Lecture 1

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Introduction

Suppose you are hired at a startup company making a new kind of nano-chip. Unfortunately, some of the nano-chips they manufacture explode after a month of use. This is a problem, of course, since they get a lot of angry customer calls. They hire you as a *data scientist* to solve their problem.

Their nano-manufacturing process introduces variability in the sizes of the chips and they believe this has something to do with the exploding problem. The first step is to collect some data: they manufacture five chips and let them run in a lab for one month. After that period they give you a dataset.

	height	**width**	**y=exploded?**
chip 1	0.8	0.8	1
chip 2	0.3	0.25	0
chip 3	0.2	0.8	0
chip 4	0.3	0.7	0
chip 5	0.9	0.7	1

Table 1: Your dataset. There is a special column (called y) that we are trying to predict using the other columns called features. Every row corresponds to one labeled nano-chip. The number of examples (aka Samples) is usually denoted by n and the number of features by p. In this example $n = 4$ and $p = 2$.

In this lecture we discuss the most common problem in statistics and machine learning, that of **prediction**. Lets recap the frequently used jargon:

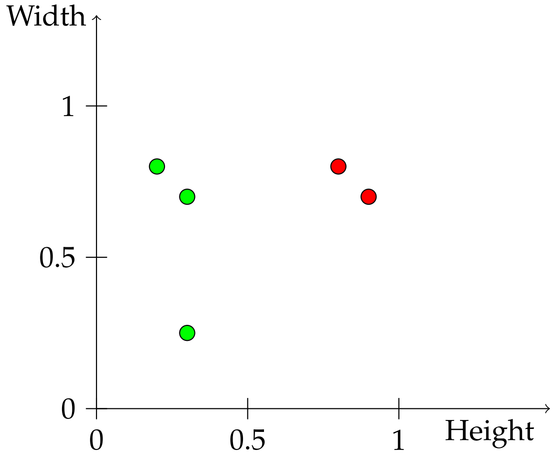
Jargon Box

The variable you are trying to predict y is called a **Label** or **Dependent variable**. Your observations (here: height and width) are called **features**, **dependent variables**,**predictors** or **covariates** in different bodies of literature.

When labels are given, it is called a **supervised** learning problem. When the labels are binary it is called **binary classification**. If we were trying to predict a continuous quantity (say y was temperature of the nano-chip) it is called **regression**.

The **Feature space** is the space where our data features live. Here it is $\mathbb{R}^2$ i.e. pairs of weight/height.

Therefore, our problem is a supervised learning problem and specifically a binary classiciation problem. Lets say we plot the data using colors for the two different labels:



It looks like the good and the bad nanochips are quite well separated on the feature space, anyone would be tempted to come up with a simple model, i.e. a simple test on the features to predict if a new nanochip will be good or bad. Before we do that, lets try to put our problem in a precise mathematical framework, to understand what we are trying to do.

1 Statistical Learning Framework

Our goal is to define what constitutes a **prediction** and to precisely define and understand **overfitting**. We will learn the concepts of **True Risk** (aka **Generalization error**) versus **Empirical Risk** (aka **Test error**). This will lead to the main algorithm used in learning: **Empirical Risk Minimization (ERM)**.

We need *a mathematical model* of how data is generated and labeled.

- We assume we are given a distribution D over the feature space. Each sample $\mathbf{x}_i$ (weight and height of a nanochip) is assumed to be randomly and independently sampled from this distribution. We use bold for $\mathbf{x}$ because it is a vector of p numbers (the features), i.e. $\mathbf{x} \in \mathbb{R}^p$.
- We assume a true labeling function h_T. The universe samples a point $\mathbf{x}_i$ and computes the true label y_i (good or faulty nano-chip) by computing $y_i = h_T(\mathbf{x}_i)$.
- We need to choose how we count errors. This is called a **Loss function** $\ell(h, \mathbf{x})$. This function takes a model h, a data point $\mathbf{x}$ and penalizes the model when it makes mistakes.

