

Applied Statistics - Notes

260236

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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**:

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

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:

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

The row vector \mathbf{x}'_j , representing the j th 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:

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

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

In general, the i th point $\mathbf{y}_i = [x_{1i}, x_{2i}, \dots, x_{ni}]$ is determined by the n -tuple of all measurements on the i th 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 $\mathbf{x}' = [x_1, x_2, \dots, x_n]$ with n components is defined by:

$$L_x = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2} \quad (4)$$

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

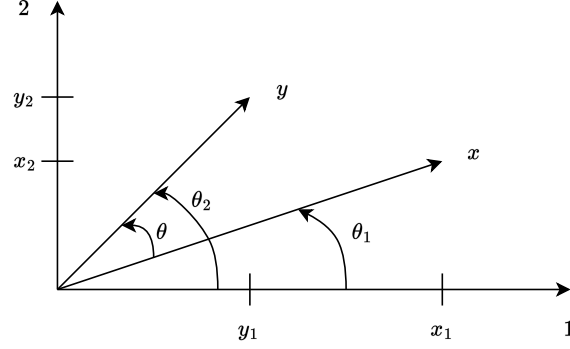


Figure 1: The angle θ between $\mathbf{x}' = [x_1, x_2]$ and $\mathbf{y}' = [y_1, y_2]$.

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

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

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

$$\cos(\theta) = \cos(\theta_2 - \theta_1) = \left(\frac{y_1}{L_y}\right)\left(\frac{x_1}{L_x}\right) + \left(\frac{y_2}{L_y}\right)\left(\frac{x_2}{L_x}\right) = \frac{x_1y_1 + x_2y_2}{L_xL_y} \quad (5)$$

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

$$\mathbf{x}\mathbf{y}' = x_1y_1 + x_2y_2$$

So let us rewrite:

- The **length** equation 4:

$$\mathbf{x}'\mathbf{x} = x_1x_1 + x_2x_2 = x_1^2 + x_2^2 \longrightarrow L_x = \sqrt{x_1^2 + x_2^2} \implies L_x = \sqrt{\mathbf{x}'\mathbf{x}} \quad (6)$$

- The **angle** equation 5:

$$\cos(\theta) = \frac{x_1y_1 + x_2y_2}{L_xL_y} \implies \cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{L_xL_y}$$

And using the rewritten length equation:

$$\cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{L_xL_y} \implies \cos(\theta) = \frac{\mathbf{x}'\mathbf{y}}{\sqrt{\mathbf{x}'\mathbf{x}} \cdot \sqrt{\mathbf{y}'\mathbf{y}}}$$

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

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

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

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

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

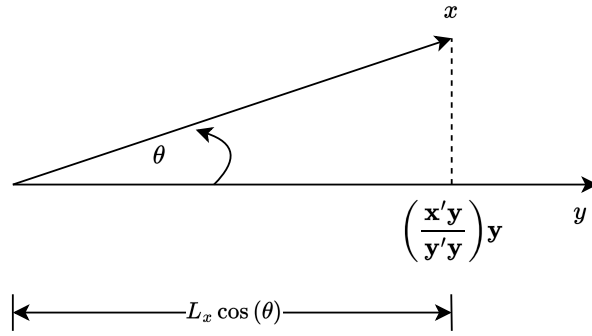


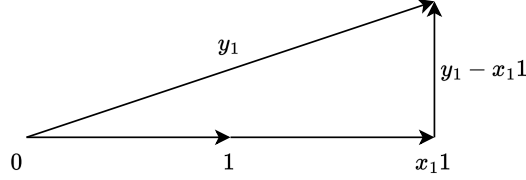
Figure 2: The projection of \mathbf{x} on \mathbf{y} .

Start by defining the $n \times 1$ vector $\mathbf{1}'_n = [1, 1, \dots, 1]$. 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 $\mathbf{y}'_i = [x_{1i}, x_{2i}, \dots, x_{ni}]$. The projection of \mathbf{y}_i on the unit vector $\left(\frac{1}{\sqrt{n}}\right)\mathbf{1}$ is:

