebra can show that

$$\begin{aligned} T_n &= n(n-1)U_{WS} + 2 \sum_{i=1}^n I(X_i > 0) - \frac{n(n+1)}{2} \\ &= n(n-1)U_{WS} + 2S_n - \frac{n(n+1)}{2} \end{aligned} \quad (6.5)$$

where S_n is the sign test statistic defined in Chapter 3.

- For large n , T_n is largely determined by $U_{WS} - 1/2$. Hence, a “large” value of $U_{WS} - 1/2$ will lead to rejection of the one-sample null hypothesis discussed in Section 3.3.

- If you want to derive (6.5) (though you don’t need to know how), I think it is helpful to note the following

$$\begin{aligned} I(X_{(i)} > 0) R_{(i)}(|\mathbf{X}|) &= \sum_{j=1}^n I(X_{(i)} > 0) I(|X_{(i)}| \geq |X_{(j)}|) = \sum_{j=1}^n I(X_{(i)} \geq |X_{(j)}|) \\ &= \sum_{j=1}^n I(X_{(i)} \geq |X_{(j)}|) = \sum_{j=1}^i I(X_{(i)} \geq -X_{(j)}) \\ &= \sum_{j=1}^i I(X_{(i)} + X_{(j)} \geq 0) \end{aligned}$$

6.3 Inference using U-statistics

- By using a large-sample approximation, you can construct a confidence interval for your U-statistic parameter of interest θ where

$$\theta = E\left\{h(X_1, \dots, X_r)\right\} \quad (6.6)$$

- While the U-statistic is a sum of random variables that are not necessarily independent, there is a type of Central Limit Theorem for U -statistics.
- Specifically, under appropriate regularity conditions:

$$\sqrt{n}(U - \theta) \longrightarrow \text{Normal}\left(0, r^2\varphi\right)$$

- The formula for φ is

$$\varphi = \text{Cov}\left(h(X_1, X_2, \dots, X_r), h(X_1, X'_2, \dots, X'_r)\right),$$

where X'_1, X'_2, \dots, X'_r are thought of as another i.i.d. sample from the same distribution as X_1, \dots, X_r .

6.4 U-statistics for Two-Sample Problems

- In two-sample problems, we have data from two groups which we label X_1, \dots, X_n and Y_1, \dots, Y_m
- A U-statistic with order (r, s) for a two-sample problem is

$$U = \frac{1}{\binom{n}{r}} \frac{1}{\binom{m}{s}} \sum_{c \in \mathcal{C}_{n,r}} \sum_{q \in \mathcal{C}_{m,s}} h(X_{c_1}, \dots, X_{c_r}, Y_{q_1}, \dots, Y_{q_s}) \quad (6.7)$$

6.4.1 The Mann-Whitney Statistic

- Consider the following U-statistic

$$U_{MW} = \frac{1}{mn} \sum_{i=1}^n \sum_{j=1}^m I(X_i \geq Y_j) \quad (6.8)$$

- This is a U-statistic of order $(1, 1)$ with kernel $h(x, y) = I(x \geq y)$.
- Hence, the U-statistic U_{MW} can be thought of as an estimate of the following parameter

$$\theta_{MW} = P(X_i \geq Y_j) \quad (6.9)$$

- If both X_i and Y_j have the same distribution, then θ_{MW} should equal $1/2$.

- The statistic mnU_{MW} is known as the **Mann-Whitney** statistic.
- The Mann-Whitney statistic has a close relation to the Wilcoxon rank sum statistic W that we defined in Section 3.2:

$$\begin{aligned}
 mnU_{MW} &= \sum_{i=1}^n \sum_{j=1}^m I(X_i \geq Y_j) \\
 &= \sum_{i=1}^n \left[\sum_{j=1}^m I(X_i \geq Y_j) + \sum_{k=1}^n I(X_i \geq X_k) \right] - \sum_{i=1}^n \sum_{k=1}^n I(X_i \geq X_k) \\
 &= \sum_{i=1}^n R_i(\mathbf{Z}) - \sum_{i=1}^n R_i(\mathbf{X}) \\
 &= W - \frac{n(n+1)}{2}
 \end{aligned} \tag{6.10}$$

- In other words, the Mann-Whitney statistic is equal to the WRS statistic minus a constant term.
- In (6.10), we are defining \mathbf{Z} as the pooled-data vector $\mathbf{Z} = (X_1, \dots, X_n, Y_1, \dots, Y_m)$.
- Also, the above derivation assumes no ties so that $\sum_{i=1}^n R_i(\mathbf{X}) = n(n+1)/2$.

- Because $W = n(n+1)/2 + mnU_{MW}$ is a linear function of U_{MW} , inference from the Wilcoxon rank sum test (when using large-sample p-values) should match inferences made from using U_{MW} to test the hypothesis $H_0 : \theta_{MW} = 1/2$.
- In other words, the two-sided Wilcoxon rank sum test can be thought of as a test of $H_0 : \theta_{MW} = 1/2$ vs. $H_A : \theta_{MW} \neq 1/2$, where θ_{MW} is the parameter defined in (6.9).

6.5 Measures of Association

- Many important measures of association are also examples of U-statistics.

- For measures of association, we have observations on n pairs of variables

$$(X_1, Y_1), \dots, (X_n, Y_n),$$

and our goal is to report some measure which quantifies the relationship between these two variables.

- In this context, we will think about U-statistics which have the form

$$U = \frac{1}{\binom{n}{r}} \sum_{c \in \mathcal{C}_{n,r}} h \left(\begin{bmatrix} X_{c_1} \\ Y_{c_1} \end{bmatrix}, \dots, \begin{bmatrix} X_{c_r} \\ Y_{c_r} \end{bmatrix} \right) \quad (6.11)$$

6.5.1 Spearman's Rank Correlation

- Spearman's sample rank correlation is defined as

$$\begin{aligned} \hat{\rho}_R &= \frac{\sum_{i=1}^n \{R_i(\mathbf{X}) - \bar{R}(\mathbf{X})\} \{R_i(\mathbf{Y}) - \bar{R}(\mathbf{Y})\}}{[\sum_{i=1}^n \{R_i(\mathbf{X}) - \bar{R}(\mathbf{X})\}^2 \sum_{i=1}^n \{R_i(\mathbf{Y}) - \bar{R}(\mathbf{Y})\}^2]^{1/2}} \\ &= \frac{12}{n(n-1)(n+1)} \sum_{i=1}^n R_i(\mathbf{X}) R_i(\mathbf{Y}) - \frac{3(n+1)}{n-1}, \end{aligned} \quad (6.12)$$

where $\bar{R}(X) = \frac{1}{n} \sum_{i=1}^n R_i(\mathbf{X})$ and $\bar{R}(\mathbf{Y}) = \frac{1}{n} \sum_{i=1}^n R_i(\mathbf{Y})$.

- Remember that $R_i(\mathbf{X})$ denotes the rank of X_i when only using the vector $\mathbf{X} = (X_1, \dots, X_n)$ to compute the rankings. Likewise, $R_i(\mathbf{Y})$ denotes the rank of Y_i when only using the vector $\mathbf{Y} = (Y_1, \dots, Y_n)$ to compute the rankings.
- Notice that $\hat{\rho}_R$ comes from applying the usual Pearson's estimate of correlation to the ranks $(R_i(\mathbf{X}), R_i(\mathbf{Y}))$ rather than the original data (X_i, Y_i) .
- As with the usual estimate of correlation, $\hat{\rho}_R$ is large (i.e., closer to 1) whenever large values of X_i tend to be associated with large values of Y_i . Similarly, $\hat{\rho}_R$ is small whenever large values of X_i tend to be associated with small values of Y_i .
- Values of $\hat{\rho}_R$ near zero indicate that there is little association between these two variables.

-
- Due to its use of ranks, $\hat{\rho}_R$ is less sensitive to outliers than Pearson's correlation.
 - Another important feature of $\hat{\rho}_R$ is that it is invariant to monotone transformations of the data.

- While Pearson's correlation is very effective for detecting linear associations between two variables, the rank correlation is very effective at detecting any monotone associations between two variables.
- $\hat{\rho}_R$ will equal 1 if Y_i is a monotone increasing function of X_i , and $\hat{\rho}_R$ will equal -1 if Y_i is a monotone decreasing function X_i .

```
xx <- pmax(rnorm(100, mean=10), 0.01)
yy <- pmax(xx + rnorm(100, sd=.5), 0.01)

## Compare the usual Pearson's correlation between
## (xx, yy) and (xx, yy^2)
round( c( cor(xx, yy), cor(xx, yy^2)), 3)
```

```
## [1] 0.896 0.900
```

```
## Now do the same for Spearman's rank correlation
round(c( cor(xx, yy, method="spearman"),
        cor(xx, yy^2, method="spearman")), 3)
```

```
## [1] 0.881 0.881
```

- $\hat{\rho}_R$ can be thought of as an estimate of the following population quantity:

$$\theta_R = 12P(X_1 \geq X_2, Y_1 \geq Y_3) - 3 \quad (6.13)$$

- To justify this, first notice that

$$\begin{aligned} V_R &= \frac{1}{n^3} \sum_{i=1}^n R_i(\mathbf{X}) R_i(\mathbf{Y}) = \frac{1}{n^3} \sum_{i=1}^n \sum_{j=1}^n I(X_i \geq X_j) \sum_{k=1}^n I(Y_i \geq Y_k) \\ &= \frac{1}{n^3} \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^n I(X_i \geq X_j) I(Y_i \geq Y_k) \end{aligned}$$

- While V_R is not exactly a U-statistic, it can be thought of as roughly a “U-statistic” with non-symmetric kernel function

$$h\left(\begin{bmatrix} X_1 \\ Y_1 \end{bmatrix}, \begin{bmatrix} X_1 \\ Y_1 \end{bmatrix}, \begin{bmatrix} X_3 \\ Y_3 \end{bmatrix}\right) = I(X_1 \geq X_2) I(Y_1 \geq Y_3)$$

- So, we should expect V_R to converge to $P\{X_1 \geq X_2, Y_1 \geq Y_3\}$ as n gets larger.

- Using (6.12) and our formula for V_R , we can write $\hat{\rho}_R$ as

$$\begin{aligned}\hat{\rho}_R &= \frac{12}{n(n-1)(n+1)} \sum_{i=1}^n R_i(\mathbf{X})R_i(\mathbf{Y}) - \frac{3(n+1)}{n-1} \\ &= 12V_R\left(\frac{n^3}{n(n-1)(n+1)}\right) - \frac{3(n+1)}{n-1}.\end{aligned}$$

Exercise 6.2. Why does θ_R equal zero when X_i and Y_i are independent? Why is $-1 \leq \theta_R \leq 1$?

6.5.2 Kendall's tau

- Ignoring the possibility of ties, Kendall's τ -statistic U_τ is given by

$$U_\tau = \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=i+1}^n \left[2 \times I\{(X_j - X_i)(Y_j - Y_i) > 0\} - 1 \right]$$

- Note that U_τ is a U-statistic of order 2 with kernel

$$h\left(\begin{bmatrix} X_1 \\ Y_1 \end{bmatrix}, \begin{bmatrix} X_2 \\ Y_2 \end{bmatrix}\right) = 2 \times I\{(X_2 - X_1)(Y_2 - Y_1) > 0\} - 1 \quad (6.14)$$

- Assuming the probability of ties is zero, Kendall's τ can be thought of as an estimate of the following quantity

$$\theta_\tau = 2P\{(X_j - X_i)(Y_j - Y_i) > 0\} - 1 \quad (6.15)$$

- Kendall's τ must be in between -1 and 1 .
- If X_i and Y_i are independent, Kendall's τ will be equal to zero (why?).

- In the context of computing U_τ , pairs of observations (X_i, Y_i) and (X_j, Y_j) are said to be **concordant** if the sign of $X_j - X_i$ agrees with the sign of $Y_j - Y_i$.
- If the sign of $X_j - X_i$ and $Y_j - Y_i$ do **not** agree, then the pairs (X_i, Y_i) and (X_j, Y_j) are said to be **discordant**.

- If either $X_j = X_i$ or $Y_j = Y_i$, then the pairs (X_i, Y_i) and (X_j, Y_j) are neither concordant or discordant.
- Let us define the following

$$\begin{aligned} n_c &= \text{the number of concordant pairs} \\ n_d &= \text{the number of discordant pairs} \\ n_n &= \text{number of pairs which are neither} \end{aligned}$$

- Here, we are counting n_c and n_d from the number of unique possible pairings. There are $n(n-1)/2$ unique pairings, and hence

$$n_c + n_d + n_n = \binom{n}{2} = \frac{n(n-1)}{2} \quad (6.16)$$

- Notice that n_c can be expressed in terms of indicator functions as

$$n_c = \sum_{i=1}^n \sum_{j=i+1}^n I\{(X_j - X_i)(Y_j - Y_i) > 0\}$$

- If we assume that there are no ties (i.e., $n_n = 0$), then U_τ can be written as

$$U_\tau = \frac{4n_c}{n(n-1)} - 1 = \frac{2n_c + 2n_c - n(n-1)}{n(n-1)} = \frac{2n_c - 2n_d}{n(n-1)} = \frac{2(n_c - n_d)}{n(n-1)}$$

- Under independence, the number of concordant and discordant pairs should be roughly equal.

- We just need ordinal data to use Kendall's τ . Kendall's τ can be computed as long you can tell if one observation is "larger" than another.
- Kendall's τ is often used in the context of assessing the agreement between different ratings.
- In this context, we might have K different judges which are rating J different objects. If r_{jk} denotes the object- j rating given by judge k , Kendall's τ from the J pairs $(r_{11}, r_{12}), \dots, (r_{J1}, r_{J2})$ would give a measure of the agreement between judges 1 and 2.

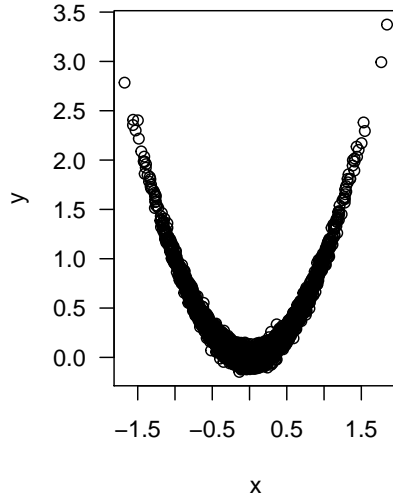
6.5.3 Distance Covariance and Correlation

- A correlation equal to zero does not imply that two random variables are independent.
- For example, if $X \sim \text{Normal}(0, 1)$, then

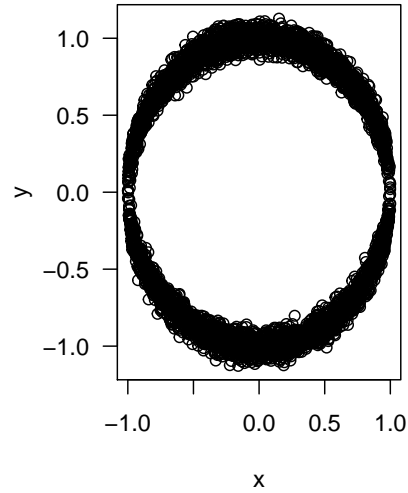
$$\text{Corr}(X, X^2) = \text{Cov}(X, X^2) = E(X^3) = 0$$

- This is also true for Spearman's rank correlation and Kendall's τ . You can have situations where $\theta_R = 0$ but X and Y are not independent. Similarly, you can have situations where $\theta_\tau = 0$ while X and Y are not independent.
- Note that the association between the two variables in the figures below is **non-monotone**.