Our goal is to find the best model h. We define the **True risk** of a model h, denoted by $L_D(h)$ as follows:

$$L_D(h) = \mathrm{E}_{\mathbf{x} \sim D}[\ell(h, \mathbf{x})].$$

The definition of true risk needs some attention: $\mathbf{x} \sim D$ means that it is now a random vector in $\mathbb{R}^p$, sampled using the distribution D. Therefore, the loss function is now a scalar random variable and we take its expectation. We will work through an example in a second.

In reality we would be only given a dataset a matrix $X \in \mathbb{R}^{n\times p}$ and labels $\mathbf{y} \in \mathbb{R}^n$. If we only have a dataset we cannot compute the true risk. Instead we try to approximate it by computing what is called **Empirical Risk** (aka Training error):

$$L_{\mathcal{S}}(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h(\mathbf{x}_i), y_i)].$$

Here we are summing over our dataset, example by example. For each i we have the feature vector $\mathbf{x}_i$ and training label y_i so we can compute if the model h is correct or not. We are simply averaging the performance of the model over the training set.

We are trying to *learn* the best model, which means find which h has the smallest empirical risk. This is called **Empirical Risk Minimization (ERM)** (aka Training).

2 Example: Computing Empirical Risk

Lets choose a simple model and compute its empirical risk. The model h_1 works as follows: It takes as input the features $\mathbf{x} = (\text{width}, \text{height})^T$ and predicts $y = 1$ if $width > 0.5$, and $y = 0$ otherwise. This is a simple decision tree of depth 1, and these short decision trees are called decision stumps. These are some of the simplest models we can define: Simply compare one feature with a threshold and assign a label. Lets repeat our dataset along with the predictions that it makes called $\hat{y_1}$. **Verify the prediction column yourself**:

	height	**width**	**y=exploded?**	**Model 1 prediction $\hat{y_1}$**
chip 1	0.8	0.8	1	1
chip 2	0.3	0.25	0	0
chip 3	0.2	0.8	0	1
chip 4	0.3	0.7	0	1
chip 5	0.9	0.7	1	1

Table 2: Your dataset $\mathcal{S}$. There is a special column (called y) that we are trying to predict using the other columns called features. Every row corresponds to one labeled nano-chip. The number of examples (aka Samples) is usually denoted by n and the number of features by p. In this example $n = 4$ and $p = 2$. The last column is the prediction of the binary decision stump h_1.

How well did model h_1 do? We want to compare y with the predictions $\hat{y}$, but that depends on the loss function we use. Lets simply use the $0 - 1$ loss now (denoted by ℓ_{01}) which simply charges 1 when the model is wrong and zero otherwise[1].

[1]Note that in a real application, shipping a faulty nano-chip may be much more expensive compared to discarding a good one, so more sophisticated loss functions can be used, depending on the application

We can now compute the empirical risk of the model h_1 on this dataset $\mathcal{S}$:

$$L_{\mathcal{S}}(h) = \frac{1}{n}\sum_{i=1}^{n} \ell_{01}(h(\mathbf{x}_i), y_i)] = \frac{1}{5}(0+0+1+1+1+0) = \frac{1}{5}3 = \frac{3}{5}.$$

Exercise

Here is another model h_2: $h_2([w,h]) = 1$ if $w \geq 0.75$, zero otherwise. In words, the model is another binary decision stump with threshold 0.75 for the feature *weight*.

- Compute the empirical risk of this model on our dataset.
- Is this a better or worse threshold for the stump?

2.1 Example: Computing True Risk

Before, we computed the empirical risk of the model h_1, which is the training error on our tiny dataset.

$$L_{\mathcal{S}}(h) = \frac{1}{n}\sum_{i=1}^{n} \ell(h_1(\mathbf{x}_i), y_i)].$$

Now we would like to compute the true risk of the model h_1:

