Machine Learning II

The learning problem

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February 8, 2022

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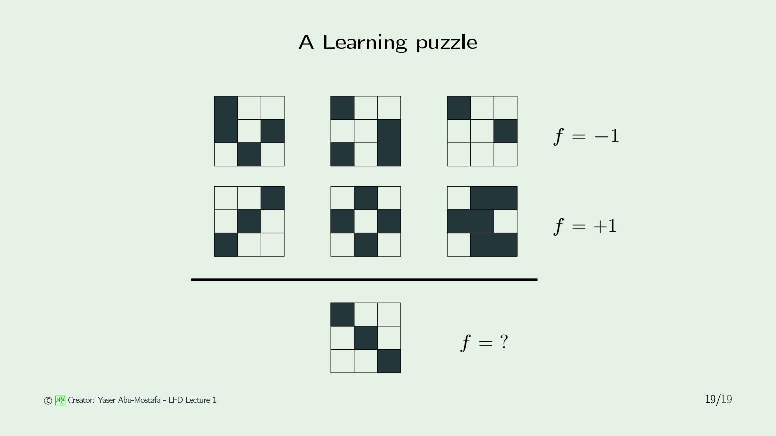
A learning puzzle



Is it -1 or +1?

Is learning feasible?

The target function is **unknown**. How could a limited data set reveal enough information to pin down the entire target function?

- More than one function fits the 6 training examples.
    - If the true f is $+1$ when the pattern is symmetric, then the solution is $+1$
    - If the true f is -1 when the top left square of the pattern is white, then the solution is -1
- We know the values of f on all the points in the training data $\mathcal{D}$. But since f is an unknown function, f remains unknown outside of $\mathcal{D}$.
- The whole purpose of learning f is to be able to predict the value of f on new points.
- Is learning feasible? Yes, in a **probabilistic sense**.

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Outline

- A related experiment
- Connection to learning
- Connection to <u>real</u> learning
- The solution

Bin and marbles

A related experiment

- Consider a 'bin' with red and green marbles.

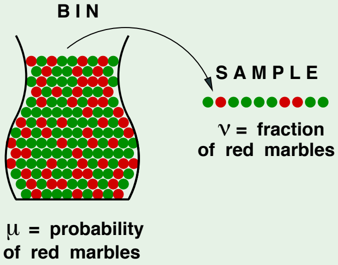
$$\mathbb{P}[\text{ picking a red marble }] = \mu$$

$$\mathbb{P}[\text{ picking a green marble }] = 1 - \mu$$

- The value of μ is unknown to us.

- We pick N marbles independently.

- The fraction of red marbles in sample $= \nu$



Bin and marbles

Does ν say anything about μ?

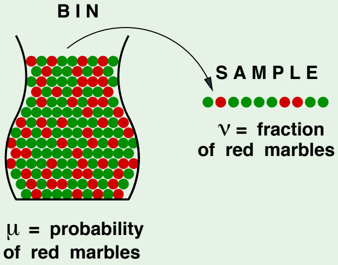
No!

Sample can be mostly green while bin is mostly red.

Yes!

Sample frequency ν is likely close to bin frequency μ.

possible versus probable



Hoefdding's inequality

What does ν say about μ?

In a big sample (large N), ν is probably close to μ (within ϵ).

Formally,

$$\mathbb{P}\left[\,|\nu - \mu| > \epsilon\,\right] \leq 2e^{-2\epsilon^2 N}$$

This is called **Hoeffding's Inequality**.

In other words, the statement "$\mu = \nu$" is P.A.C.

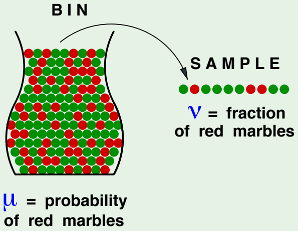
P.A.C = Probably Approximately Correct

We want the probability of the "bad event" (ν far from μ) to be small.