Sample Pearson Corr. = -0.022'



Sample Pearson Corr. = 0.0016



6.5.3.1 Definition

- **Distance covariance** and **distance correlation** are two measures of dependence that have been developed much more recently (see Székely et al. (2007)).
- The interesting thing about these two measures is that: if they equal zero then it implies that the two random variables are independent.

- Moreover, the measures have a relatively straightforward formula, and they have easily computable estimates.
- For i.i.d. bivariate random variables $(X_1, Y_1), \dots, (X_n, Y_n)$, the squared distance covariance parameter is defined as

$$\begin{aligned}\theta_{dCov,XY}^2 &= E\{|X_1 - X_2||Y_1 - Y_2|\} + E\{|X_1 - X_2|\}E\{|Y_1 - Y_2|\} \\ &\quad - 2E\{|X_1 - X_2||Y_1 - Y_3|\}\end{aligned}$$

- The distance correlation between X_i and Y_i is then defined as

$$\rho_{d,XY} = \frac{\theta_{dCov,XY}}{\theta_{dCov,XX}\theta_{dCov,YY}}$$

- Notice that we must have $\theta_{dCov,XY} \geq 0$ and $\rho_{d,XY} \geq 0$.
- There is no notion of a negative correlation when using distance correlation.
- The interpretation of $\theta_{dCov,XY}^2$ is perhaps not as clear as the usual correlation parameter. Nevertheless, $\theta_{dCov,XY} = 0$ implies independence, and larger values of $\theta_{dCov,XY}$ imply that X_i and Y_i have some form of “greater” association.

Example

- Let us consider the example we had before where we compared X and X^2 .
- Specifically, suppose we have observed pairs $(X_1, Y_1), \dots, (X_n, Y_n)$ where $X_i \sim \text{Normal}(0, 1)$ and $Y_i = X_i^2$.
- In this case, the distance covariance turns out to be

$$\begin{aligned}\theta_{dCov,XY}^2 &= E\{|X_1 - X_2||Y_1 - Y_2|\} + E\{|X_1 - X_2|\}E\{|Y_1 - Y_2|\} - 2E\{|X_1 - X_2||Y_1 - Y_3|\} \\ &= E\{|X_1 - X_2||X_1^2 - X_2^2|\} + E\{|X_1 - X_2|\}E\{|X_1^2 - X_2^2|\} - 2E\{|X_1 - X_2||X_1^2 - X_3^2|\}\end{aligned}$$

- It could be a lot work to compute the above expectation exactly. However, we can estimate it pretty closely using simulation:

```

set.seed(4157)
nreps <- 500000 ## number of simulation replications
term1 <- term2 <- term3 <- term4 <- rep(0, nreps)
for(k in 1:nreps) {
  xx <- rnorm(3)
  term1[k] <- abs(xx[1] - xx[2])*abs(xx[1]^2 - xx[2]^2)
  term2[k] <- abs(xx[1] - xx[2])
  term3[k] <- abs(xx[1]^2 - xx[2]^2)
  term4[k] <- abs(xx[1] - xx[2])*abs(xx[1]^2 - xx[3]^2)
}
dcov.sq.est <- mean(term1) + mean(term2)*mean(term3) - 2*mean(term4)
dcov.sq.est

```

```
## [1] 0.137895
```

- The squared distance covariance for this example seems to be about 0.14.
- Thus, the distance covariance is positive for this example where the two variables are dependent while the usual covariance between these two variables is zero.

-
- **Exercise 6.2.** For the example where we have observed pairs $(X_1, Y_1), \dots, (X_n, Y_n)$ with $X_i \sim \text{Normal}(0, 1)$ and $Y_i = X_i^2$, compute Kendall's τ parameter θ_τ .
-

6.5.3.2 Estimation of Distance Covariance and Distance Correlation

- The distance covariance and correlation are estimated by using a bunch of pairwise distances between our observations.
- The pairwise distances a_{ij} and b_{ij} for the X_i and Y_i are defined as

$$\begin{aligned} a_{ij} &= |X_i - X_j| \\ b_{ij} &= |Y_i - Y_j| \end{aligned}$$

- We then construct the $n \times n$ matrix \mathbf{A} (with elements A_{ij}) and the $n \times n$ matrix \mathbf{B} (with elements B_{ij}) in the following way

$$A_{ij} = \begin{cases} a_{ij} - \frac{1}{n-2}a_{i.} - \frac{1}{n-2}a_{.j} + \frac{1}{(n-1)(n-2)}a_{..} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

$$B_{ij} = \begin{cases} b_{ij} - \frac{1}{n-2}b_{i.} - \frac{1}{n-2}b_{.j} + \frac{1}{(n-1)(n-2)}b_{..} & \text{if } i \neq j \\ 0 & \text{if } i = j \end{cases}$$

where $a_{i.} = \sum_{k=1}^n a_{ik}$, $a_{.j} = \sum_{k=1}^n a_{kj}$, and $a_{..} = \sum_{k=1}^n \sum_{l=1}^n a_{kl}$.

- In other words, \mathbf{A} is a matrix containing “centered” pairwise distances.

- The estimate of the squared distance covariance parameter is then given by

$$\hat{\theta}_{dCov,XY}^2 = \frac{1}{n(n-3)} \sum_{i=1}^n \sum_{j=1}^n A_{ij} B_{ij} \quad (6.17)$$

- The estimate of the distance correlation is

$$\hat{\rho}_{d,XY} = \frac{\hat{\theta}_{dCov,XY}}{\hat{\theta}_{dCov,XX} \hat{\theta}_{dCov,YY}} \quad (6.18)$$

- It turns out that $\hat{\theta}_{dCov,XY}^2$ is a U-statistic of order 4 (see Huo and Székely (2016) for a justification of this). It has kernel function

$$h\left(\begin{bmatrix} X_1 \\ Y_1 \end{bmatrix}, \begin{bmatrix} X_1 \\ Y_1 \end{bmatrix}, \begin{bmatrix} X_3 \\ Y_3 \end{bmatrix}, \begin{bmatrix} X_4 \\ Y_4 \end{bmatrix}\right) = \frac{1}{4} \sum_{i=1}^4 \sum_{j=1}^4 A_{ij} B_{ij} \quad (6.19)$$

- You can compute distance covariances and distance correlations using the **energy** package in **R**.

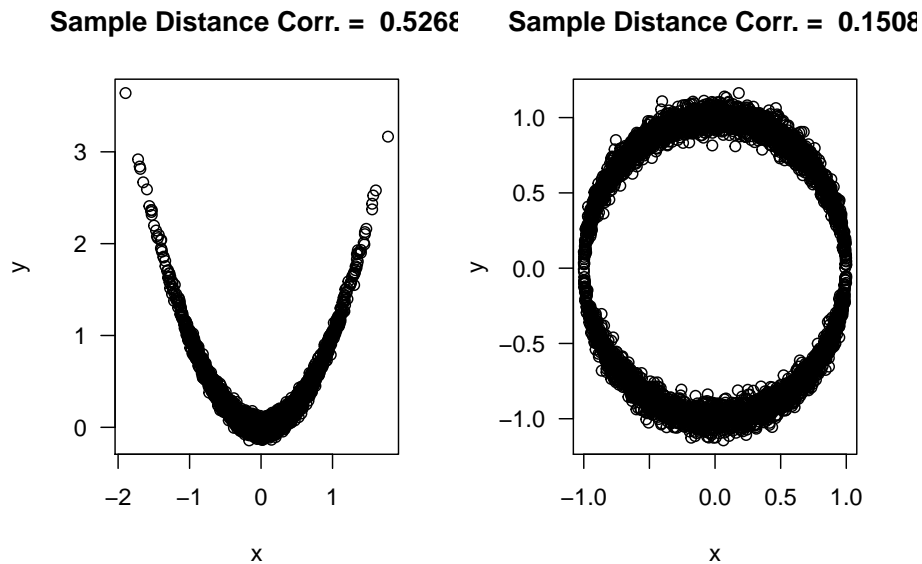
```
library(energy)

n <- 5000
## generate "parabola" data
xx1 <- rnorm(n, sd=0.5)
yy1 <- xx1^2 + rnorm(n, sd=0.05)

## generate circle data
xx2 <- runif(n, min=-1, max=1)
yy2 <- sample(c(-1,1), size=n, replace=TRUE)*sqrt(1 - xx2^2) + rnorm(n, sd=.05)

d.cor1 <- dcor(xx1, yy1)
d.cor2 <- dcor(xx2, yy2)
```

```
par(mfrow=c(1,2))
plot(xx1, yy1, xlab="x", ylab="y", main=paste("Sample Distance Corr. = ",
                                              round(d.cor1, 4)), las=1)
plot(xx2, yy2, xlab="x", ylab="y", main=paste("Sample Distance Corr. = ",
                                              round(d.cor2, 4)), las=1)
```



```
## Let's just compare the values of distance correlation and Pearson's
## for both examples
p.cor1 <- cor(xx1, yy1)
p.cor2 <- cor(xx2, yy2)

kend.cor1 <- cor(xx1, yy1, method="kendall")
kend.cor2 <- cor(xx2, yy2, method="kendall")

spear.cor1 <- cor(xx1, yy1, method="spearman")
spear.cor2 <- cor(xx2, yy2, method="spearman")

# Pearson, Kendall's-tau, Rank, Distance Correlation
round(c(p.cor1, kend.cor1, spear.cor1, d.cor1), 4) ## parabola
```

```
## [1] -0.0124 0.0077 0.0109 0.5268
```



```
round(c(p.cor2, kend.cor2, spear.cor2, d.cor2), 4) ## circle
```

```
## [1] 0.0134 0.0041 0.0138 0.1508
```


Part II

Nonparametric Estimation

Chapter 7

The Empirical Distribution Function

7.1 Definition and Basic Properties

- Every random variable has a cumulative distribution function (cdf).
- The cdf of a random variable X is defined as

$$F(t) = P(X \leq t) \tag{7.1}$$

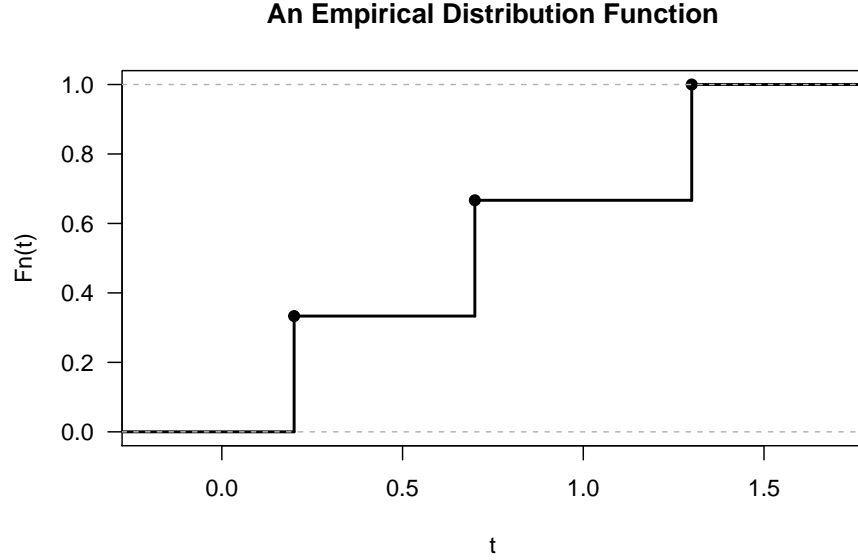
- The empirical distribution function or empirical cumulative distribution function (ecdf) estimates $F(t)$ by computing the proportion of observations which are less than or equal to t .
- For i.i.d. random variables X_1, \dots, X_n with cdf F , the empirical distribution function is defined as

$$\hat{F}_n(t) = \frac{1}{n} \sum_{i=1}^n I(X_i \leq t)$$

- Note that the empirical distribution function can be computed for any type of data without making any assumptions about the distribution from which the data arose.
- The only assumption we are making is that X_1, \dots, X_n constitute an i.i.d. sample from some common distribution function F .

- For example, if we observed $X_1 = 0.7$, $X_2 = 0.2$, and $X_3 = 1.3$, the corresponding empirical distribution function would be

$$\hat{F}_3(t) = \begin{cases} 0 & \text{for } t < 0.2 \\ 1/3 & \text{for } 0.2 \leq t < 0.7 \\ 2/3 & \text{for } 0.7 \leq t < 1.3 \\ 1 & \text{for } t \geq 1.3 \end{cases} \quad (7.2)$$



7.2 Confidence intervals for $F(t)$

- For a fixed value of t , the distribution of $n\hat{F}_n(t)$ is

$$n\hat{F}_n(t) \sim \text{Binomial}(n, F(t)) \quad (7.3)$$

- This is because, for a fixed t , $n\hat{F}_n(t)$ is the sum of n independent Bernoulli random variables W_1^t, \dots, W_n^t

$$n\hat{F}_n(t) = \sum_{i=1}^n W_i^t = \sum_{i=1}^n I(X_i \leq t) \quad (7.4)$$

- The probability that $W_i^t = 1$ is

$$P(W_i^t = 1) = P(X_i \leq t) = F(t)$$

Pointwise Confidence Intervals

- Because $\hat{F}_n(t)$ is a mean of independent random variables, we can say that

$$\frac{\sqrt{n}(\hat{F}_n(t) - F(t))}{\sqrt{\hat{F}_n(t)(1 - \hat{F}_n(t))}} \rightarrow \text{Normal}(0, 1)$$

- The above asymptotic statement is the basis for constructing **pointwise confidence intervals** for $F(t)$.
- For a fixed t , a $100 \times (1 - \alpha)\%$ confidence interval for $F(t)$ is the following

$$\begin{aligned} CI_\alpha^{pw}(t) &= [L_\alpha^{pw}(t), U_\alpha^{pw}(t)] \\ L_\alpha^{pw}(t) &= \max \left\{ \hat{F}_n(t) - z_{1-\alpha/2} \sqrt{\frac{\hat{F}_n(t)(1 - \hat{F}_n(t))}{n}}, 0 \right\} \\ U_\alpha^{pw}(t) &= \min \left\{ \hat{F}_n(t) + z_{1-\alpha/2} \sqrt{\frac{\hat{F}_n(t)(1 - \hat{F}_n(t))}{n}}, 1 \right\} \end{aligned} \quad (7.5)$$

- Plotting $CI_\alpha^{pw}(t)$ for different values of t , would give pointwise confidence intervals for the distribution function. Plotting pointwise confidence intervals for $F(t)$ or for survival functions $S(t) = 1 - F(t)$ is fairly common in practice.
 - However, these pointwise confidence intervals only hold for each point separately.
-

Simultaneous Confidence Bands

- Simultaneous confidence bands can be thought of as two functions $L_\alpha^{band}(t)$ and $U_\alpha^{band}(t)$ such that we are “ $100 \times (1 - \alpha)\%$ confident” that all of $F(t)$ is contained within the bands $L_\alpha^{band}(t)$ and $U_\alpha^{band}(t)$.
- Specifically, we want the statement

$$L_\alpha^{band}(t) \leq F(t) \leq U_\alpha^{band}(t) \quad \text{for all } t \quad (7.6)$$

to hold with at least $1 - \alpha$ probability.