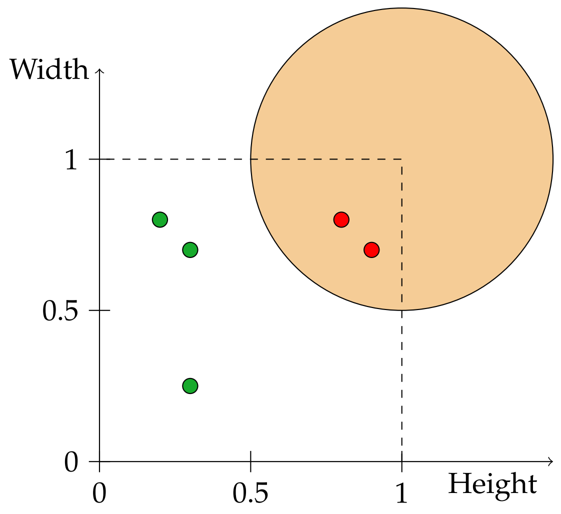
$$L_D(h) = \mathrm{E}_{\mathbf{x}\sim D}[\ell(h, \mathbf{x})].$$

We cannot compute this expectation using only our dataset. We need to know the true distribution D that generates the data and also the true labeling function h_T. In this example lets assume:
• $D \sim$ Uniform$[0,1]x[0,1]$. In words, the weight and the height of the nano-chips are selected randomly uniformly and independently in $[0,1]$.

• Lets also assume a true labeling function:

$$h_T(w,h) = \begin{cases} 1 & \text{if } (w-1)^2 + (h-1)^2 \leq \frac{1}{4}, \\ 0 & \text{otherwise.} \end{cases}$$

This function will label nanochips as $h_T = 1$ (*exploding*) if their weight,height combination is within distance $1/2$ from the point $[1,1]$.



What is the true risk of the decision stump model h_1? Recall how h_1 labels points:

$$h_1(w, h) = \begin{cases} 1 & \text{if } w \geq 0.5, \\ 0 & \text{otherwise.} \end{cases}$$

Our goal is to compute the true risk:

$$L_D(h) = \mathrm{E}_{\mathbf{x} \sim D}[\ell_{01}(h, \mathbf{x})].$$

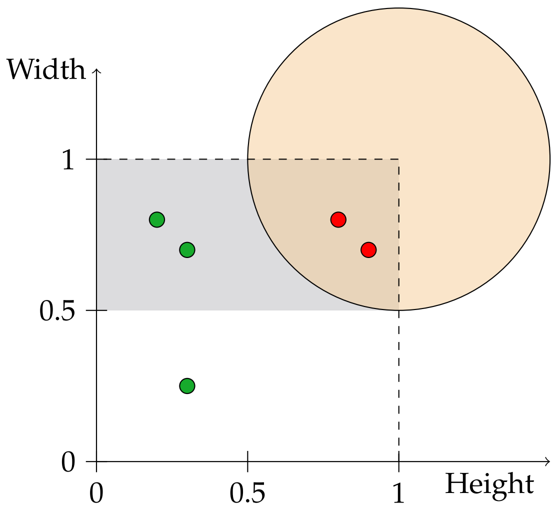
We are using the zero-one loss ℓ_{01} which takes as input a prediction $\hat{y}$ and a true value y and charges 1 when the prediction is wrong and zero otherwise:

$$\ell_{01}(\hat{y}, y) = \begin{cases} 0 & \text{if } \hat{y} = y, \\ 1 & \text{otherwise.} \end{cases}$$

Note that when the point $\mathbf{x}$ is chosen randomly from D, ℓ_{01} is a random variable that takes the values zero or one.

The probability $\mathbb{P}[\ell_{01} = 1]$ is just the probability that the random nanochip features land in the area of the feature space where h_1 is wrong, i.e. disagrees with h_T.

Lets draw the decision region where h_1 labels nanochips as exploding:



The light grey area is where h_1 labels exploding and the orange circle are true exploding, i.e. h_T labels exploding. The stump region h_1 is misclassifying the two green points on the upper left. Since the nanochip features are selected unformly in the $[0,1]$ square, the probability that the loss is 1 is equal to the area of the grey rectangle minus the area of the quarter disk:

$$\mathbb{P}[\ell_{01}=1] = 0.5 \times 1 - \frac{1}{4}\pi(\frac{1}{2})^2 = 0.30\ldots.$$

This exactly the true risk of the model h_1:

$$L_D(h) = \mathrm{E}_{\mathbf{x}\sim D}[\ell_{01}(h,\mathbf{x})] = 1 \times \mathbb{P}[\ell_{01}=1] + 0 \times \mathbb{P}[\ell_{01}=0] = 0.30\ldots.$$