Applied Statistics - Notes

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Preface

Every theory section in these notes has been taken from two sources:

- An Introduction to Statistical Learning [1]
- Applied Multivariate Statistical Analysis (sixth edition). [2]

About:

GitHub repository

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1 Sample Geometry

1.1 The Geometry of the Sample

A single **multivariate observation** is the **collection of measurements on p different variables taken on the same item or trial**. If n **observations** have been obtained, the entire data set can be placed in an $n \times p$ array (or matrix), also called **data frame**:

$$\underset{(n\times p)}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} \tag{1}$$

Each **row** of $\mathbf{X}$ represents a **multivariate observation**. Since the entire data frame is often one particular realization of what might have been observed, we say that the data frame are a **sample of size n from a p-variate "population"**. The sample then consists of n measurements, each of which has p components.

Look at the matrix, n measurements (rows), each of which has p components (columns). In mathematics, each n row contains p columns and vice versa.

The data frame can be plotted in two different ways:

1. p-dimensional scatter plot, where the rows represent n points in p-dimensional space;

2. Geometrical representation, p vectors in n-dimensional space.

1.1.1 Scatter plot

For the **p-dimensional scatter plot**, the rows of $\mathbf{X}$ represent n points in p-dimensional space:

$$\underset{(n\times p)}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \\ \vdots \\ \mathbf{x}_n' \end{bmatrix} \begin{array}{l} \leftarrow \text{1st (multivariate) observation} \\ \\ \\ \leftarrow n\text{th (multivariate) observation} \end{array} \tag{2}$$

The row vector $\mathbf{x}_j'$, representing the jth observation, contains the coordinates of a point. The **scatter plot** of n points in p-dimensional space **provides information** on the **locations and variability of the points**.

Note: when p (dimensional space) is greater than 3, the **scatter plot** representation cannot actually be graphed. Yet the consideration of the data as n points in p dimensions provides **insights that are not readily available from algebraic expressions**.

1.1.2 Geometrical representation

The alternative **geometrical representation** is constructed by considering the data as p **vectors in n-dimensional space**. Here we take the elements of the columns of the data frame to be the coordinates of the vectors:

$$\underset{(n\times p)}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix} = [\mathbf{y}_1 \mid \mathbf{y}_2 \mid \cdots \mid \mathbf{y}_p] \tag{3}$$

Then the **coordinates** of the first point $\mathbf{y}_1 = [x_{11}, x_{21}, \ldots, x_{n1}]$ **are the** n **measurements** on the first variable.

In general, the ith point $\mathbf{y}_i = [x_{11}, x_{21}, \ldots, x_{n1}]$ is determined by the n-tuple of all measurements on the ith variable.

Geometrical representations usually **facilitate understanding** and lead to further insights. The ability to **relate algebraic expressions to the geometric concepts** of length, angle and volume is therefore **very important**.

1.1.3 Geometrical interpretation of the process of finding a sample mean

Before starting the explanation, you need to understand a few things.

- The **length** of a vector $\mathbf{x}' = [x_1, x_2, \ldots, x_n]$ with n components is defined by:

  $$L_x = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} \tag{4}$$

  Multiplication of a vector $\mathbf{x}$ by a scalar c changes the length:

  $$\begin{aligned} L_{cx} &= \sqrt{c^2 \cdot x_1^2 + c^2 \cdot x_2^2 + \cdots + c^2 \cdot x_n^2} \\ &= |c| \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} \\ &= |c|\, L_x \end{aligned}$$

  So, for example, in $n = 2$ dimensions, the vector:

  $$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

  The length of $\mathbf{x}$, written L_x, is defined to be:

  $$L_x = \sqrt{x_1^2 + x_2^2}$$

- Another important concept is **angle**. Consider two vectors in a plane and the angle θ between them: The value θ can be represented as the

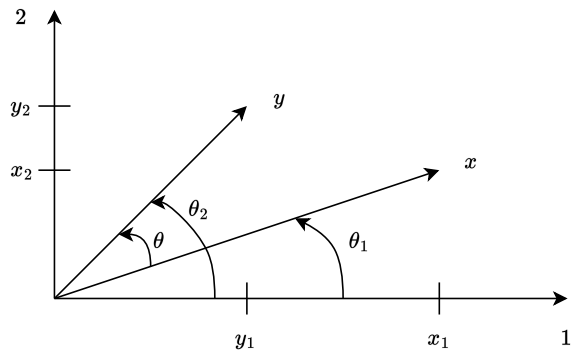


Figure 1: The angle θ between $\mathbf{x}' = [x_1, x_2]$ and $\mathbf{y}' = [y_1, y_2]$.

difference between the angles θ_1 and θ_2 formed by the two vectors and the first coordinate axis. Since, by definition:

$$\cos(\theta_1) = \frac{x_1}{L_x} \quad \cos(\theta_2) = \frac{y_1}{L_y}$$
$$\sin(\theta_1) = \frac{x_2}{L_x} \quad \sin(\theta_2) = \frac{y_2}{L_y}$$
$$\cos(\theta) = \cos(\theta_2 - \theta_1) = \cos(\theta_2)\cos(\theta_1) + \sin(\theta_2)\sin(\theta_1)$$

The angle θ between the two vectors $\mathbf{x}' = [x_1, x_2]$ and $\mathbf{y}' = [y_1, y_2]$ is specified by:

$$\cos(\theta) = \cos(\theta_2 - \theta_1) = \left(\frac{y_1}{L_y}\right)\left(\frac{x_1}{L_x}\right) + \left(\frac{y_2}{L_y}\right)\left(\frac{x^2}{L_x}\right) = \frac{x_1 y_1 + x_2 y_2}{L_x L_y} \tag{5}$$

- With the angle equation 5, it's convenient to introduce the **inner product** of two vectors:

$$\mathbf{x}\mathbf{y}' = x_1 y_1 + x_2 y_2$$

So let us rewrite:

  - The **length** equation 4:

$$\mathbf{x}'\mathbf{x} = x_1 x_1 + x_1 x_1 = x_1^2 + x_2^2 \longrightarrow L_x = \sqrt{x_1^2 + x_2^2} \Longrightarrow L_x = \sqrt{\mathbf{x}'\mathbf{x}} \tag{6}$$

  - The **angle** equation 5:

$$\cos(\theta) = \frac{x_1 y_1 + x_2 y_2}{L_x L_y} \Longrightarrow \cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{L_x L_y}$$

