Big Data Analytics

The learning problem

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Table of contents

1

Table of contents

A learning puzzle

A Learning puzzle

$f = -1$

$f = +1$

$f = ?$

Is it -1 or +1?

3

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**.

Table of contents

Outline

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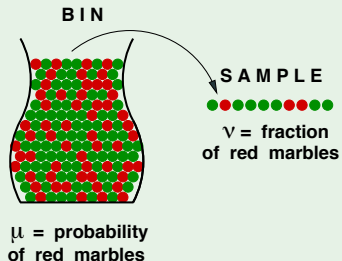- Connection to <u>real</u> learning
- The solution

A related experiment

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

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

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

- The value of μ is <u>unknown</u> to us.

- We pick N marbles independently.

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

BIN

SAMPLE

ν = **fraction of red marbles**

μ = **probability of red marbles**

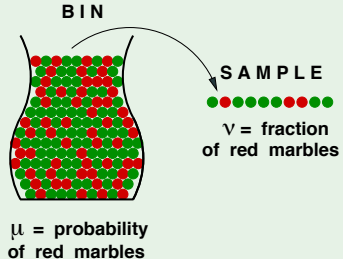Does ν say anything about μ?

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

BIN

SAMPLE

ν = fraction
of red marbles

μ = probability
of red marbles

What <u>does</u> 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.
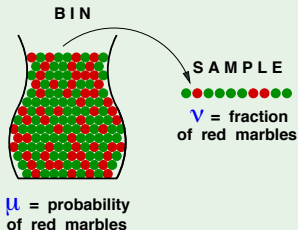
In other words, the statement "$\mu = \nu$" is P.A.C.

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P.A.C = Probably Approximately Correct

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

9

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

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

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

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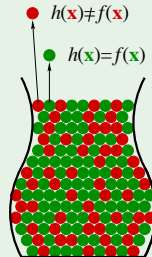\end{aligned}
$$

Table of contents

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 $h(\mathbf{x}){\neq}f(\mathbf{x})$

Back to the learning diagram

The bin analogy:
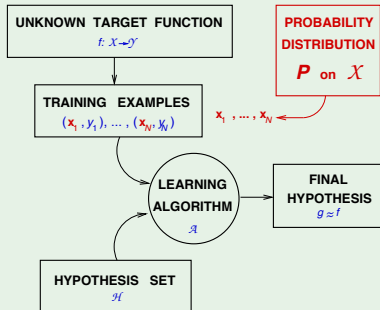
$\mathcal{X}$

UNKNOWN TARGET FUNCTION
$f: \mathcal{X} \to \mathcal{Y}$

PROBABILITY DISTRIBUTION
P on $\mathcal{X}$

TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_N, y_N)$

$\mathbf{x}_1, \dots, \mathbf{x}_N$

LEARNING ALGORITHM
$\mathcal{A}$

FINAL HYPOTHESIS
$g \approx f$

HYPOTHESIS SET
$\mathcal{H}$

16

Table of contents

Are we done?

Not so fast! h is fixed.

For <u>this</u> h, ν generalizes to μ.

'verification' of h, not learning

No guarantee ν will be small.

We need to choose from multiple h's.

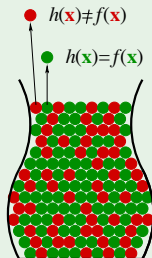$\bullet$ $h(\mathbf{x}) \neq f(\mathbf{x})$

$\bullet$ $h(\mathbf{x}) = f(\mathbf{x})$
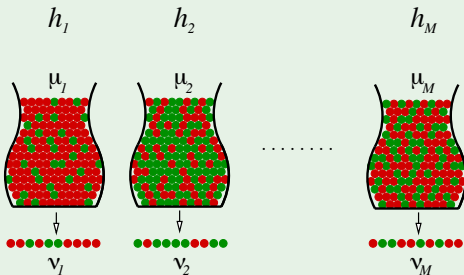
Multiple bins

