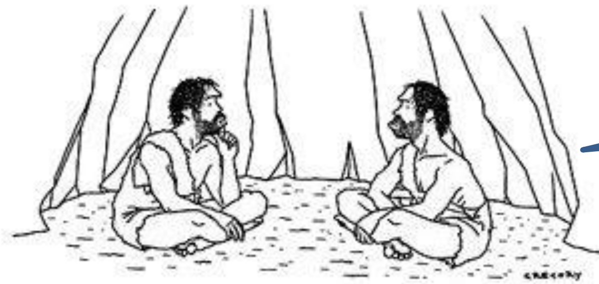


"Something's just not right—our air is clean, our water is pure, we all get plenty of exercise, everything we eat is organic and free-range, and yet nobody lives past thirty."

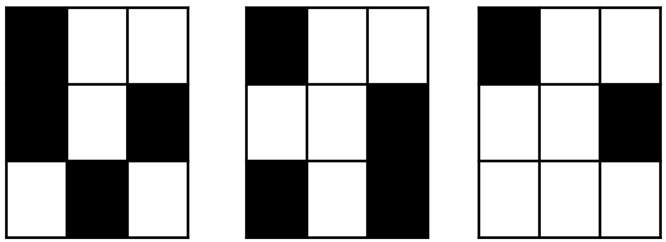
Learning general rules from experience

Fundamental of Inductive Learning:

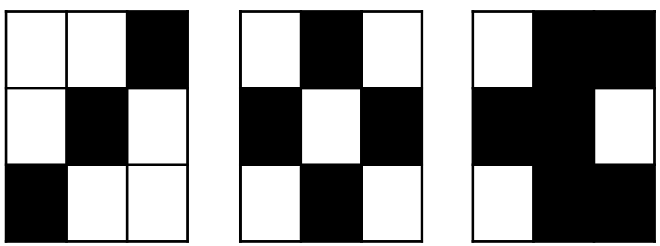
The Empirical Risk Minimization(ERM) rule

Is Inductive Learning Feasible?

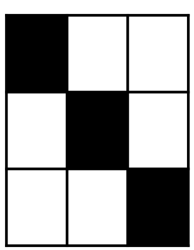
- Let us consider the following two examples:



f = -1



f = 1



f = ?

$$f: \{0,1\}^3 \rightarrow \{0,1\}$$

We know f only partially in its domain

0 0 0	**0**
0 0 1	**1**
0 1 0	**1**
0 1 1	**0**
1 0 0	**1**
1 0 1	**?**
1 1 0	**?**
1 1 1	**?**

How is f in the last 3 elements?

It is Not...

	g	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
0 0 0	0	0	0	0	0	0	0	0	0
0 0 1	1	1	1	1	1	1	1	1	1
0 1 0	1	1	1	1	1	1	1	1	1
0 1 1	0	0	0	0	0	0	0	0	0
1 0 0	1	1	1	1	1	1	1	1	1
1 0 1	?	0	0	0	0	1	1	1	1
1 1 0	?	0	0	1	1	0	1	0	1
1 1 1	?	0	1	0	1	0	0	1	1

- We can't learn this function !
- Try to verify that the eight solutions are equivalent, this is, all provide the same error.
  - Fix one of them as true solution and count how many of the others provide one, two o three errors on the unknown values.

What then ?

- **Inductive Learning** is a hopeless approach:

In a strict sense learning out of the sample is not possible!!

(see Inductivist Turkey (Bertrand Russell) ☺)

Is there any hope to know anything about f outside the data set **without making assumptions** about f ?

Yes, if we are willing to give up "for sure".

Try to learn something less exigent than the proper **unknown** function,

i.e. some useful property about the **unknown** function

Let’s try to exploit randomness….

- NEW Hypothesis: items inside $\mathcal{D}$ are i.i.d samples from a probability distribution $\mathcal{P}$

- **Consequences:**
  - $\mathcal{D}$ **is the output of a random variable (vector)**
  - **It is not realistic to expect that every sample** $\mathcal{D}$ represent equally well the distribution $\mathcal{P}$
  - **The function *g* depends on** $\mathcal{D}$, hence its election is also a random process .

- **Where is the novelty ?**
  - **Probability theory shows that there are probabilistic dependencies between a random variable and a sample of it (under conditions).**
    - **Example : Confidence interval for the sample mean** $P(|\bar{x}-\mu|<\epsilon)>1-\delta, \quad \delta(\epsilon) \ll 1$

But is probability sufficient?

- MAIN QUESTION:

  There is a learning algorithm A and a sample size m such that for each distribution P if A receives m i.i.d. samples from P, is there exists a high probability that it will generate a predictor g with a low error?

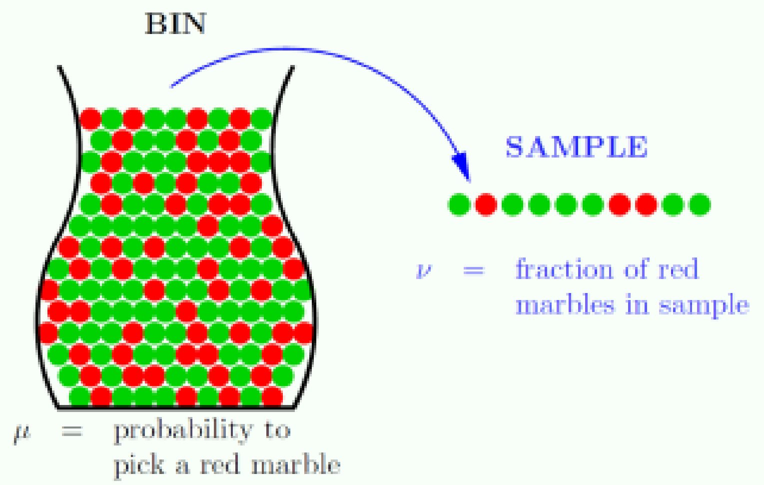
- No-Free-Lunch (NFL) Theorem (Informal): "For every algorithm there exist a $\mathcal{P}$ on which it fails, even though that $\mathcal{P}$ can be sucessfully learned by another learner. Moreover, all algorithms are equivalent in average on all possible target functions f"

- Conclusion: In order to succeed each learner ($\mathcal{A}, \mathcal{H}$) must be applied on the class of distributions $\mathcal{P}$ that it can learn.

