## Chapter 1

# A Case Study in Learning

## 1.1 What is Learning?

Here are some definitions of learning:<sup>1</sup>

• "Learning involves strengthening correct responses and weakening incorrect responses. Learning involves adding new information to your memory. Learning involves making sense of the presented material by attending to relevant information, mentally reorganizing it, and connecting it with what you already know."

From eLearning and the Science of Instruction by Ruth C. Clark and Richard E. Mayer

• "Learning is the relatively permanent change in a person's knowledge or behavior due to experience. This definition has three components: 1) the duration of the change is long-term rather than short-term; 2) the locus of the change is the content and structure of knowledge in memory or the behavior of the learner; 3) the cause of the change is the learner's experience in the environment rather than fatigue, motivation, drugs, physical condition or physiologic intervention."

From Learning in Encyclopedia of Educational Research, Richard E. Mayer

There are three basic types of learning in psychology:

**Classical conditioning** (for example, Pavlov's dogs- the sound of a bell leads to a salivation response). In this case, a neutral stimulus is paired with a natural response.

**Operant conditioning**: A response is increased or decreased due to reinforcement or punishment.

**Observational learning**: Learning through observation and imitation of others.

And there are generally three important stages of learning (learning as information processing)

Acquisition. An initial stage, when new information is presented and a response is established.

**Retention**: Transferring what we have learned into long term memory.

**Recall**: Use the knowledge we have obtained when it is needed (recalling a fact or performing a skill).

Consider these as we proceed into learning for machines:

<sup>&</sup>lt;sup>1</sup>Downloaded from http://theelearningcoach.com/learning/10-definitions-learning/

### Machine Learning

There are a lot of ways we might define machine learning, but consider the following<sup>2</sup>:

A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

For example, suppose we want to classify email as being "spam" or not (this is our task T). Then we'll need a database of emails labeled as to whether or not they are spam. This dataset then represents our experience E. We'll then need to decide on a performance measure- we'd probably choose the percent correct as the measure P.

There are three categories of machine learning: Supervised, unsupervised, and reinforcement learning.

• Supervised learning

Supervised learning is characterized by having labeled data with access to direct feedback (performance measure). The idea is that the computer has access to an "expert", and the computer is building up a model that mimics to behavior of the expert in such a way that it is able to predict the output of unforeseen input in the same way as the expert would have predicted it (testing on data that has not been seen is critical).

We might see that there could be issues here- If the computer simply memorizes all the input-output pairs, is that learning?

(Trade-off between accuracy and generalizability, or in statistical terms, it is a trade-off between bias and variance- more on this later).

• Unsupervised learning

Unsupervised learning is characterized by data with no labels or targets, but only a general goal. In this case, there is no "expert" available. We might be finding hidden structures in data, for example.

Data clustering is an example of unsupervised learning. Feature extraction is another example.

• Reinforcement learning

One classical example is the "truck backer-upper": We have a tractor-trailer and we need to back up the trailer into a loading dock. Think about what the space might be, what are the decisions we need to make, and what is "success"?

As another example, suppose there is a room with n slot machines. What is the strategy of play that will maximize your winning? (We'll look at this problem a bit later) In reinforcement learning, we have to expore the domain space in order to figure out the actions, so we have several things to keep track of.

#### **1.1.1** Questions for Discussion:

- 1. Consider the concept of *superstition*: This is a belief that one must engage in certain behaviors in order to gain a certain outcome, where in reality, the outcome did not depend on those behaviors. Is it possible for a computer to engage in superstitious activity? Discuss in terms of the supervised versus unsupervised learning paradigms.
- 2. A signal light comes on and is followed by one of two other lights. The goal is to predict which of the lights comes on given that the signal light comes on. The experimenter is free to arrange the pattern of the two response lights in any way- for example, one might come on 75% of the time.

Let  $E_1, E_2$  denote the event that the first (second) light comes on, and let  $A_1, A_2$  denote the prediction that the first (second) light comes on (respectively). Let  $\pi$  be the probability that  $E_1$  occurs.