Notation for learning

Both μ and ν depend on which hypothesis h

$\quad\quad \nu$ is 'in sample' denoted by $E_{\text{in}}(h)$

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

The Hoeffding inequality becomes:

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

$E_{\text{out}}(h)$

$E_{\text{in}}(h)$

20
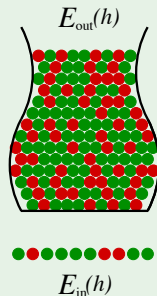
Notation with multiple bins
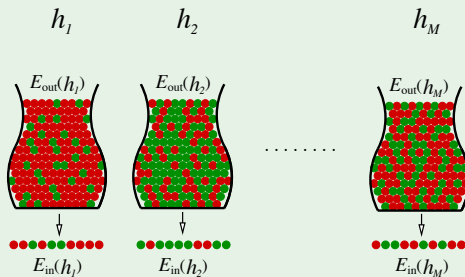
h_1 h_2 h_M

$E_{\text{out}}(h_1)$ $E_{\text{out}}(h_2)$ $E_{\text{out}}(h_M)$

. . . .

$E_{\text{in}}(h_1)$ $E_{\text{in}}(h_2)$ $E_{\text{in}}(h_M)$

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?

$P(10 \text{ heads in 10 tosses})$

$= P(\text{first toss is head and ... and tenth toss is head})$

$= P(\text{first toss is head}) \times \cdots \times P(\text{tenth toss is head})$

$= [P(\text{a toss is head})]^{10}$

$= 1/2^{10}$

$\approx 1/1000$

$= 0.1\%$

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?

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

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

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

<div align="center">

Coin analogy

</div>

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 some coin will get 10 heads?

Answer: $\approx 63\%$

25

From coins to learning

26
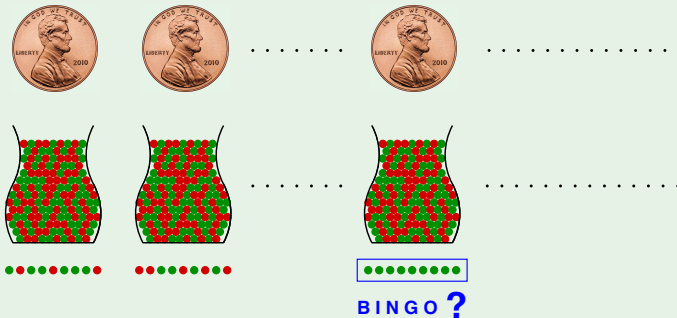
From coins to learning

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**

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

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

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

A simple solution

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

$$\implies$$

$$|E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon$$
$$\text{or } |E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon$$
$$\ldots$$
$$\text{or } |E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon$$

A simple solution

$$\mathbb{P}[\,|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\,] \leq \mathbb{P}[\quad |E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon$$

$$\text{or } |E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon$$

$$\cdots$$

$$\text{or } |E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon\,]$$

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

The final verdict

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

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

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

31

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

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

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

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

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,

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

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 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 <u>effective</u> 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

Table of contents

Feasibility of learning

- If we insist on a deterministic answer, i.e. $\mathcal{D}$ tells us something <u>certain</u> about f outside of $\mathcal{D}$, then the answer is no.

- If we accept a probabilistic answer, i.e. $\mathcal{D}$ tells us something <u>likely</u> about f outside of $\mathcal{D}$, then the answer is yes.

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

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

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 two questions of learning

The complexity of $\mathcal{H}$.

Question 1: According to the Hoeffding Inequality, a larger M increases the risk that $E_{in}(g)$ will be a poor estimate of $E_{out}(g)$ $\implies$ 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 two questions of learning

The complexity of f.

Question 1: If we fix the hypothesis set and the number of training examples, the inequality provides the same bound $\implies$ 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 $E_{\text{in}}(g)$.

Learning theory

What the theory will achieve

Characterizing the feasibility of learning for infinite M

Characterizing the tradeoff:

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

out-of-sample error

model complexity

Error

in-sample error

d_{VC}^* VC dimension, d_{VC}