



# MACHINE LEARNING

LEARNINGTHEORY

# AGENDA

## 01 Preliminaries

Risk minimization, union bound, and Hoeffding inequality.

## 02 The case of finite $\mathcal{H}$

Uniform convergence, sample complexity, error bound, bias-variance tradeoff.

## 03 The case of infinite $\mathcal{H}$

VC dimension





# AI

**PRELIMINARIES**

# LEARNING THEORY

## PRELIMINARIES



We want to answer three main questions:

1. **Can we make formal the bias/variance tradeoff?**
2. **Why should doing well on the training set tell us anything about generalization error?**
3. **Are there conditions under which we can actually prove that learning algorithms will work well?**

# LEARNING THEORY

## PRELIMINARIES



We are going to **define** a **binary classifier**:

$$h_w(x) = g(w^T x)$$

$$g(z) = \mathbf{1}\{z \geq 0\}$$

We establish our **training set** as:

$$S = \{(x^{(i)}, y^{(i)})\}_{i=1}^m, S \sim_{iid} D$$

# LEARNING THEORY

## PRELIMINARIES



We are going to define the **training error**  $\hat{\epsilon}_S$  of a hypothesis  $h_w$  in a **simple way**:

$$\hat{\epsilon}_S(h_w) = \frac{1}{m} \sum_{i=1}^m \mathbf{1}\{h_w(x^{(i)}) \neq y^{(i)}\}$$

**Fraction of data points where the hypothesis is wrong.**

The **training error** is also called **RISK**.

# LEARNING THEORY

## PRELIMINARIES



As always, our **objective** consists in **minimizing** the **risk** (training error):

$$\hat{w} = \underset{w}{\operatorname{argmin}} \hat{\mathcal{E}}_S(h_w)$$

**Minimizing** this **expression** deals with a **non-convex optimization problem**.  
**Logistic regression** and **SVM** are **convex approximations** to this **problem**.

# LEARNING THEORY

## PRELIMINARIES



We are going to **change** the **problem**. Now, the **objective** will reside in **choosing** the **hypothesis** function  $h_w$  instead of the **parameters**  $w$ .

Thus, we define the **hypothesis class**  $\mathcal{H}$  as the **class** of all **linear classifiers** that the **algorithm** is **choosing** from.

$$\mathcal{H} = \{h_w: h_w(x) = \mathbf{1}\{w^T x \geq 0\}, w \in \mathbb{R}^{n+1}\}$$

Therefore, **empirical risk minimization** is **redefined** as:

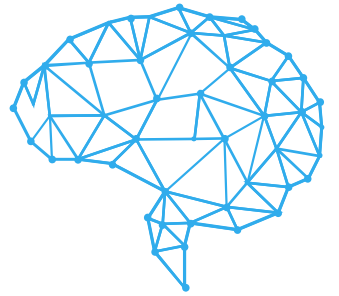
$$\widehat{h}_w = \operatorname{argmin}_{h_w \in \mathcal{H}} \widehat{\mathcal{E}}_S(h_w)$$

**NOTE:** the **hypothesis class**  $\mathcal{H}$  can represent any set of functions.



# LEARNING THEORY

## PRELIMINARIES



Let us remember that the **main goal** resides in the **generalization error not** in the **training error**. The **generalization error** would be **defined as**:

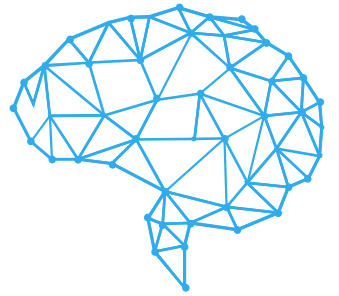
$$\mathcal{E}(h_w) = P_{(x,y) \sim D}(h_w(x) \neq y)$$

**Probability** that, if we now **draw a new example**  $(x, y)$  from the **distribution D**,  $h$  will **misclassify** it.

We want to **make an estimation**  $\hat{\mathcal{E}}_S$  (**training error**) to get **close** to the **generalization error**  $\mathcal{E}(h_w)$ .