<sup>&</sup>lt;sup>2</sup>Prof. T. Mitchell, CMU

- (a) If the goal is to maximize your reward through accurate predictions, what should you do in this experiment? Just give a heuristic answer- you do not have to formally justify it.
- (b) How would you program a machine to maximize it's prediction accuracy? Can you state this in mathematical terms?
- (c) What do you think happens with actual subject (human) trials?

## Chapter 2

# **Statistics**

## 2.1 Quantities and Measures for Random Data

The most basic way to characterize a numerical data set is through one number- the mean (or median or mode).

• The sample mean for a discrete set of m numbers,  $x_1, \ldots, x_m$  is given by:

$$\bar{x} = \frac{1}{m} \sum_{k=1}^{m} x_k$$

• The mean of a set of m vectors in  $\mathbb{R}^n$ :

Suppose we have m vectors in  $\mathbb{R}^n$ . We can similarly define the (sample) mean by replacing the scalar  $x_k$  with the  $k^{\text{th}}$  vector:

$$\bar{\boldsymbol{x}} = \frac{1}{m} \sum_{k=1}^{m} \boldsymbol{x}^{(k)}$$

The  $j^{\text{th}}$  element of the sample mean vector is just the sample mean of the (scalar) data in the  $j^{\text{th}}$  dimension of your collection of vectors.

- Note that we can also define the mean for a collection of  $m \times n$  matrices, as well. For example, if I have a collection of k photos that are each  $m \times n$  pixels, then I can compute the mean photo by summing the matrices together, then dividing by k.
- In fact, matrices have different properties that we can consider- A matrix can be thought of as a collection of column vectors, or as a collection of row vectors, or simply a collection of numbers.

Similarly, we can compute a mean of over the columns (and getting a column), or the mean over all rows (and get a row), or we can compute the mean over all the numerical values of the matrix, which is called the **grand mean**.

- Computing the mean in Matlab, Python and R:
  - Matlab:
    - \* If x is a row or column vector (example): x=[1,2,3,4,5]; mean(x)
    - \* If X is an  $m \times n$  matrix (example):

```
X = [1, 2, 3; 4, 5, 6];
     mean(X)
                    %Returns a row vector as default
     m=mean(X,1); %Returns a row vector 1 x n
     m=mean(X,2); %Returns a column vector m x 1
     m=mean(mean(X)); % Returns the grand mean (a scalar)
- Python: First, import numpy: import numpy as np
    * If x is a row or column vector- two methods are shown below:
     x=np.array([1,2,3,4,5]) #Example vector
     np.mean(x) #Returns a scalar
     x.mean(0)
                  #Returns an array- a scalar or a vector
   * If X is an m \times n array
     X=np.array([[1,2,3],[4,5,6]])
     X.mean(0) # Output: array([2.5, 3.5, 4.5])
     X.mean(1) # Output: array([2., 5.])
                 # Output the grand mean: 3.5
     X.mean()
     Alternatively, for the row, column means respectively:
     Xr=np.mean(X,axis=0)
```

Xm=np.mean(X,axis=1)

– R

```
* If \boldsymbol{x} is a row or column vector: then
  x<-c(1,2,3,4,5)
  np.mean(x) #Returns a scalar
               #Returns an array- a scalar or a vector
  x.mean(0)
* If X is an m \times n array
  x<-array(1:6,c(2,3)) #x is a 2 x 3 matrix</pre>
  colMeans(x)
                      #Returns: 1.5 3.5 5.5
  rowMeans(x)
                      #Returns: 3 4
  Alternatively,
  apply(x,1,mean)
                      #Returns: 3 4
  apply(x,2,mean)
                      #Returns: 1.5 3.5 5.5
```

A note about language: Should "row mean" be the mean found by summing the rows together, and producing a row, or should "row mean" be the sum through the rows, producing a column? I will typically mean the former, but I see that R uses the latter (the command colMeans produces the mean down the columns and returns a row, for example).

Just be sure you're consistent with whichever method you want to define.

• The *Median* is a number so that exactly half the data is above that number, and half the data is below that number. Although the median does not have to be unique, we follow the definitions below if we are given a finite sample:

If there are an odd number of data points, the median is the middle point. If there is an even number of data points, then there are two numbers in the middle- the median is the average of these.

The syntax for the median works in very much the same way as the mean.