Hoefdding's inequality

$$\mathbb{P}\left[|\nu - \mu| > \epsilon\right] \leq 2e^{-2\epsilon^2 N}$$

- Valid for all N and ϵ
- Bound does not depend on μ
- Tradeoff: N, ϵ, and the bound.
- $\nu \approx \mu \quad \Longrightarrow \quad \mu \approx \nu \quad$ ☺



Two rules of probability

Let $\mathcal{B}_1, \mathcal{B}_2$ be any two events. If $\mathcal{B}_1 \implies \mathcal{B}_2$ (i.e. event $\mathcal{B}_1$ implies event $\mathcal{B}_2$ or equivalently, $\mathcal{B}_1 \subseteq \mathcal{B}_2$), then

$$\mathbb{P}(\mathcal{B}_1) \leq \mathbb{P}(\mathcal{B}_2).$$

Let $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_M$ be <u>any</u> M events, then

$$\mathbb{P}(\mathcal{B}_1 \text{ or } \mathcal{B}_1 \text{ or } \ldots \text{ or } \mathcal{B}_M) \leq \mathbb{P}(\mathcal{B}_1) + \mathbb{P}(\mathcal{B}_2) + \cdots + \mathbb{P}(\mathcal{B}_M).$$

The second rule is known as the *union bound* or *Boole's inequality*.

Exercise I

If the probability of red marbles is $\mu = 0.9$, what is the probability that a sample of $N = 10$ marbles will have a fraction of red marbles $\nu \leq 0.1$? [Hint: use a binomial distribution]

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Solution. If X is the number of red marbles among $N = 10$ marbles, we have that

$$\nu \leq 0.1 \iff X \leq 1,$$

Then, we can write

$$\mathbb{P}(X \leq 1) = \mathbb{P}(X = 0) + \mathbb{P}(X = 1) = 9.2 \times 10^{-9},$$

where

$$\mathbb{P}(X = x) = \binom{N}{x} \mu^x (1 - \mu)^{N-x}, \quad x = 0, 1, \dots, N,$$

since $X \sim \text{Binomial}(N, \mu)$.

Exercise II

If the probability of red marbles is $\mu = 0.9$, use the Hoeffding Inequality to bound the probability that a sample of 10 marbles will have a fraction of red marbles $\nu \leq 0.1$ and compare the answer to the previous exercise. [Hint: Use one of the previous rule]

Exercise II

If the probability of red marbles is $\mu = 0.9$, use the Hoeffding Inequality to bound the probability that a sample of 10 marbles will have a fraction of red marbles $\nu \leq 0.1$ and compare the answer to the previous exercise. [Hint: Use one of the previous rule]

Solution. If $\mu = 0.9$ and $\nu \leq 0.1$, it implies that $|\nu - \mu| \geq 0.8$ (or $|\nu - \mu| > 0.8^{-}$, the largest number less than 0.8). We can write

$$\begin{aligned} \mathbb{P}(\nu \leq 0.1) &\leq \mathbb{P}(|\nu - \mu| \geq 0.8) \\ &= \mathbb{P}(|\nu - \mu| > 0.8^{-}) \\ &\leq 2e^{-2\times(0.8^{-})^2\times 10} = 5.52 \times 10^{-6} \end{aligned}$$

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From marbles to learning

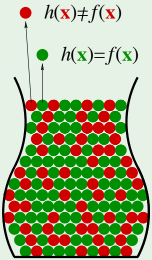
Connection to learning

Bin: The unknown is a number μ

Learning: The unknown is a function $f : \mathcal{X} \to \mathcal{Y}$

Each marble ● is a point $\mathbf{x} \in \mathcal{X}$

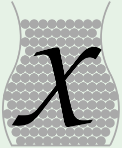
- ● : Hypothesis got it right $h(\mathbf{x}) = f(\mathbf{x})$
- ● : Hypothesis got it wrong $h(\mathbf{x}) \neq f(\mathbf{x})$

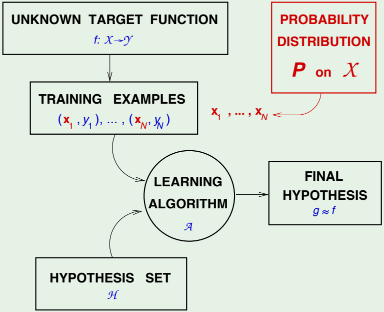


Learning diagram updated

Back to the learning diagram

The bin analogy:





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Verification vs learning

Are we done?

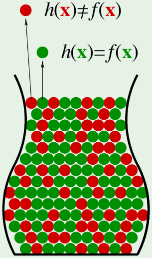
Not so fast! h is fixed.

For this h, ν generalizes to μ.

'verification' of h, not **learning**

No guarantee ν will be small.

