





Can Machine Learning solve my problem?

9th BCD ISHEP Cargèse School - part I 28 March 2024 - Cargèse, France

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What impressive things machine learning can and/or will be able to do?



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Can Machine Learning solve my problem? I do not know

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https://www.general-staff.com/wp-content/uploads/2019/03/MathWarning-300x193.jpg



https://www.meme-arsenal.com/en/create/meme/1868835

What is learning ?

"A relatively permanent change in behaviour due to past experiences."

D. Coon, Introduction to psychology: exploration and application (1983)

Start from the beginning ...

Supervised Learning Learn by example



Question:

List 2 animals that you believe are capable of learning.





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Rat bait shyness - I



Rat bait shyness - II



Rzóska, J. (1953). Bait shyness, a study in rat behavior. British Journal of Animal Behaviour, 1, 128–135

Question:

 Do you believe the rat will learn the correlation between bad food ⇒ shock and/or sound ⇒ nausea?



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Question:

 What aspect of the rat learning model prevents it from understanding the input ⇒ output correlation?

Pigeon superstition



Skinner, B. F. "Superstition' in the Pigeon", Journal of Experimental Psychology#38, 1947

Take home message

Priors knowledge is crucial for effective learning

Papaya tasting

Binary classification





Papaya tasting



X: set of all features, x = [softness, color]
Y: set of possible labels, y = [tasty, not tasty]

- Training sample
 - Tasty
 - Not tasty

A controlled example:

Papaya tasting



X: set of all features, x = [softness, color]Y: set of possible labels, y = [tasty, not tasty]D: data generation model, $D \Longrightarrow P(X)$

Training sample

- Tasty
- Not tasty

A controlled example:

Tasty

Not tasty

Papaya tasting



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Papaya tasting



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S: training sample: $[x_i, y_i]$, $i \in training$ m: number of objects for training

Training sample

- Tasty
- Not tasty

Papaya tasting



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Papaya tasting



Training sample

- Tasty
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X: set of all features, x = [softness, color]Y: set of possible labels, y = [tasty, not tasty]D: data generation model, $D \Longrightarrow P(X)$ True Labelling function: y = f(x)

S: training sample: $[x_i, y_i]$, $i \in training$ m: number of objects for training h_s learner: $y_{est;i} = h_s(x_i)$ L metric: $L(y_{true;i} - y_{est;i})$, $i \in training$

Papaya tasting



X: set of all features, x = [softness, color]Y: set of possible labels, y = [tasty, not tasty] *D*: data generation model, $D \Longrightarrow P(X)$ *True Labelling function:* y = f(x)S: training sample: $[x_i, y_i]$, $i \in training$ *m: number of objects for training*

 $\begin{array}{ll} h_{S} & \text{learner: } y_{est;i} = h_{S}(x_{i}) \\ L & \text{metric: } L \left(y_{true;i} - y_{est;i} \right), i \in \\ training \end{array}$

 $L \rightarrow fraction \ of \ incorrect \ predictions$

Papaya tasting



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$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$

A controlled example:

Papaya tasting

Proposed learner:

$$h_S(x) = \begin{cases} y_i & \text{if } x = x_i \mid \{x_i \in S\} \\ 0 & \text{otherwise} \end{cases}$$



- *X*: set of all features, x = [softness, color]Y: set of possible labels, y = [tasty, not tasty] *D*: data generation model, $D \Longrightarrow P(X)$ *True Labelling function:* y = f(x)S: training sample: $[x_i, y_i]$, $i \in training$ *m: number of objects for training* h_s learner: $y_{est:i} = h_s(x_i)$
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Toy model ...



X: set of all features, x = [softness, color]Y: set of possible labels, *y* = [tasty, not tasty] D: data generation model, $D \Longrightarrow P(X)$ *True Labelling function:* y = f(x)S: training sample: $[x_i, y_i]$, $i \in training$ *m*: number of objects for training learner: $y_{est:i} = h_s(x_i)$ h_{s} metric: $L(y_{true:i} - y_{est:i}), i \in$ L training

$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$

Question:

Training sample

Tasty

Not tasty

Proposed learner:

 $h_S(x) = \begin{cases} y_i & \text{if } x = x_i \mid \{x_i \in S\} \\ 0 & \text{otherwise} \end{cases}$ -1 0.5 Color 0 -0.5 1 -0.5 0.5 -1 Softness

[tasty, not tasty] = [1, 0]

What is the expected loss when this model is applied to an arbitrary test sample?