• The *Mode* is the value taken the most number of times. In the case of ties, the data is multi-modal. We typically would not use the mode unless there is a special reason to do so.

#### 2.1.1 Matlab note, Linear Algebra

We'll be subtracting a row vector from each row of a matrix, and similarly, we'll subtract a column vector from each column of a matrix. You'll note that, if A is a matrix, r is a row, and c is a column, then writing something like:

 $A - r \qquad A - c$ 

would not be defined in linear algebra, and for older versions of Matlab, this was the case as well. This changed several years ago, so that "Matrix - Row" is assumed to be row subtraction for each row of the matrix, and "Matrix - Column" is assumed to be carried out column-wise on the matrix. We'll see this below.

#### 2.1.2 Centering and Double Centering Data

Let matrix A be  $m \times n$ , which may be considered n points in  $\mathbb{R}^m$  (this looks at the data column-wise) or m points in  $\mathbb{R}^n$  (looking at the data row-wise). If we wish to look at A both ways, a double-centering may be appropriate.

The result of the double-centering will be that (in Matlab), we determine A so that

 $mean(\hat{A}, 1) = 0, mean(\hat{A}, 2) = 0$ 

There are a couple of ways to do this. Here is onw algorithm, where the means are computed first.

#### Algorithm for Double Centering

- Given matrix A:
  - Compute the mean of the rows. Call this row r.
  - Compute the mean of the columns. Call this column c.
  - Compute the grand mean. Call this scalar g.
- Output the matrix: A r c + g.

Here is the implementation in Matlab, Python and R:

Matlab	Python	R
A=[1,2,3;4,5,6];	A=np.array([[1,2,3],[4,5,6]])	A<-array(1:6,c(2,3))
<pre>r=mean(A,1);</pre>	r=A.mean(0)	r=apply(A,2,mean)
<pre>c=mean(A,2);</pre>	c=A.mean(1)	c=apply(A,1,mean)
	c=c[:,np.newaxis]	
<pre>g=mean(mean(A));</pre>	g=A.mean()	g=mean(apply(A,1,mean))
B=A-r-c+g	B=A-r-c+g	B1=sweep(A,2,r)
		B2=sweep(B1,1,c)
		B=B2+g

#### Python Note about Vector Subtraction

In the Python code, we needed to "reshape" the size of the column representing the mean across A. In the first line, c=A.mean(1), we see that the shape of c is (2,). After the next line, the shape of c is (2,1). We didn't need to do that for r, although we probably should have- That is, the current shape of r is (3,), but we really wanted a row vector, so we could reshape it as r=r[np.newaxis,:] so that the shape is (1,3). Why? If you leave c and r as defined in the code above, what happens with c-r? You get a matrix- That is,

$$c - r - \begin{bmatrix} 2\\5 \end{bmatrix} - \begin{bmatrix} 2.5, 3.5, 4.5 \end{bmatrix} = \begin{bmatrix} -0.5 & -1.5 & -2.5\\2.5 & 1.5 & 0.5 \end{bmatrix}$$

So we need to be careful when we think we're subtracting vectors. Now back to the text...

As a final note, double centering is only suitable if it is reasonable that the  $m \times n$  matrix may be data in either  $\mathbb{R}^n$  or  $\mathbb{R}^m$ . For example, you probably would not double center a matrix that is 5000 × 2- Treat this as 5000 points in  $\mathbb{R}^2$ , so that the mean is in  $\mathbb{R}^2$ .

## 2.2 Variance and Standard Deviation

The number that is used to describe the spread of the data about its mean is the *variance*. As with the mean, we rarely know the underlying distribution, so again we'll focus on the sample variance.

Let  $\{x_1, \ldots, x_m\}$  be *m* real numbers, and  $\bar{x}$  its sample mean. Then the sample variance is:

$$s^{2} = \frac{1}{m-1} \sum_{k=1}^{m} (x_{k} - \bar{x})^{2}$$

If we think of the data as a vector of length m, then this formula becomes:

$$s^2 = \frac{1}{m-1} \| \boldsymbol{x} - \bar{x} \|^2$$

The standard deviation is the square root of the variance, so the standard deviation is s.