- In other words, we want less than α probability for any part of the path of $F(t)$ going outside of the bands.

- One choice of $L_\alpha^{band}(t)$ and $U_\alpha^{band}(t)$ which has this property is the following

$$L_\alpha^{band}(t) = \max\{\hat{F}_n(t) - \delta_{\alpha,n}, 0\} \quad U_\alpha^{band}(t) = \min\{\hat{F}_n(t) + \delta_{\alpha,n}, 1\}, \quad (7.7)$$

where $\delta_{\alpha,n}$ is given by

$$\delta_{\alpha,n} = \sqrt{\frac{1}{2n} \ln\left(\frac{2}{\alpha}\right)}$$

- The reason this choice of confidence band works is the Dvoretzky-Kiefer-Wolfowitz (DKW) inequality. The DKW inequality states that

$$P\left(\sup_t |F(t) - \hat{F}_n(t)| > \varepsilon\right) \leq 2e^{-2n\varepsilon^2}$$

- Our choice of confidence bands (7.7) then works because

$$\sup_t |F(t) - \hat{F}_n(t)| \leq \delta_{\alpha,n}$$

is equivalent to

$$L_\alpha^{band}(t) \leq F(t) \leq U_\alpha^{band}(t) \quad \text{for all } t$$

- Then, from the DKW inequality we have

$$\begin{aligned} P\left(L_\alpha^{band}(t) \leq F(t) \leq U_\alpha^{band}(t) \quad \text{for all } t\right) &= P\left(\sup_t |F(t) - \hat{F}_n(t)| \leq \delta_{\alpha,n}\right) \\ &\geq 1 - 2e^{-2n\delta_{\alpha,n}^2} \\ &= 1 - \alpha. \end{aligned}$$

- Confidence bands will almost always be wider than the pointwise confidence intervals.
- This extra width is due to the fact that we are requiring the coverage probability to hold for the entire path of $F(t)$ rather than at just a single point.

7.3 The Empirical Distribution Function in R

- We will see how to work with empirical distribution functions in **R** by using data from a study on kidney function.
- This dataset has 157 observations which has the age of each study participant and a measure of overall kidney function. The data can be obtained at https://web.stanford.edu/~hastie/CASI_files/DATA/kidney.txt
- We will only look at the **tot** variable in this chapter.

```
kidney <- read.table("https://web.stanford.edu/~hastie/CASI_files/DATA/kidney.txt",  
                    header=TRUE)  
head(kidney)
```

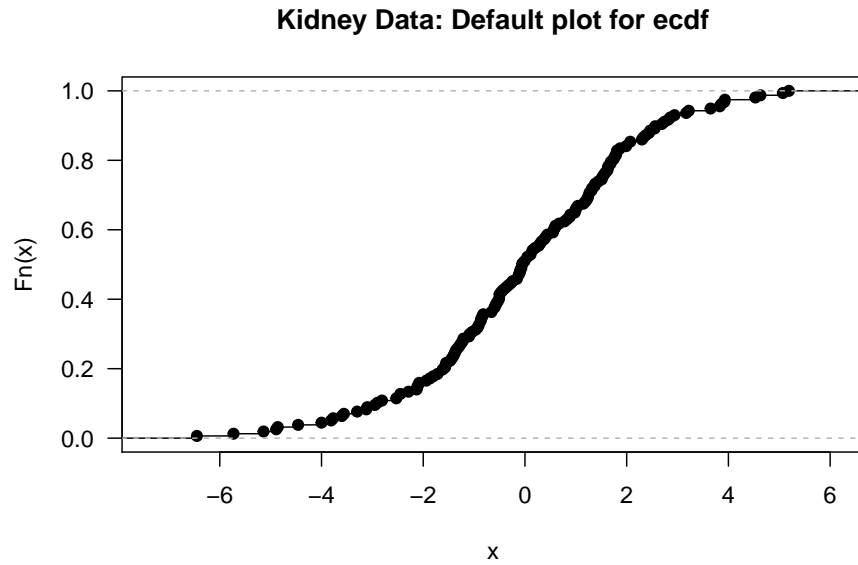
```
##   age  tot  
## 1  18  2.44  
## 2  19  3.86  
## 3  19 -1.22  
## 4  20  2.30  
## 5  21  0.98  
## 6  21 -0.50
```

- The **ecdf** function is the main function which computes the empirical distribution function in **R**
- The **ecdf** function will create an **ecdf** object. To create an ecdf object for the kidney totals, use the following code:

```
kidney.Fhat <- ecdf(kidney$tot)
```

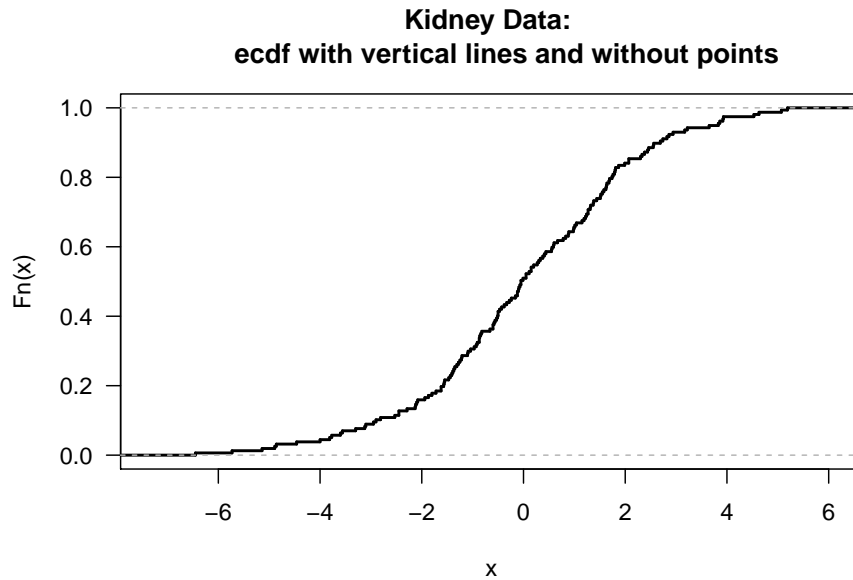
- You can plot the ecdf for the kidney totals by just calling **plot(ecdf)**

```
plot(kidney.Fhat, main = "Kidney Data: Default plot for ecdf", las=1)
```



- If you don't like the look of the points in the ecdf plot, you can use add the argument **do.points = FALSE** when calling plot. Also, you can add the argument **verticals = TRUE** if you want the plot to draw vertical lines whenever there is a jump in the empirical distribution function.

```
plot(kidney.Fhat, do.points=FALSE, verticals=TRUE, main = "Kidney Data:  
ecdf with vertical lines and without points", las=1, lwd=2)
```



-
- A nice feature of the `ecdf` function is that `ecdf` object can be treated as a function which computes the empirical distribution function. For example,

```
kidney.Fhat <- ecdf(kidney$tot)
```

```
kidney.Fhat(0)
```

```
## [1] 0.5095541
```

```
kidney.Fhat( c(-1,1,4) )
```

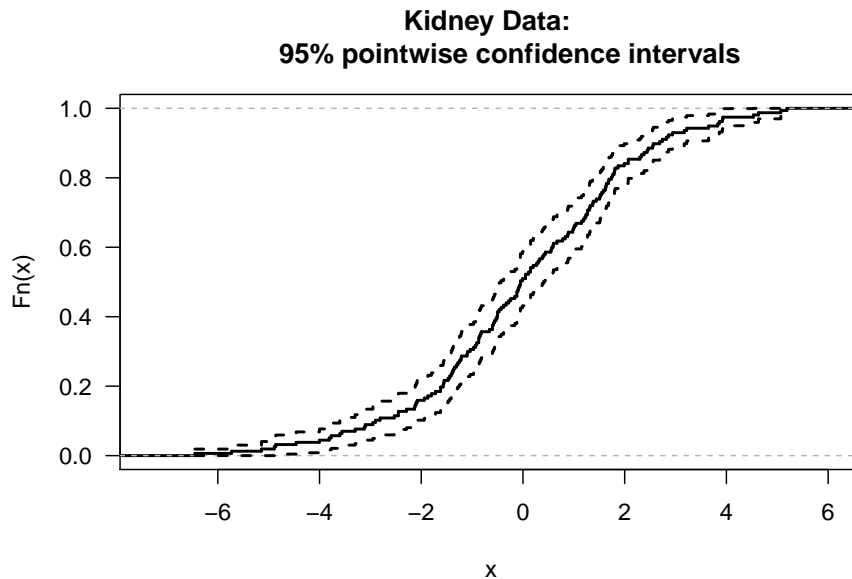
```
## [1] 0.3057325 0.6560510 0.9745223
```

- **R** does not plot confidence intervals when plotting the empirical distribution function.
- We can do this ourselves, by using the pointwise confidence interval formula shown in (7.5)

```
## 1. First, we will compute the standard errors at each of the
##     observed time points
tt <- sort(unique(kidney$tot))
std.err <- sqrt(kidney.Fhat(tt)*(1 - kidney.Fhat(tt))/ length(kidney$tot))

## 2. Now, compute the confidence intervals at each time point
ci.low <- pmax(kidney.Fhat(tt) - qnorm(.975)*std.err, 0)
ci.upper <- pmin(kidney.Fhat(tt) + qnorm(.975)*std.err, 1)

## 3. Now, plot the results. Note that type="s" in the lines function produces
##     "step functions" which pass through the provided points.
plot(kidney.Fhat, do.points=FALSE, verticals=TRUE, main = "Kidney Data:
      95% pointwise confidence intervals", las=1, lwd=2)
lines(tt, ci.low, type="s", lty=2, lwd=2)
lines(tt, ci.upper, type="s", lty=2, lwd=2)
```

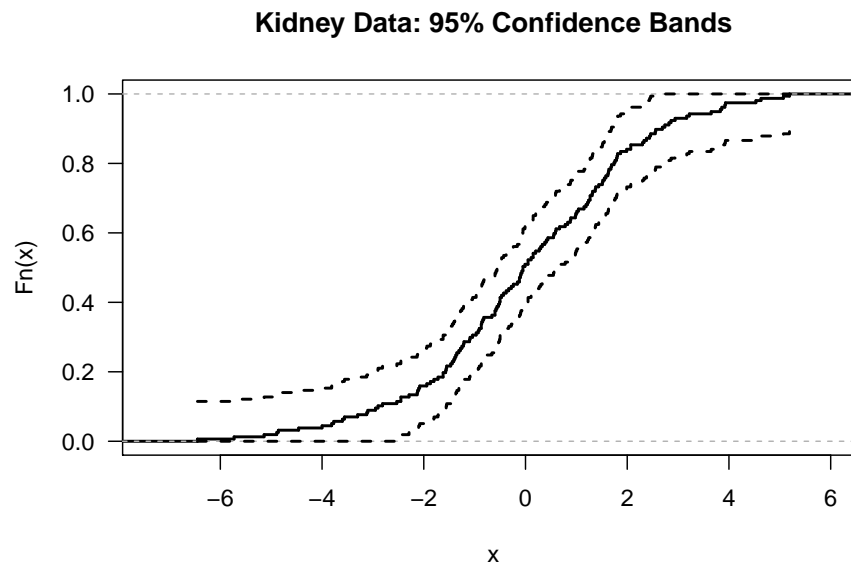


- We could plot the confidence bands as well.

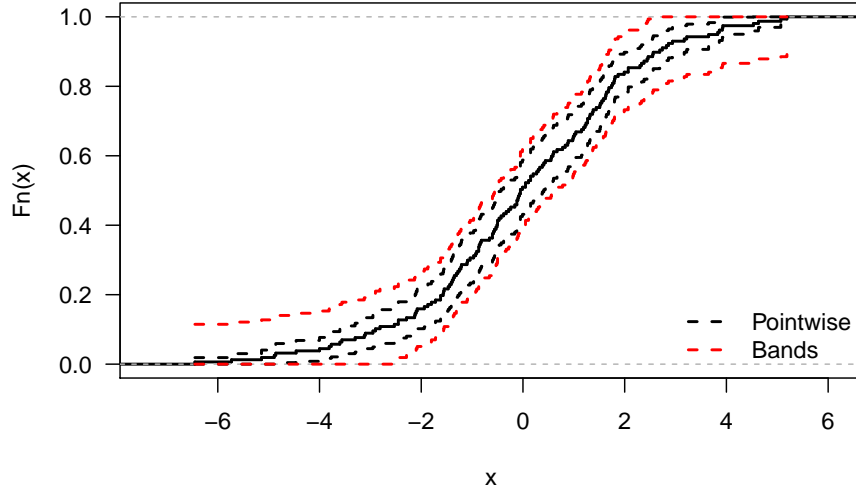
```
n <- length(kidney$tot)

## Compute the confidence bands at each time point
ci.band.low <- pmax(kidney.Fhat(tt) - sqrt(log(2/0.05)/(2*n)), 0)
ci.band.upper <- pmin(kidney.Fhat(tt) + sqrt(log(2/0.05)/(2*n)), 1)
```

```
plot(kidney.Fhat, do.points=FALSE, verticals=TRUE,  
     main = "Kidney Data: 95% Confidence Bands", las=1, lwd=2)  
lines(tt, ci.band.low, type="s", lty=2, lwd=2)  
lines(tt, ci.band.upper, type="s", lty=2, lwd=2)
```



- Comparing the pointwise confidence intervals and the simultaneous confidence bands in the same plot shows how much wider the confidence bands are:

Kidney Data: Confidence Bands and Pointwise Confidence Interval:**7.4 The Kolmogorov-Smirnov Test**

- The one-sample Kolmogorov-Smirnov (KS) test is a type of goodness-of-fit test that is based on the empirical distribution function.
- The KS test will test whether or not our data X_1, \dots, X_n comes from a specific distribution of interest F_0 .
- Supposing our data X_1, \dots, X_n are an i.i.d. sample with distribution function F , the hypothesis test of interest can be stated as

$$H_0 : F = F_0 \quad \text{vs.} \quad H_A : F \neq F_0 \quad (7.8)$$

- The one-sample KS test could be used, for example, as a test of normality.

- The one-sample Kolmogorov-Smirnov test statistic $KS_n^{(1)}$ looks at the maximum distance between the empirical distribution function and F_0

$$KS_n^{(1)} = \sup_t |\hat{F}_n(t) - F_0(t)|$$

- Large values of $KS_n^{(1)}$ provide evidence against the null hypothesis.

- Under H_0 , $\sqrt{n}KS_n^{(1)}$ converges in distribution to a **Kolmogorov distribution** as n goes to infinity.
- The Kolmogorov distribution has the following cumulative distribution function:

$$F_{Kolmo}(t) = 1 - 2 \sum_{j=1}^{\infty} (-1)^{(j+1)} e^{-2j^2 t^2}$$

- The one-sample KS test can be performed in **R** using the **ks.test** function. For one-sample tests, you have to provide the “name” of the distribution function that you are choosing for F_0 .

```
xx <- rt(100, df=2) ## generate 100 observations from a t-dist with 2 d.f.
ks.test(xx, y="pnorm") ## test that these data follow Normal(0, 1)
```

```
##
## One-sample Kolmogorov-Smirnov test
##
## data: xx
## D = 0.19459, p-value = 0.001028
## alternative hypothesis: two-sided
```

- You can even test that the data follow some other $\text{Normal}(\mu, \sigma^2)$ by just providing **mean** and **sd** arguments.

```
ks.test(xx, y="pnorm", mean=1, sd=2)
```

```
##
## One-sample Kolmogorov-Smirnov test
##
## data: xx
## D = 0.21328, p-value = 0.0002239
## alternative hypothesis: two-sided
```

- Suppose we have data from two groups: $X_1, \dots, X_n \sim F_X$ and $Y_1, \dots, Y_m \sim F_Y$. The two-sample KS test performs a test of the following hypothesis

$$H_0 : F_X = F_Y \quad \text{vs.} \quad H_A : F_X \neq F_Y.$$

- In this case, we are only testing whether the distributions of the two groups are different. We are not testing whether observations from group 1 tend to be larger (or smaller) than those from group 2.