- This highlights the need for **exploiting problem-specific knowledge** to achieve better than random performance (inductive bias)
  - Geometric constraint
  - Finite class $\mathcal{H}$
  - Finite VC dimension
  - …. many others

Can we infer something outside the data using only $\mathcal{D}$?: The PAC answer

Population Mean from Sample Mean



The BIN Model

- Bin with red and green marbles.
- Pick a sample of N marbles *independently*.
- μ: probability to pick a red marble.
  ν: fraction of red marbles in the sample.

$$\begin{array}{rcccl} \text{Sample} & \longrightarrow & \text{the data set} & \longrightarrow & \nu \\ \text{BIN} & \longrightarrow & \text{outside the data} & \longrightarrow & \mu \end{array}$$

Can we guarantee anything about ***μ* (outside the data)** after observing ***v* (the data)**?
ANSWER: No. It is possible for the sample to be all green marbles and the bin to be mostly red.

Then, why do we trust polling (e.g. to predict the outcome of a presidential election).
ANSWER: The bad case is possible, but **not probable**.

Hoeffding's Inequality

Hoeffding/Chernoff proved that, most of the time, **for a fixed μ**, ν cannot be too far from μ

$$\mathbb{P}(\mathcal{D}\colon |\mu - \nu| > \epsilon) \leq 2e^{-2\epsilon^2 N} \qquad \text{for any } \epsilon > 0$$

$$\mathbb{P}(\mathcal{D}\colon |\mu - \nu| \leq \epsilon) \geq 1 - 2e^{-2\epsilon^2 N} \qquad \text{for any } \epsilon > 0$$

Question: What does the value of ν tell us on μ: $\mu \approx \nu \Leftrightarrow \nu \approx \mu$

Example: $N = 1,000$; draw a sample and observe ν.

99% of the time	$\mu - 0.05 \leq \nu \leq \mu + 0.05$	$(\epsilon = 0.05)$
99.9999996% of the time	$\mu - 0.10 \leq \nu \leq \mu + 0.10$	$(\epsilon = 0.10)$

What does this mean? If I repeatedly pick a sample of size 1,000, observe ν and claim that

$$\mu \in [\nu - 0.05, \nu + 0.05], \qquad \text{(the error bar is } \pm 0.05\text{)}$$

I will be right 99% of the time. On any particular sample you **may** be wrong, but not often.

We learned *something*. From ν, we reached outside the data to μ.

Hoeffding's Inequality: Remarkable facts

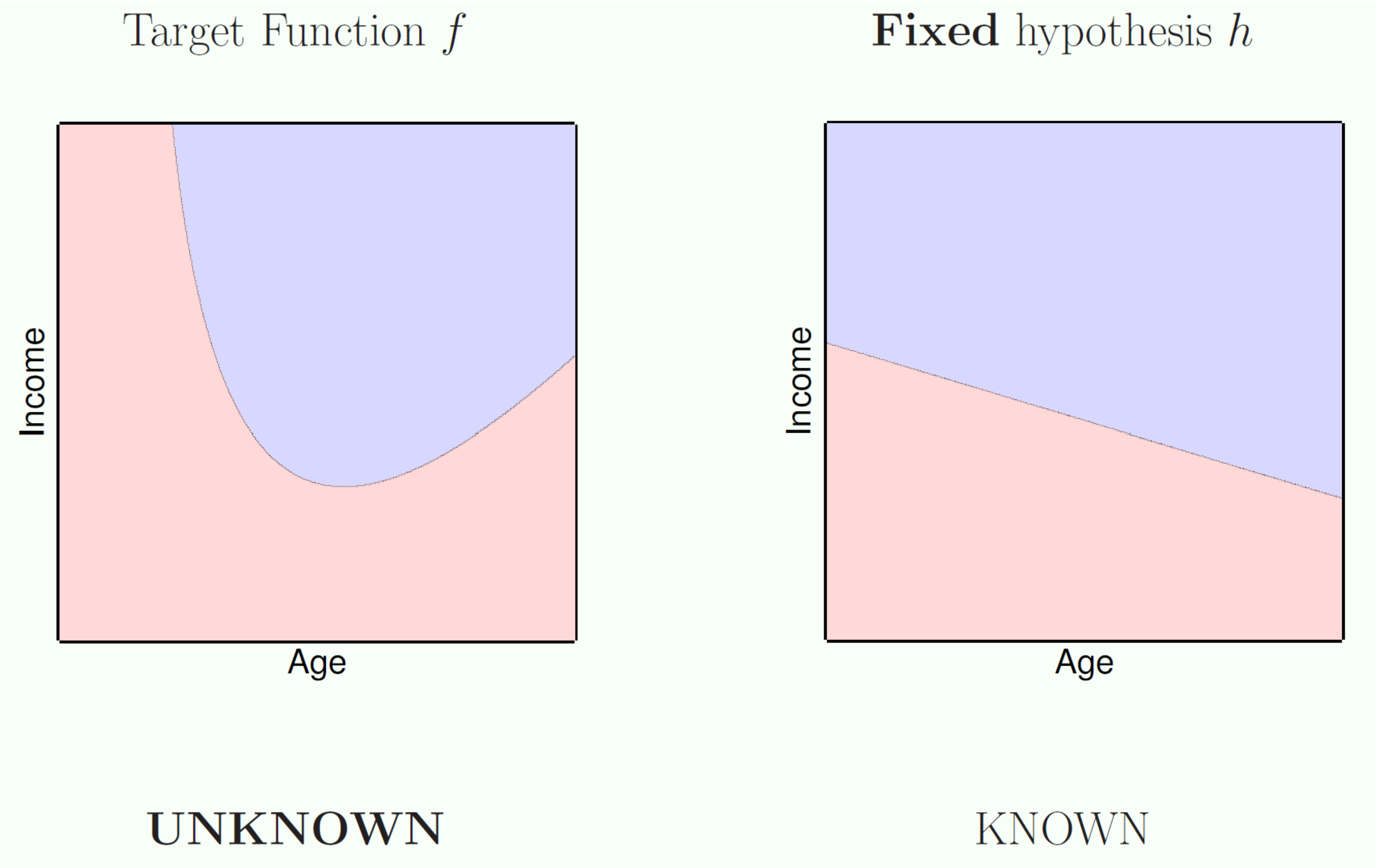
- The key ingredient: samples must be i.i.d.
  - If the sample is constructed in some arbitrary fashion, then indeed we cannot say anything.
  - Even with independence, ν can take on arbitrary values; but some values are more likely than others.
  - This is what allows us to learn something – it is likely that $\nu \approx \mu$.