    And using the rewritten length equation:

$$\cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{L_x L_y} \Longrightarrow \cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{\sqrt{\mathbf{x}'\mathbf{x}} \cdot \sqrt{\mathbf{y}'\mathbf{y}}}$$

- The **projection** (or shadow) of a vector $\mathbf{x}$ on a vector $\mathbf{y}$ is:

$$\frac{(\mathbf{x}'\mathbf{y})}{\mathbf{y}'\mathbf{y}}\mathbf{y} = \frac{(\mathbf{x}'\mathbf{y})}{L_y}\frac{1}{L_y}\mathbf{y} \tag{7}$$

Where the vector $\frac{1}{L_y}\mathbf{y}$ has unit length. The **length of the projection** is:

$$\frac{|\mathbf{x}'\mathbf{y}|}{L_y} = L_x \left|\frac{\mathbf{x}'\mathbf{y}}{L_x L_y}\right| = L_x \left|\cos(\theta)\right| \tag{8}$$

Where θ is the angle between $\mathbf{x}$ and $\mathbf{y}$:

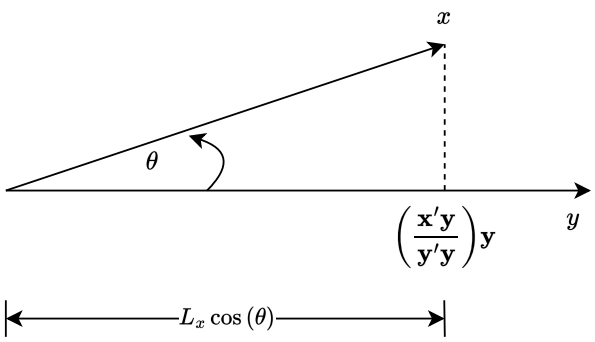


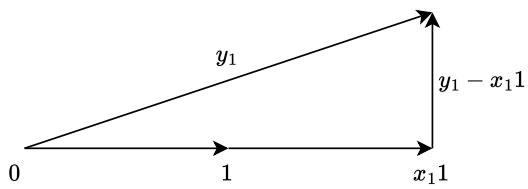
Figure 2: The projection of $\mathbf{x}$ on $\mathbf{y}$.

Start by defining the $n \times 1$ vector $\mathbf{1}'_n = [1, 1, \ldots, 1]$. The vector $\mathbf{1}$ forms equal angles with each of the n coordinates axes, so the vector $\left(\frac{1}{\sqrt{n}}\right)\mathbf{1}$ has unit length in the equal-angle direction. Consider the vector $\mathbf{y}'_i = [x_{1i}, x_{2i}, \ldots, x_{ni}]$. The projection of $\mathbf{y}_i$ on the unit vector $\left(\frac{1}{\sqrt{n}}\right)\mathbf{1}$ is:

$$\mathbf{y}'_i\left(\frac{1}{\sqrt{n}}\mathbf{1}\right)\frac{1}{\sqrt{n}}\mathbf{1} = \frac{x_{1i} + x_{2i} + \cdots + x_{ni}}{n}\mathbf{1} = \overline{x}_i\mathbf{1} \tag{9}$$

Although it may seem like a complex equation at first glance, it is nothing more than the mean! In fact, the **sample mean** $\overline{\mathbf{x}}_i = \frac{(x_{1i} + x_{2i} + \cdots + x_{ni})}{n} = \frac{\mathbf{y}'_i\mathbf{1}}{n}$ corresponds to the multiple of $\mathbf{1}$ required to give the projection of $\mathbf{y}_i$ onto the line determined by $\mathbf{1}$.

Furthermore, using the projection, you can obtain the **deviation** (**mean corrected**). For each $\mathbf{y}_i$ we have the decomposition:



Where $\overline{x}_i\mathbf{1}$ is perpendicular to $y_i - \overline{x}_i\mathbf{1}$. The **deviation**, or **mean corrected**, vector is:

$$\mathbf{d}_i = \mathbf{y}_i - \overline{x}_i\mathbf{1} = \begin{bmatrix} x_{1i} - \overline{x}_i \\ x_{2i} - \overline{x}_i \\ \vdots \\ x_{ni} - \overline{x}_i \end{bmatrix} \tag{10}$$

The **elements** of $\mathbf{d}_i$ are the **deviations of the measurements on the ith variable from their sample mean**.

Using the length rewritten with inner product (equation 6) and the deviation (equation 10), we obtain:

$$L^2_{\mathbf{d}_i} = \mathbf{d}_i'\mathbf{d}_i = \sum_{j=1}^{n} (x_{ji} - \overline{x}_i)^2 \tag{11}$$

$$(\text{Length of deviation vector})^2 = \text{sum of squared deviations}$$

From the sample standard deviation, we see that the **squared length is proportional to the variance** of the measurements on the ith variable. Equivalently, the **length is proportional to the standard deviation**. So longer vectors represent more variability than shorter vectors.

Furthermore, for any two deviation vectors $\mathbf{d}_i$ and $\mathbf{d}_k$:

$$\mathbf{d}_i'\mathbf{d}_k = \sum_{j=1}^{n} (x_{ji} - \overline{x}_i)(x_{jk} - \overline{x}_k) \tag{12}$$

And with a few mathematical operations, we can get it:

$$r_{ik} = \frac{s_{ik}}{\sqrt{s_{ii}}\sqrt{s_{kk}}} = \cos(\theta_{ik}) \tag{13}$$

Where the **cosine** of the angle is the **sample correlation coefficient**. Note: s_{ik} is the **sample covariance**:

$$s_{ik} = \frac{1}{n}\sum_{j=1}^{n} (x_{ji} - \overline{x}_i)(x_{jk} - \overline{x}_k) \qquad i = 1, 2, \ldots, p, \quad k = 1, 2, \ldots, p \tag{14}$$

Thus:

- If the two deviation vectors have **nearly the same orientation**, the sample correlation will be close to 1;

- If the two vectors are **nearly perpendicular**, the sample correlation will be approximately zero;
- If the two vectors are oriented in **nearly opposite directions**, the sample correlation will be close to -1.

1.2 Generalized Variance

Before starting the explanation, you need to understand what is a sample variance.

