Applied Statistics - Notes

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March 2024

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]

Contents

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 **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 **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

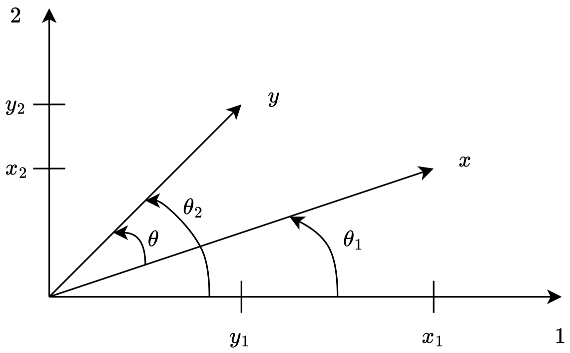


Figure 1: The angle θ between $\mathbf{x}' = [x_1, x_2]$ and $\mathbf{y}' = [y_1, y_2]$.

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 shadown) 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:

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

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

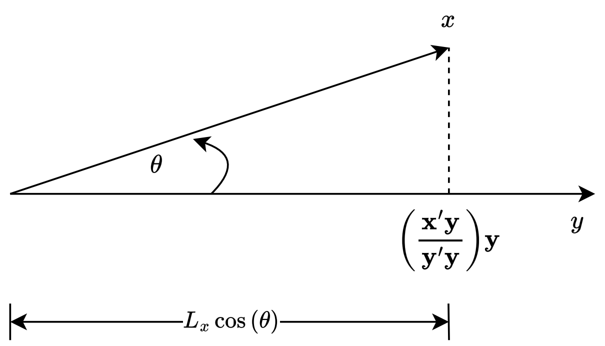


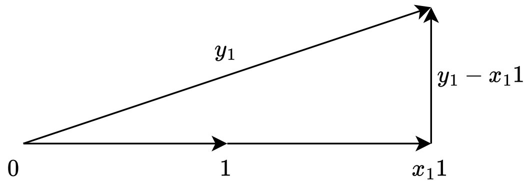
Figure 2: The projection of $\mathbf{x}$ on $\mathbf{y}$.

Start by defining the $n \times 1$ vector $\mathbf{1}_n' = [1, 1, \dots, 1]$. 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:

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

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** i**th variable from their sample mean**.

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

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

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

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 $\mathbf{d}_k$:

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

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

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

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

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

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:

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

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.

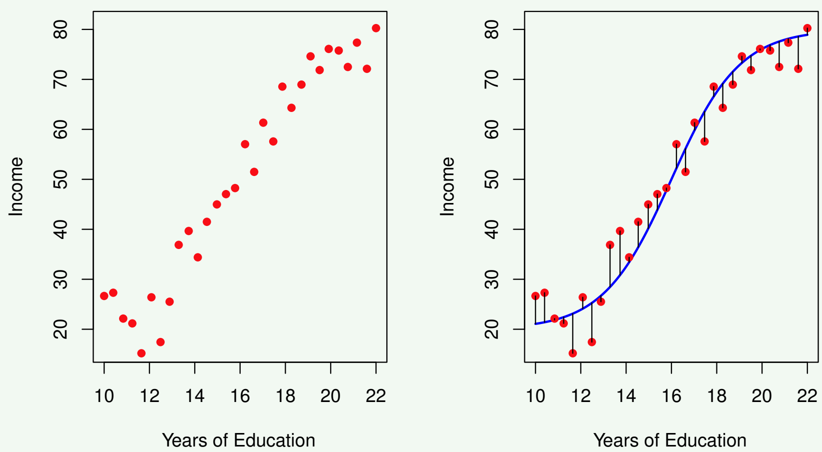


Figure 3: The `Income` data set. [1]

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:

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

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

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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