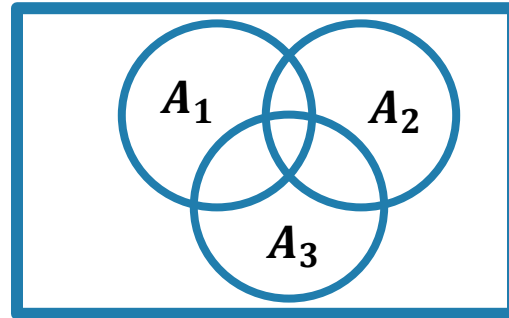
# LEARNING THEORY

## PRELIMINARIES



To **reduce** the **generalization error** we will **need two lemmas**:

1. **Union bound**: Let  $A_1, A_2, \dots, A_k$  be  $k$  **different events** (that may not be independent). Then  $P(A_1 \cup \dots \cup A_k) \leq P(A_1) + \dots + P(A_k)$ .



2. **Hoeffding inequality**: let  $Z_1, \dots, Z_n$  be  $n$  **independent and identically distributed (iid) random variables** drawn from a **Bernoulli( $\phi$ ) distribution** with **mean  $\phi$** . Therefore,  $P(Z_i = 1) = \phi$  and  $P(Z_i = 0) = 1 - \phi$ . Let  $\hat{\phi} = \frac{1}{m} \sum_{i=1}^m z_i$  and let any  $\gamma > 0$  be fixed. Then

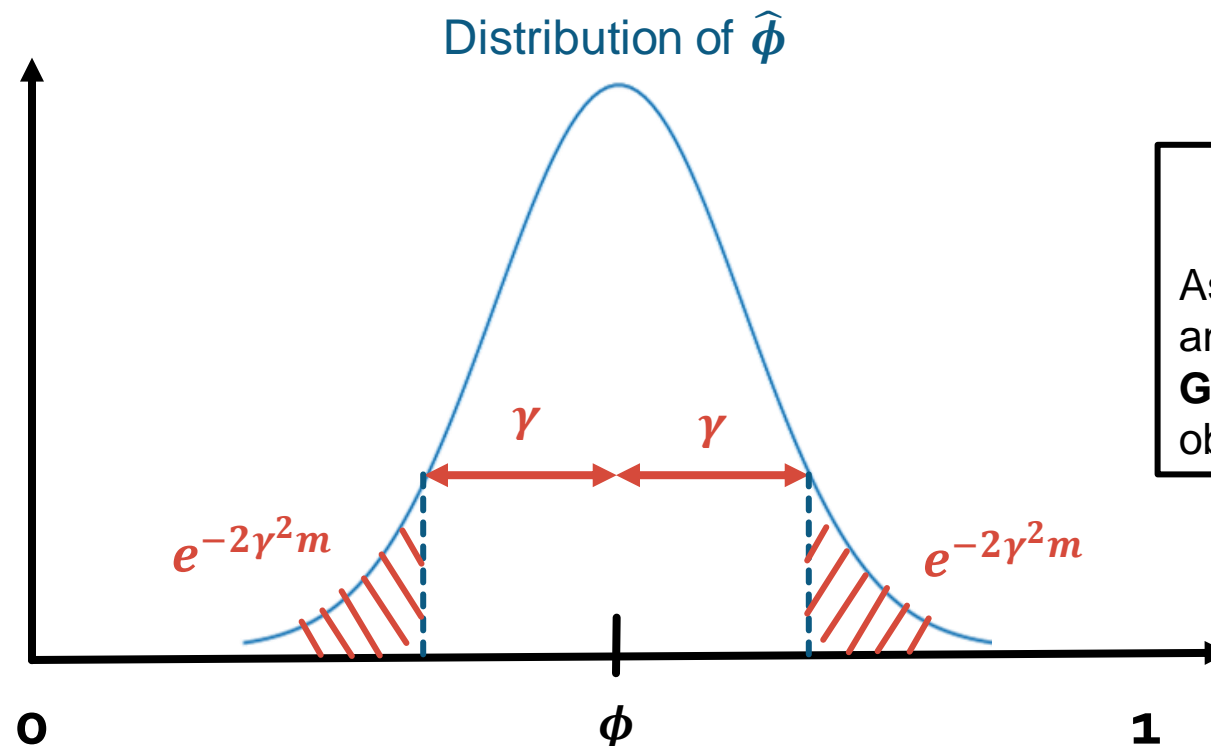
$$P(|\phi - \hat{\phi}| > \gamma) \leq 2e^{-2\gamma^2 m}$$

# LEARNING THEORY

## PRELIMINARIES



The **Hoeffding inequality** says that if we take  $\hat{\phi}$  (the **average** of  $m$  **Bernoulli**( $\phi$ ) **random variables**) to be our **estimate** of  $\phi$ , then the **probability** of our **being far from the true value** is **small**, so long as  $m$  is **large**.