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loss = fraction of incorrect predictions

$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m} \quad {}_{26}$$

Papaya tasting

Proposed learner:

$$h_S(x) = \begin{cases} y_i & \text{if } x = x_i \mid \{x_i \in S\} \\ 0 & \text{otherwise} \end{cases}$$

Answer:



- Training sample Not tasty **Answer:** $L_S(h_S) = 0.0$ $L_D(h_S) = 0.25$
- *X*: set of all features, x = [softness, color]Y: set of possible labels, *y* = [tasty, not tasty] = [1, 0] D: data generation model, $D \Longrightarrow P(X)$ *True Labelling function:* y = f(x)S: training sample: $[x_i, y_i]$, $i \in training$ *m*: number of objects for training learner: $y_{est:i} = h_S x_i$ $h_{\rm s}$ metric: $L(y_{true,i} - y_{est;i}), i \in$ L

training

$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$

Papaya tasting

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Answer:



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Question:

• How can we avoid overfitting?

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by adding prior knowledge ...

Choosing the learner

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Hypothesis class (\mathcal{H}):

 $h: \mathcal{X} \longrightarrow \mathcal{Y}; \qquad h \in \mathcal{H}$

 $\operatorname{ERM}_{\mathcal{H}}(S) \in \operatorname{argmin}_{h \in \mathcal{H}} L_S(h),$

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 $f \in \mathcal{H}$

Choosing the learner

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True Labelling function: y = *f*(*x*)

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Machine Learning:

(a personal favorite) Supervised definition
Hypothesis: x --- Nature

► У

Breiman, L., Statistical Modeling: The Two Cultures, Stat. Sci, Volume 16 (2001)





Algorithmic modeling:



Breiman, L., Statistical Modeling: The Two Cultures, Stat. Sci, Volume 16 (2001)



Breiman, L., Statistical Modeling: The Two Cultures, Stat. Sci, Volume 16 (2001)

Representativeness

Probability distribution, P



 (μ_P, σ_P)

Sample, S1



 $(\mu_{S_1}, \sigma_{S_1})$

Representativeness



Representativeness



Representativeness



Representativeness



Representativeness



Representativeness

- A sample S1 is said to be representative of a probability distribution P if one can draw accurate conclusions about P from S1
- If two samples S1 and S2 are representative of P, S1 and S2 are representative in relation to each other

Representativeness

- A sample S1 is said to be representative of a probability distribution P if one can draw accurate conclusions about P from S1
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Question:

If a sample S_1 identically independently distributed (i.i.d.) from a distribution P, is this enough to guarantee that S_1 is representative of P?

Model assumptions

 $\chi: \text{ set of all features,} \\ x = [softness, color] \\ Y: \text{ set of possible labels,} \\ y = [tasty, not tasty] \\ D: data generation model, \\ D \Rightarrow P(\chi) \\ True Labelling function: <math>y = f(x) \\ S: \text{ training sample: } [x_i, y_i], i \in training \\ h_S \quad \text{learner: } y_{est,i} = h_S(x_i) \\ \end{bmatrix}$

$$h_S(x) = \begin{cases} y_i & \text{if } \exists i \in [m] \text{ s.t. } x_i = x \\ 0 & \text{otherwise.} \end{cases}$$

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Bad samples and hypothesis

Bad samples and hypothesis

 $\delta \rightarrow$ probability of non-representative (bad) samples

Bad hypothesis and samples

- $\delta \ \rightarrow \mbox{ probability of non-representative (bad) samples }$
- 1 $\delta \rightarrow$ confidence parameter

Bad hypothesis and samples

 $\delta \ \rightarrow \mbox{ probability of non-representative (bad) samples }$

- 1 $\delta \rightarrow$ confidence parameter
- $\epsilon \rightarrow$ contamination. A failure will occur when $L_D(h_S) \geq \epsilon$

Good
hypothesis:
$$\mathcal{H}_G \coloneqq [h \in \mathcal{H} : L_S(h_S) = 0 \& L_D(h_S) < \epsilon]$$

Bad hypothesis: $\mathcal{H}_B := [h \in \mathcal{H} : L_S(h_S) = 0 \& L_D(h_S) \ge \epsilon]$

Bad hypothesis and samples

 $\delta \ \rightarrow \mbox{ probability of non-representative (bad) samples }$

- 1 $\delta \rightarrow$ confidence parameter
- $\epsilon \rightarrow$ contamination. A failure will occur when $L_D(h_S) \geq \epsilon$

Good
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$$\mathcal{H}_G :=$$
 $[h \in \mathcal{H} : L_S(h_S) = 0$ & $L_D(h_S) < \epsilon]$ Bad
hypothesis: $\mathcal{H}_B :=$ $[h \in \mathcal{H} : L_S(h_S) = 0$ & $L_D(h_S) \ge \epsilon]$