A **sample variance** is defined as:

$$s_k^2 = s_{kk} = \frac{1}{n-1} \sum_{j=1}^{n} (x_{jk} - \overline{x}_k)^2 \qquad k = 1, 2, \ldots, p \tag{15}$$

With a single variable, the **sample variance is often used to describe the amount of variation in the measurements on that variable**. When p variables are observed on each unit, the variation is described by the **sample variance-covariance matrix**:

$$\mathbf{S} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix} = \left\{ s_{ik} = \frac{1}{n-1} \sum_{j=1}^{n} (x_{ji} - \overline{x}_i)(x_{jk} - \overline{x}_k) \right\} \tag{16}$$

The sample covariance matrix contains p variances and $\frac{1}{2}p(p-1)$ potentially different covariances. Sometimes it's desirable to **assign a single numerical value for the variation expressed by S**. One choice for a value is the determinant of $\mathbf{S}$, which reduces to the usual sample variance of a single characteristic when $p = 1$. This determinant is called the **generalized sample variance**:

$$\text{Generalized sample variance} = \det(\mathbf{S}) = |\mathbf{S}| \tag{17}$$

2 Statistical Learning

2.1 Introduction

Suppose that we observe a quantitative response Y and p different predictors, $X_1, X_2, \ldots, X_p$. We assume that there is some relationship between Y and $X = (X_1, X_2, \ldots, X_p)$, which can be written in the general form:

$$Y = f(X) + \varepsilon \tag{18}$$

Where ε is an **error term**, which is **independent** of X and has **mean zero**. The function f represents the **systematic information** that X provides about Y. The **function** f that connects the input variables to the output variable **is in general unknown**.

Example 1

For **example**, on the left-hand panel of figure 3, a plot `income` versus `years of education` for 30 individuals in the Income data set.

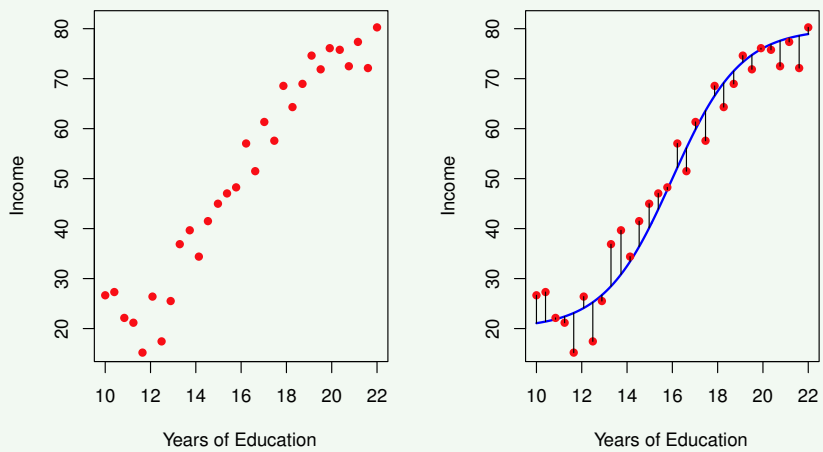


Figure 3: The `Income` data set. [1]

As you can see, the plot suggests that one might be able to predict `income` using `years of education`. Since `Income` is a simulated data set, the function f is known and is shown by the blue curve in the right-hand panel. The **vertical lines** represent the **error terms** ε. We note that some of the 30 observations lie above the blue curve and some lie below it; overall, the **errors have approximately mean zero**.

In essence, **statistical learning refers to a set of approaches for estimating** f. In this chapter we outline some of the key theoretical concepts that arise in estimating f.

2.2 Why Estimate f (systematic information provided by a predictor about a quantitative response)?

There are two main reasons that we may wish to estimate f: **prediction** and **inference**.

2.2.1 Prediction

In many situations, a set of inputs X are readily available, but the output Y cannot be easily obtained. In this setting, since the error term ε averages to zero, we can predict Y using:

$$\hat{Y} = \hat{f}(X) \tag{19}$$

- $\hat{f}$ represents our **estimate for f**
- $\hat{Y}$ represents **prediction** for Y

The function $\hat{f}$ is often treated as a **black box**, in the sense that one is not typically concerned with the exact form of $\hat{f}$, provided that **it yields accurate predictions for Y**.

Example 2

As an **example**, suppose that:

- $X_1, \ldots, X_p$ are **characteristics of a patient's blood sample** that can be easily measured in a lab.
- Y is a variable encoding the **patient's risk for a severe adverse reaction to a particular drug**.

It is natural to seek to predict Y using X, since we can then avoid giving the drug in question to patients who are at high risk of an adverse reaction. That is, patients for whom the estimate of Y is high.

The accuracy of $\hat{Y}$ as a prediction for Y depends on two quantities: **reducible error** and **irreducible error**.

- In general, $\hat{f}$ will not be a perfect estimate for f, and this **inaccuracy** will introduce some error. This is a **reducible error** because we can potentially **improve the accuracy of $\hat{f}$ by using the most appropriate statistical learning technique to estimate f**.
- Even if it were possible to form a perfect estimate for f, so that our estimated response took the form $\hat{Y} = f(X)$, our prediction would still have some error in it! This is because Y is also a function of ε (error term), which, by definition, cannot be predicted using X. Therefore, variability associated with ε also affects the accuracy of our predictions. This is the **irreducible error**, because **no matter how well we estimate f, we cannot reduce the error introduced by ε**.

The real question is: *why is the irreducible error larger than zero?* Well, the quantity ε may contain unmeasured variables that are useful in predicting Y: since we don't measure them, f cannot use them for its prediction. The quantity ε may also contain unmeasurable variation.

Example 3

For **example**, the risk of an adverse reaction might vary for a given patient on a given day, depending on manufacturing variation in the drug itself or the patient's general feeling of well-being on that day.

Consider a given estimate $\hat{f}$ and a set of predictors X, which yields the prediction $\hat{Y} = \hat{f}(X)$. Assume for a moment that both $\hat{f}$ and X are fixed, so that the only variability comes from ε (error term). Then, it's easy to show that:

$$\begin{aligned} E\left(Y - \hat{Y}\right)^2 &= E\left[f(X) + \varepsilon - \hat{f}(X)\right]^2 \\ &= \underbrace{\left[f(X) - \hat{f}(X)\right]^2}_{\text{Reducible}} + \underbrace{\text{Var}(\varepsilon)}_{\text{Irreducible}} \end{aligned} \tag{20}$$

- $\left[f(X) - \hat{f}(X)\right]^2$ represents the **squared difference between the predicted and actual value of Y**
- $E\left(Y - \hat{Y}\right)^2$ represents the **average**, or **expected value**
- $\text{Var}(\varepsilon)$ represents the **variance associated with the error term ε**

The focus of this course is on *techniques* for estimating f with the aim of **minimizing the reducible error**. It is important to keep in mind that the irreducible error will always provide an upper bound on the accuracy of our prediction for Y. Unfortunately, this bound is almost always unknown in practice.