- The two-sample KS test compares the empirical distribution functions from these two groups.
- The two-sample KS test statistic is defined as the maximum distance between the two empirical distribution functions:

$$KS_{n,m}^{(2)} = \sup_t |\hat{F}_{n,X}(t) - \hat{F}_{m,Y}(t)|$$

Here, $\hat{F}_{n,X}(t) = \frac{1}{n} \sum_{i=1}^n I(X_i \leq t)$ and $\hat{F}_{m,Y}(t) = \frac{1}{m} \sum_{j=1}^m I(Y_j \leq t)$ denote the empirical distribution functions from the X and Y samples.

- The two-sample KS test statistic also converges to the same limit as the one-sample KS test statistic. In particular, under H_0 :

$$\sqrt{\frac{nm}{n+m}} KS_{n,m}^{(2)} \rightarrow \text{Kolmogorov} \quad \text{as } n, m \rightarrow \infty$$

- The **ks.test** function in **R** also performs two-sample KS tests.

```
xx <- rnorm(100)
yy <- rlogis(100)
ks.test(xx, yy)
```

```
##
## Two-sample Kolmogorov-Smirnov test
##
## data:  xx and yy
## D = 0.21, p-value = 0.02431
## alternative hypothesis: two-sided
```

- We can compute the KS statistic ourselves and check that this matches the value of the KS statistic returned by the **ks.test** function:

```
zz <- c(xx, yy)
zz.order <- sort(zz)
F.x <- ecdf(xx)
F.y <- ecdf(yy)

KS.stat <- max( abs( F.x(zz.order) - F.y(zz.order) ) )
KS.stat

## [1] 0.21
```


-
- **Exercise 7.1.** Why does

$$KS_{n,m}^{(2)} = \max_{1 \leq i \leq n+m} |\hat{F}_{n,X}(Z_{(i)}) - \hat{F}_{n,Y}(Z_{(i)})|,$$

where $\mathbf{Z} = (Z_1, \dots, Z_{n+m})$ denotes the pooled sample and $Z_{(1)}, \dots, Z_{(n+m)}$ denote the order statistics from \mathbf{Z} ?

7.5 The empirical distribution function and statistical functionals

- In many areas of mathematics, it is common to refer to a function which is a “functions of functions” as a **functional**.
- For example, $T(f)$ which is defined as

$$T(f) = \int_0^1 f^2(x) dx \quad (7.9)$$

is a functional because $T(f)$ takes arguments which are functions and outputs real numbers.

- Many common parameters that we encounter in statistics can be thought of as functionals where the input of the functional is usually a distribution function.
- For example, the mean is an example of a functional

$$\mu(F) = \int x dF(x) = \int x f(x) dx$$

As indicated by the notation $\mu(F)$, the value of the mean depends on the underlying distribution function F .

- Also, the variance is an example of a functional

$$\sigma^2(F) = \int (x - \mu(F))^2 dF(x) = \int x^2 dF(x) - \mu^2(F)$$

- The median is an example of a functional

$$\text{med}(F) = F^{-1}(1/2)$$

- The tail probability $P(X_i > c)$ is also a functional

$$\theta_c(F) = \int I(x > c) dF(x)$$

- Many common estimators can be thought of as coming from “plugging in” the empirical cdf into the appropriate statistical functional.
- For example, plugging in the empirical cdf into the mean functional gives:

$$\mu(\hat{F}_n) = \int x d\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n X_i = \bar{X}$$

- Plugging in the empirical cdf into the tail probability functional gives

$$\theta_c(\hat{F}_n) = \int I(x > c) d\hat{F}_n(x) = \frac{1}{n} \sum_{i=1}^n I(X_i > c) = 1 - \hat{F}_n(c)$$

- The sample variance is not quite a plug-in estimate for $\sigma^2(F)$ but it is very close

$$\begin{aligned} \sigma^2(\hat{F}_n) &= \int x^2 d\hat{F}_n(x) - \mu^2(\hat{F}_n) = \frac{1}{n} \sum_{i=1}^n X_i^2 - \bar{X}^2 \\ &= \frac{1}{n} \sum_{i=1}^n (X_i - \bar{X})^2 = \frac{n-1}{n} \hat{\sigma}^2 \end{aligned}$$

- This notation for statistical functionals will be useful when we discuss the bootstrap later in the course.
- The notation for statistical functionals is also very useful in the context of influence functions and robust statistics, but we will not discuss these topics in this course.

7.6 Additional Reading

- Additional reading which covers the material discussed in this chapter includes:
 - Chapter 2 from Wasserman (2006)

Chapter 8

Density Estimation

8.1 Introduction

- In this section, we focus on methods for estimating a **probability density function** (pdf) $f(x)$.
- For a continuous random variable X , areas under the probability density function are probabilities

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

and $f(x)$ is related to the cumulative distribution function via $f(x) = F'(x)$.

- With parametric approaches to density estimation, you only need to estimate several parameters as these parameters completely determine the form of $f(x)$.
- For example, with a Gaussian distribution you only need to find μ and σ^2 to determine the form of $f(x)$.
- In a nonparametric approach to estimating a pdf, we will assume that our observations X_1, \dots, X_n are an independent identically distribution sample from a distribution with pdf $f(x)$, but otherwise we will make few assumptions about the particular form of $f(x)$.

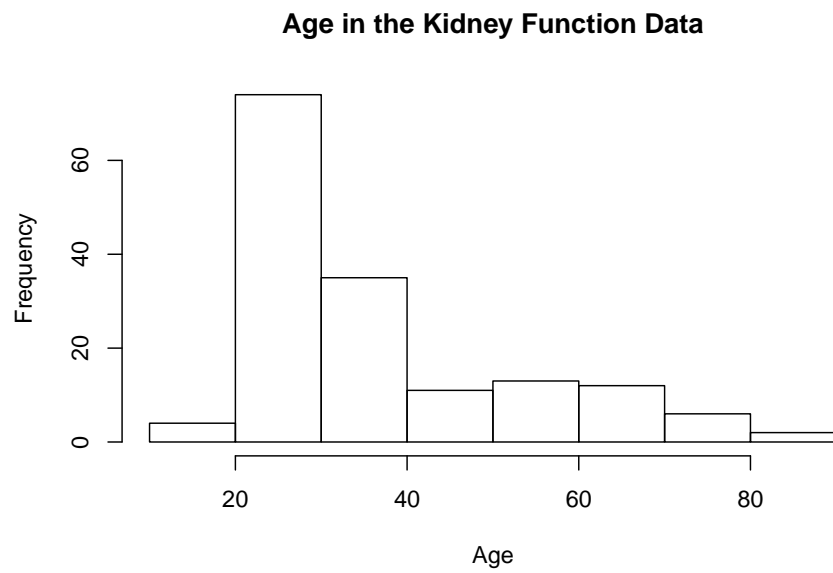


Figure 8.1: Histogram of ages from kidney function data. Data retrieved from: https://web.stanford.edu/~hastie/CASI_files/DATA/kidney.txt

8.2 Histograms

8.2.1 Definition

- While histograms are often thought of as mainly a visualization tool, a histogram can also be thought of as an estimate of the density $f(x)$.
- To construct a histogram, you first need to define a series of “bins”: B_1, \dots, B_{D_n} .
- Each bin is a left-closed interval. That is, the bins have the form $B_k = [x_0 + (k-1)h_n, x_0 + kh_n)$:

$$\begin{aligned} B_1 &= [x_0, x_0 + h_n) \\ B_2 &= [x_0 + h_n, x_0 + 2h_n) \\ &\vdots \\ B_{D_n} &= [x_0 + (D_n - 1)h_n, x_0 + D_n h_n) \end{aligned}$$

- x_0 - the origin
- h_n - bin width
- D_n - number of bins
- Histograms are based on the counts n_k of observations that fall into each bin:

$$\begin{aligned} n_k &= \# \text{ of observations falling into the } k^{th} \text{ bin} \\ &= \sum_{i=1}^n I(x_0 + (k-1)h_n \leq X_i < x_0 + kh_n) \end{aligned}$$

- From the counts n_k , the histogram estimate of the density at a point x in the k^{th} bin (that is if $x_0 + (k-1)h_n \leq x < x_0 + kh_n$), is defined as

$$\hat{f}_{h_n}^H(x) = \frac{n_k}{nh_n}$$

- **Note:** Histogram plots often show the actual bin counts n_k rather than the values of $\hat{f}_{h_n}^H(x)$.

- To see the motivation for the histogram estimate, notice that if we choose a relatively small value of $h_n > 0$

$$P(a < X_i < a + h_n) = \int_a^{a+h_n} f(t)dt \approx h_n f(c),$$

for any point $a \leq c \leq a + h_n$.

- So, for a point $x \in B_k$, the expected value of $\hat{f}_{h_n}^H(x)$ is

$$\begin{aligned}
 E\{\hat{f}_{h_n}^H(x)\} &= \frac{1}{nh_n} E\{n_k\} \\
 &= \frac{1}{nh_n} \sum_{i=1}^n P(x_0 + (k-1)h_n \leq X_i < x_0 + kh_n) \\
 &= \frac{1}{h_n} P(x_0 + (k-1)h_n \leq X_i < x_0 + kh_n) \\
 &\approx f(x)
 \end{aligned}$$

8.2.2 Histograms in R

- In **R**, histograms are computed using the **hist** function

```
hist(x, breaks, probability, plot, ...)
```

- The **breaks** argument
 - Default is “Sturges”. This is a method for finding the bin width.
 - Can be a name giving the name of an algorithm for computing bin width (e.g., “Scott” and “FD”).
 - Can also be a single number. This gives the number of bins used.
 - Could be a vector giving the breakpoints between bins.
 - Could also be a function which computes the number of bins.
- The **probability** argument. If this is set to **FALSE**, then the bin counts are shown in the histogram. If set to **TRUE**, then the bin counts divided by nh_n are shown in the histogram.
- The **plot** argument. If **TRUE**, a histogram is plotted whenever **hist** is called. If **FALSE**, a histogram is not plotted when **hist** is called.

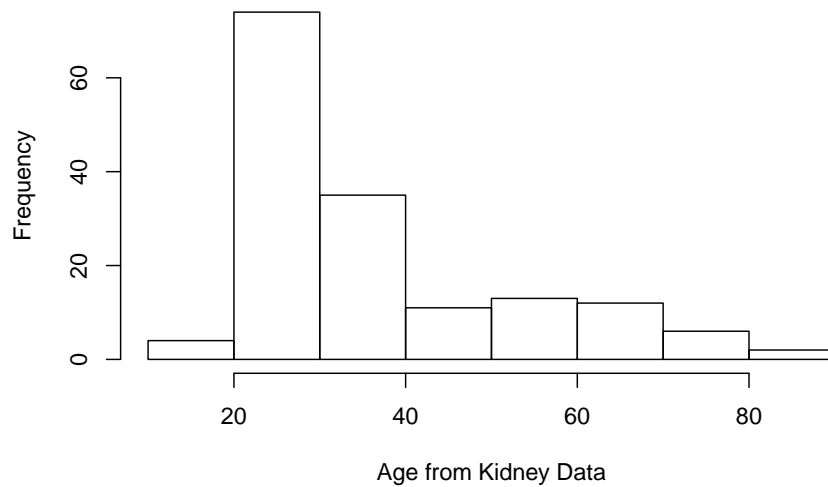
Note: The default for R, is to use right-closed intervals $(a, b]$. This can be changed using the **right** argument of the **hist** function.

- Let’s use the kidney function data again to demonstrate the use of histograms in **R**. This time we will focus on the **age** variable.

```
kidney <- read.table("https://web.stanford.edu/~hastie/CASI_files/DATA/kidney.txt",
                     header=TRUE)
```

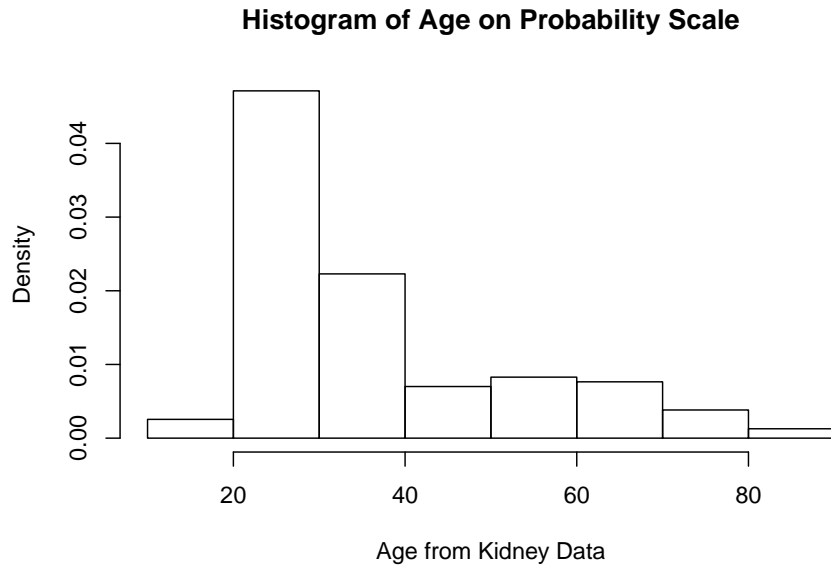
- You can plot a histogram of **age** just by calling the **hist** function.

```
kidney.hist <- hist(kidney$age, main="", xlab="Age from Kidney Data")
```



- Use the **probability = TRUE** argument to plot the density-estimate version of the histogram. This histogram should integrate to 1.

```
kidney.hist2 <- hist(kidney$age, main="Histogram of Age on Probability Scale",  
                     xlab="Age from Kidney Data", probability=TRUE)
```



-
- In addition to generating a histogram plot, the `histogram` function also returns useful stuff.

```
names(kidney.hist)
```

```
## [1] "breaks" "counts" "density" "mids" "xname" "equidist"
```

- **breaks**
 - the boundaries for the histogram bins. The bins are of the form (`breaks[k]`, `breaks[k+1]`]
- **counts**
 - the number of observations falling into each bin
- **density**
 - the value of the estimated density within each of the bins
- **mids**
 - the midpoint of each of the bins


```
kidney.hist$breaks
```

```
## [1] 10 20 30 40 50 60 70 80 90
```

```
kidney.hist$counts
```

```
## [1] 4 74 35 11 13 12 6 2
```

```
## The following sum should match the first element of kidney.hist$counts[1]
sum(kidney.hist$breaks[1] < kidney$age & kidney$age <= kidney.hist$breaks[2])
```

```
## [1] 4
```

- Let's check that the density values returned by `hist` match our definition of the histogram density estimate in (8.1).

```
binwidth <- kidney.hist$breaks[2] - kidney.hist$breaks[1]
kidney.hist$density
```

```
## [1] 0.002547771 0.047133758 0.022292994 0.007006369 0.008280255 0.007643312
## [7] 0.003821656 0.001273885
```

```
kidney.hist$counts/(length(kidney$age)*binwidth)
```

```
## [1] 0.002547771 0.047133758 0.022292994 0.007006369 0.008280255 0.007643312
## [7] 0.003821656 0.001273885
```

8.2.3 Performance of the Histogram Estimate and Bin Width Selection

8.2.3.1 Bias/Variance Decomposition

- It is common to evaluate the performance of a density estimator through its **mean-squared error** (MSE).
- In general, MSE is a function of bias and variance

$$\text{MSE} = \text{Bias}^2 + \text{Variance}$$

- We will first look at the mean-squared error of $\hat{f}_{h_n}^H(x)$ at a single point x

$$\begin{aligned}
 \text{MSE}\{\hat{f}_{h_n}^H(x)\} &= E\left(\{\hat{f}_{h_n}^H(x) - f(x)\}^2\right) \\
 &= E\left(\left[\hat{f}_{h_n}^H(x) - E\{\hat{f}_{h_n}^H(x)\} + E\{\hat{f}_{h_n}^H(x)\} - f(x)\right]^2\right) \\
 &= E\left(\left[\hat{f}_{h_n}^H(x) - E\{\hat{f}_{h_n}^H(x)\}\right]^2\right) + E\left(\left[E\{\hat{f}_{h_n}^H(x)\} - f(x)\right]^2\right) \\
 &\quad + 2E\left(\left[\hat{f}_{h_n}^H(x) - E\{\hat{f}_{h_n}^H(x)\}\right]\left[E\{\hat{f}_{h_n}^H(x)\} - f(x)\right]\right) \\
 &= \underbrace{\text{Var}\{\hat{f}_{h_n}^H(x)\}}_{\text{Variance}} + \underbrace{\left(E\{\hat{f}_{h_n}^H(x)\} - f(x)\right)^2}_{\text{Bias Squared}}
 \end{aligned}$$

- In general, as the bin width h_n increases, the histogram estimate will have less variation but will become more biased.