### Central Limit Theorem

As you take more  $m$  samples and **average** them, a **Gaussian** distribution is obtained.



# AI

THE CASE OF FINITE  $\mathcal{H}$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



Let us consider that we have a **finite hypothesis class**  $\mathcal{H} = \{h_1, \dots, h_k\}$  consisting of  **$k$  hypotheses** or **functions** mapping from  $\mathcal{X}$  to  $\{0, 1\}$ .

**Risk** minimization will **choose** the **hypothesis** with the **lowest training error**.

We are going to **prove** that:

1.  $\hat{\epsilon}_S \approx \epsilon$ .
2. There is an upper-bound to  $\hat{\epsilon}_S$ .

Therefore, if we **minimize** the **training error**, the **generalization error will decrease** as well.

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



We are going to take a **fixed hypothesis**  $h_j \in \mathcal{H}$  and will consider a **Bernoulli** random variable  $Z_i \underset{iid}{\sim} D$  which **misclassifies** an **example**  $Z_i = \mathbf{1}\{h_j(x^{(i)}) \neq y^{(i)}\} \in \{0, 1\}$ .

The **probability** that, from a **fixed hypothesis**  $h_j$ , we **misclassify** an **example** is the **expected value** (mean of the distribution) or **generalization error**:

$$P(Z_i = 1) = \varepsilon(h_j)$$

On the other hand, we know that the **training error** is computed as the **fraction** of **misclassified examples** (mean of the sample):

$$\hat{\varepsilon}_S(h_j) = \frac{1}{m} \sum_{i=1}^m Z_i = \frac{1}{m} \sum_{i=1}^m \mathbf{1}\{h_j(x^{(i)}) \neq y^{(i)}\}$$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



We will use the **Hoeffding inequality** to look at the **difference between the generalization and training errors**:

$$P(|\varepsilon(h_j) - \hat{\varepsilon}(h_j)| > \gamma) \leq 2e^{-2\gamma^2 m}$$

We have **proved** that for a **fixed hypothesis  $h_j$**  and a **large training set**, the **training error** will **approximate** the **generalization error** with a **high probability**.

Now, let us **prove** this statement for **all  $h \in \mathcal{H}$** .

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



Let us think of  $A_j$  as an event  $|\mathcal{E}(\mathbf{h}_j) - \widehat{\mathcal{E}}(\mathbf{h}_j)| > \gamma$ , thus  $P(A_j) \leq 2e^{-2\gamma^2 m}$ . Using the union bound lemma we have:

$$P(\exists \mathbf{h}_j \in \mathcal{H} / |\mathcal{E}(\mathbf{h}_j) - \widehat{\mathcal{E}}(\mathbf{h}_j)| > \gamma) = P\left(A_1 \cup \dots \cup A_k\right)$$

$$P(\exists \mathbf{h} \in \mathcal{H} / |\mathcal{E}(\mathbf{h}_j) - \widehat{\mathcal{E}}(\mathbf{h}_j)| > \gamma) \leq \sum_{i=1}^k P(A_i)$$

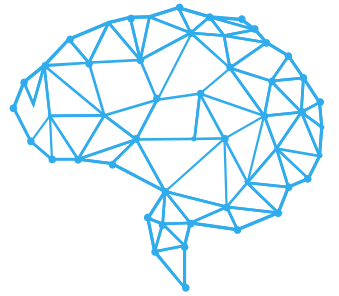
$$P(\exists \mathbf{h} \in \mathcal{H} / |\mathcal{E}(\mathbf{h}_j) - \widehat{\mathcal{E}}(\mathbf{h}_j)| > \gamma) \leq \sum_{i=1}^k 2e^{-2\gamma^2 m}$$

$$P(\exists \mathbf{h} \in \mathcal{H} / |\mathcal{E}(\mathbf{h}_j) - \widehat{\mathcal{E}}(\mathbf{h}_j)| > \gamma) \leq 2ke^{-2\gamma^2 m}$$



# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



The **probability** that such **hypothesis does not exist** is defined as:

$$P(\neg \exists h_j \in \mathcal{H} / |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| > \gamma) = 1 - P(\exists h_j \in \mathcal{H} / |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| > \gamma)$$

$$P(\neg \exists h_j \in \mathcal{H} / |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| > \gamma) = P(\forall h_j \in \mathcal{H} / |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| \leq \gamma)$$

$$P(\neg \exists h_j \in \mathcal{H} / |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| > \gamma) \geq 1 - 2ke^{-2\gamma^2 m}$$

We have proved that with **probability at least**  $1 - 2ke^{-2\gamma^2 m}$ , the **generalization error**  $\mathcal{E}(h_j)$  will be **within a distance**  $\gamma$  of the **training error**  $\widehat{\mathcal{E}}(h_j)$  for all  $h \in \mathcal{H}$ .