Example 4

Consider a company that is interested in conducting a direct-marketing campaign.
The *goal* is to identify individuals who are likely to respond positively to a mailing, based on observations of demographic variables measured on each individual.
In this case:

- The demographic variables serve as *predictors*;
- Response to the marketing campaign (either positive or negative) serves as the *outcome*.

The company is <u>not</u> interested in obtaining a deep understanding of the relationships between each individual predictor and the response; instead, the company simply **wants to accurately predict the response using the predictors**.
This is an example of **modeling for prediction**.

2.2.2 Inference

We are often interested in understanding the association between Y (quantitative response) and $X_1, \ldots, X_p$ (p-predictors). In this situation we wish to estimate f (systematic information), but our goal is not necessarily to make predictions for Y. Now it's obviously that $\hat{f}$ cannot be treated as a black box, because we need to know its exact form. In this setting, one may be interested in **answering the following questions**:

- ***Which predictors are associated with the response?*** It is often the case that only a small fraction of the available predictors are substantially associated with Y. So, **identifying** the few **important predictors among a large set of possible variables can be extremely useful**.
- ***What is the relationship between the response and each predictor?*** Larger values of the predictor are associated with larger values of Y. Other predictors may have the opposite relationship. The relationship between the response and the given predictor may **depend** on:
  - The **complexity** of f;
  - The **values of the other predictors**.
- ***Can the relationship between Y and each predictor be adequately summarized using a linear equation, or is the relationship more complicated?*** Historically, **most methods** for estimating f **have** taken **linear form**. But often the true relationship is more complicated, in which case a **linear model may not provide an accurate representation** of the relationship between the input and the output variables.

Example 5

Modeling the brand of a product that a customer might purchased based on variables such as:

- Price
- Store
- Location
- Discount levels
- Competition price

And so forth. In this situation one might really be most interested in the **association between each variable and the probability of purchase**. For instance, *to what extent is the product's price associated with sales?*
This is an example of **modeling for inference**.

Example 6

Consider the following figure:

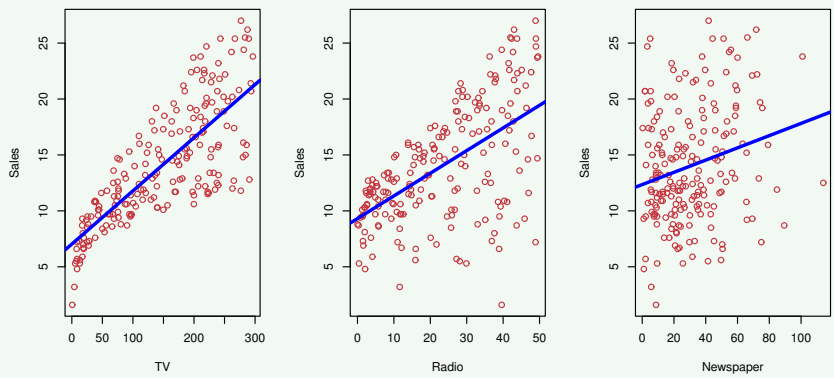


Figure 4: The `Advertising` data set. The plot displays `sales`, in thousands of units, as a function of `TV`, `radio`, and `newspaper` budgets, in thousands of dollars, for 200 different markets. In each plot we show the simple least squares fit of `sales` to that variable. In other words, each blue line represents a simple model that can be used to predict `sales` using `TV`, `radio`, and `newspaper`, respectively.

One may be interested in answering questions such as:

- *Which media are associated with sales?*
- *Which media generate the biggest boost in sales?*
- *How large of an increase in sales is associated with a given increase in TV advertising?*

This situation falls into the **inference model**.

2.2.3 Difference between prediction and inference

Example 7

In a real estate setting, one may seek to relate values of homes to inputs such as:

- Crime rate
- Zoning
- Distance from a river
- Air quality
- Schools
- Income level of community
- Size of houses

And so forth. In this case one might be interested in the association between each individual input variable and housing price. For instance, *how much extra will a house be worth if it has a view of the river?* This is an **inference problem**.

But attention! Alternatively, one may simply be interested in predicting the value of a home given its characteristics: *is this house under or over valued?* And this is a **prediction problem**.

So, as you can see from the example, the difference between a prediction problem and an inference problem is so small. A problem can change its nature because the ultimate goal is also changing.

2.3 How do we estimate f?

We will always assume that we have observed a set of n different data points. For example, in figure 3 at page 10 we observed $n = 30$ data points. These observations are called **training data** because we will **use these observations to train, or teach, our method how to estimate f**.

Let:

- x_{ij} represent the value of the jth predictor, or input, for observation i, where $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, p$
- y_i represent the response variable for the ith observation.

Then, our training data consist of:

$$\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

Where $x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$.

Our goal is to **apply a statistical learning method to the training data in order to estimate the unknown function f**. In other words, we want to find a function $\hat{f}$ such that $Y \approx \hat{f}(X)$ for any observations (X, Y). Most statistical learning methods for this task can be characterized as either **parametric** or **non-parametric**.

2.3.1 Parametric Methods

The **parametric methods** involve a two-step model-based approach:

1. Select a model.

   (a) **Make an assumption about the functional form**, or shape, of f. For **example**, one very simple assumption is that f is linear in X:

   $$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p \tag{21}$$

   This is a **linear model** (that will be discussed in the future). Once we have assumed that f is linear, **the problem of estimating f is greatly simplified**. Instead of having to estimate an entirely arbitrary p-dimensional function $f(X)$, one only needs to **estimate the $p+1$ coefficients** $\beta_0, \beta_1, \ldots, \beta_p$.

2. Use training data to fit/train the model.

   (b) After a model has been selected, we need a **procedure that uses the training data to fit the model** or **train the model**. In the case of the linear method, we need to estimate the parameters $\beta_0, \beta_1, \ldots, \beta_p$. So, we want to find values of these parameters such that:

   $$Y \approx \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

   The most **common approach to fitting** the (linear) model is referred to as (**ordinary**) **least squares** (that will be discussed in the future). However, the least squares is one of many possible ways to fit the linear model.