8.2.3.2 Bias and Variance of the Histogram Estimate

- Recall that, for a histogram estimate, we have D_n bins where the k^{th} bin takes the form

$$B_k = [x_0 + (k-1)h_n, x_0 + kh_n)$$

- For a point $x \in B_k$, that “belongs” to the k^{th} bin, the histogram density estimate is

$$\hat{f}_n^H(x) = \frac{n_k}{nh_n}, \quad \text{where } n_k = \text{number of observations falling into bin } B_k$$

- To better examine what happens as n changes, we will define the function $A_{h_n, x_0}(x)$ as the function which returns the index of the interval to which x belongs.
- For example, if $x_0 = 0$, $h_n = 1/3$, and $x = 1/2$, then $A_{h_n, x_0}(x) = 2$.
- So, we can also write the histogram density estimate at the value x as

$$\hat{f}_{h_n}^H(x) = \frac{n_{A_{h_n, x_0}(x)}}{nh_n}$$

-
- **Exercise 8.1.** Suppose $x_0 = -2$ and $h_n = 1/2$. What are the values of $A_{h_n, x_0}(-1)$, $A_{h_n, x_0}(1.3)$, and $A_{h_n, x_0}(0.75)$?
-

- Note that we can express $n_{A_{h_n, x_0}(x)}$ as

$$n_{A_{h_n, x_0}(x)} = \sum_{i=1}^n I(X_i \in B_{A_{h_n, x_0}(x)})$$

- Hence, is a binomial random variable with n trials and success probability $p_{h_n, x_0}(x)$ (why?)

$$n_{A_{h_n}(x)} \sim \text{Binomial}\{n, p_{h_n, x_0}(x)\}$$

- The success probability $p_{h_n, x_0}(x)$ is defined as

$$\begin{aligned} p_{h_n, x_0}(x) &= P\{X_i \text{ falls into bin } B_{A_{h_n, x_0}(x)}\} \\ &= \int_{x_0 + (A_{h_n, x_0}(x)-1)h_n}^{x_0 + A_{h_n, x_0}(x)h_n} f(t) dt. \end{aligned}$$

- Because $n_{A_{h_n, x_0}(x)}$ follows a binomial distribution, we know that

$$\begin{aligned} E(n_{A_{h_n, x_0}(x)}) &= np_{h_n, x_0}(x) \\ \text{Var}(n_{A_{h_n, x_0}(x)}) &= np_{h_n, x_0}(x)\{1 - p_{h_n, x_0}(x)\} \end{aligned}$$

- So, we can express the bias of the histogram density estimate $\hat{f}_{h_n}^H(x) = n_{A_{h_n, x_0}(x)}/(nh_n)$ as

$$\begin{aligned} \text{Bias}\{\hat{f}_{h_n}^H(x)\} &= E\{\hat{f}_{h_n}^H(x)\} - f(x) \\ &= \frac{1}{nh_n} E(n_{A_{h_n, x_0}(x)}) - f(x) \\ &= \frac{p_{h_n, x_0}(x)}{h_n} - f(x), \end{aligned}$$

and we can express the variance as:

$$\begin{aligned} \text{Var}\{\hat{f}_{h_n}^H(x)\} &= \frac{1}{n^2 h_n^2} \text{Var}(n_{A_{h_n, x_0}(x)}) \\ &= \frac{p_{h_n, x_0}(x)\{1 - p_{h_n, x_0}(x)\}}{nh_n^2} \end{aligned}$$

- Using the approximation $f(t) \approx f(x) + f'(x)(t - x)$ for t close to x , we have that

$$\begin{aligned}
\frac{p_{h_n, x_0}(x)}{h_n} &= \frac{1}{h_n} \int_{x_0 + (A_{h_n, x_0}(x) - 1)h_n}^{x_0 + A_{h_n, x_0}(x)h_n} f(t) dt \\
&\approx \frac{1}{h_n} \int_{x_0 + (A_{h_n, x_0}(x) - 1)h_n}^{x_0 + A_{h_n, x_0}(x)h_n} f(x) dt + \frac{f'(x)}{h_n} \int_{x_0 + (A_{h_n, x_0}(x) - 1)h_n}^{x_0 + A_{h_n, x_0}(x)h_n} (t - x) dt \\
&= f(x) + \frac{f'(x)}{2h_n} \left[(t - x)^2 \right]_{x_0 + (A_{h_n, x_0}(x) - 1)h_n}^{x_0 + A_{h_n, x_0}(x)h_n} \\
&= f(x) + \frac{f'(x)}{2h_n} \left[(x_0 + A_{h_n, x_0}(x)h_n)^2 - (x_0 + (A_{h_n, x_0}(x) - 1)h_n)^2 - 2xh_n \right] \\
&= f(x) + \frac{f'(x)}{2h_n} \left[2x_0 A_{h_n, x_0}(x)h_n + A_{h_n, x_0}^2(x)h_n^2 - 2x_0(A_{h_n, x_0}(x) - 1)h_n \right. \\
&\quad \left. - (A_{h_n, x_0}(x) - 1)^2 h_n^2 - 2xh_n \right] \\
&= f(x) + \frac{f'(x)}{2h_n} \left[2x_0 h_n + 2A_{h_n, x_0}(x)h_n^2 - h_n^2 - 2xh_n \right] \\
&= f(x) + f'(x) \left[h_n/2 - [x - x_0 - \{A_{h_n, x_0}(x) - 1\}h_n] \right]
\end{aligned}$$

- So, the bias of the histogram density estimate $\hat{f}_{h_n}^H(x)$ is

$$\begin{aligned}
\text{Bias}\{\hat{f}_{h_n}^H(x)\} &= \frac{p_{h_n, x_0}(x)}{h_n} - f(x) \\
&\approx f'(x) \left[h_n/2 - [x - x_0 - \{A_{h_n, x_0}(x) - 1\}h_n] \right] \quad (8.1)
\end{aligned}$$

- Choosing a very small bin width h_n will result in a small bias because the left endpoint of the bin $x_0 + (A_{h_n}(x) - 1)h_n$ will always be very close to x .

- Now, let us turn to the variance of the histogram estimate at x :

$$\begin{aligned}
\text{Var}\{\hat{f}_{h_n}^H(x)\} &= \frac{p_{h_n, x_0}(x)}{nh_n^2} \{1 - p_{h_n, x_0}(x)\} \\
&\approx \frac{f(x) + f'(x) \left\{ \frac{h_n}{2} - [x - x_0 - (A_{h_n, x_0}(x) - 1)h_n] \right\}}{nh_n} \{1 - p_{h_n, x_0}(x)\} \\
&\approx \frac{f(x)}{nh_n} \quad (8.2)
\end{aligned}$$

- For a more detailed description of the above approximation see Scott (1979) or Chapter 6 of Wasserman (2006).
- Note that large bin widths will reduce the variance of $\hat{f}_{h_n}^H(x)$.

8.2.3.3 Pointwise Approximate Mean Squared Error

- Using (8.2) and (8.1), the approximate mean-squared error (AMSE) of the histogram density estimate at a particular point x is given by

$$\begin{aligned}
 \text{MSE}\{\hat{f}_{h_n}^H(x)\} &= E\left(\{\hat{f}_{h_n}^H(x) - f(x)\}^2\right) \\
 &= \left(\text{Bias}\{\hat{f}_{h_n}^H(x)\}\right)^2 + \text{Var}\{\hat{f}_{h_n}^H(x)\} \\
 &\approx \frac{h_n^2 [f'(x)]^2}{4} - h_n f'(x) [x - x_0 - \{A_{h_n, x_0}(x) - 1\} h_n] \\
 &\quad + [f'(x)]^2 \left(x - x_0 - \{A_{h_n, x_0}(x) - 1\} h_n\right)^2 + \frac{f(x)}{n h_n} \\
 &= \text{AMSE}\{\hat{f}_{h_n}^H(x)\} \tag{8.3}
 \end{aligned}$$

- For any approach to bin width selection, we should have $h_n \rightarrow 0$ and $n h_n \rightarrow \infty$.
- This MSE approximation depends on a particular choice of x .
- Difficult to use (8.3) as a criterion for selecting the bandwidth because the best choice of h_n will usually depend on your choice of x .

8.2.3.4 Integrated Mean Squared Error and Optimal Histogram Bin Width

- Using the approximate mean integrated squared error (AMISE) allows us to find an optimal bin width that does not depend on a particular choice of x .
- The AMISE is defined as

$$\begin{aligned}
 \text{AMISE}\{\hat{f}_{h_n}^H\} &= E\left\{\int_{-\infty}^{\infty} \{\hat{f}_{h_n}^H(x) - f(x)\}^2 dx\right\} \\
 &= \int_{-\infty}^{\infty} \text{MSE}\{\hat{f}_{h_n}^H(x)\} dx
 \end{aligned}$$

Using the previously derived approximation (8.3) for the AMSE, it can be shown that

$$\text{MISE}\{\hat{f}_{h_n}^H\} \approx \frac{1}{n h_n} + \frac{h_n^2}{12} \int_{-\infty}^{\infty} [f'(x)]^2 dx \tag{8.4}$$

-
- To select the optimal bin width, we minimize the MISE as a function of h_n .
 - Minimizing (8.4), as a function of h_n yields the following formula for the optimal bin width

$$h_n^{opt} = \left(\frac{6}{n \int_{-\infty}^{\infty} [f'(x)]^2 dx} \right)^{1/3} = Cn^{-1/3} \quad (8.5)$$

- Notice that $h_n^{opt} \rightarrow 0$ and $nh_n^{opt} \rightarrow \infty$ as $n \rightarrow \infty$.
- Notice also that the optimal bin width depends on the unknown quantity $\int_{-\infty}^{\infty} [f'(x)]^2 dx$.

8.2.4 Choosing the Histogram Bin Width

- We will mention three rules for selecting the bin width of a histogram.
 - Scott rule: (based on the optimal bin width formula (8.5))
 - Friedman and Diaconis (FD) rule (also based on the optimal bin width formula (8.5))
 - Sturges rule: (based on wanting the histogram to look Gaussian when the data are in fact Gaussian-distributed)
-

- Both the Scott and the FD rule are based on the optimal bin width formula (8.5).
- The main problem with using the formula (8.5) is the presence of $\int_{-\infty}^{\infty} [f'(x)]^2 dx$.
- **Solution:** See what this quantity looks like if we assume that $f(x)$ corresponds to a $\text{Normal}(\mu, \sigma^2)$ density.
- With the assumption that $f(x) = \text{Normal}(\mu, \sigma^2)$:

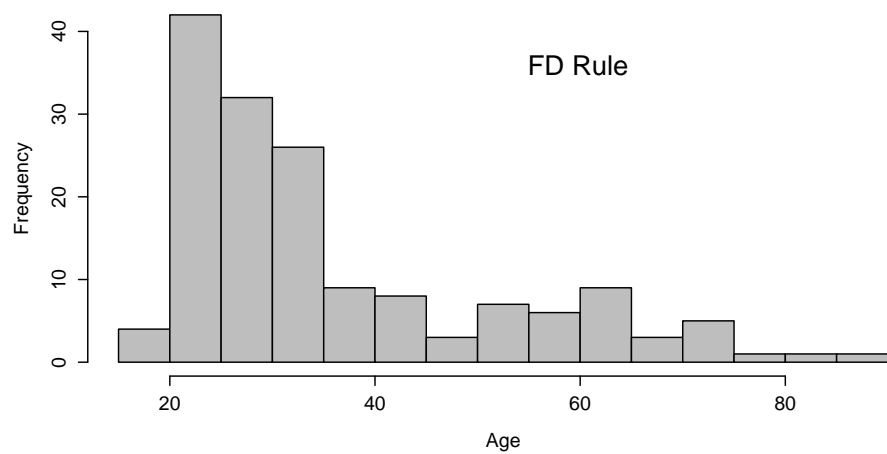
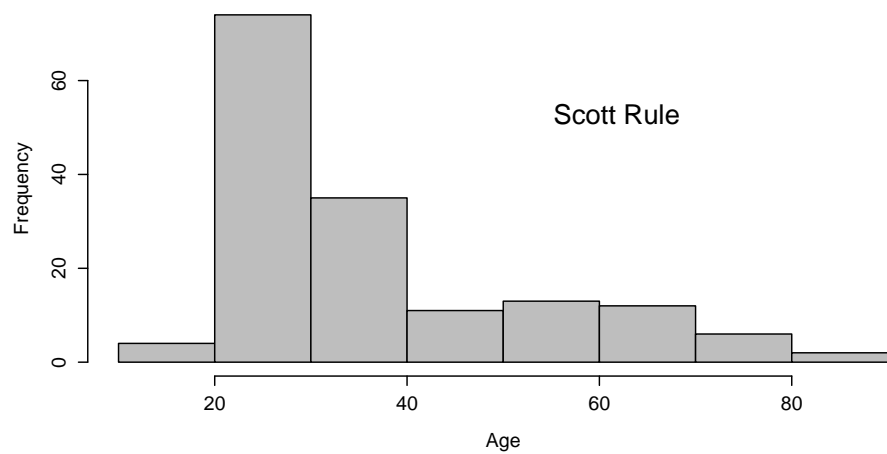
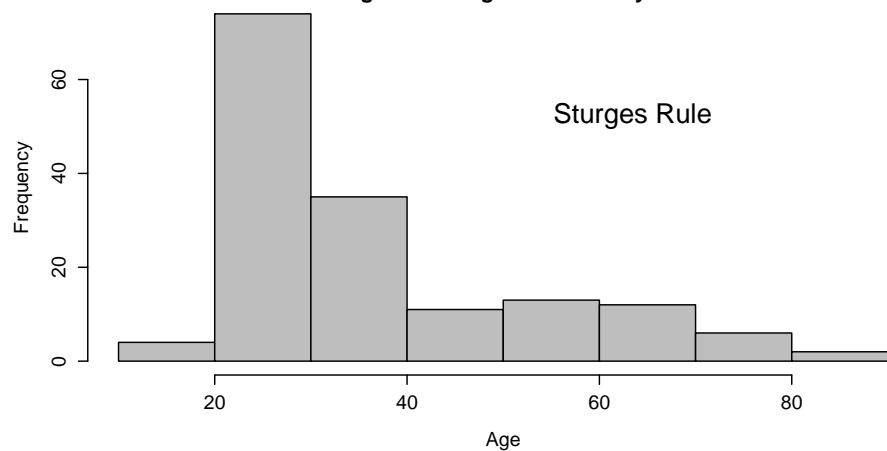
$$h_n^{opt} = 3.5\sigma n^{-1/3}$$

- **Scott rule:** Use $h_n^* = 3.5\hat{\sigma}n^{-1/3}$, where $\hat{\sigma}$ denotes the sample standard deviation.