- The bound $2e^{-2\epsilon^2 N}$ does not depend on μ or the size of the bin
  - The bin can be infinite.
  - It's great that it does not depend on μ because μ is **unknown**.

- The key player in the bound $2e^{-2\epsilon^2 N}$ is N.
  - If $N \to \infty$, $\mu \approx \nu$ with very very very . . . high probabilty, but not for sure.
  - Can you live with 10^{-100} probability of error?

$$\boxed{\mathbb{P}(\mathcal{D}\colon\ |\mu - \nu| > \epsilon) \leq 2e^{-2\epsilon^2 N}}$$

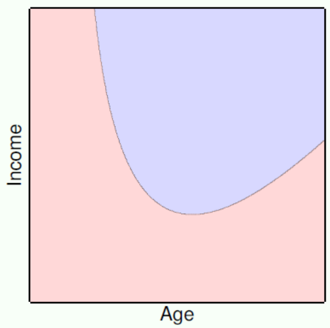
Learning setup



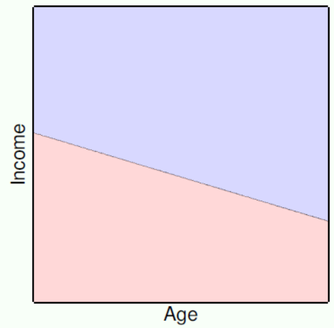
In learning, the unknown is an entire function *f*; in the bin it was a single number μ.

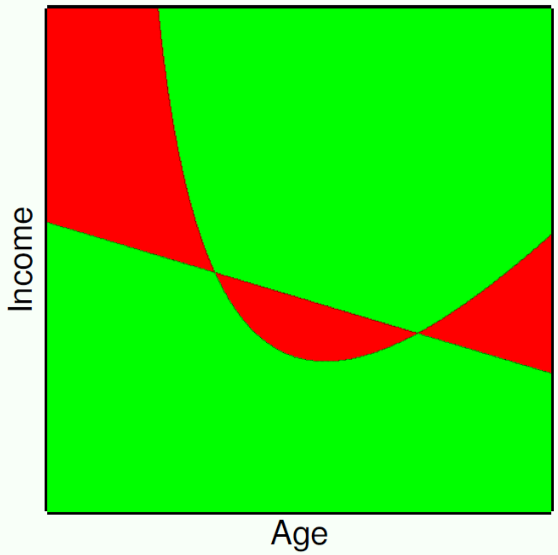
The Learning Error Function

Target Function f



Fixed hypothesis h





UNKNOWN

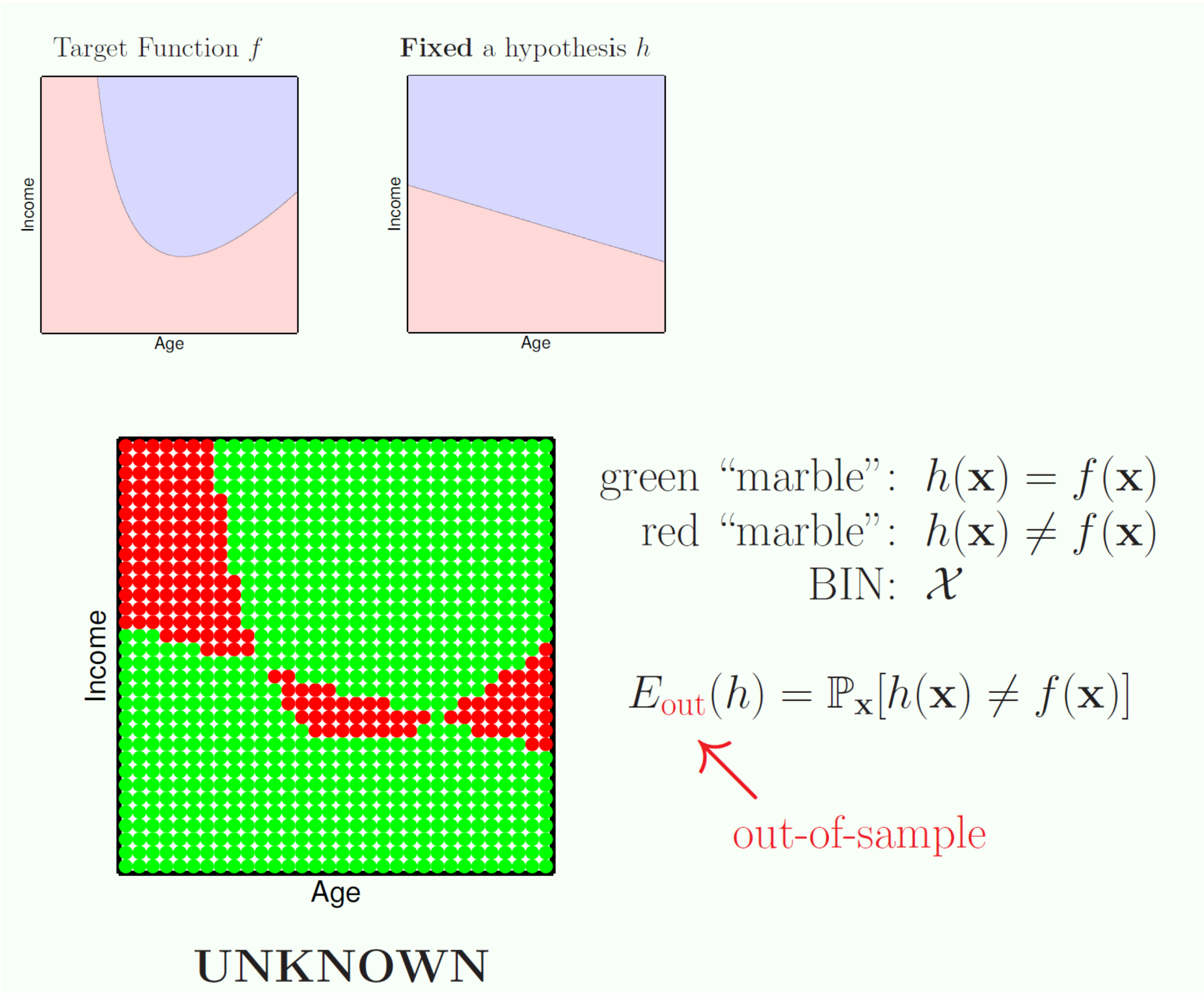
$$\text{green:} \quad h(\mathbf{x}) = f(\mathbf{x})$$
$$\text{red:} \quad h(\mathbf{x}) \neq f(\mathbf{x})$$