The parametric model-based reduces the problem of estimating f down to one of **estimating a set of parameters**. In fact, assuming a parametric form for f simplifies the problem of estimating f because it is generally much easier to estimate a set of parameters in the linear model, than it is to fit an entirely arbitrary function f.

⚠ Potential disadvantage

The **model** we choose will **usually not match the true unknown form of f**. If the chosen model is **too far** from the true f, then our **estimate will be poor**.

✔ Possible (partial) solution

We can try to address this problem by **choosing flexible models** that can **fit many different possible functional forms for f**. But fitting a more flexible model **requires estimating a greater number of parameters**.

These more complex models (**flexible models**) can lead to a phenomenon known as **overfitting** the data, which essentially means **they follow the errors**, or **noise**, **too closely** (these issues are discussed throughout this course).

2.3.2 Non-Parametric Methods

The **non-parametric** methods do not make explicit assumptions about the functional form of f. Instead they seek an **estimate of f that gets as close to the data points as possible without being too rough or wiggly**.

✔ Major advantage over parametric approaches

By avoiding the assumption of a particular functional form for f, non-parametric approaches have the **potential to accurately fit a wider range of possible shapes** for f. Any parametric approach brings with it the possibility that the functional form used to estimate f is very different from the true f, in which case the resulting model will not fit the data well.

⚠ Disadvantage

Since non-parametric approaches do not reduce the problem of estimating f to a small number of parameters, **a very large number of observations** (far more than is typically needed for a parametric approach) **is required in order to obtain an accurate estimate** for f.

2.4 Supervised and Unsupervised Learning

Most statistical learning problems fall into one of two categories: **supervised learning** or **unsupervised learning**.

Supervised learning

The examples that we have discussed in this chapter all fall into the **supervised learning** domain. For each observation of the predictor measurement(s) $x_i, i = 1, \ldots, n$ there is an associated response measurement y_i.

We wish to **fit a model that relates the response to the predictors**, with the aim of:

- **Accurately predicting the response for future observations** (prediction, section 2.2.1)
- **Better understanding the relationship between the response and the predictors** (inference, section 2.2.2)

Unsupervised learning

The **unsupervised learning** describes the somewhat more challenging situation in which **for every observation** $i = 1, \ldots, n$, **we observe a vector of measurements** x_i **but no associated response** y_i.

In this setting, we are in some sense *working blind*; the situation is referred to as **unsupervised** because **we lack a response variable that can supervise our analysis**. We can **seek to understand the relationships between the variables or between the observations**.

2.5 Assessing Model Accuracy

The aim of this section is to decide which method will give the best results for a given set of data.

2.5.1 Measuring the Quality of Fit (MSE)

In order to evaluate the performance of a statistical learning method on a given data set, we need some way to measure how well its predictions actually match the observed data. We need to **quantify the extent to which the predicted response value for a given observation is close to the true response value for that observation**. The most commonly-used measure is the **mean squared error (MSE)**:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{f}\left(x_i\right)\right)^2 \tag{22}$$

- $\hat{f}\left(x_i\right)$ is the prediction that $\hat{f}$ gives for the ith observation
- y_i the ith true response

Obviously,the MSE will be:

- **Small** if the predicted responses are very close to the true responses;
- **Large** if for some of the observations, the predicted and true responses differ substantially.

In general, we do not really care how well the method works on the training data. Rather, **we are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen test data**.

Example 8

Suppose that we are interested in developing an algorithm to predict a stock's price based on previous stock returns.

We can train the method using stock returns from the past 6 months. But we <u>don't</u> really care how well our method predicts last week's stock price.
We instead **care about how well it predict tomorrow's price or next month's price**.

Example 9

Suppose that we have clinical measurements (e.g. weight, blood pressure, height, age, family history of disease) for a number of patients, as well as information about whether each patient has diabetes.

We can use these patients to train a statistical learning method to predict risk of diabetes based on clinical measurements.

In practice, **we want this method to accurately predict diabetes risk for *future patients* based on their clinical measurements**. Again, we are not very interested in whether or not the method accurately predicts diabetes risk for patients used to train the mode, since we already know which of those patients have diabetes!

In mathematical terms, suppose that we fit our statistical learning method on our training observations:

$$\{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

And we obtain the estimate $\hat{f}$. We can then compute:

$$\hat{f}(x_1), \hat{f}(x_2), \ldots, \hat{f}(x_n)$$

If these are approximately equal to:

$$y_1, y_2, \ldots, y_n$$

Then **the training MSE is small**.

However, we are really not interested in whether $\hat{f}(x_i) \approx y_i$; instead, we want to know whether $\hat{f}(x_0)$ is approximately equal to y_0, where (x_0, y_0) is a **previously unseen test observation not used to train the statistical learning method**.

We **want to choose the method that gives the lowest test mean squared error (MSE)**, as opposed to the lowest training MSE. In other words, if we had a large number of test observations, we could compute:

$$\text{Ave}\left(y_0 - \hat{f}(x_0)\right)^2 \tag{23}$$

The **average squared prediction error for these test observations** (x_0, y_0).

⚠ Problem to find the lowest training MSE

There is no guarantee that the method with the lowest training MSE will also have the lowest test MSE.

The problem is that **many statistical methods specifically estimate coefficients so as to minimize the training set MSE**. For these methods, the **training set MSE can be quite small**, **but the test MSE is often much larger**.

Example 10

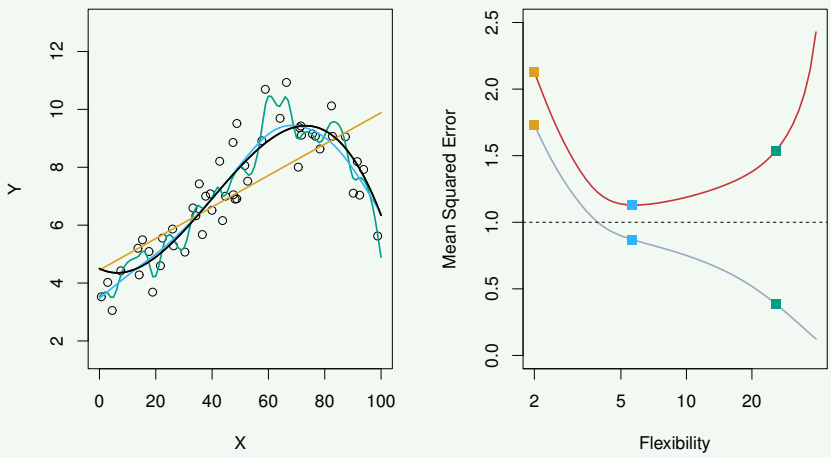


Figure 5: On the left: *data simulated from f, shown in black. Three estimates of f are shown: the linear regression (orange curve), and two smoothing spline fits (blue and green curves).* Right: *Training MSE (grey curve), test MSE (red curve), and minimum possible test MSE over all methods (dashed line). Squares represent the training and test MSEs for the three fits shown in the left-hand panel.* [1]

In the left-hand panel we have generated observations from the (error term) equation 18 with the true f given by the black curve.
The orange, blue and green curves illustrate three possible estimates for f obtained using methods with increasing levels of flexibility.