Realizability assumption, $f \in \mathcal{H}$

Constructing misleading samples

The world



Bad samples

For 1 element in the training sample

$$x_i \mid h(x_i) = y_i$$

Constructing misleading samples

The world



Bad samples For 1 element in the training sample $x_i \mid h(x_i) = y_i$ $P(x_i \in \mathcal{D} : h(x_i) = y_i) = 1 - L_{\mathcal{D},f}(h)$

Constructing misleading samples

The world



Bad samples For 1 element in the training sample $x_i \mid h(x_i) = y_i$ $P(x_i \in \mathcal{D} : h(x_i) = y_i) = 1 - L_{\mathcal{D},f}(h)$ $P(x_i \in \mathcal{D} : h(x_i) = y_i) \le 1 - \epsilon$

Constructing misleading samples

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Bad samples For 1 element in the training sample $x_i \mid h(x_i) = y_i$ $P(x_i \in \mathcal{D} : h(x_i) = y_i) = 1 - L_{\mathcal{D},f}(h)$ $P(x_i \in \mathcal{D} : h(x_i) = y_i) \le 1 - \epsilon$

For *m* elements in the training sample

Since all elements in training are i.i.d.,

$$P(S_m : L_S(h) = 0) \le \prod_{i=1}^m (1-\epsilon) = (1-\epsilon)^m$$

Considering bad hypothesis

For 1 hypothesis

$$P(S_m : L_S(h) = 0) \leq (1 - \epsilon)^m$$



Considering bad hypothesis

For 1 hypothesis

$$P(S_m : L_S(h) = 0) \leq (1 - \epsilon)^m$$

The sum rule

$$P(A \cup B) \leq P(A) + P(B)$$



Considering bad hypothesis

$$P(S_m : L_S(h) = 0) \leq (1 - \epsilon)^m$$

For 1 hymothesis

The sum rule $P(A \cup B) \leq P(A) + P(B)$

For all bad hypothesis

$$\delta = P(L_S(h) = 0, \forall h \in \mathcal{H}_B) \leq \sum_{h \in \mathcal{H}_B} (1 - \epsilon)^m$$

Considering bad hypothesis

$$P(S_m : L_S(h) = 0) \leq (1 - \epsilon)^m$$

For 1 hymothesis

The sum rule $P(A \cup B) \leq P(A) + P(B)$

For all bad hypothesis

$$\delta = P(L_S(h) = 0, \forall h \in \mathcal{H}_B) \leq \sum_{h \in \mathcal{H}_B} (1 - \epsilon)^m$$

using...

$$(1-x)^y \le \exp\left(-xy\right)$$

Considering bad hypothesis

$$P(S_m : L_S(h) = 0) \leq (1 - \epsilon)^m$$

For 1 hypothesis

The sum rule $P(A\cup B) \leq P(A)+P(B)$

 $\delta \le N_{\mathcal{H}} \exp(-\epsilon m)$

For all bad hypothesis $\delta = P(L_S(h) = 0, \forall h \in \mathcal{H}_B) \leq \sum_{h \in \mathcal{H}_B} (1 - \epsilon)^m$

using...

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L. Valiant. A theory of the learnable. Communications of the ACM, 27, 1984.

PAC learning model

$$\delta \le N_{\mathcal{H}} \exp(-\epsilon m)$$



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PAC learning model

$$\delta \le N_{\mathcal{H}} \exp(-\epsilon m)$$

 $\begin{array}{ll} \textbf{P}robably & \longrightarrow \text{ with confidence 1 - } \delta \text{ over } m \text{ samples} \\ \textbf{A}pproximately & \longrightarrow \text{ within a contamination level} \leq \epsilon \\ \textbf{C}orrect & \end{array}$

If, $m_{\mathcal{H}}(\epsilon, \delta) \geq \frac{\ln(N_{\mathcal{H}}/\delta)}{\epsilon} \longrightarrow L_{(\mathcal{D},f)}(h_S) \leq \epsilon.$

L. Valiant. A theory of the learnable. Communications of the ACM, 27, 1984.

Remember what is behind this!!