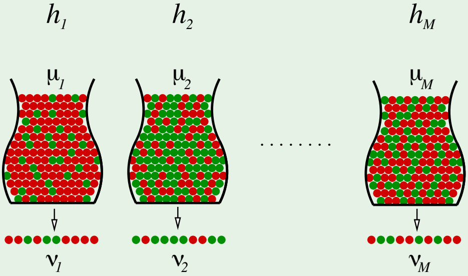
We need to **choose** from multiple h's.



Multiple bins

Multiple bins

Generalizing the bin model to more than one hypothesis:



Notation for learning

Notation for learning

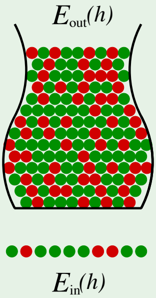
Both μ and ν depend on which hypothesis h

ν is '**in sample**' denoted by $E_{\text{in}}(h)$

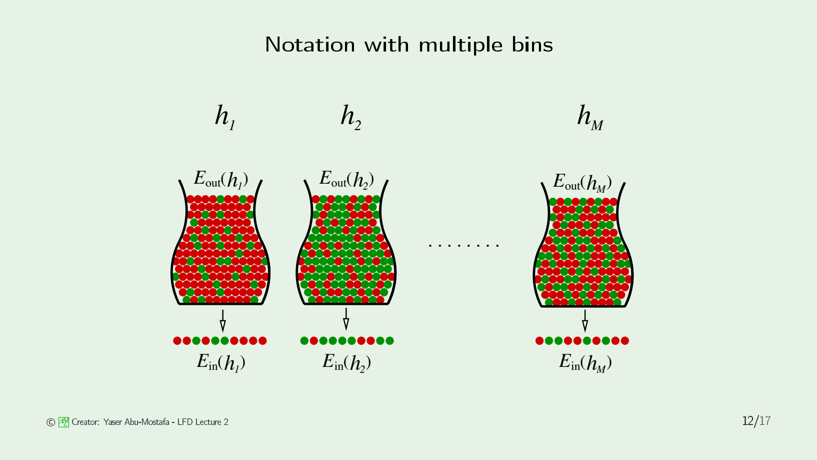
μ is '**out of sample**' denoted by $E_{\text{out}}(h)$

The Hoeffding inequality becomes:

$$\mathbb{P}\left[\, |E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon \,\right] \;\leq\; 2e^{-2\epsilon^2 N}$$



Notation with multiple bins



Hoefdding does not apply to multiple bins - coin analogy

Hoefdding does not apply to multiple bins!

- If you toss one fair coin 10 times, what is the probability that you will get 10 heads?
- If you toss 1000 fair coins 10 times each, what is the probability that some coin will get 10 heads?

Hoefdding does not apply to multiple bins - coin analogy

If you toss one fair coin 10 times, what is the probability that you will get 10 heads?

$$
\begin{aligned}
& P(\text{10 heads in 10 tosses}) \\
& = P(\text{first toss is head and ... and tenth toss is head}) \\
& = P(\text{first toss is head}) \times \cdots \times P(\text{tenth toss is head}) \\
& = [P(\text{a toss is head})]^{10} \\
& = 1/2^{10} \\
& \approx 1/1000 \\
& = 0.1\%
\end{aligned}
$$

Hoefdding does not apply to multiple bins - coin analogy

If you toss 1000 fair coins 10 times each, what is the probability that some coin will get 10 heads?

$$
\begin{aligned}
& P(\text{ no heads in 10 tosses for one coin}) \\
& = 1 - P(\text{10 heads in 10 tosses for one coin}) \\
& = 1 - 1/1000
\end{aligned}
$$

$$
\begin{aligned}
& P(\text{ no heads in 10 tosses for 1000 coins}) \\
& = (1 - 1/1000)^{1000} \\
& \approx 0.37
\end{aligned}
$$

$$P(\text{10 heads in 10 tosses for at least one coin}) = 1 - 0.37 \approx 0.63$$