It is clear that as the **level of flexibility increases**, the **curves fit the observed data more closely**.
The *green curve* is the most flexible and matches the data very well; however, we observe that it fits the true f (shown in black) poorly because it is too wiggly.
By **adjusting the level of flexibility** of the smoothing spline fit, we can **produce many different fits to this data**.

Example 10

Referring to Figure 5

We now move on to the right-hand panel. The grey curve displays the average training MSE as a function of flexibility, or more formally the **degrees of freedom**[a], for a number of smoothing splines.
The orange, blue and green squares indicate the MSEs associated with the corresponding curve in the left-hand panel.
A more restricted and hence smoother curve has fewer degrees of freedom than a wiggly curve. The *linear regression* is at the most restrictive end, with two degrees of freedom.

The **training MSE declines monotonically as flexibility increases**. In this example, the true f is non-linear, and so the orange linear fit is not flexible enough to estimate f well.
The *green curve* has the lowest training MSE of all three methods, since it corresponds to the most flexible of the three curves fit in the left-hand panel.

The test MSE is displayed using the red curve. As with the training MSE, the test MSE initially declines as the level of flexibility increases. At some point, the test MSE levels off and then starts to increase again. Consequently, the orange and green curves both have high test MSE. The blue curve minimizes the test MSE, which should not be surprising given that visually it appears to estimate f the best in the left-hand panel.
The horizontal dashed line indicates $\mathrm{Var}(\varepsilon)$, the **irreducible error** (eq. 20), which **corresponds to the lost achievable test MSE among all possible methods**. Hence, the smoothing spline represented by **the blue curve is close to optimal**.

[a] The degrees of freedom is a **quantity that summarizes the flexibility of a curve**.

In the right-hand panel of figure 5, as the flexibility of the Statistical learning method increases, we observe a **monotone decrease in the training MSE and a U-shape** in the test MSE. This is a **fundamental property** of statistical learning that holds regardless of the particular data set at hand and regardless of the Statistical method being used.

As model flexibility increases, the training MSE will decrease, but the test MSE may not. **When a given method yields a small training MSE but a large test MSE**, we are said to be **overfitting** the data.

Why does this phenomenon happen?

This happens because our **statistical learning procedure** is working too hard to find patterns in the training data, and **may be picking up some patterns that are just caused by random chance** rather than by true properties of the unknown function f.

So when we *overfit* the training data, the **test MSE** will be **very large because the supposed patterns that the method found in the training data simply don't exist in the test data**.

We almost always expect the **training MSE to be smaller than the test MSE** because most **statistical learning methods** either directly or indirectly seek to **minimize the training MSE**. *Overfitting* refers specifically to the test case in which a **less flexible model would have yielded a smaller test MSE**.

Example 11

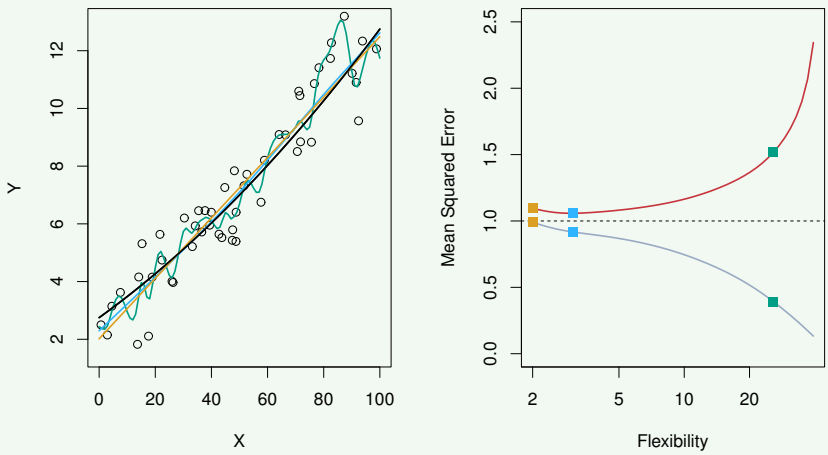


Figure 6: Details are as in Figure 5, using a different true f that is much closer to linear. In this setting, linear regression provides a very good fit to the data. [1]

This figure provides another **example** in which the true f is approximately linear. Again we observe that the training MSE decreases monotonically as the model flexibility increases, and that there is a *U-shape* in the test MSE.

However, because the truth is close to linear, the **test MSE only decreases slightly before increasing again**, so that the **orange least squares fit is substantially better than the highly flexible green curve**.

Example 12

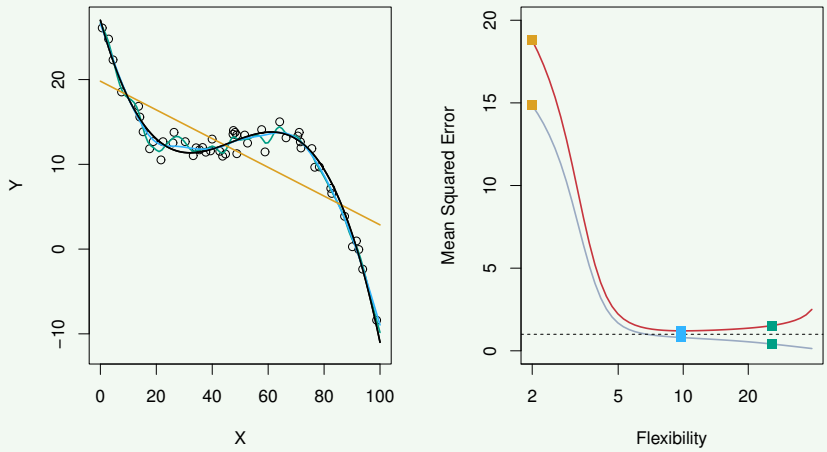


Figure 7: Details are as in Figure 5, using a different true f that is far from linear. In this setting, linear regression provides a very poor fit to the data. [1]

Finally, this figure displays an **example** in which f is highly non-linear.