- **FD rule:** Use $h_n^* = 2 \times IQR \times n^{-1/3}$. This is a somewhat more robust choice of h_n as it is not as sensitive to outliers.

- **Sturges rule:** The bin width is chosen so that we have $1 + \log_2(n)$ bins. This choice tends to give wide intervals.

Histograms for Age in the Kidney Data



8.3 A Box-type Density Estimate

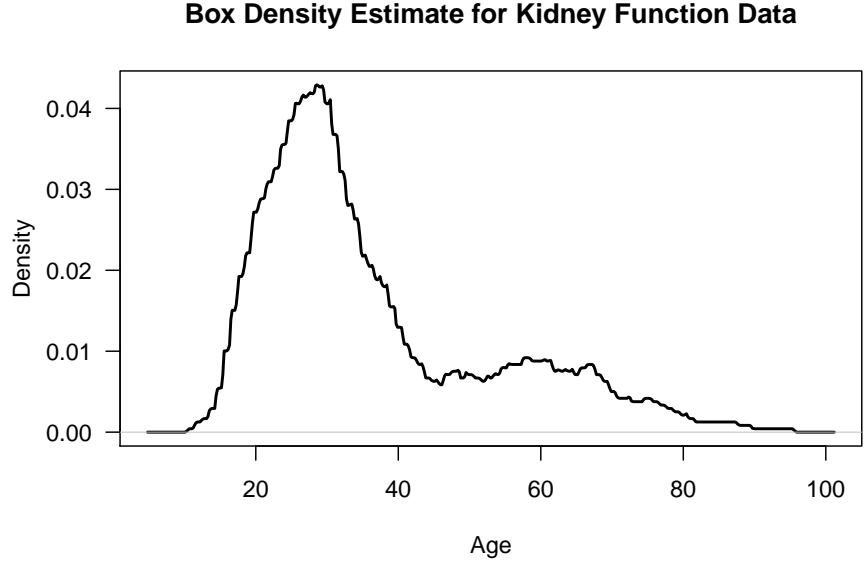
- A related estimator $\hat{f}_{h_n}^B$ of the density $f(x)$ uses a “sliding bin” at each point x to calculate the estimate of $f(x)$.
- Specifically, the “box estimate” $\hat{f}_{h_n}^B(x)$ at the point x is defined as

$$\begin{aligned}\hat{f}_{h_n}^B(x) &= \frac{1}{2nh_n} \left[\# \text{ of observations falling in the interval } (x - h_n, x + h_n) \right] \\ &= \frac{1}{2nh_n} \sum_{i=1}^n I(x - h_n < X_i < x + h_n)\end{aligned}$$

- In other words, for each x we are forming a bin of width $2h_n$ around x , and we are counting the number of observations that fall in this bin.
- You can think of each point x as being the center of its own bin.
- The expectation of the box estimator at the point x is

$$E\{\hat{f}_{h_n}^B(x)\} = \frac{1}{2h_n} P(x - h_n < X_i < x + h_n) \approx f(x)$$

- Unlike the histogram, the box estimate does not require the density estimate to be constant within each bin.
- Also, histograms can have dramatic changes near the bin edges while the box estimate suffers less from this problem.
- However, plots of the box estimate will still largely be non-smooth and have a “jagged” appearance.

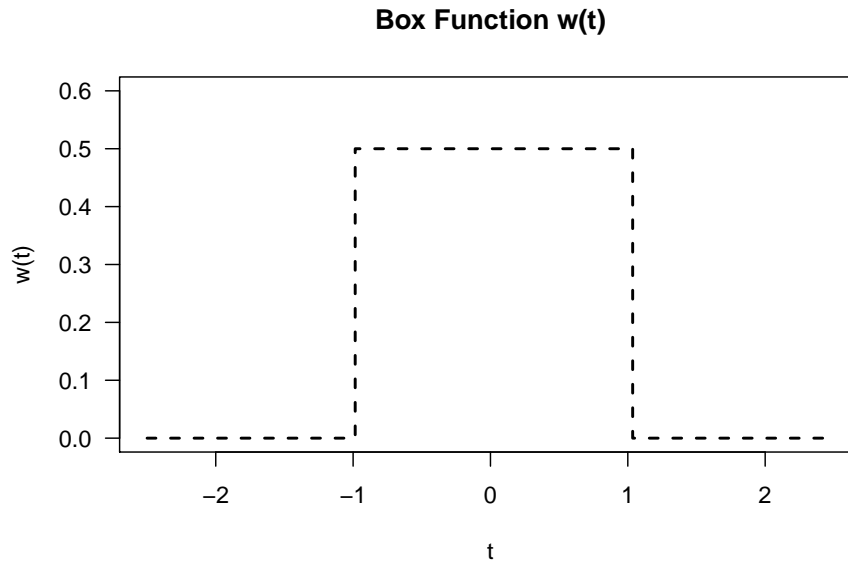


-
- We can also express $\hat{f}_{h_n}^B(x)$ in the following way:

$$\hat{f}_{h_n}^B(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h_n} w\left(\frac{X_i - x}{h_n}\right), \quad (8.6)$$

where $w(t)$ is defined as the following “box function”

$$w(t) = \begin{cases} \frac{1}{2} & \text{if } |t| < 1 \\ 0 & \text{otherwise} \end{cases}$$



- While the estimator $\hat{f}_{h_n}^B$ does seem reasonable, it always results in density estimates which are not “smooth.”
- Most kernel density estimates are formed by replacing the box function $w(t)$ with a smoother function.

- **Exercise 8.2.** Write an **R** function which computes the $\hat{f}_{h_n}^B(x)$ at a collection of specified points.
- **Exercise 8.3.** Suppose we have observations $(X_1, X_2, X_3, X_4) = (-1, 0, 1/2, 1)$. Assuming $h_n = 1/2$, plot $w(\frac{X_i - x}{h_n})/nh_n$ for $i = 1, \dots, 4$ and plot the box density estimate $\hat{f}_{h_n}^B(x)$.
- **Exercise 8.4.** Suppose we have i.i.d. observations $X_1, \dots, X_n \sim F$ where the cdf F is assumed to be continuous. What is $\text{Var}\{\hat{f}_{h_n}^B(x)\}$?

8.4 Kernel Density Estimation

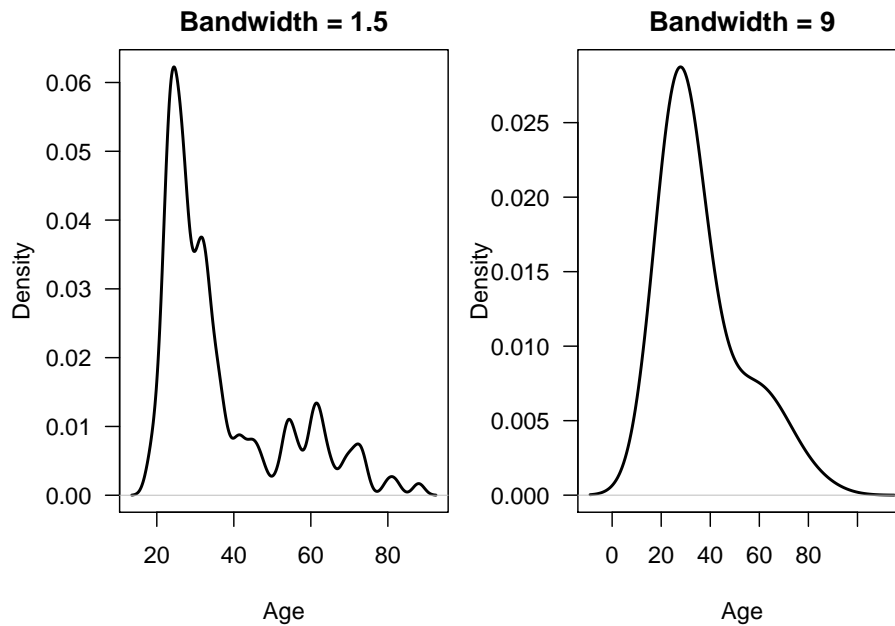
8.4.1 Definition

- Kernel density estimates are a generalization of the box-type density estimate $\hat{f}_{h_n}^B(x)$.
- With kernel density estimation, we replace the “box function” in (8.6) with a function $K(\cdot)$ which is much smoother.
- The function $K(\cdot)$ will also give higher weight to observations which are closer to x than those that are further away from x .

-
- A kernel density estimator $\hat{f}_{h_n}(x)$ of the density $f(x)$ is defined as

$$\hat{f}_{h_n}(x) = \frac{1}{nh_n} \sum_{i=1}^n K\left(\frac{x - X_i}{h_n}\right) \quad (8.7)$$

- The function $K(\cdot)$ is referred to as the **kernel function**.
- The scalar term $h_n > 0$ is called the **bandwidth**.
- The value of the bandwidth h_n largely determines how “bumpy” the density estimate will appear.
- The appearance and the statistical performance of $\hat{f}_{h_n}(x)$ depend much more on the value of h_n than on the choice of kernel function.



- Kernel functions are usually chosen so that

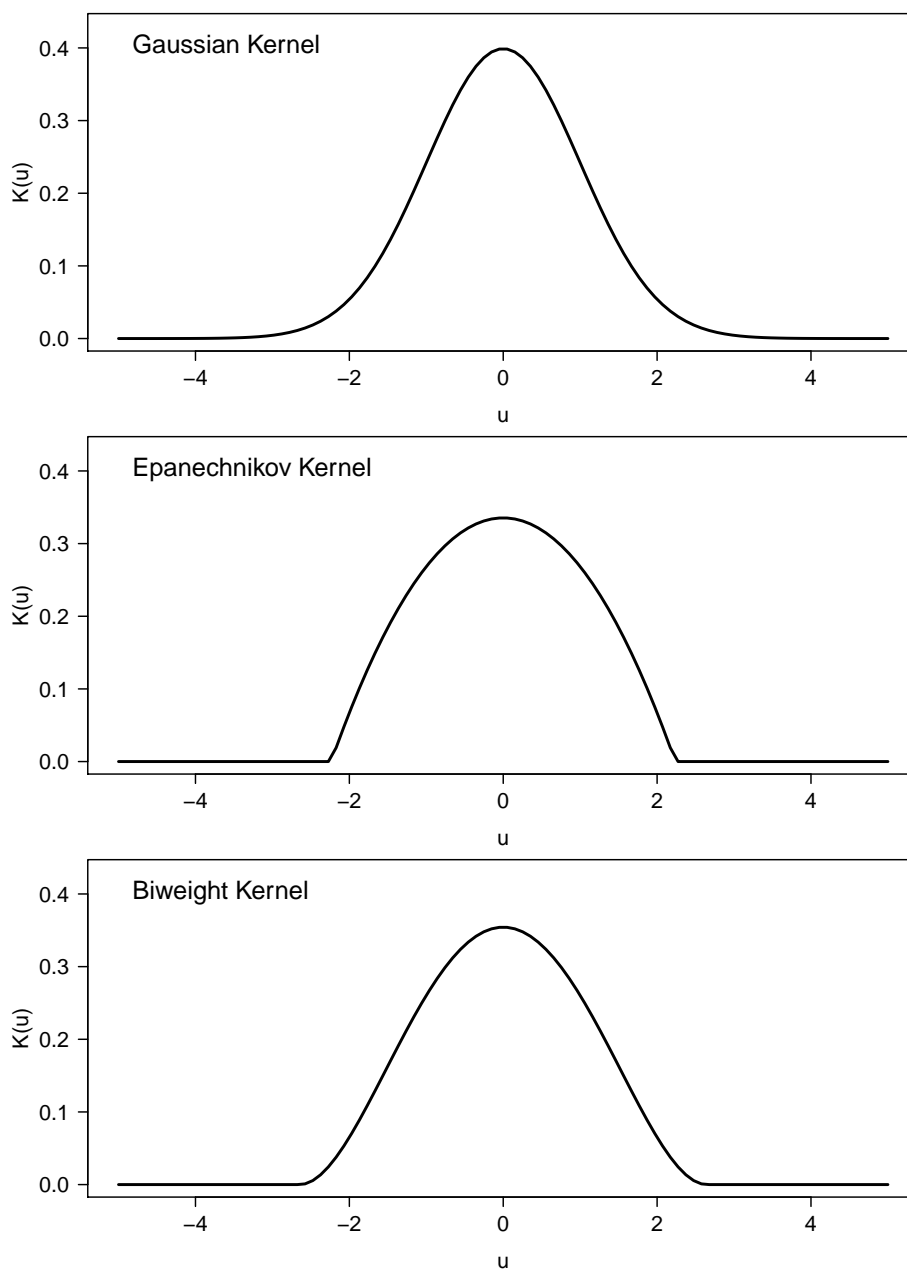
$$K(t) \geq 0 \quad \text{for all } t$$

and that they also satisfy the following properties:

$$K(t) = K(-t) \quad \int_{-\infty}^{\infty} K(t) dt = 1 \quad \int_{-\infty}^{\infty} K^2(t) dt < \infty$$

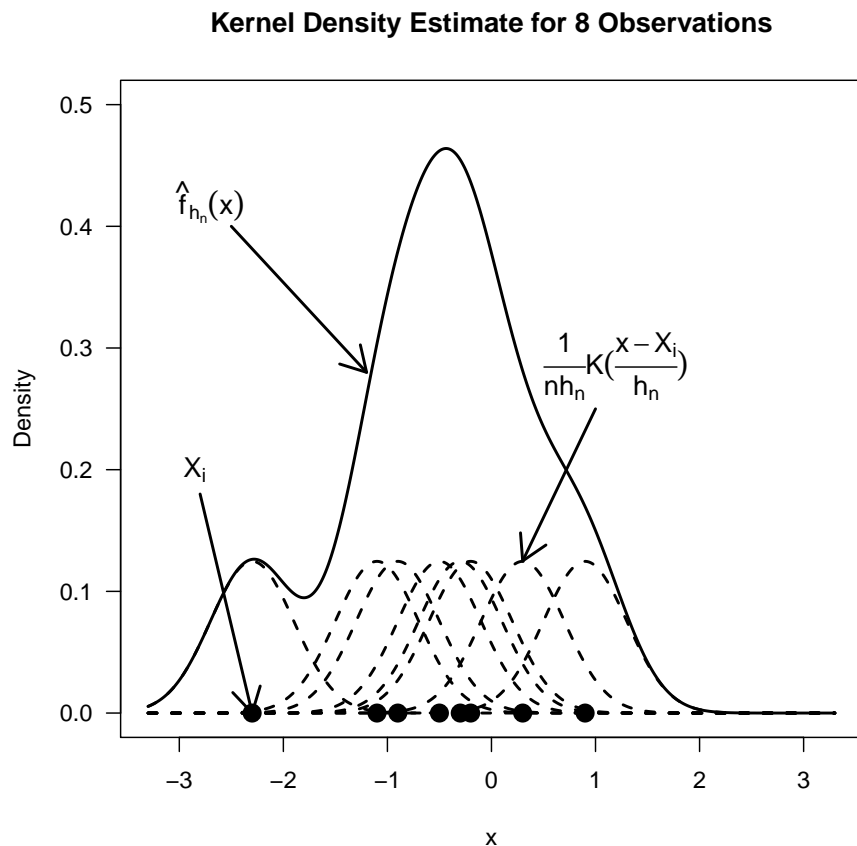
- You can think of $K(u)$ as a probability density function which is symmetric around 0.
- Some of the most common choices of kernel functions include

Gaussian :	$K(u) = \exp(-u^2/2)/\sqrt{2\pi}$
Epanechnikov :	$K(u) = \frac{3}{4\sqrt{5}}(1 - \frac{1}{5}u^2)I(u < \sqrt{5})$
biweight :	$K(u) = \frac{15}{16\sqrt{7}}(1 - \frac{1}{7}u^2)^2I(u < \sqrt{7})$



- When plotting $\frac{1}{nh_n} K\left(\frac{x-X_i}{h_n}\right)$ as a function of x , it should look like a “small hill” centered around X_i .
- As h_n decreases, $\frac{1}{nh_n} K\left(\frac{x-X_i}{h_n}\right)$ becomes more strongly concentrated around X_i and has a higher peak.