Hoefdding does not apply to multiple bins - coin analogy

Coin analogy

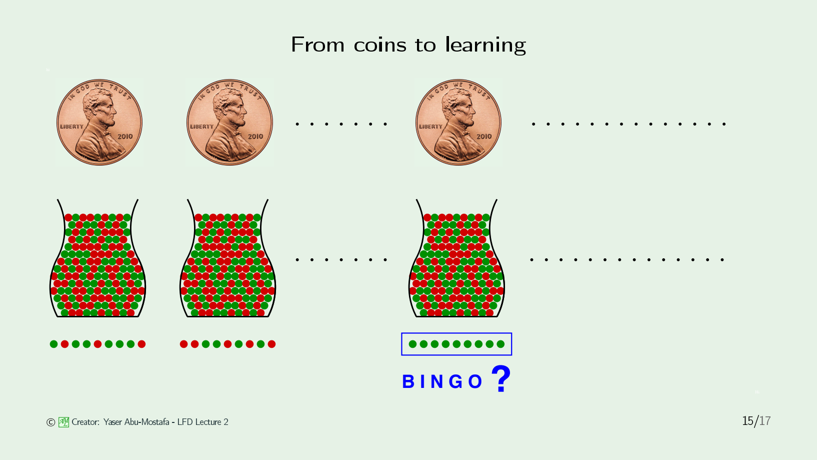
Question: If you toss a fair coin 10 times, what is the probability that you will get 10 heads?

Answer: $\approx 0.1\%$

Question: If you toss 1000 fair coins 10 times each, what is the probability that <u>some</u> coin will get 10 heads?

Answer: $\approx 63\%$

From coins to learning



From coins to learning

The Hoeffding inequality applies to each bin individually. The inequality states that

$$\mathbb{P}[|E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon] \leq 2e^{-2\epsilon^2 N} \quad \text{for any} \;\; \epsilon > 0$$

where

1. the hypothesis h is fixed before the data is generated,
2. the probability is with respect to random data sets $\mathcal{D}$.

The assumption "h is fixed before the data set is generated" is critical to the validity of the bound.

From coins to learning

In learning, we consider an entire hypothesis set, say $\mathcal{H} = \{h_1, h_2, \ldots, h_M\}$ (with a finite number of hypotheses), instead of just one hypothesis h. Then, the learning algorithm picks the final hypothesis $g \in \mathcal{H}$ based on $\mathcal{D}$.

The statement we would like to make is **not**

$$\mathbb{P}[|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon] \text{ is small for any fixed } h_m \in \mathcal{H},$$

where $m = 1, 2, \ldots, M$, but **rather**

$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \text{ is small for the final hypothesis } g.$$

A simple solution

$$|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon$$

$$\Longrightarrow$$

$$\begin{aligned} &|E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon \\ \text{or } &|E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon \\ \cdots \\ \text{or } &|E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon \end{aligned}$$

A simple solution

A simple solution

$$
\begin{aligned}
\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ \mathbb{P}[\quad & |E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon \\
& \textbf{or } |E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon \\
& \cdots \\
& \textbf{or } |E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon\ ] \\
\leq\ & \sum_{m=1}^{M} \mathbb{P}\left[|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon\right]
\end{aligned}
$$

The final verdict

The final verdict

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \le\ \sum_{m=1}^{M} \mathbb{P}\left[|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon\right]$$

$$\le\ \sum_{m=1}^{M} 2e^{-2\epsilon^2 N}$$

$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \le 2{\color{red}M}e^{-2\epsilon^2 N}$$

Generalization error

- The **out-of-sample error** E_{out} measures how well our training on $\mathcal{D}$ has generalized to unseen data points. E_{out} is based on the performance over the entire input space $\mathcal{X}$.
- The **in-sample error** E_{in} is based on the training data points.
- The **generalization error** is the discrepancy between E_{in} and E_{out}. Generalization error is also used as another name for E_{out} (but not here).
- The Hoeffding inequality provides a way to *charaterize the generalization error* with a probabilistic bound.

Generalization bound

The Hoeffding inequality states that

$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N} \quad \text{for any} \quad \epsilon > 0$$

This can be rephrased as follows. Pick a tolerance level δ, for example $\delta = 0.01$, and assert with probability at least $1 - \delta$ that

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{1}{2N} \ ln\left(\frac{2M}{\delta}\right)}.$$

This is called a *generalization bound* since it bounds E_{out} in terms of E_{in}.