**UNIFORM CONVERGENCE**  
(Holds for all hypotheses)

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



There are **three quantities of interest**:  $m$ ,  $\gamma$ , and the **probability of error**  $\delta$ . We can **bound one** in terms of the other two.

Given  $\delta$  and  $\gamma$ , we can obtain the **size of the training set**  $m$  for which the **training error** will be **within**  $\gamma$  of the **generalization error** with at least probability  $1 - \delta$ .

$$\delta = 2ke^{-2\gamma^2 m}$$

$$m \geq -\frac{1}{2\gamma^2} \log\left(\frac{\delta}{2k}\right)$$

$$m \geq \frac{1}{2\gamma^2} \log\left(\left(\frac{\delta}{2k}\right)^{-1}\right)$$

$$m \geq \frac{1}{2\gamma^2} \log\left(\frac{2k}{\delta}\right)$$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



Therefore, we need a **training set size** of  $m \geq \frac{1}{2\gamma^2} \log \left( \frac{2k}{\delta} \right)$  to guarantee that with **probability of at least  $1 - \delta$** , we have that the **training error  $\hat{\epsilon}(h_j)$**  is within  $\gamma$  of the **generalization error  $\epsilon(h_j)$** . Formally

$$|\epsilon(h_j) - \hat{\epsilon}(h_j)| \leq \gamma, \forall h \in \mathcal{H}$$

### SAMPLE COMPLEXITY

(Number of training examples needed to achieve a certain bounding error)

**NOTE:** we can see that **even** if we **increase** the **number** of **hypotheses  $k$**  in the class  $\mathcal{H}$ , the **number** of **training examples  $m$**  needed will **remain small**.

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



If we hold  $m$  and  $\delta$  **fixed**, we can get the **following**:

$$\delta = 2ke^{-2\gamma^2 m}$$

$$\gamma = \sqrt{\frac{1}{2m} \log\left(\frac{2k}{\delta}\right)}$$

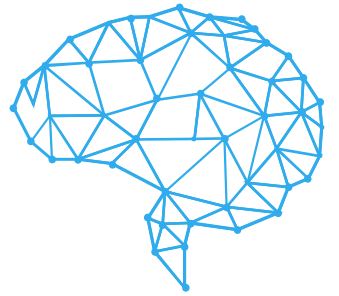
We want to make  $\gamma$  the **upper bound error**, thus

$$|\varepsilon(\mathbf{h}_j) - \widehat{\varepsilon}(\mathbf{h}_j)| \leq \gamma$$

$$|\varepsilon(\mathbf{h}_j) - \widehat{\varepsilon}(\mathbf{h}_j)| \leq \sqrt{\frac{1}{2m} \log\left(\frac{2k}{\delta}\right)}$$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



Let us assume that the **uniform convergence**  $\forall h \in \mathcal{H}, |\mathcal{E}(h_j) - \widehat{\mathcal{E}}(h_j)| \leq \gamma$  holds.

Is there something that we can **prove** about the **generalization error**  $\mathcal{E}$  using the **estimated hypothesis**  $\widehat{h}$  with **empirical risk minimization**? Remembering that:

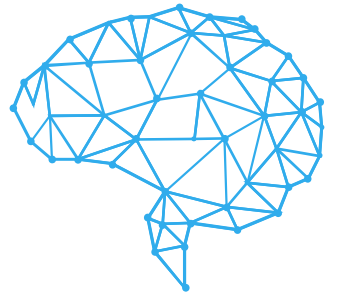
$$\widehat{h} = \operatorname{argmin}_{h \in \mathcal{H}} \widehat{\mathcal{E}}(h)$$

Now, we are going to define the **best hypothesis** as the hypothesis that **minimizes** the **generalization error**:

$$h^* = \operatorname{argmin}_{h \in \mathcal{H}} \mathcal{E}(h)$$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