- The kernel density estimate $\hat{f}_{h_n}(x)$ is a sum of all these “small hills”.



- The nice thing about (8.7) is that it guarantees that $\hat{f}_{h_n}(x)$ is a probability density function

$$\begin{aligned}
 \int_{-\infty}^{\infty} \hat{f}_{h_n}(x) dx &= \int_{-\infty}^{\infty} \frac{1}{nh_n} \sum_{i=1}^n K\left(\frac{x - X_i}{h_n}\right) dx \\
 &= \frac{1}{n} \sum_{i=1}^n \int_{-\infty}^{\infty} \frac{1}{h_n} K\left(\frac{x - X_i}{h_n}\right) dx \\
 &= 1
 \end{aligned}$$

- Also, formula (8.7) guarantees that $\hat{f}_{h_n}(x)$ inherits the smoothness properties of $K(u)$

$$\hat{f}'_{h_n}(x) = \frac{1}{n} \sum_{i=1}^n \frac{1}{h_n^2} K'\left(\frac{x - X_i}{h_n}\right)$$

8.4.2 Bias, Variance, and AMISE of Kernel Density Estimates

- As with the bin width in histogram estimation, the bias/variance tradeoff drives the best choice of the bandwidth h_n in kernel density estimation.

Approximate Bias

- The exact expectation of a kernel density estimate $\hat{f}_{h_n}(x)$ is

$$\begin{aligned} E\{\hat{f}_{h_n}(x)\} &= \frac{1}{nh_n} \sum_{i=1}^n E\left\{K\left(\frac{x - X_i}{h_n}\right)\right\} \\ &= \frac{1}{h_n} E\left\{K\left(\frac{x - X_1}{h_n}\right)\right\} \\ &= \frac{1}{h_n} \int_{-\infty}^{\infty} K\left(\frac{x - t}{h_n}\right) f(t) dt \\ &= \int_{-\infty}^{\infty} K(u) f(x - uh_n) du \end{aligned}$$

Above, we used the substitution $u = (x - t)/h_n$.

- Thus, the exact bias of $\hat{f}_{h_n}(x)$ is

$$\begin{aligned} \text{Bias}\{\hat{f}_{h_n}(x)\} &= \int_{-\infty}^{\infty} K(u) f(x - uh_n) du - f(x) \\ &= \int_{-\infty}^{\infty} K(u) \{f(x - uh_n) - f(x)\} du \end{aligned} \quad (8.8)$$

- The expression for bias shown in (8.8) will only have a closed form for special choices of $K(\cdot)$ and $f(\cdot)$.
- Nevertheless, we can get a reasonable approximation of this bias for small h_n .

- To approximate the bias for small h_n , we can use the following Taylor series approximation

$$f(x - uh_n) - f(x) \approx -uh_nf'(x) + \frac{u^2h_n^2}{2}f''(x)$$

Plugging this approximation into our expression for the bias in (8.8) gives:

$$\begin{aligned} \text{Bias}\{\hat{f}_{h_n}(x)\} &\approx -h_nf'(x) \int_{-\infty}^{\infty} uK(u)du + \frac{h_n^2f''(x)}{2} \int_{-\infty}^{\infty} u^2K(u)du \\ &= \frac{h_n^2f''(x)}{2} \int_{-\infty}^{\infty} u^2K(u)du \\ &= \frac{h_n^2f''(x)\mu_2(K)}{2} \quad \text{where } \mu_2(K) = \int_{-\infty}^{\infty} u^2K(u)du \\ &= \text{ABias}\{\hat{f}_{h_n}(x)\} \end{aligned} \tag{8.9}$$

Here, $\text{ABias}\{\hat{f}_{h_n}(x)\}$ stands for the approximate bias.

- Formula (8.9) shows the direct dependence of the magnitude of bias on the value of the bandwidth.
- Formula (8.9) also shows the effect of the curvature $f''(x)$ of the density on the magnitude of bias.

Approximate Variance

- The exact variance of a kernel density estimate $\hat{f}_{h_n}(x)$ is

$$\begin{aligned} \text{Var}\{\hat{f}_{h_n}(x)\} &= \frac{1}{n^2h_n^2} \sum_{i=1}^n \text{Var}\left\{K\left(\frac{x-X_i}{h_n}\right)\right\} \\ &= \frac{1}{nh_n^2} \text{Var}\left\{K\left(\frac{x-X_1}{h_n}\right)\right\} \\ &= \frac{1}{nh_n^2} \int_{-\infty}^{\infty} K^2\left(\frac{x-t}{h_n}\right)f(t)dt - \frac{1}{n} \left[\frac{1}{h_n} E\left\{K\left(\frac{x-X_1}{h_n}\right)\right\} \right]^2 \\ &= \frac{1}{nh_n} \int_{-\infty}^{\infty} K^2(u)f(x-uh_n)du - \frac{1}{n} \left[\text{Bias}\{\hat{f}_{h_n}(x)\} + f(x) \right]^2 \end{aligned}$$

- We will ignore the last term because it is of order $1/n$. Then, if we use the Taylor series approximation $f(x - uh_n) = f(x) - uh_nf'(x) + \dots$, we

have:

$$\begin{aligned}
 \text{Var}\{\hat{f}_{h_n}(x)\} &\approx \frac{f(x)}{nh_n} \int_{-\infty}^{\infty} K^2(u)du - \frac{f'(x)}{n} \int_{-\infty}^{\infty} uK^2(u)du + \dots \\
 &\approx \frac{f(x)\kappa_2(K)}{nh_n} \quad \text{where } \kappa_2(K) = \int_{-\infty}^{\infty} K^2(u)du \\
 &= \text{AVar}\{\hat{f}_{h_n}(x)\}
 \end{aligned}$$

Approximate Mean Integrated Squared Error (AMISE)

- Using our approximations for the bias and variance, we can get an approximate expression for the mean-squared error of $\hat{f}_{h_n}(x)$ at the point x

$$\begin{aligned}
 \text{MSE}\{\hat{f}_{h_n}(x)\} &\approx \text{AVar}\{\hat{f}_{h_n}(x)\} + \left(\text{ABias}\{\hat{f}_{h_n}(x)\}\right)^2 \\
 &= \frac{f(x)\kappa_2(K)}{nh_n} + \frac{h_n^4[f''(x)]^2\mu_2^2(K)}{4} \quad (8.10)
 \end{aligned}$$

- Notice that if we want the MSE to go to 0 as $n \rightarrow \infty$, we need the following two things to happen:
 - $h_n \rightarrow 0$ as $n \rightarrow \infty$
 - $nh_n \rightarrow \infty$ as $n \rightarrow \infty$

- The approximate mean integrated squared error (AMISE) of the kernel density estimator is obtained by integrating the approximation (8.10) for MSE across x

$$\begin{aligned}
 \text{AMISE}\{\hat{f}_{h_n}\} &= \frac{\kappa_2(K)}{nh_n} \int_{-\infty}^{\infty} f(x)dx + \frac{h_n^4\mu_2^2(K)}{4} \int_{-\infty}^{\infty} [f''(x)]^2dx \\
 &= \frac{\kappa_2(K)}{nh_n} + \frac{h_n^4\mu_2^2(K)}{4} \int_{-\infty}^{\infty} [f''(x)]^2dx \quad (8.11)
 \end{aligned}$$

8.4.3 Bandwidth Selection with the Normal Reference Rule and Silverman's "Rule of Thumb"

- If we differentiate the formula for AMISE given in (8.11) with respect to h_n and set it to zero, we get the following equation for h_n^{opt} which would be the bandwidth minimizing $\text{AMISE}\{\hat{f}_{h_n}\}$:

$$0 = \frac{-\kappa_2(K)}{n(h_n^{opt})^2} + (h_n^{opt})^3\mu_2^2(K) \int_{-\infty}^{\infty} [f''(x)]^2dx$$

- The solution of the above equation gives the optimal bandwidth:

$$h_n^{opt} = n^{-1/5} \left(\int_{-\infty}^{\infty} [f''(x)]^2 dx \right)^{-1/5} \kappa_2(K)^{1/5} \mu_2(K)^{-2/5}$$

- For the case of a Gaussian kernel,

$$\begin{aligned} \kappa_2(K) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-u^2} du = \frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{\sqrt{2}}{\sqrt{2\pi}} e^{-u^2} du = \frac{1}{2\sqrt{\pi}} \\ \mu_2(K) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u^2 e^{-u^2/2} du = 1 \end{aligned}$$

so that, in the case of a Gaussian kernel, the optimal bandwidth is given by

$$h_n^{opt} = n^{-1/5} (2\sqrt{\pi})^{-1/5} \left(\int_{-\infty}^{\infty} [f''(x)]^2 dx \right)^{-1/5}$$

- However, the optimal bandwidth h_n^{opt} for a kernel density estimate depends on the unknown quantity

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

- Similar to the Scott and FD rules for choosing the bin width of histogram, one way of setting the bandwidth h_n of a kernel density estimate is to use the value of $\int_{-\infty}^{\infty} [f''(x)]^2 dx$ when it is assumed that $f(x)$ is the density of a Normal($0, \sigma^2$) random variable.
- If $f(x) = \text{Normal}(0, \sigma^2)$, then

$$\int_{-\infty}^{\infty} [f''(x)]^2 dx = \frac{3}{8\sqrt{\pi}\sigma^5}$$

- If we use this assumption about $f''(x)$ and assume a Gaussian kernel, the formula for the optimal bandwidth becomes bandwidth is

$$h_n^{opt} = n^{-1/5} (2\sqrt{\pi})^{-1/5} \left(\frac{3}{8\sqrt{\pi}\sigma^5} \right)^{-1/5} = \sigma n^{-1/5} \sigma \left(\frac{4}{3} \right)^{1/5} \approx 1.06 \sigma n^{-1/5}$$

- The rule $h_n^{opt} = 1.06 \sigma n^{-1/5}$ works pretty well if the true density has a roughly Gaussian shape. For example, unimodal, non-heavy tails, not too strong skewness, etc.

- The **Normal reference rule** for the bandwidth is

$$h_n^{NR} = 1.06\tilde{\sigma}n^{-1/5}$$

- Here, $\tilde{\sigma}$ is usually either $\tilde{\sigma} = \hat{\sigma}$ or $\tilde{\sigma} = s$.
- $h_n = 1.06\hat{\sigma}n^{-1/5}$ is typically too large if $f(x)$ is multimodal or if $f(x)$ has substantial skewness.
- This oversmoothing effect of $h_n = 1.06\hat{\sigma}n^{-1/5}$ can be reduced somewhat by replacing $\hat{\sigma}$ with

$$s = \min\left\{\hat{\sigma}, \frac{IQR}{1.34}\right\}$$

- For multimodal distributions, we typically have $\hat{\sigma} \leq IQR/1.34$ while for strongly skewed distributions such as the log-normal distribution we typically have $\hat{\sigma} \geq IQR/1.34$.
- For these reasons, $\tilde{\sigma} = s$ is often suggested when using the Normal reference rule.

- Silverman's "rule-of-thumb" for the bandwidth is

$$h_n^{SR} = 0.9sn^{-1/5}$$

(see Chapter 3 of Silverman (2018)).

- This rule is just an adjustment for the fact that $1.06sn^{-1/5}$ is still too large for many skewed or multimodal distribution and using 0.9 instead of 1.06 reduces this problem.

- **Exercise 8.5** Assuming that $f(x) = \frac{1}{\sqrt{2\pi}\sigma}e^{-x^2/2\sigma^2}$, show that

$$\int_{-\infty}^{\infty} [f''(x)]^2 dx = \frac{3}{8\sqrt{\pi}\sigma^5}$$

- **Exercise 8.6** Suppose $X_1, \dots, X_n \sim N(0, \sigma^2)$. Suppose that we have density estimate $\hat{f}_{h_n}(x)$ that uses the Gaussian kernel.

- Compute the exact values of $E\{\hat{f}_{h_n}(x)\}$ and $\text{Var}\{\hat{f}_{h_n}(x)\}$.
- Compute $\text{AMISE}\{\hat{f}_{h_n}\}$. Can you get an expression for the value of h_n which minimizes AMISE?

8.5 Cross-Validation for Bandwidth Selection

8.5.1 Squared-Error Cross-Validation

- The usual goal in bandwidth selection is to choose the bandwidth which minimizes the mean integrated squared error (MISE)

$$\text{MISE}(h) = E \left[\int \{\hat{f}_h(x) - f(x)\}^2 dx \right] \quad (8.12)$$

or some related criterion which also measures an expected discrepancy between $\hat{f}_h(x)$ and $f(x)$.

- The MISE can be rewritten as

$$\text{MISE}(h) = E \left[\int \hat{f}_h^2(x) dx \right] - 2 \int E \left[\hat{f}_h(x) \right] f(x) dx + \int f^2(x) dx \quad (8.13)$$

- If the goal is to minimize $\text{MISE}(h)$, we can ignore the last term since it does not depend on h .

- Our goal will be to find a bandwidth that minimizes an estimate of $\text{MISE}(h)$ (an estimate which ignores the last term in (8.13)), and this estimate will use a technique called leave-one-out **cross-validation**.
- Regarding the first term in (8.13), we can just estimate this expectation with

$$\int \hat{f}_h^2(x) dx$$

- The second term in (8.13) is trickier because it has $f(x)$ in it.
- We can simplify this term though

$$\int E \left[\hat{f}_h(x) \right] f(x) dx = E \left[\frac{1}{h} K \left(\frac{X_1 - X_2}{h} \right) \right]$$

(why is this true?)