$$E(h) = \mathbb{P}_{\mathbf{x}}[h(\mathbf{x}) \neq f(\mathbf{x})]$$

("size" of the red region)

The function h defines an unknown but fixed probability error E(h)

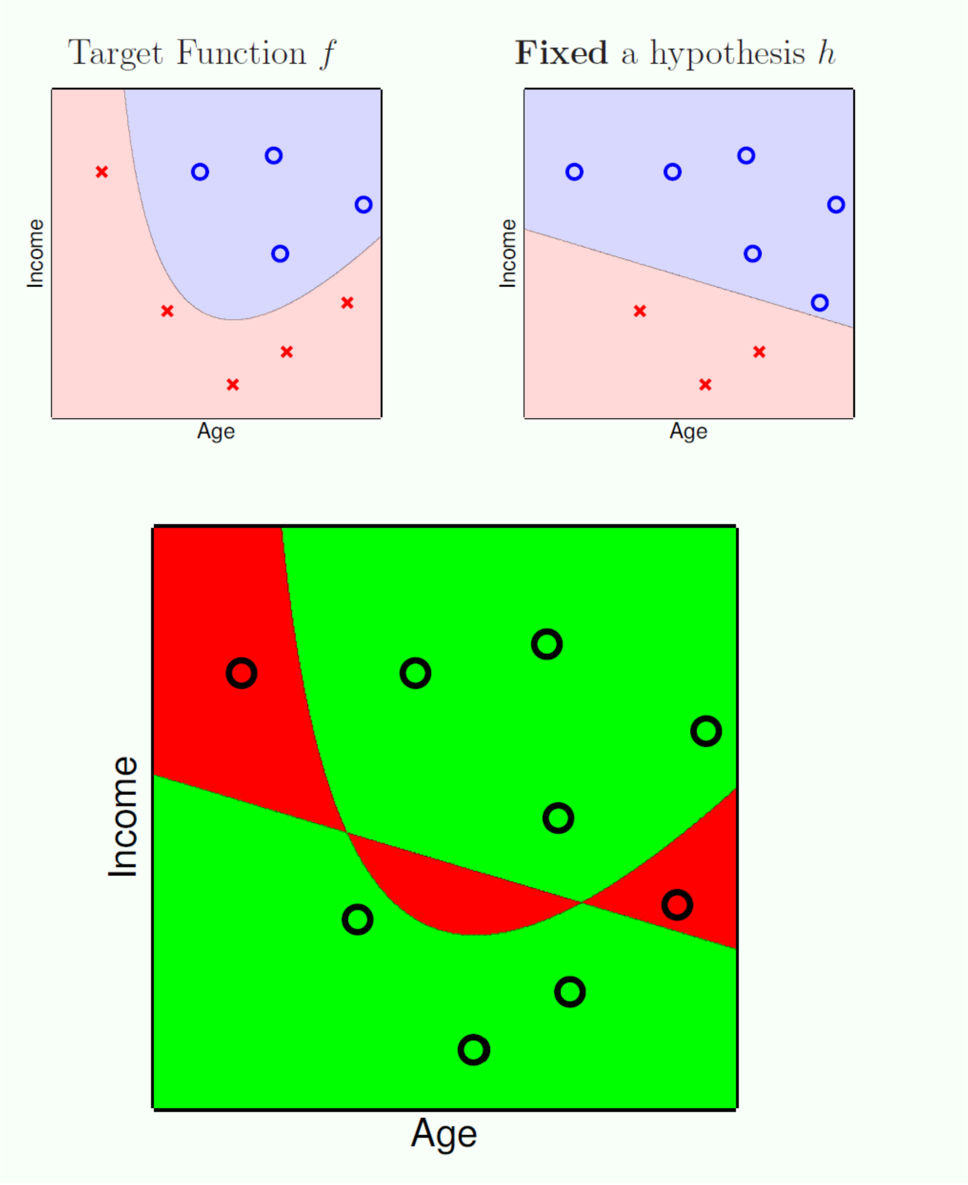
Relating the Bin to Learning



Let´s consider all possible sample points

Now a Bin Model is defined by *h* and *f*

Relating the Bin to Learning - the Data

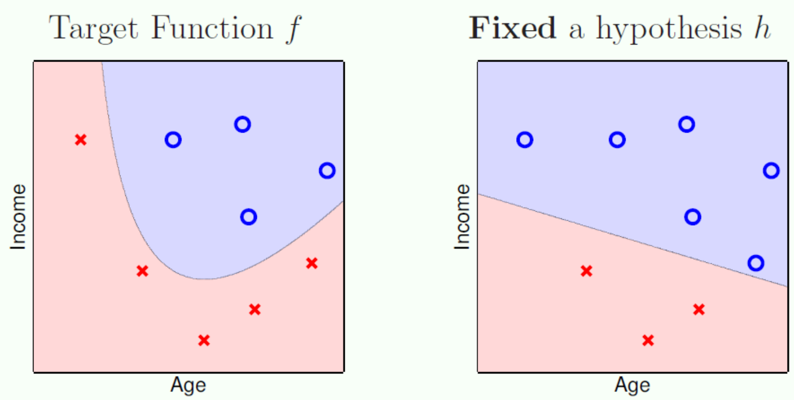


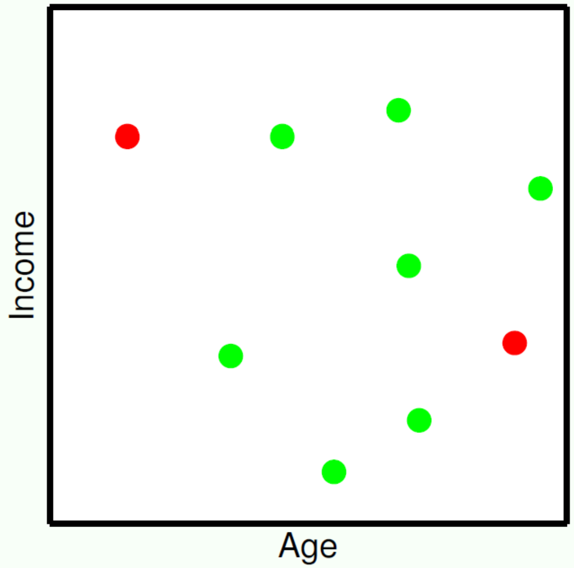
On the same sample, the target function f and the hypothesis h provides us with different labels

We have points in different zones of the error function.

If the sample is draw independently acccording to $\mathbb{P}$, each point will be red with probability μ and green with probability $1- \mu$

Relating the Bin to Learning - the Data





green data: $h(\mathbf{x}_n) = f(\mathbf{x}_n)$

red data: $h(\mathbf{x}_n) \neq f(\mathbf{x}_n)$

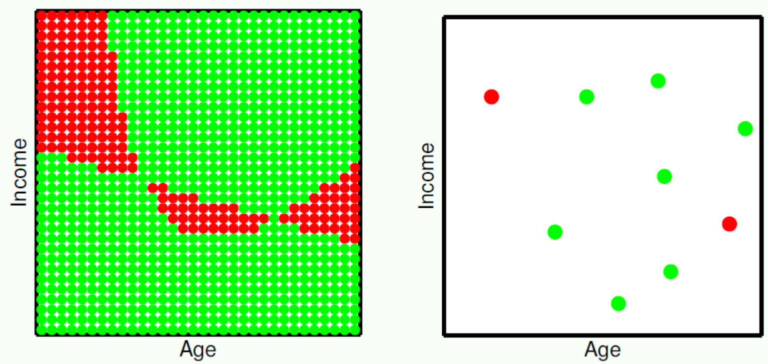
$E_{\text{in}}(h) =$ fraction of red data

in-sample

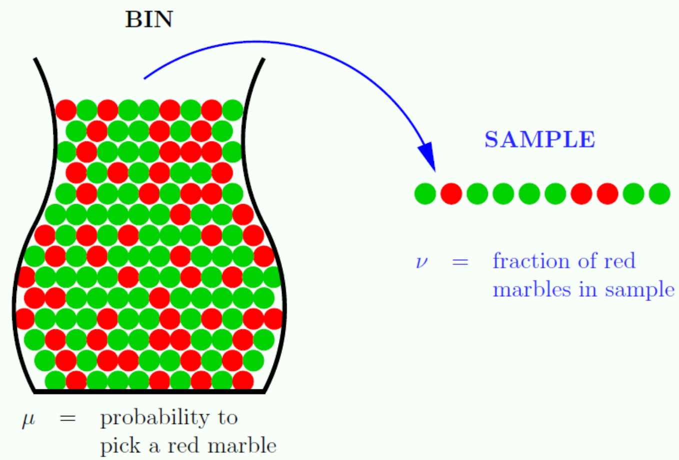
misclassified

KNOWN!

Bin Model and Learning



Unknown f and $P(\mathbf{x})$, **fixed** h



Learning	**Bin Model**
input space $\mathcal{X}$	Bin
$\mathbf{x}$ for which $h(\mathbf{x}) = f(\mathbf{x})$	green marble
$\mathbf{x}$ for which $h(\mathbf{x}) \neq f(\mathbf{x})$	red marble
$P(\mathbf{x})$	randomly picking a marble
data set $\mathcal{D}$	sample of N marbles