The training and test MSE curves still exhibit the same general patterns, but now there is a rapid decrease in both curves before the test MSE start to increase slowly.

2.5.2 The Bias-Variance Trade-Off

The U-shape observed in the test MSE curves (Figures: 5, 6, 7) turns out to be the result of two competing properties of statistical learning methods.

The expected test MSE, for a given value x_0, can always be decomposed into the sum of three fundamental quantities:

- The **variance** of $\hat{f}(x_0)$
- The squared **bias** of $\hat{f}(x_0)$
- The **variance of the error terms ε**

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \mathrm{Var}\left(\hat{f}(x_0)\right) + \left[\mathrm{Bias}\left(\hat{f}(x_0)\right)\right]^2 + \mathrm{Var}(\varepsilon) \tag{24}$$

Where $E\left(y_0 - \hat{f}(x_0)\right)^2$ defines the **expected test MSE** at x_0 and refers to the **average test MSE** that we would obtain if we **repeatedly estimated f using a large number of training sets, and tested each at x_0**.

The equation 24 tell us that in order to minimize the expected test error, we need to **simultaneously select a statistical learning method that** achieves **<u>low</u> variance and <u>low</u> bias**. Note that variance is inherently a nonnegative quantity, and squared bias is also nonnegative. Hence, we see that the expected test MSE can never lie below $\mathrm{Var}(\varepsilon)$, the irreducible error (equation 20).

☆ Meaning of the variance

The **variance** refers to the **amount by which $\hat{f}$ would change if we estimated it using a different training data set**. So different training data sets will result in a different $\hat{f}$. But ideally the estimate for f should not vary too much between training sets. However, **if a method has high variance then small changes in the training data can result in large changes in $\hat{f}$**.
In general, **more flexible statistical methods have higher variance**.

Example 13

Consider the green and the orange curves in Figure 5 at page 22.

The flexible green curve is following the observations very closely. It has high variance because changing any one of these data points may cause the estimate $\hat{f}$ to change considerably.

In contrast, the orange least squares line is relatively inflexible and has low variance, because moving any single observations will likely cause only a small shift in the position of the line.

☆ Meaning of the bias

The **bias** refers to the **error that is introduced by approximating a real-life problem, which may be extremely complicated, by a much simpler model**.

Example 14

For **example**, linear regression assumes that there is a linear relationship between Y and $X_1, X_2, \ldots, X_p$. It is unlikely that any real-life problem truly has such a simple linear relationship, and so performing linear regression will undoubtedly result in some bias in the estimate of f.

In the Figure 7 on page 25, the true f is substantially non-linear, so no matter how many training observations we are given, it will not be possible to produce an accurate estimate using linear regression. In other words, linear regression results in high bias in this example.

However, in Figure 6 on page 24 the true f is very close to linear, and so given enough data, it should be possible for linear regression to produce an accurate estimate.

Generally, as we use **more flexible methods**, the **variance will increase** and the **bias will decrease**.

As we increase the flexibility of a class of methods, the bias tends to initially decrease faster than the variance increases. Consequently, the expected test MSE declines. However, at some point increasing flexibility has little impact on the bias but starts to significantly increase the variance. When this happens the test MSE increases. Note that we observed this pattern of decreasing test MSE followed by increasing test MSE in the right-hand panels of Figures 5, 6, 7. In summary:

1. We increase the flexibility of a class of methods;
2. The bias tends to initially decrease faster than the variance increases;
3. The expected test MSE declines;
4. At some point increasing flexibility has little impact on the bias but starts to significantly increase the variance;
5. The test MSE increases.

Example 15

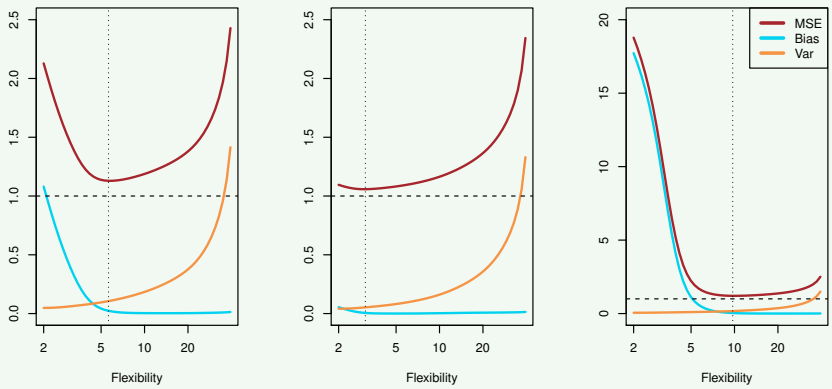


Figure 8: Squared bias (blue curve), variance (orange curve), $\mathrm{Var}(\varepsilon)$ (dashed line), and test MSE (red curve) for the three data sets in Figures 5, 6, 7. The vertical dotted line indicates the flexibility level corresponding to the smallest test MSE. [1]

Three plots illustrate equation 24 on page 26 for the examples in Figure 5, 6, 7.
In each case the blue solid curve represents the squared bias, for different levels of flexibility, while the orange curve corresponds to the variance. The horizontal dashed line represents $\mathrm{Var}(\varepsilon)$, the irreducible error. Finally, the red curve, corresponding to the test set MSE, is the sum of these three quantities.

In all three cases, the variance increases and the bias decreases as the method's flexibility increases. However, the flexibility level corresponding to the optimal test MSE differs considerably among the three data sets, because the squared bias and variance change at different rates in each of the data sets.

In the left-hand panel of this Figure, the bias initially decreases rapidly, resulting in an initial sharp decrease in the expected test MSE.

On the other hand, in the center panel of this Figure the true f is close to linear, so there is only a small decrease in bias as flexibility increases, and the test MSE only declines slightly before increasing rapidly as the variance increases.

Finally, in the right-hand panel of this Figure, as flexibility increases, there is a dramatic decline in bias because the true f is very non-linear. There is also very little increase in variance as flexibility increases. Consequently, the test MSE declines substantially before experiencing a small increase as model flexibility increases.

☆ Meaning of the bias-variance trade-off

The relationship between bias, variance, and test set MSE given in equation 24 on page 26 and displayed in the Figure 8 (previous example) is referred to as the **bias-variance trade-off**.