Starting with the **uniform convergence assumption** we have:

$$|\varepsilon(\mathbf{h}_j) - \widehat{\varepsilon}(\mathbf{h}_j)| \leq \gamma$$

$$\varepsilon(\widehat{\mathbf{h}}) - \widehat{\varepsilon}(\widehat{\mathbf{h}}) \leq \gamma$$

$$\varepsilon(\widehat{\mathbf{h}}) \leq \widehat{\varepsilon}(\widehat{\mathbf{h}}) + \gamma$$

Because we obtained  $\widehat{\mathbf{h}}$  with **empirical risk minimization**, there is **no other hypothesis** with **less training error** than  $\widehat{\mathbf{h}}$ , thus  $\widehat{\varepsilon}(\widehat{\mathbf{h}}) \leq \widehat{\varepsilon}(\mathbf{h}^*)$  and the **inequality remains true**:

$$\varepsilon(\widehat{\mathbf{h}}) \leq \widehat{\varepsilon}(\mathbf{h}^*) + \gamma$$

$$\varepsilon(\widehat{\mathbf{h}}) \leq \widehat{\varepsilon}(\mathbf{h}^*) + 2\gamma$$

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



### Theorem:

Let  $|H| = k$ , and let any  $n, \delta$  be fixed. Then with **probability at least  $1 - \delta$** , we have that

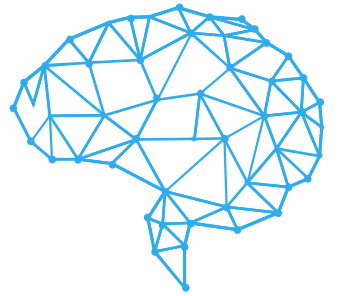
$$\varepsilon(\hat{h}) \leq \hat{\varepsilon}(h^*) + 2\gamma$$

$$\varepsilon(\hat{h}) \leq \min_{h \in \mathcal{H}} \varepsilon(h) + 2 \sqrt{\frac{1}{2m} \log \left( \frac{2k}{\delta} \right)}$$

Thus, our **generalization error** of the **hypothesis** obtained with **ERM**  $\varepsilon(\hat{h})$  will be at most  **$2\gamma$  higher** than the **training error** of the **best possible hypothesis**  $\hat{\varepsilon}(h^*)$ .

# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



By **analyzing** the **theorem** we can see the following:

$$\varepsilon(\hat{h}) \leq \min_{h \in \mathcal{H}} \varepsilon(h) + 2 \sqrt{\frac{1}{2m} \log \left( \frac{2k}{\delta} \right)}$$