Out-of-sample Error: $E_{\text{out}}(h) = \mathbb{P}_{\mathbf{x}}[h(\mathbf{x}) \neq f(\mathbf{x})]$	μ = probability of picking a red marble
In-sample Error: $E_{\text{in}}(h) = \frac{1}{N}\sum_{n=1}^{N} [\![h(\mathbf{x}) \neq f(\mathbf{x})]\!]$	ν = fraction of red marbles in the sample

Hoeffding inequality in Learning

- $\mathcal{H}$={h}, only one function, and f(x) is the unknown true function.
- Let's $[\![f(x) = h(x)]\!]$ and $[\![f(x) \neq h(x)]\!]$ represent binary variables in the population and $\mu = \Pr([\![f(x) \neq h(x)]\!])$
- For any training sample $\mathcal{D}$ of size N , $\nu = \text{Fraction}([\![f(x) \neq h(x)]\!])$ on $\mathcal{D}$
- Now μ and ν represent the population and sample error respectively.
- Let's denote by $\mathrm{E}_{out}(h) = \mu$ *and* $\mathrm{E}_{in}(h) = \nu$ the h's global and sample error respectively
- The Hoeffding inequality can be rewritten as:

$$P(\mathcal{D}: |\mathrm{E}_{out}(h) - \mathrm{E}_{in}(h)| > \epsilon) \leq 2e^{-2\epsilon^2 N} \text{ for any } \epsilon > 0$$

This is called a "Probably Aproximately Correct (PAC)" result

- IMPORTANT: Note that $\mathcal{H}$ is set before knowing the data sample.

Hoeffding says that $E_{\text{in}}(h) \approx E_{\text{out}}(h)$

$$\mathbb{P}(\mathcal{D}\colon |\mu - \nu| > \epsilon) \le 2e^{-2\epsilon^2 N} \quad \Longleftrightarrow \quad \mathbb{P}(\mathcal{D}\colon |E_{\text{out}}(h) - E_{\text{in}}(h)| > \epsilon) \le 2e^{-2\epsilon^2 N}$$

E_{in} is random, but known; E_{out} fixed, but unknown.