Good test set performance of a statistical learning method requires low variance as well as low squared bias. This is referred to as a **trade-off** because it is **easy to obtain a method with extremely low bias but high variance**[1] or **a method with very low variance but high bias** (by fitting a horizontal line to the data).

The **challenge lies in finding a method for which both the variance and the squared bias are low**. This trade-off is one of the most important recurring themes in this course.

[1] For **instance**, by drawing a curve that passes through every single training observation

2.6 Algorithm: K-Nearest Neighbors (KNN)

Many approaches attempt to **estimate the conditional distribution of Y given X**, and **then classify a given observation to the class** with **highest estimated probability**. One such method is the **K-nearest neighbors (KNN)** classifier.

In mathematical terms, given a positive integer K and a test observation x_0 the KNN classifier:

1. **Identifies** the K points in the training data that are closest to x_0, represented by $\mathcal{N}_0$.
2. It then **estimates** the conditional probability for class j as the fraction of points in $\mathcal{N}_0$ whose response values equal j:

$$\Pr\left(Y = J \mid X = x_0\right) = \frac{1}{K} \sum_{i \in \mathcal{N}_0} I\left(y_i = j\right) \tag{25}$$

3. Finally, KNN **classifies** the test observation x_0 to the class with the largest probability from the previous equation.

Example 16

Suppose that we choose $K = 3$. Then KNN algorithm:

1. Identify the three observations that are closet to the cross. As you can see in the Figure 9 on page 31, this neighborhood is shown as a circle. It consists of two blue points and one orange point, resulting in estimated probabilities of $\frac{2}{3}$ for the blue class and $\frac{1}{3}$ for the orange class.
2. Hence, KNN will predict that the black cross belongs to the blue class.

Example 17

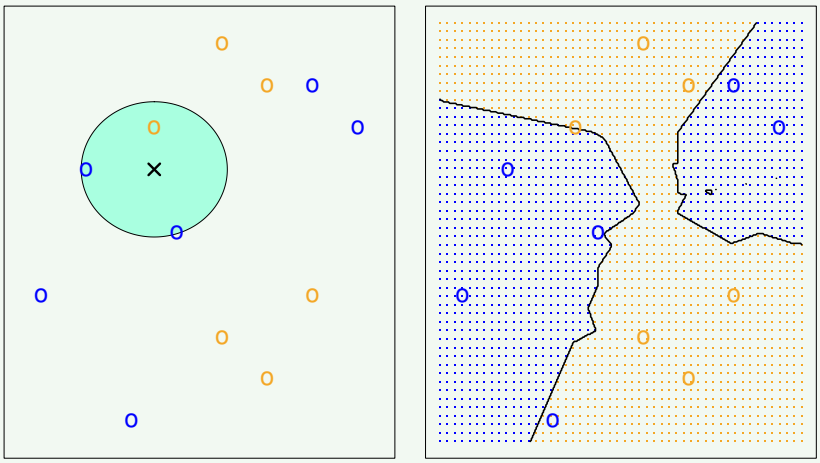


Figure 9: The KNN approach, using $K = 3$, is illustrated in a simple situation with six blue observations and six orange observations. Left: *a test observation at which a predicted class label is desired is shown as a black cross. The three closest points to the test observation are identified, and it is predicted that the test observation belongs to the most commonly-occurring class, in this case blue.* Right: *the KNN decision boundary for this example is shown in black. The blue grid indicates the region in which a test observation will be assigned to the blue class, and the orange grid indicates the region in which it will be assigned to the orange class.*

This figure provides an illustrative example of the KNN approach. In the left-hand panel, we have plotted a small training data set consisting of six blue and six orange observations. Our goal is to make a prediction for the point labeled by the black cross.

In the right-hand panel, we have applied the KNN approach with $K = 3$ at all of the possible values for X_1 and X_2, and have drawn in the corresponding KNN decision boundary.

Example 18

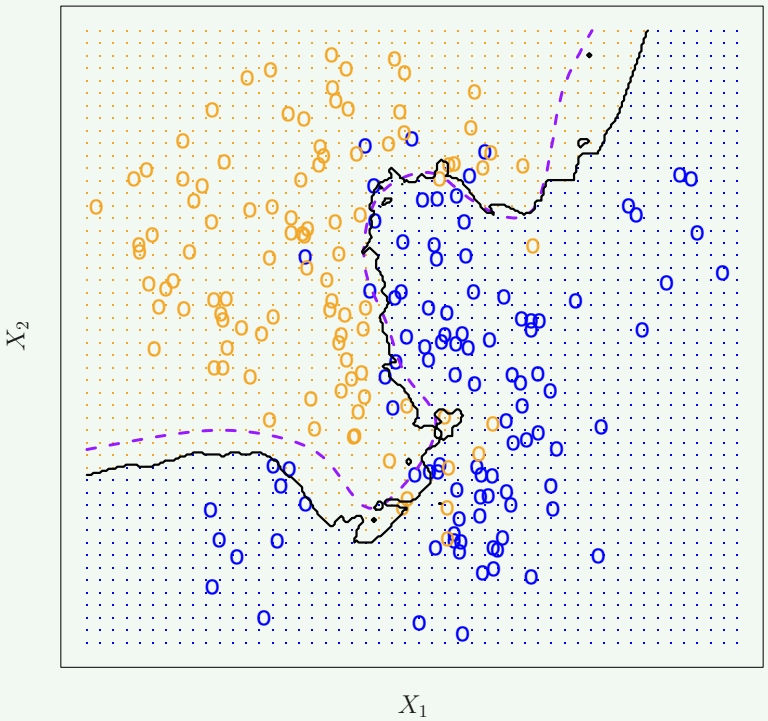


Figure 10: The black curve indicates the KNN decision boundary on the data, using $K = 10$. The Bayes decision boundary is shown as a purple dashed line. The KNN and Bayes decision boundaries are very similar.

This Figure displays the KNN decision boundary, using $K = 10$, when applied to the larger simulated data set.

References

[1] G. James, D. Witten, T. Hastie, and R. Tibshirani. *An Introduction to Statistical Learning: with Applications in R*. Springer Texts in Statistics. Springer New York, 2013.

[2] R.A. Johnson and D.W. Wichern. *Applied Multivariate Statistical Analysis*. Applied Multivariate Statistical Analysis. Pearson Prentice Hall, 2007.

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