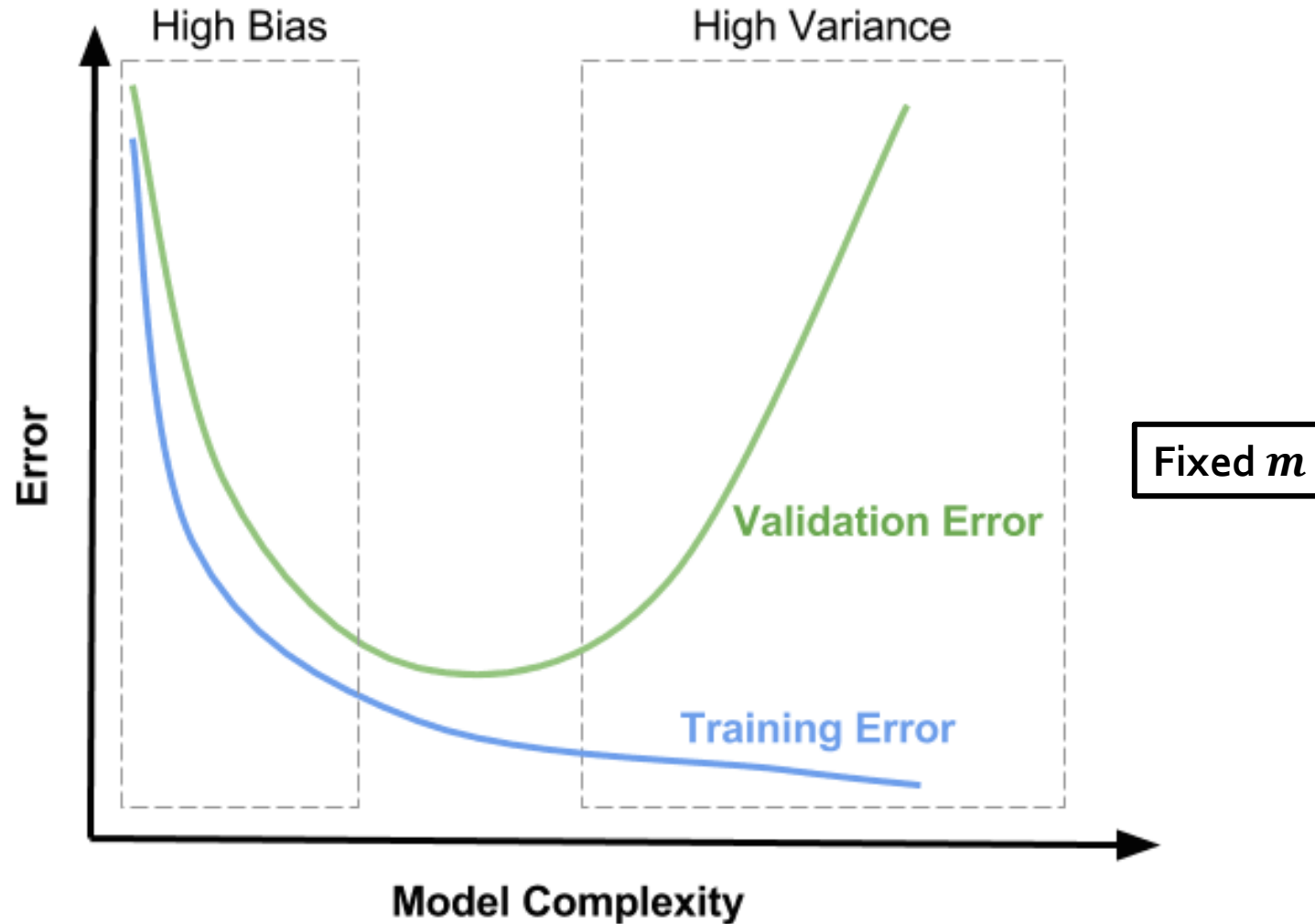
If we switch to a **larger hypothesis class**  $\mathcal{H}' \supseteq \mathcal{H}$  (i.e. quadratic), then  $\min_{h \in \mathcal{H}} \varepsilon(h)$  will **decrease** because we have a larger set of hypothesis for which we can obtain the minimum, thus we **reduce the bias**.

On the other hand,  $k$  will **become larger** resulting in an **increase** of the **second term**, thus **increasing the variance**.



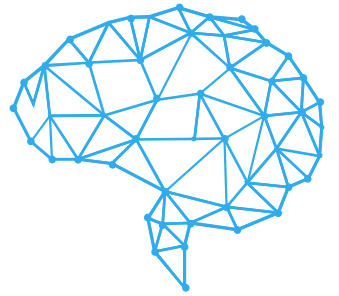
# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



# LEARNING THEORY

## THE CASE OF FINITE $\mathcal{H}$



By looking at the **training set size**  $m$ , we can obtain the following **complexity bound**:

**Corollary:** Let  $|\mathcal{H}| = k$ , and let any  $\delta, \gamma$  be fixed. Then for  $\varepsilon(\hat{h}) \leq \min_{h \in H} \varepsilon(h) + 2\gamma$  to hold with **probability at least**  $1 - \delta$ , it suffices that:

$$m > \frac{1}{2\gamma^2} \log\left(\frac{2k}{\delta}\right)$$

$$m = O\left(\frac{1}{\gamma^2} \log\left(\frac{k}{\delta}\right)\right)$$

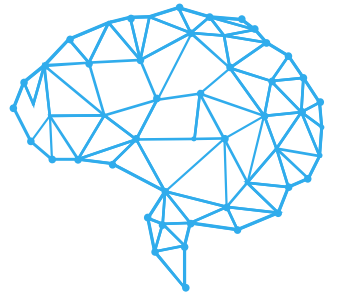


# AI

THE CASE OF INFINITE  $\mathcal{H}$

# LEARNING THEORY

## THE CASE OF INFINITE $\mathcal{H}$



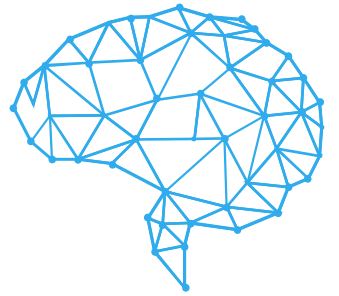
Many **hypothesis classes** contain an **infinite** number of **functions** (i.e. **any function parametrized** by **real** numbers). We want to **prove** the **previous results** for this **infinite space** of functions.