- If $E_{\text{in}}(h) \approx 0 \overset{N \gg 1}{\Longrightarrow} E_{out}(h) \approx 0$ (with high probability), i.e. $\mathbb{P}_{\mathcal{X}}[h(\mathbf{x}) \neq f(\mathbf{x})] = 0$
  – We have learned something about the *entire* $f: f \approx h$ *over* $\mathcal{X}$ (outside $\mathcal{D}$)

- If $E_{\text{in}} \gg 0$, we're out of luck.
  – But, we have still learned something about the *entire* $f: f \not\approx h$ *over* $\mathcal{X}$; it is not very useful though.

Questions:

1. Suppose that E_{in} = 1, have we learned something about the entire f that is useful?
2. What is the worst E_{in} for inferring about f ?

Understanding PAC results

$$P(\mathcal{D}: |\mathrm{E}_{out}(h) - \mathrm{E}_{in}(h)| > \epsilon) \leq 2e^{-2\epsilon^2 N} \text{ for any } \epsilon > 0$$

- Let's consider $\delta = 2e^{-2\epsilon^2 N}$ then

$$P(\mathcal{D}: |\mathrm{E}_{out}(h) - \mathrm{E}_{in}(h)| > \epsilon) \leq \delta \Leftrightarrow P(\mathcal{D}: |\mathrm{E}_{out}(h) - \mathrm{E}_{in}(h)| \leq \epsilon) > 1 - \delta$$

- Or equivalently:

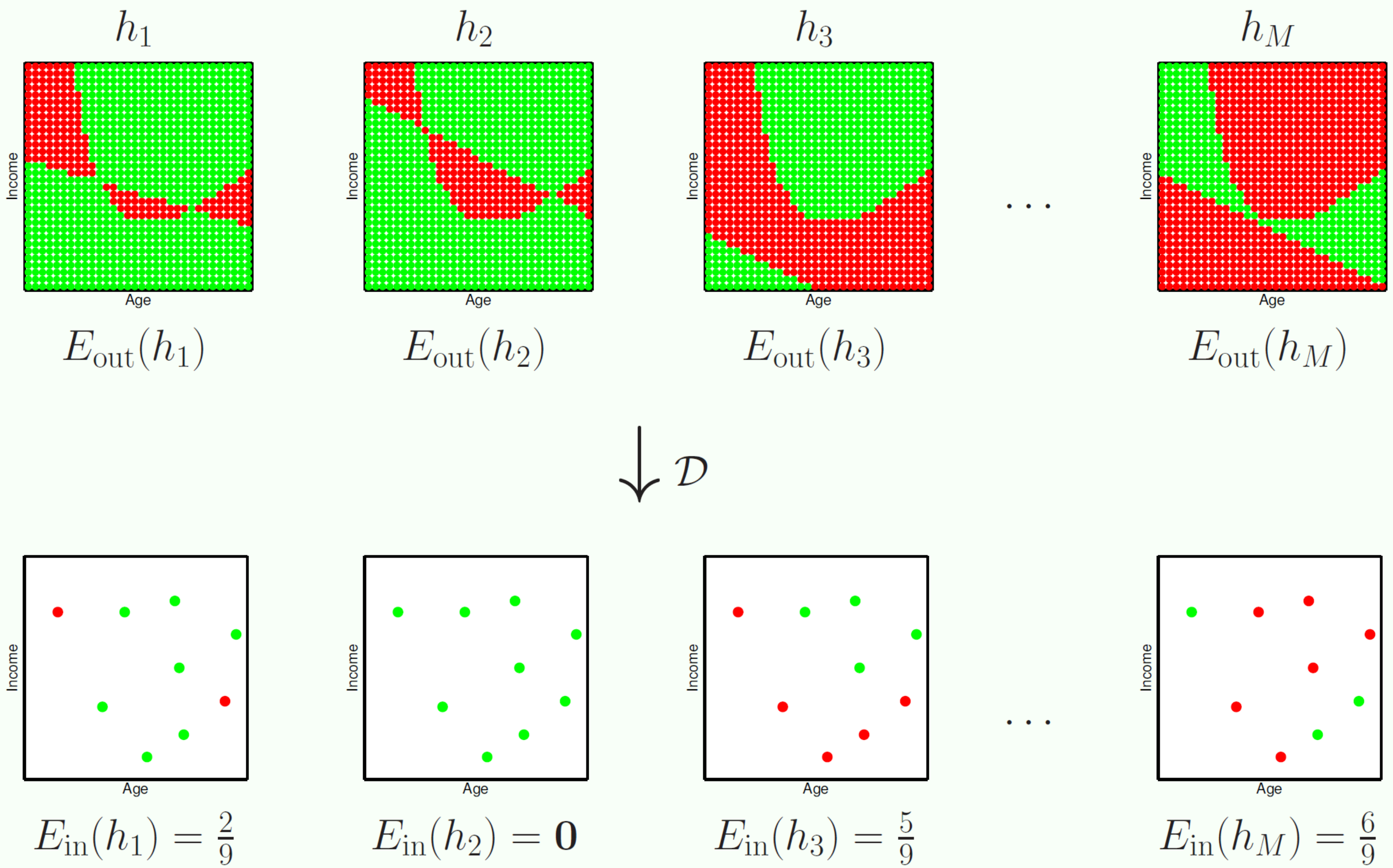
$$\mathrm{E}_{out}(h) \leq \mathrm{E}_{in}(h) + \epsilon \text{ , } \textit{with probability at least } 1 - \delta \text{ on } \mathcal{D}$$

- Let's write ϵ as a function of N and δ, then

$$\mathrm{E}_{out}(h) \leq \mathrm{E}_{in}(h) + \sqrt{\frac{1}{2N}\log\frac{2}{\delta}} \quad \textit{with probability at least } 1 - \delta \textit{ on } \mathcal{D}$$

- The higher N the narrow the interval (The sample size is important !!)
- The smaller δ the larger the interval (The higher guarantee the lesser accuracy)

Real Learning – Finite Learning Model



Pick the hypothesis with minimum E_{in}; will E_{out} be small?