Generalization bound

We can rewrite the Hoeffding inequality as follows

$$\begin{aligned}
&\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq 2Me^{-2\epsilon^2 N} \\
\implies\ &1 - \mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| \leq \epsilon] \leq 2Me^{-2\epsilon^2 N} \\
\implies\ &\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| \leq \epsilon] \geq 1 - 2Me^{-2\epsilon^2 N}
\end{aligned}$$

In other words, with probability at least $1 - 2Me^{-2\epsilon^2 N}$, we have

$$|E_{\text{in}}(g) - E_{\text{out}}(g)| \leq \epsilon,$$

or, equivalently,

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \epsilon \textbf{ and } E_{\text{out}}(g) \geq E_{\text{in}}(g) - \epsilon.$$

Generalization bound

If $\delta = 2Me^{-2\epsilon^2 N}$, then we have $\epsilon = \sqrt{\frac{1}{2N}\ ln\left(\frac{2M}{\delta}\right)}$.

Since $E_{\text{out}}(g) \leq E_{\text{in}}(g) + \epsilon$, we can say that, with probability at least $1 - \delta$,

$$E_{\text{out}}(g) \leq E_{\text{in}}(g) + \sqrt{\frac{1}{2N}\ ln\left(\frac{2M}{\delta}\right)}.$$

In other words, the hypothesis g that we choose will continue to do well out of sample.

We also want to be sure that there is no other hypothesis $h \in \mathcal{H}$ where $E_{\text{out}}(h)$ is significantly better than $E_{\text{out}}(g)$. The other direction of the bound (i.e. $E_{\text{out}}(g) \geq E_{\text{in}}(g) - \epsilon$) assures us that it is unlikely that any other hypothesis in $\mathcal{H}$ was unlucky on the trainng set but is acutally much better than the g we have chosen.

The VC inequality

- The error bound depends on M, the size of the hypothesis set $\mathcal{H}$
- If $\mathcal{H}$ is an infinite set, the bound goes to infinity and becomes useless
- M can be replaced with something finite (the effective number of hypotheses), so that the bound is meaningful.

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ 4\ m_{\mathcal{H}}(2N)\ e^{-\frac{1}{8}\epsilon^2 N}$$

The Vapnik-Chervonenkis Inequality

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Feasibility of learning

- If we insist on a deterministic answer, i.e. $\mathcal{D}$ tells us something certain about f outside of $\mathcal{D}$, then the answer is no.
- If we accept a probabilistic answer, i.e. $\mathcal{D}$ tells us something likely about f outside of $\mathcal{D}$, then the answer is yes.

What we know so far

Learning is feasible. It is likely that

$$E_{\text{out}}(g) \approx E_{\text{in}}(g).$$

Is this learning? We need $g \approx f$, which means

$$E_{\text{out}}(g) \approx 0.$$

The two questions of learning

$E_{\text{out}}(g) \approx 0$ is achieved through

$$E_{\text{out}}(g) \approx E_{\text{in}}(g) \textbf{ and } E_{\text{in}}(g) \approx 0$$

Learning can be reduced to two questions:

1. Can we make sure that $E_{\text{out}}(g)$ is close enough to $E_{\text{in}}(g)$?
2. Can we make $E_{\text{in}}(g)$ small enough?

- The Hoeffding Inequality addresses the **first question** only.
- We answer the **second question** after running the learning algorithm on the the training data.

The complexity of $\mathcal{H}$.

Question 1: According to the Hoeffding Inequality, a larger M increases the risk that $E_{\text{in}}(g)$ will be a poor estimate of $E_{\text{out}}(g)$ $\implies$ we need to control M (a measure of the complexity of $\mathcal{H}$).

Question 2: We stand a better chance if $\mathcal{H}$ is more complex $\implies$ a more complex $\mathcal{H}$ gives us more flexibility in finding some g that fits the data well.

The complexity of f.

Question 1: If we fix the hypothesis set and the number of training examples, the inequality provides the same bound $\Longrightarrow$ The complexity of f does not affect how well $E_{\text{in}}(g)$ approximates $E_{\text{out}}(g)$.

Question 2: The data from a complex f are harder to fit than the data from a simple f (large $E_{\text{in}}(g)$). We can increase the complexity of $\mathcal{H}$, but then $E_{\text{out}}(g)$ will not be as close to $E_{\text{in}}(g)$.

What the theory will achieve

Characterizing the feasibility of learning for infinite M

Characterizing the tradeoff:

Model complexity $\uparrow$	E_{in}	$\downarrow$
Model complexity $\uparrow$	$E_{\text{out}} - E_{\text{in}}$	$\uparrow$