#### **Quick Example**

Let's take some template data to look at what the variance (and standard deviation) measure: Consider the data:

$$-\frac{2}{n}, -\frac{1}{n}, 0, \frac{1}{n}, \frac{2}{n}$$

If n is large, our data is tightly packed together about the mean, 0. If n is small, the data are spread out. The variance and standard deviation of this sample is:

$$s^{2} = \frac{1}{4} \left( \frac{4+1+0+1+4}{n^{2}} \right) = \frac{5}{2} \frac{1}{n^{2}}, \qquad s = \sqrt{\frac{5}{2}} \frac{1}{n}$$

and this is in agreement with our heuristic: If n is large, our data is tightly packed about the mean, and the standard deviation is small. If n is small, our data is loosely distributed about the mean, and the standard deviation is large. Another way to look at the standard deviation is in linear algebra terms: If the data is put into a vector of length m (call it x), then the (sample) standard deviation can be computed as:

$$s = \frac{\|\boldsymbol{x} - \bar{x}\|}{\sqrt{m-1}}$$

#### 2.2.1 Covariance and Correlation Coefficients

If we have two data sets, sometimes we would like to compare them to see how they relate to each other. In this case, it is important that the two data sets be ordered so that  $x_1$  is being compared to  $y_1$ , then  $x_2$  is compared to  $y_2$ , and so on.

**Definition:** Let  $X = \{x_1, \ldots, x_n\}, Y = \{y_1, \ldots, y_n\}$  be two ordered data sets with means  $m_x, m_y$  respectively. Then the sample covariance of the data sets is given by:

$$Cov(X,Y) = s_{xy}^2 = \frac{1}{n-1} \sum_{k=1}^n (x_k - m_x)(y_k - m_y)$$

There are exercises at the end of the chapter that will reinforce the notation and give you some methods for manipulating the covariance. In the meantime, it is easy to remember this formula if you think of the following:

If X and Y have mean zero, and we think of X and Y as vectors  $\boldsymbol{x}$  and  $\boldsymbol{y}$ , then the covariance is just the dot product between the vectors, divided by n-1:

$$\operatorname{Cov}(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{n-1} \boldsymbol{x}^T \boldsymbol{y}$$

We can then interpret what it means for X, Y to have a covariance of zero: x is "orthogonal" to y. Continuing with this analogy, if we normalized by the size of x and the size of y, we'd get the cosine of the angle between them. This is the definition of the correlation coefficient, and gives the relationship between the covariance and correlation coefficient:

**Definition:** The correlation coefficient between the data ordered in vector x and data in y is given by:

$$r_{xy} = \frac{s_{xy}^2}{s_x s_y} = \frac{\sum_{k=1}^n (x_k - m_x)(y_k - m_y)}{\sqrt{\sum_{k=1}^n (x_k - m_x)^2 \cdot \sum_{k=1}^n (y_k - m_y)^2}}$$

If the data in x and y have been mean subtracted, then the formula is reminiscent of something from linear algebra:

$$r_{xy} = rac{oldsymbol{x}^Toldsymbol{y}}{\|oldsymbol{x}\| \cdot \|oldsymbol{y}\|} = \cos( heta)$$

This works out so nicely because we have a  $\frac{1}{n-1}$  in both the numerator and denominator, so they cancel each other out.

We also see immediately that  $r_{xy}$  can only take on the real numbers between -1 and 1. Some interesting values of  $r_{xy}$ :

If $r_{xy}$ is:	Then the data is:
1	Perfectly correlated $(\theta = 0)$
0	Uncorrelated $(\theta = \frac{\pi}{2})$
-1	Perfectly (negatively) correlated ( $\theta = \pi$ )

One last comment before we leave this section: The covariance  $s_{xy}^2$  and correlation coefficient  $r_{xy}$  only look for *linear* relationships between data sets!

For example, we know that  $\sin(x)$  and  $\cos(x)$ , either as functions, or as data points sampled at equally spaced intervals, will be uncorrelated, but, because  $\sin^2(x) + \cos^2(x) = 1$ , we see that  $\sin^2(x)$  and  $\cos^2(x)$  are perfectly correlated.

This difference is the difference between the words "correlated" and "statistically independent". Statistical independence (not defined here) and correlations are not the same thing. We will look at this difference closely in a later section.