The Hoeffding inequality for multiple hypothesis

NOW IS DIFFERENT: In Hoeffding's inequality h is fixed before knowing the data, BUT in REAL PROBLEMS the chosen hypothesis, $g \in \mathcal{H}$ is identified using the data.

SEARCH CAUSES SELECTION BIAS: THE COIN ANALOGY

Question: if toss one **fair coin** ten times, what is the probability that you will get ten heads ?

Answer: $\approx$ **0.1** (try it)

Question: if toss 1000 **fair coins** ten times, what is the probability that some coin will get ten heads ?

Answer: $\approx$ **0.63** (try it)

Identifying coins with functions: the higher the size of $\mathcal{H}$ the higher the probability of having a hypothesis with $E_{in} \approx 0$ error , BUT can we expect E_{out} to be small ?

Guaranties for $\mathcal{H}$-finite

- Adapting the Hoeffding's inequality to the case of finite $\mathcal{H}$
  1. Hoeffding: ***g* should be fixed before knowing the data sample**. (MANDATORY CONDITION)
  2. Now, the Learning Algorithm uses the training data to search for $\boldsymbol{g}$.
  3. How to establish valid guarantees for any class element?

- A simple solution is to consider an event valid for all functions in $\mathcal{H}$.
  - Let g denote a generic hypothesis solution then,

$$\{\mathcal{D}: |E_{in}(g) - E_{out}(g)| > \epsilon\} = \bigcup_{h_i \in H} (\mathcal{D}: |E_{in}(h_i) - E_{out}(h_i)| > \epsilon)$$

  - Using $P\left(\bigcup_{i=1:|\mathcal{H}|} B_i\right) \leq \sum_{i=1}^{|\mathcal{H}|} P(B_i)$

$$P(\mathcal{D}: |\mathrm{E}_{in}(g) - \mathrm{E}_{out}(g)| > \epsilon) < 2|\mathcal{H}|e^{-2\epsilon^2 N} \text{ for any } \epsilon > 0$$

Uniform Convergence with N

Interpreting the bound

$$\mathbb{P}(\mathcal{D}: |\mathrm{E}_{in}(\boldsymbol{g}) - \mathrm{E}_{out}(\boldsymbol{g})| > \epsilon) \leq 2|\mathcal{H}|e^{-2\epsilon^2 N} \qquad \text{for any } \epsilon > 0$$

$$\mathbb{P}(\mathcal{D}: |\mathrm{E}_{in}(\boldsymbol{g}) - \mathrm{E}_{out}(\boldsymbol{g})| \leq \epsilon) \geq 1 - 2|\mathcal{H}|e^{-2\epsilon^2 N} \qquad \text{for any } \epsilon > 0$$

Generalization bar error

Result: With probability at least $1 - \boldsymbol{\delta}$, $E_{out}(g) \leq E_{in}(g) + \sqrt{\frac{1}{2N}\ln\frac{2|\mathcal{H}|}{\delta}}$

To do that, denote $\delta = 2|\mathcal{H}|e^{-2\epsilon^2 N}$ and writes ϵ as a function of N, δ and $|\mathcal{H}|$

E_{in} reaches outside to E_{out} when $|\mathcal{H}|$ is small $\qquad E_{out}(g) \leq E_{in}(g) + \mathcal{O}\left(\sqrt{\frac{\ln|\mathcal{H}|}{N}}\right)$

if $N \gg \ln|\mathcal{H}|$, then $E_{out}(g) \approx E_{in}(g)$

- This bound does not depend on $\mathcal{X}$, $\mathbb{P}$(x), f or how g is found. (i.e. a worst case bound)
- Only requires $\mathbb{P}$(x) to generate the data points independently *including* the test point.

A particular case: The Realizability Hypothesis

- Definition ($\mathcal{H}$ -realizable): There exist $h^* \in \mathcal{H}$ $s.t.$ $E_{out_{\mathcal{P},f}}(h^*) = 0$

- This means that the class of functions $\mathcal{H}$ includes at least a function with error zero for any $\mathcal{P}$ and f.

- Being a mathematical hypothesis can be applied in real tasks.
  - Example: Separated clases in classification

- Under this hyphotesis can be shown that the ERM rule on finite clases $\mathcal{H}$ always provides a function h_S s.t. $E_{in}(h_S) = 0$, obtaining the smallest error bound

$$\mathrm{E}_{out}(h_S) \leq \frac{1}{N} \log \frac{|\mathcal{H}|}{\delta} \quad \textit{with probability al least } 1 - \delta$$

Formal Definition of PAC-Learning

- A hypothesis class $\mathcal{H}$ is PAC learnable if there exist a function $m_{\mathcal{H}}(\epsilon, \delta) \rightarrow \mathbb{N}$ and a learning algorithm $\mathcal{A}$ with the following property:
  - For every, $\epsilon, \delta \in (0,1)$
  - For every distribution $\mathcal{P}$ over $\mathcal{X}$
  - For every labeling function f

  if the realizable assumption holds with respect to $\mathcal{H}, \mathcal{P}, f$ then when running the learning algorithm on $\mathrm{N} \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d samples generated by $\mathcal{P}$ and labeled by f, the algorithm returns a hypothesis h such that , with probability al least 1- δ (over the choice of the m training samples)

$$ERM_{\mathcal{P},f}(h) \leq \epsilon$$

This means the learning algorithm always return a hypothesis h with error close to zero.

(*Understanding Machine Learning,* Shalev-Shwartz and Ben-David, 2014, free pdf)

Sample Complexity in PAC-Learnability

- How many examples are required to guarantee a PAC solution in realizable classes?