PAC Assumptions

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S: training sample: $[x_i, y_i]$, $i \in training$ m: number of objects for training

 $h_{S} \quad \text{learner: } y_{est;i} = h_{S}(x_{i})$ $h_{S}(x) = \begin{cases} y_{i} & \text{if } \exists i \in [m] \text{ s.t. } x_{i} = x \\ 0 & \text{otherwise.} \end{cases}$ $L: \text{ loss: } L(y_{true;i} - y_{est;i}), i \in \text{training}$ $L_{\mathcal{D}}(h_{S}) = \frac{|\{x \in \mathcal{D} : h_{S}(x) \neq f(x)\}|}{m}$

Hypothesis class (${\cal H}$):

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Papaya tasting



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S: training sample: $[x_i, y_i]$, $i \in training$ m: number of objects for training \mathcal{H} : hypothesis class:

axis aligned squares in steps of 0.05

$$N_{_{H}} = 20$$


Papaya tasting



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axis aligned squares in steps of 0.05

$$N_{H} = 20$$

L: loss: $L(y_{true;i} - y_{est;i}), i \in training$

$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$



Question:



Data model: uniform distribution [-1,1] in both axis

- $1 \delta = 0.95 \leftarrow \text{ confidence}$
- ϵ = 0.05 \leftarrow contamination
- $N_H = 20 \leftarrow \text{number of possible}$ squares

m = ??



Join at menti.com with code: 7907 6385

What would you guess is the number of examples necessary for training?

Question:



Data model: uniform distribution [-1,1] in both axis

- $1 \delta = 0.95 \leftarrow \text{ confidence}$
- ϵ = 0.05 \leftarrow contamination
- $N_H = 20 \leftarrow \text{number of possible}$ squares

m~120



Question:

-1



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True labelling function

Data model: uniform distribution [-1,1] in both axis



Generalization ...

Agnostic PAC learning

- $\chi: \text{ set of all features,} \\ x = [softness, color] \\ Y: \text{ set of possible labels,} \\ y = [tasty, not tasty] \\ D: data generation model, \\ D \Longrightarrow P(\chi, Y) \\ True Labelling function: y = f([x,y]) \\ S: \text{ training sample: } [x_i, y_i], i \in training \\ m: number of objects for training \\ h_s \qquad \text{learner: } y_{est;i} = h_s(x_i, y_i) \\ \end{cases}$
 - L: loss

$$L_{\mathcal{D}}(h) \stackrel{\text{def}}{=} \mathbb{E}_{(x,y)\sim\mathcal{D}}(h(x)-y)^2$$

Hypothesis class:

 $h: \mathcal{X} \longrightarrow \mathcal{Y}; \qquad h \in \mathcal{H}$

$$\operatorname{ERM}_{\mathcal{H}}(S) \in \operatorname{argmin}_{h \in \mathcal{H}} L_S(h),$$

- $m \rightarrow$ number of objects in training
- \mathcal{H} is finite, N_{H} = number of hypothesis
- The true labelling function may not be part of *H*:

 $f^{{}{}\oplus{}} \mathcal{H}$

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

Important remark!

Representativeness

in machine learning

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or Uniform Convergence

$$\forall h \in \mathcal{H}, |L_S(h) - L_\mathcal{D}(h)| \le \epsilon$$

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Representativeness

in machine learning

or Uniform Convergence

$$\forall h \in \mathcal{H}, |L_S(h) - L_\mathcal{D}(h)| \le \epsilon$$

It can be shown that, if \mathcal{H} has uniform convergence, $\text{ERM}_{\mathcal{H}}$ is a successful agnostic PAC learner of \mathcal{H} .

Can machine learning solve my problem?

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• If your data satisfy all the necessary conditions;

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- If your data satisfy all the necessary conditions;
- If you have enough training sample to fulfill your expectations;

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Then.. probably (1-δ), approximately (ε) : yes

Many of these requirements are difficult to fulfill, e.g.

What about practical situations?

If you are using a classical learner whose class under your training sample and loss function are representative (has uniform convergence), you are probably getting reasonable results... **but not all the time**! Many of these requirements are difficult to fulfill, e.g.

What about practical situations?

If you are using a classical learner whose class under your training sample and loss function are representative (has uniform convergence), you are probably getting reasonable results... **but not all the time**!

So why does it seem to work in everything around us?

Best guess: we do not know how to model real data...

There is plenty room for improvement!

Progress will only be possible through interdisciplinary collaboration!

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Machine learning is a wonderful field of research, which has already shown its potential in many fields! We should definitely take advantage of its results .. however ...

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References:

This talk is a rough summary of chapters 1-4:

Shai Shaley-Shiwartz and Shai Ben-David

UNDERSTANDING MACHINE LEARNING

FROM THEORY TO ALGORITHMS



Free download - with agreement from the editor:

https://www.cse.huji.ac.il/~shais/UnderstandingMachineLearning/index.html

23 lectures of 1.5 hours each on youtube:

https://www.youtube.com/playlist?list=PLPW2keNyw-usgvmR7FTQ3ZRjfLs5jT4BO