## 2.3 The Covariance Matrix

Suppose we have a collection of n columns, where each column represents data in one dimension. And suppose each column has p elements. The  $p \times n$  matrix X can be thought of as either p points in  $\mathbb{R}^n$  or n points in  $\mathbb{R}^p$ . Thinking of have p points in dimension i and p points in dimension j, we can compute the variance between those dimensions.

Continuing, we can compute the covariance between all pairings of the *n* dimensions resulting in an  $n \times n$  matrix (note that the diagonal entries would be the covariance of a set of data with itself- which is the regular variance). Such a matrix is known as the covariance matrix.

In the formulas below, we'll assume that X has been demean-subtracted (subtract the row representing the mean from all rows of X). The  $(i, j)^{\text{th}}$  entry in the covariance matrix is then defined as the covariance between the  $i^{\text{th}}$  and  $j^{\text{th}}$  dimensions:

$$s_{ij}^{2} = \frac{1}{p-1} \sum_{k=1}^{p} X(k,i) \cdot X(k,j)$$

Computing this for all i, j will result in an  $n \times n$  symmetric matrix, C, for which  $C_{ij} = s_{ij}^2$ .

In the exercises, you'll show that an alternative way of computing the covariance matrix is by using what we'll refer to as its definition below.

**Definition:** Let X denote a matrix of data, so that, if X is  $p \times n$ , then we have p data points in  $\mathbb{R}^n$ . Furthermore, we assume that the data in X has been mean subtracted (so the mean in  $\mathbb{R}^n$  is the zero vector). Then the  $n \times n$  covariance matrix associated with X is given by:

$$C = \frac{1}{p-1} X^T X$$

In the language of your choice, it is straightforward to compute the covariance matrix- but be sure to keep in mind the dimensions.

Matlab	Python	R
X=rand(10,3);	X=np.random.rand(10,3)	X<-matrix(runif(30),nrow=10)
C=cov(X);	C=np.cov(X.T,bias=False)	C<-cov(X)

You might note that in Python, the default matrix arrangement is reversed, and the default number to divide by is n rather than n-1, unless you include the "bias" option.

### 2.4 Exercises

1. Compute the covariance between the following data sets:

- 2. Let's explore some of the things mentioned in the text. Use a computer program to verify the following:
  - (a) "If t is a vector of equally spaced points, the sin(t) and cos(t) (computer notation) will be uncorrelated". Show this by example using Matlab, Python or R.
  - (b) Continuing, show that  $\sin^2(t)$  and  $\cos^2(t)$  are perfectly correlated (again, using Matlab, Python or R).
  - (c) Take the vector t, and let y = 2t 5. Show that the vectors t and y have a correlation of 1.
  - (d) Redo the previous experiment, but use any negative slope. What is the correlation coefficient?
- 3. Let  $\boldsymbol{x}$  be a vector of data with mean  $\bar{\boldsymbol{x}}$ , and let  $\boldsymbol{a}, \boldsymbol{b}$  be scalars.
  - (a) Show, using the definition of the mean, that the mean of  $a\mathbf{x}$  is  $a\bar{\mathbf{x}}$ .
  - (b) Similarly, find a formula for the mean of ax + b in terms of the mean of x.
- 4. Let  $\boldsymbol{x}$  be a vector of data with variance  $s_x^2$ , and let a, b be scalars.

(a) Show, using the definition of variance, that the variance of ax is  $a^2s_x^2$ . You might start with:

$$s_{(ax)}^2 = \frac{1}{m-1} \sum_{i=1}^m (ax_i - \overline{ax_i})^2$$

(b) Similarly, find a formula for the variance of ax + b in terms of the variance of x.

The exercises below explore the notion that the correlation tries to find linear relationships between data.