We are going to make some **statements** that are **not correct** at all but **will help** with the **understanding** of the **proof**.

Let us say that the class  $\mathcal{H}$  is parametrized by  $d$  **real** numbers. Because we are constrained by computers that **use 64 bits** to represent floating-point numbers, we have **at most**  $k = 2^{64d}$  **different hypotheses**.

# LEARNING THEORY

## THE CASE OF INFINITE $\mathcal{H}$



To **hold** the **theorem**  $\varepsilon(\hat{h}) \leq \hat{\varepsilon}(h^*) + 2\gamma$  as **valid** with at least **probability**  $1 - \delta$ , we need to suffice the corollary:

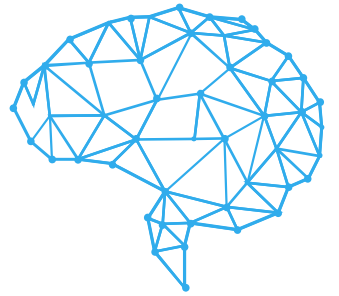
$$m = \mathcal{O}\left(\frac{1}{\gamma^2} \log\left(\frac{k}{\delta}\right)\right)$$

$$m = \mathcal{O}\left(\frac{1}{\gamma^2} \log\left(\frac{2^{64d}}{\delta}\right)\right) = \mathcal{O}\left(\frac{d}{\gamma^2} \log\left(\frac{1}{\delta}\right)\right)$$

Therefore, the **number** of **training examples needed** is **at most linear** in the **parameters** of the **model**  $d$ .

# LEARNING THEORY

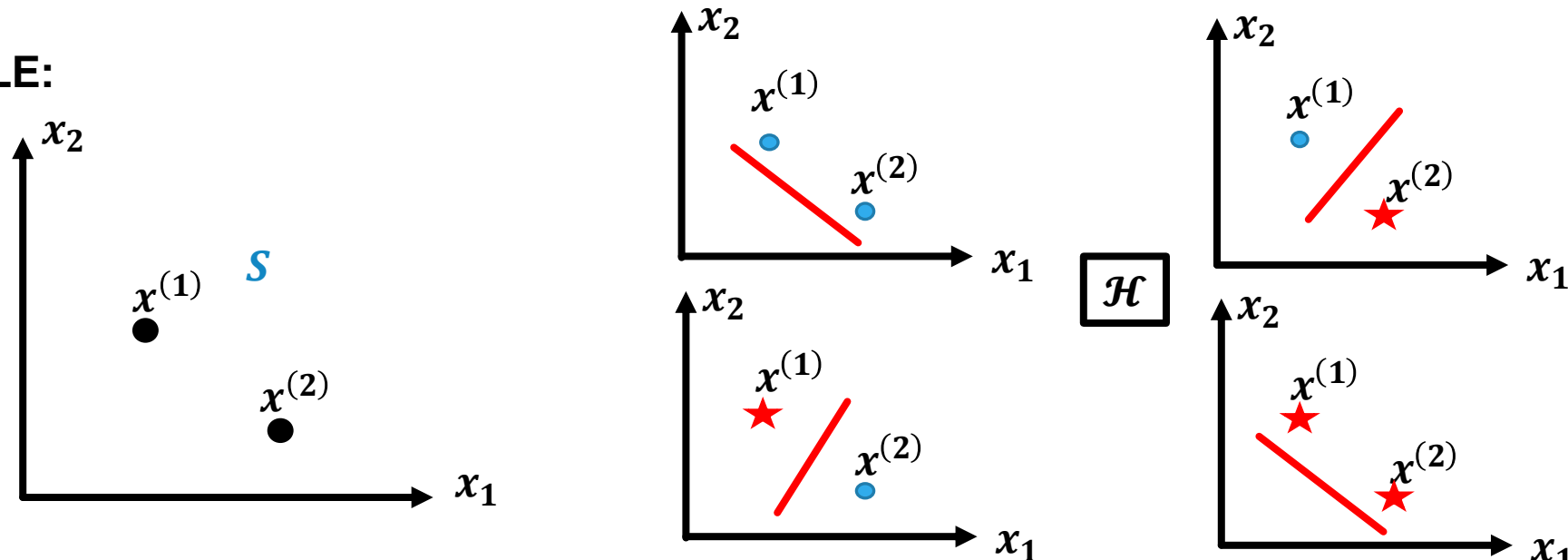
## THE CASE OF INFINITE $\mathcal{H}$



We will introduce a **definition** to make the **proof** for infinite classes  $\mathcal{H}$ .