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

Although it may seem like a complex equation at first glance, it is nothing more than the mean! In fact, the **sample mean** $\bar{x}_i = \frac{(x_{1i} + x_{2i} + \dots + x_{ni})}{n} = \frac{\mathbf{y}'_i\mathbf{1}}{n}$ 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 $\bar{x}_i \mathbf{1}$ is perpendicular to $\mathbf{y}_i - \bar{x}_i \mathbf{1}$. The **deviation**, or **mean corrected**, vector is:

$$\mathbf{d}_i = \mathbf{y}_i - \bar{x}_i \mathbf{1} = \begin{bmatrix} x_{1i} - \bar{x}_i \\ x_{2i} - \bar{x}_i \\ \vdots \\ x_{ni} - \bar{x}_i \end{bmatrix} \quad (10)$$

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

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

$$L_{\mathbf{d}_i}^2 = \mathbf{d}_i' \mathbf{d}_i = \sum_{j=1}^n (x_{ji} - \bar{x}_i)^2 \quad (11)$$

(Length of deviation vector)² = 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 i th 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 :

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

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

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

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

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

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:

$$s_k^2 = s_{kk} = \frac{1}{n-1} \sum_{j=1}^n (x_{jk} - \bar{x}_k)^2 \quad k = 1, 2, \dots, p \quad (15)$$

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**:

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

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 \mathbf{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**:

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

2 Statistical Learning

2.1 Introduction

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

$$Y = f(X) + \varepsilon \quad (18)$$

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.

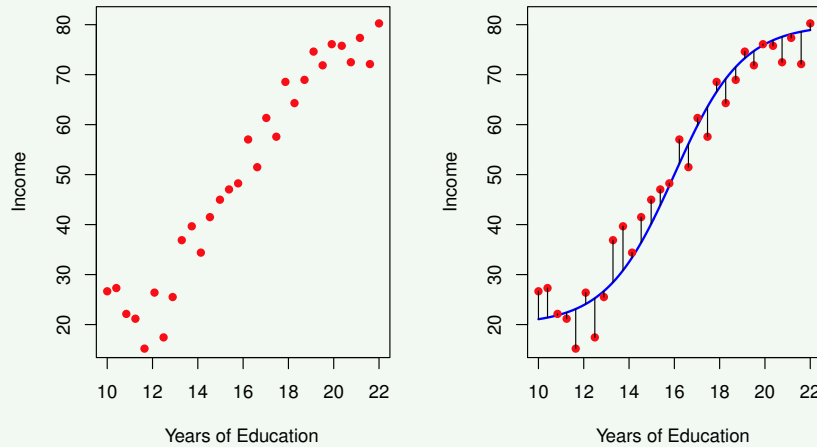


Figure 3: The Income data set. [1]

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:

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

- \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, \dots, 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:

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

- $[f(X) - \hat{f}(X)]^2$ represents the **squared difference between the predicted and actual value of Y**
- $E(Y - \hat{Y})^2$ 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 not 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, \dots, 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:

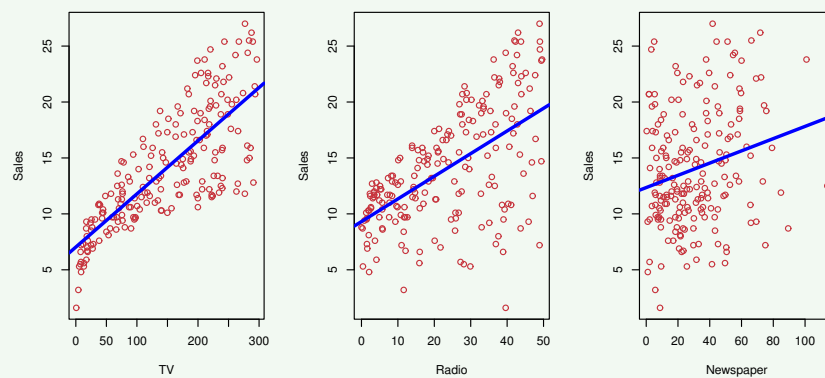


Figure 4: The **Advertising** data set. The plot displays **sales**, in thousands of units, as a function of **TV**, **radio**, and **newspaper** budgets, in thousands of dollars, for 200 different markets. In each plot we show the simple least squares fit of **sales** to that variable. In other words, 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 j th predictor, or input, for observation i , where $i = 1, 2, \dots, n$ and $j = 1, 2, \dots, p$
- y_i represent the response variable for the i th observation.

Then, our training data consist of:

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

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

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

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 :

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

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** $\beta_0, \beta_1, \dots, \beta_p$.

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 $\beta_0, \beta_1, \dots, \beta_p$. 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

TODO.

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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