

# Lectures on Data Science and Engineering

## Lecture 2

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### Introduction

In the previous lecture we learned what is the Training error (Empirical Risk) and the Generalization Error (True Risk) and how to compute it for a model  $h$ .

Recall: We are given a dataset  $\mathcal{S}$  of  $n$  labeled examples and the Empirical Risk is

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

which is averaging the loss over our training set. We hope that this will be a good approximation to the **True risk** of a model  $h$ , denoted by  $L_D(h)$  as follows:

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

For any given model we can compute its training error. The challenge of training is to find the *best possible model*. In other words, we would ideally like to search over all possible models (*i.e.* search over all possible python functions that take the features  $\mathbf{x}$  and produce a label  $y$ ) to choose the one with the smallest empirical risk on the training set  $\mathcal{S}$ . This is called Empirical Risk Minimization (ERM):

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

where we are searching over all models to find the one that minimizes the loss.

Let's remember our dataset  $\mathcal{S}$ :

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

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

	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  $\mathcal{S}$ . 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  $p = 2$ .

### Exercise 1

How small can you make the training error for this dataset  $\mathcal{S}$  for the zero-one loss  $\ell_{01}$ ? You can use any model  $h$  you want.

Think about the previous exercise before continuing.

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The problem is that we can always make the training error zero. One way to do this is by a model  $h$  that **memorizes** the dataset  $\mathcal{S}$  and produces labels as follows:

### Stupid Memorization Model $h_m$

- For a given input  $\mathbf{x}$ , if the same feature vector  $\mathbf{x}$  is in the training set, output the training label as a prediction:  $h_m(\mathbf{x}) = y$ .
- For a given input  $\mathbf{x}$  that is not in the training set, make the prediction  $h_m(\mathbf{x}) = 0$

This model  $h_m$  achieves zero empirical loss but is a terrible model that will always predict 0 unless it has seen the example before. Using the framework of the previous lecture you can compute the true risk of  $h_m$  (for the  $D$  and true labeling function  $h_T$  given in Lect.1) and you will find that it is 1, i.e. the worst possible risk. This model has simply memorized the training set but has no predictive power: This is an example of **overfitting**.

# 1 How to avoid overfitting: Inductive Bias

The way we usually avoid overfitting is through **hope**: the hope that the universe is simple. Instead of minimizing the empirical risk over *all possible models* we limit our search within *simple models*. We critically assume here that the true labeling function  $h_T$  is also simple and hence our search over simple models will find it, or find a model close to it<sup>1</sup>.

## 1.1 Example: ERM over Stumps

In this example we will search over all decision stumps that look only at the variable *width*: Lets consider decision stumps  $h_\theta$  that label points as follows:

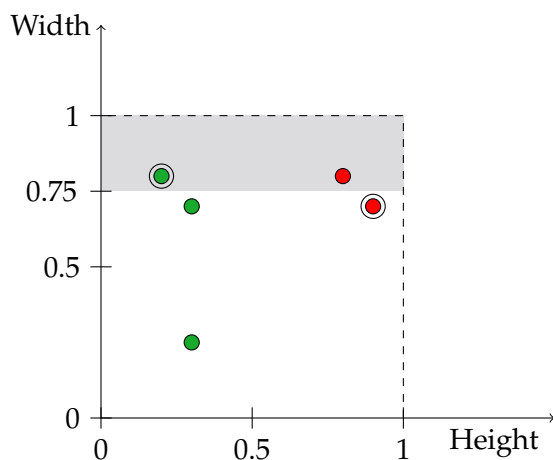
$$h_\theta(w, h) = \begin{cases} 1 & \text{if } w \geq \theta, \\ 0 & \text{otherwise.} \end{cases}$$

This is now a family of models  $\mathcal{H}$ . This is called a *hypothesis class* and this particular one is quite simple and is parametrized by one scalar parameter  $\theta$ , the threshold we use.

We will now perform ERM over this hypothesis class:

$$\min_{h \in \mathcal{H}} L_S(h_\theta) = \min_{\theta \in [0,1]} L_S(h_\theta).$$

Lets draw the decision region for  $h_\theta$  when  $\theta = 0.75$ :

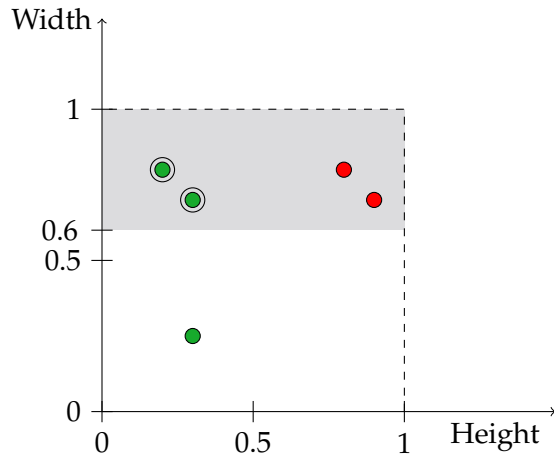


For  $\theta = 0.75$  the model is misclassifying two points shown circled. So the empirical risk is  $L_S(h_{0.75}) = \frac{1}{5} \cdot 2$ .

If we choose  $\theta = 0.6$  we have the decision region:

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<sup>1</sup>This is all formalized in the field of learning theory, where complexity is measured by the concept of VC dimension and its extensions.



For  $\theta = 0.6$  the model is misclassifying again two points shown circled. So the empirical risk is the same:  $L_S(h_{0.75}) = \frac{1}{5} 2$ .

You can see that for this dataset, there is no decision stump on the feature *width* that will misclassify fewer than 2 points. So  $\theta^* = 0.6$  or  $\theta^* = 0.7$  can be selected as an ERM optimum. If instead one uses a decision stump on the variable height, thresholding height on 0.5 will produce zero training error.

### Exercise 2

- Think of an algorithm for training binary decision stump models.
- What is the running time in terms of the number of samples  $n$  and number of features  $p$ ?

### Exercise 3

Assume a data generation model as in Lecture 1:

- $D \sim \text{Uniform}[0, 1] \times [0, 1]$ . In words, the weight and the height of the nano-chips are selected randomly uniformly and independently in  $[0, 1]$ . Assume the true labeling function to be:

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

This function will label nanochips as  $h_T = 1$  (*exploding*) if their weight,height combination is within distance  $1/2$  from the point  $[1, 1]$ . We are using 0-1 loss throughout.

- Perform true risk minimization to find  $\theta^*$  for stumps on *width*.
- Perform true risk minimization over either *width* or *height*. What is the lowest possible true risk?