- This depend on ϵ, δ, $\mathcal{H}$ and the loss function range

- If $\mathcal{H}$ is a PAC-realizable, there exist many functions $m_{\mathcal{H}}(\epsilon, \delta)$ that satisfy the requirements given in the definition of Realizable PAC learnability

- The sample complexity for learning $\mathcal{H}$ is defined as the "minimal integer" $m_{\mathcal{H}}(\epsilon, \delta)$ that satisfies the requirements of realizable PAC learning with accuracy ϵ and confidence δ

- Result for loss function with range in [0,1]: every realizable finite hypothesis class is PAC learnable with sample complexity

$$m_H(\varepsilon, \delta) \leq \left\lceil \frac{1}{\epsilon} \log \frac{|\mathcal{H}|}{\delta} \right\rceil$$

Formal Definition of Agnostic PAC-Learning

- A hypothesis class $\mathcal{H}$ is agnostic PAC learnable if there exist a function $m_{\mathcal{H}}(\epsilon, \delta) \to \mathbb{N}$ and a learning algorithm $\mathcal{A}$ with the following property:
  - For every, $\epsilon, \delta \in (0,1)$
  - For every distribution $\mathcal{P}$ over $\mathcal{X}$

  When running the learning algorithm on $\mathrm{N} \geq m_{\mathcal{H}}(\epsilon, \delta)$ i.i.d samples generated by $\mathcal{P}$, the algorithm returns a hypothesis h such that , with probability al least 1- δ (over the choice of the *m* training samples)

$$E_{in\,\mathcal{P}}(h) \leq \min_{h' \in \mathcal{H}} E_{in\,\mathcal{P}}(h') + \epsilon$$

This means the learning algorithm always return a hypothesis h closer to the best possible inside of the class $\mathcal{H}$

The ERM rule is a succesful agnostic PAC learner for finite classes $\mathcal{H}$

Agnostic-PAC Sample Complexity

- How many examples are required to guarantee a PAC solution?
- This depend on ϵ, δ, $\mathcal{H}$ and the loss function range
- If $\mathcal{H}$ es PAC learnable, there exist many functions $m_{\mathcal{H}}(\epsilon, \delta)$ that satisfy the requirements given in the definition of PAC learnability
- The sample complexity of learning $\mathcal{H}$ is defined as the "minimal integer" $m_{\mathcal{H}}(\epsilon, \delta)$ that satisfies the requirements of PAC learning with accuracy ε and confidence δ
- Result for loss function with range in [0,1]: every finite hypothesis class is PAC learnable with sample complexity

$$m_H(\varepsilon, \delta) \leq \left\lceil \frac{2}{\epsilon^2} \log \frac{2|\mathcal{H}|}{\delta} \right\rceil$$

- Compare this new expression with that in the PAC-realizable case!

Feasibility of Learning vs Complexity

- Learning is possible in a probabilistic setting (under conditions):
  - Samples from $\mathcal{X}$ **must be i.i.d**
  - Same probability distribution in training and test

- To be succesful in learning means to find a function g, s.t. $\mathrm{E}_{out}(g) \approx 0$
- Nevertheless, we are only able to guarantee,

$$P(\mathcal{D}\colon |\mathrm{E}_{in}(g) - \mathrm{E}_{out}(g)| > \epsilon) < 2|\mathcal{H}|e^{-\epsilon^2 N} \text{ for any } \epsilon > 0$$

- Feasibility of Learning must answer two questions:
  1. Can we make sure that $\mathrm{E}_{out}(g)$ is close enough to $\mathrm{E}_{in}(g)$?
  2. Can we make $\mathrm{E}_{in}(g)$ small enough?

- What is the relationship between Feasibility of Learning and the complexity of $\mathcal{H}$ and f?

Feasibility of learning : $E_{out} \approx 0$

Two conditions:

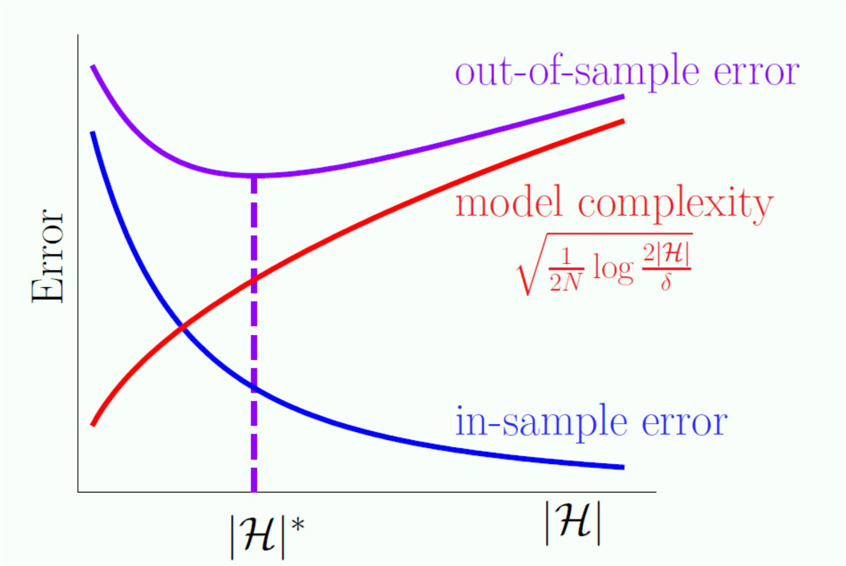
(1) $E_{in} \approx E_{out}$ $\longrightarrow$ Is verified thank to the Hoeffding's inequality

(2) $E_{in} \approx 0$ $\longrightarrow$ Is achieved through the learning algorithm

Together, these ensure $E_{out} \approx 0$

BUT there is a tradeoff on $\mathcal{H}$:

- **Small $|\mathcal{H}|$** $\Rightarrow E_{in} \approx E_{out}$
- **Large $|\mathcal{H}|$** $\Rightarrow E_{in} \approx 0$ is more likely



What about the UNKNOWN complexity of f :

- Simple f $\Rightarrow$ can use small $\mathcal{H}$ to get $E_{in} \approx 0$ (need smaller N).
- Complex f $\Rightarrow$ need large $\mathcal{H}$ to get $E_{in} \approx 0$ (need larger N).

The Fundamental theorem of PAC learning

Let $\mathcal{H}$ be a hyphotesis class of functions from a domain $\mathcal{X}$ to [0,1] ad let the loss functions be the 0--1 loss. Then the following are equivalent:

- $\mathcal{H}$ has the uniform convergence properties
- Any ERM rule is a successful agnostic PAC learner for $\mathcal{H}$
- $\mathcal{H}$ is agnostic PAC learnable
- $\mathcal{H}$ is PAC learnable
- Any ERM rule is a successful PAC learner for $\mathcal{H}$
- $\mathcal{H}$ has a finite VC-dimension