5. Show that, for data in vectors  $\boldsymbol{x}, \boldsymbol{y}$  and a real scalar a,

$$\operatorname{Cov}(ax, y) = a\operatorname{Cov}(x, y) = \operatorname{Cov}(x, ay)$$

- 6. For a and b fixed scalars, and data in vector  $\boldsymbol{x}$  find a formula for the Cov(x, ax + b) in terms of the variance of  $\boldsymbol{x}$ .
- 7. For a and b fixed scalars, and data in vector  $\boldsymbol{x}$ , let  $\boldsymbol{y} = a\boldsymbol{x} + b$ , find the correlation coefficient  $r_{xy}^2$  and simplify as much as possible. What do you get?
- 8. Let X be a  $p \times n$  matrix of data, where we n columns of p data points (you may assume each column has zero mean). Show that the (i, j)<sup>th</sup> entry of  $\frac{1}{p-1}X^T X$  is the covariance between the i<sup>th</sup> and j<sup>th</sup> columns of X. HINT: It might be convenient to write X in terms of its columns,

$$X = [\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n]$$

Also show that  $\frac{1}{p-1}X^T X$  is a symmetric matrix.

## 2.5 Line of Best Fit

In this section, we examine the simplest case of fitting data to a function. We are given p pairs of data (t is for "target", we'll use y for something else):

$$(x_1, t_1), (x_2, t_2), \dots (x_p, t_p)$$

We wish to find a line through the data. That is, we want to find scalars m, b so that

$$mx_i + b = t_i$$

for each pair  $(x_i, t_i)$ . Of course, if the data actually was on a line, we would not need p points- only two are needed.

Therefore we assume that there is something going on so that the data is not exactly on the line- for each point, we now have an error. We are distinguishing now between the point on the line:

$$y_i = mx_i + b$$

and the *desired* value  $t_i$ . Now the error at the *i*th point is defined as:

$$(t_i - y_i)^2 = (t_i - (mx_i + b))^2$$

and the overall error is the sum of squares error (summed over the p points):

$$E(m,b) = \sum_{k=1}^{p} (t_k - (mx_k + b))^2$$

We have now translated our problem into a Calculus problem- Find the minimum of E(m, b). Here are some exercises to lead you to the solution:

#### Exercises with the Error

1. E is a function of m and b, so the minimum value occurs where

$$\frac{\partial E}{\partial m} = 0 \qquad \frac{\partial E}{\partial b} = 0$$

Show that this leads to the system of equations: (the summation index is 1 to p)

$$m\sum x_k^2 + b\sum x_k = \sum x_k t_k$$
$$m\sum x_k + bn = \sum t_k$$

2. With linear algebra, the line of best fit becomes the matrix-vector equation below that has **no solution**. Therefore, we are looking for the least squares solution.

$mx_1 + b$ $mx_2 + b$ $mx_2 + b$	$= t_1$ $= t_2$ $= t_3$		$x_1$ $x_2$	1 1 1	$\begin{bmatrix} m \end{bmatrix}$	$\begin{bmatrix} t_1 \\ t_2 \end{bmatrix}$		
$ \begin{array}{c} mx_3 + b \\ \vdots \\ mx_p + b \end{array} $	$= t_3$ $\vdots$ $= t_p$	⇒	$\begin{array}{c} x_3\\ \vdots\\ x_p \end{array}$	:	$\begin{bmatrix} b \end{bmatrix} =$	$\begin{array}{c} \vdots \\ t_p \end{array}$	$\Rightarrow$	Ac = t

In this case, the error is the norm of the difference between the matrix product Ac = y and the known target vector t, but usually we square that difference to get the "least squares" solution. In other words, we try to find c that minimizes:

$$E(c) = \|t - y\|^2 = \|t - Ac\|^2$$

For now, we can solve this problem using the **normal equations**. That is, we will multiply both sides of our equation by  $A^T$  to get:

$$A\boldsymbol{c} = \boldsymbol{t} \quad \Rightarrow \quad A^T A \boldsymbol{c} = A^T \boldsymbol{t}$$

Originally, A was  $p \times 2$ , so now  $A^T A$  is  $2 \times 2$ , which we can invert. EXERCISE: Show that this system of two equations in two variables is the same as the system we obtained by setting the partial derivatives to zero.

3. (Toy problem) Find the line of best fit through the data:

#### A word of caution:

The line of best fit is **mathematically a unique answer**. That is, given a specific set of data, we get one answer using our technique. However, what we have not considered is whether or not the data is actually linear!

Students of statistics will recognize that this is the issue that you spend a good amount of time studyingtests for goodness of fit exist, but would take us too far afield for now.