**DEFINITION:** given a set  $S = \{x^{(1)}, \dots, x^{(D)}\}$  of **points**  $x^{(i)} \in \mathcal{X}$ , we say that  $\mathcal{H}$  **SHATTERS**  $S$  if  $\mathcal{H}$  can realize any labeling on  $S$ . That is, if **for any set of labels**  $\{y^{(1)}, \dots, y^{(D)}\}$ , there **exists some**  $h \in \mathcal{H}$  so that  $h(x^{(i)}) = y^{(i)}$  **for all**  $i = 1, \dots, D$ .

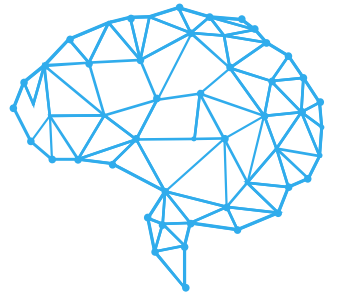
**EXAMPLE:**



**SHATTER:** for any possible labeling of these points, we can find a linear classifier that obtains “zero training error” on them.

# LEARNING THEORY

## THE CASE OF INFINITE $\mathcal{H}$



### DEFINITION:

The **Vapnik-Chervonenkis dimension** of  $\mathcal{H}$ , ( $VC(\mathcal{H})$ ) is the **size** of the **largest set** shattered by  $\mathcal{H}$ .

### EXAMPLE:

If  $\mathcal{H} = \{\text{linear classifiers in 2D}\}$ , therefore  $VC(\mathcal{H}) = 3$ . There is **no set of size 4** that it could **shatter**.

In a **general form** we have that if  $\mathcal{H} = \{\text{linear classifiers in } n \text{ Dimensions}\}$ , therefore  $VC(\mathcal{H}) = n + 1$ .

# LEARNING THEORY

## THE CASE OF INFINITE $\mathcal{H}$



### THEOREM:

Let  $\mathcal{H}$  be given and let  $D = VC(\mathcal{H})$ . Then with **probability at least  $1 - \delta$** , we have that for all  $h \in \mathcal{H}$ ,

$$|\varepsilon(h) - \hat{\varepsilon}(h)| \leq o\left(\sqrt{\frac{D}{m} \log\left(\frac{m}{D}\right) + \frac{1}{m} \log\left(\frac{1}{\delta}\right)}\right)$$

With probability at least  $1 - \delta$ , we also have that:

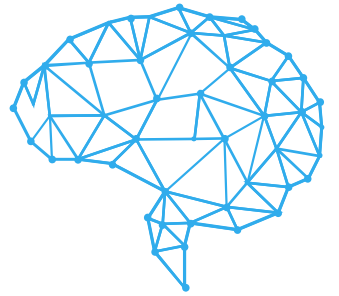
$$\hat{\varepsilon}(h) \leq \varepsilon(h^*) + o\left(\sqrt{\frac{D}{m} \log\left(\frac{m}{D}\right) + \frac{1}{m} \log\left(\frac{1}{\delta}\right)}\right)$$

**If a hypothesis class has finite VC dimension, then uniform convergence occurs as  $m$  becomes large.**



# LEARNING THEORY

## THE CASE OF INFINITE $\mathcal{H}$



### COROLLARY:

For  $|\mathcal{E}(\mathbf{h}) - \widehat{\mathcal{E}}(\mathbf{h})| \leq \gamma$  to hold for all  $\mathbf{h} \in \mathcal{H}$  (and hence  $\mathcal{E}(\widehat{\mathbf{h}}) \leq \mathcal{E}(\mathbf{h}^*) + 2\gamma$ ) with probability at least  $1 - \delta$ , it suffices that  $n = \mathcal{O}_{\gamma, \delta}(D)$ .

Thus, **sample complexity** is **upper-bounded** by the **VC dimension**. Also, for “most” hypothesis classes, the **VC dimension** is also **roughly linear** in the **number of parameters**.

We **conclude** that for a **given hypothesis class**  $\mathcal{H}$ , the **number of training examples needed** to **achieve generalization error close** to that of the **optimal classifier** is usually **roughly linear** in the **number of parameters of**  $\mathcal{H}$ .