- We can construct an estimate of (8.13) by first defining the following “leave-one-out” estimate

$$\hat{f}_{h,-i}(x) = \frac{1}{(n-1)h} \sum_{j \neq i} K \left(\frac{x - X_j}{h} \right)$$

- In other words, $\hat{f}_{h,-i}(x)$ is a density estimate constructed from using bandwidth h and all the data except for the i^{th} observation.
- Then, we are going use the following quantity to estimate $\int E[\hat{f}_h(x)]f(x)dx$

$$\frac{1}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i) = \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} \frac{1}{h} K\left(\frac{X_i - X_j}{h}\right)$$

- The term $\frac{1}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i)$ is referred to as a leave-one-out cross-validation estimate.
- The expectation of this quantity is

$$\begin{aligned} E\left\{\frac{1}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i)\right\} &= \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} E\left\{\frac{1}{h} K\left(\frac{X_i - X_j}{h}\right)\right\} \\ &= E\left\{\frac{1}{h} K\left(\frac{X_1 - X_2}{h}\right)\right\} \end{aligned}$$

- The leave-one-out **cross-validation estimate of the MISE** (ignoring the irrelevant $\int f^2(x)dx$) is

$$\hat{J}_{MISE}(h) = \int \hat{f}_h^2(x)dx - \frac{2}{n} \sum_{i=1}^n \hat{f}_{h,-i}(X_i)$$

- The integrated squared error cross-validation choice of the bandwidth $h_{n,cv}$ is the value of $h > 0$ which minimizes $\hat{J}_{MISE}(h)$

$$h_{n,cv} = \arg \min_{h>0} \hat{J}_{MISE}(h)$$

8.5.2 Computing the Cross-validation Bandwidth

- **R** does have built-in capabilities for finding the bandwidth through cross-validation, but let's do an example ourselves to see how the process works.
- First, we can build a function called `J_mise` that has input and output:
 - Input: a value of the bandwidth h and a vector of data
 - Output: the value of $\hat{J}_{MISE}(h)$

```

J_mise <- function(h, x) {
  n <- length(x)
  loo.val <- rep(0, n)
  for(k in 1:n) {
    ## compute the leave-one-out density estimate
    ## only focus on density on interval (18, 90)
    loo.fhat <- density(x[-k], bw=h, from=18, to=90)
    loo.fhat.fn <- approxfun(loo.fhat$x, loo.fhat$y)
    loo.val[k] <- loo.fhat.fn(x[k])
  }
  fhat <- density(x, bw=h, from=18, to=90)
  fhat.sq.fn <- approxfun(fhat$x, fhat$y^2)

  ans <- integrate(fhat.sq.fn, lower=18, upper=90)$value - 2*mean(loo.val)
  return(ans)
}

```

- Now, we want to use our **R** function to compute $\hat{J}(h_j)$ over a grid of bandwidth values

$$h_{min} \leq h_1 < \dots < h_q \leq h_{max}$$

- The smallest and largest possible bandwidths h_{min} and h_{max} can be chosen by looking at plots of the density for different bandwidths.
- h_{min} should correspond to a density estimate which is very nonsmooth while h_{max} should correspond to a density which is oversmoothed.
- For the ages from the kidney data, $h_{min} = 1/2$ and $h_{max} = 5$ seem like reasonable choices.
- Let us compute $\hat{J}(h)$ for a grid of 100 bandwidths between 1/2 and 5:

```

h.grid <- seq(1/2, 5, length.out=100)
CV.est <- rep(0, 100)
for(j in 1:100) {
  CV.est[j] <- J_mise(h=h.grid[j], x=kidney$age)
}

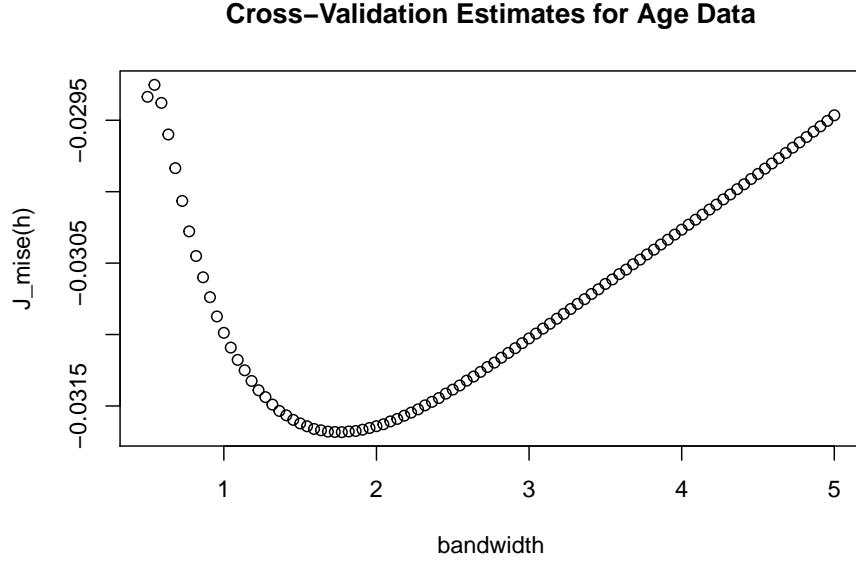
```

- Now, if we plot $\hat{J}(h)$ vs. h , we can see what the best value of the bandwidth is. From the graph, it appears that a bandwidth of roughly $h = 1.8$ minimizes $\hat{J}(h)$

```

plot(h.grid, CV.est, xlab="bandwidth", ylab="J_mise(h)",
     main = "Cross-Validation Estimates for Age Data")

```



- The specific value of the bandwidth where $\hat{J}(h_j)$ reaches its minimum is:

```
h.grid[ which.min(CV.est) ]
```

```
## [1] 1.772727
```

8.5.3 Likelihood Cross-Validation

- An alternative to MISE is the **Kullback-Leibler (KL) divergence**

$$\begin{aligned} \text{KL}(h) &= \int \log\left(\frac{f(x)}{\hat{f}_h(x)}\right) f(x) dx \\ &= - \int \log\{\hat{f}_h(x)\} f(x) dx + \int \log\{f(x)\} f(x) dx \end{aligned}$$

- We only need to get an estimate of $\int \log\{\hat{f}_h(x)\} f(x) dx$ because $\int \log\{f(x)\} f(x) dx$ does not depend on h .
- We can use the same approach as we did for integrated squared error cross-validation to estimate $\int \log\{\hat{f}_h(x)\} f(x) dx$.
- The leave-one-out **cross-validation estimate of the KL divergence** (ignoring the irrelevant $\int \log\{f(x)\} f(x) dx$ term) is

$$\hat{J}_{KL}(h) = -\frac{1}{n} \sum_{i=1}^n \log\{\hat{f}_{h,-i}(X_i)\}$$

- Choosing the bandwidth which minimizes $\hat{J}_{KL}(h)$ is often referred to as **likelihood cross-validation**.
- An **R** function which can compute $\hat{J}_{KL}(h)$ is given below:

```
J_KL <- function(h, x) {
  n <- length(x)
  loo.val <- rep(0, n)
  for(k in 1:n) {
    ## compute the leave-one-out density estimate
    ## only focus on density on interval (18, 90)
    loo.fhat <- density(x[-k], bw=h, from=18, to=90)
    loo.fhat.fn <- approxfun(loo.fhat$x, loo.fhat$y)
    loo.val[k] <- (-1)*log(loo.fhat.fn(x[k]))
  }
  return(mean(loo.val))
}
```

-
- **Exercise 8.7** Using the **age** variable from the kidney function data, find the best bandwidth using a Gaussian kernel and likelihood cross-validation.
-

8.6 Density Estimation in R

- In **R**, kernel density estimates are computed using the **density** function

```
density(x, bw, kernel, n, ...)
```

- **x** - the vector containing the data
- **bw** - the value of the bandwidth.
 - **bw** = **nrd0** gives the default bandwidth rule. This is Silverman's rule-of-thumb $h_n = 0.9sn^{-1/5}$
 - **bw** = **nrd** gives the bandwidth $h_n = 1.06\hat{\sigma}n^{-1/5}$
 - **bw** = **ucv** or **bw** = **bcv** find the bandwidth using cross-validation
- **kernel** - the choice of kernel function. The default kernel is the Gaussian kernel.

- Be careful, some of the non-Gaussian kernels used in the `density` function are scaled differently than the definitions you might often see in textbooks or on-line resources.
- `n` - the number of equally spaced points at which the density is to be estimated. The default is 512

-
- In this section, we will use the `galaxies` dataset in the `MASS` package. The first few observations of the `galaxies` dataset look like:

```
library(MASS)
galaxies[1:5]
```

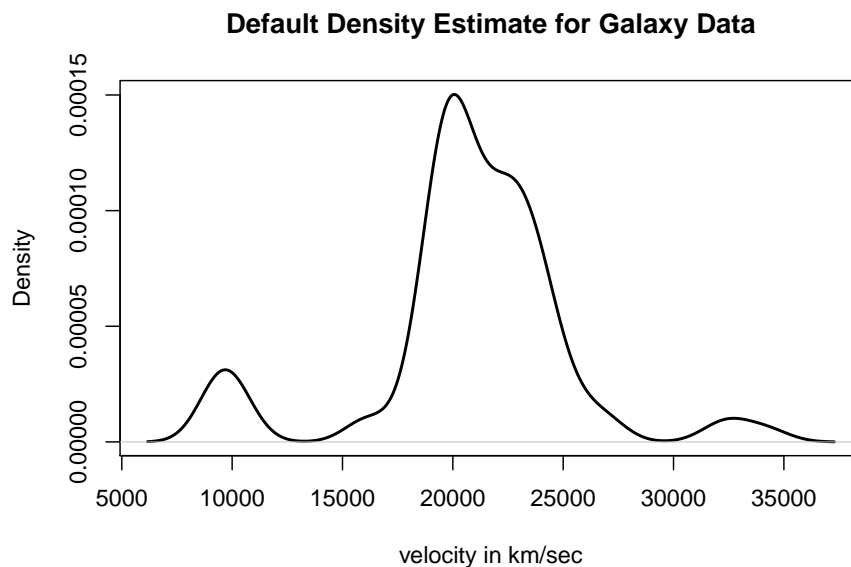
```
## [1] 9172 9350 9483 9558 9775
```

- Kernel density estimates can be computed in **R** using the `density` function

```
galax.dens <- density(galaxies)
```

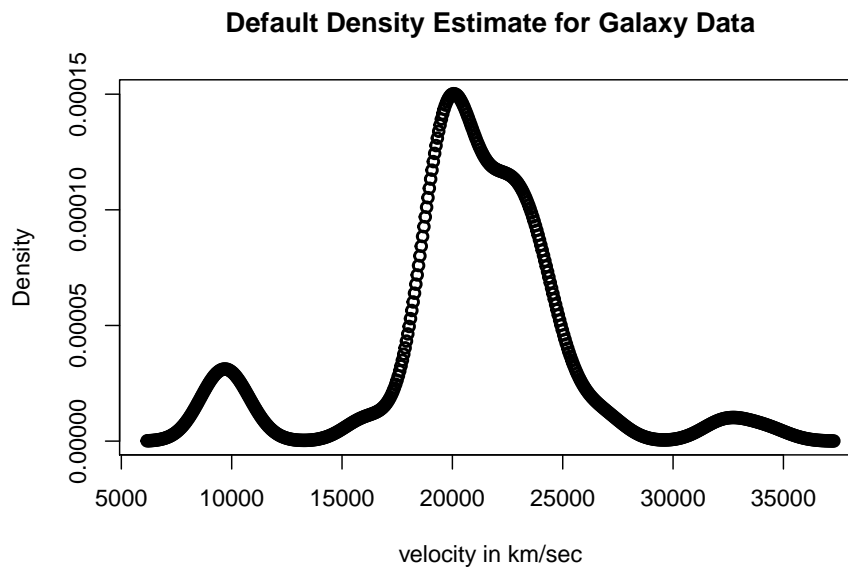
- You can display a density plot just by applying the `plot` function to our `galax.dens` object

```
plot(galax.dens, main="Default Density Estimate for Galaxy Data",
     xlab="velocity in km/sec", ylab="Density", lwd=2)
```



- The density function returns vectors `x` and `y` as components
 - `x` - the vector of points at which the density was estimated
 - `y` - the value of the estimated density at each of the `x` points
- So, just plotting the `(x, y)` should give you a plot of the density estimate

```
plot(galax.dens$x, galax.dens$y, main="Default Density Estimate for Galaxy Data",  
     xlab="velocity in km/sec", ylab="Density", lwd=2)
```



- The default in **R** is to estimate the density at 512 points. Thus, `galax.dens$x` and `galax.dens$y` should each have length 512.

- The `bw` component returned by the `density` function is the bandwidth used to estimate the density.

```
galax.dens$bw
```

```
## [1] 1001.839
```

- The default bandwidth selection rule in **R** is Silverman’s rule-of-thumb $h_n^{SR} = 0.9sn^{-1/5}$.
- We can check that this is true with the following code:

```
0.9*min(sd(galaxies), IQR(galaxies)/1.34)/(length(galaxies)^(1/5))

## [1] 1001.839
```

-
- The **R** function **approxfun** is useful if you want to compute the (approximate) value of the density estimate at a particular point. This approximation will be very close to the true value since the **density** function returns the value of the density over a dense grid of points.
 - **approxfun** just linearly interpolates between a set of x and y values.
 - Note that, as a default, **approxfun** returns NA values if you try to evaluate the function at points which are either less than the minimum x value or greater than maximum x value.
 - For example, suppose we want to know the value of the density estimate at the points 18000 and 33000. This could be done with the following code

```
galaxy.fn <- approxfun(galax.dens$x, galax.dens$y)
galaxy.fn(18000)
```

```
## [1] 4.73857e-05
```

```
galaxy.fn(33000)
```

```
## [1] 1.004542e-05
```

-
- **Exercise 8.8** Plot the density estimate for the galaxy dataset using the following three rules for finding the bandwidth: (1) **bw = nrd**, (2) **bw=nrd0**, (3) **bw=ucv**. Based on these plots, how many distinct “clusters” or “groups” would you say the galaxy observations fall into.

- **Exercise 8.9** Consider a density estimate of the form

$$\tilde{f}(x) = \sum_{k=1}^4 \pi_k \frac{1}{\sigma_k} K\left(\frac{x - \mu_k}{\sigma_k}\right),$$

where $\sigma_k > 0$ and the π_k represent probabilities, that is, $\pi_k \geq 0$ with $\pi_1 + \pi_2 + \pi_3 + \pi_4 = 1$. Can you guess values for π_k , μ_k , and σ_k that fit the galaxy data well? Try finding the best values of (π_k, μ_k, σ_k) by plotting $\tilde{f}(x)$ next to the kernel density estimate returned by the `density` function in R.

8.7 Additional Reading

- Additional reading which covers the material discussed in this chapter includes:
 - Chapters 2-3 from Silverman (2018)
 - Chapter 6 from Wasserman (2006)
 - Chapters 2-3 from Härdle et al. (2012)
 - Chapter 4 from Izenman (2008)
 - Sheather (2004)

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