Can Machine Learning solve my problem?

Michigan Cosmology Summer School - part I

7 June 2023 - Ann Arbor, USA

Emille E. O. Ishida

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Clermont Ferrand, France

LPC Particules pLasmas Univers applicationS
Laboratoire de Physique de Clermont

UCA UNIVERSITÉ Clermont Auvergne

cnrs

Truffade

COIN Cosmostatistics Initiative

SNAD

FINK

LSST Large Synoptic Survey Telescope

Puy-de-Dome

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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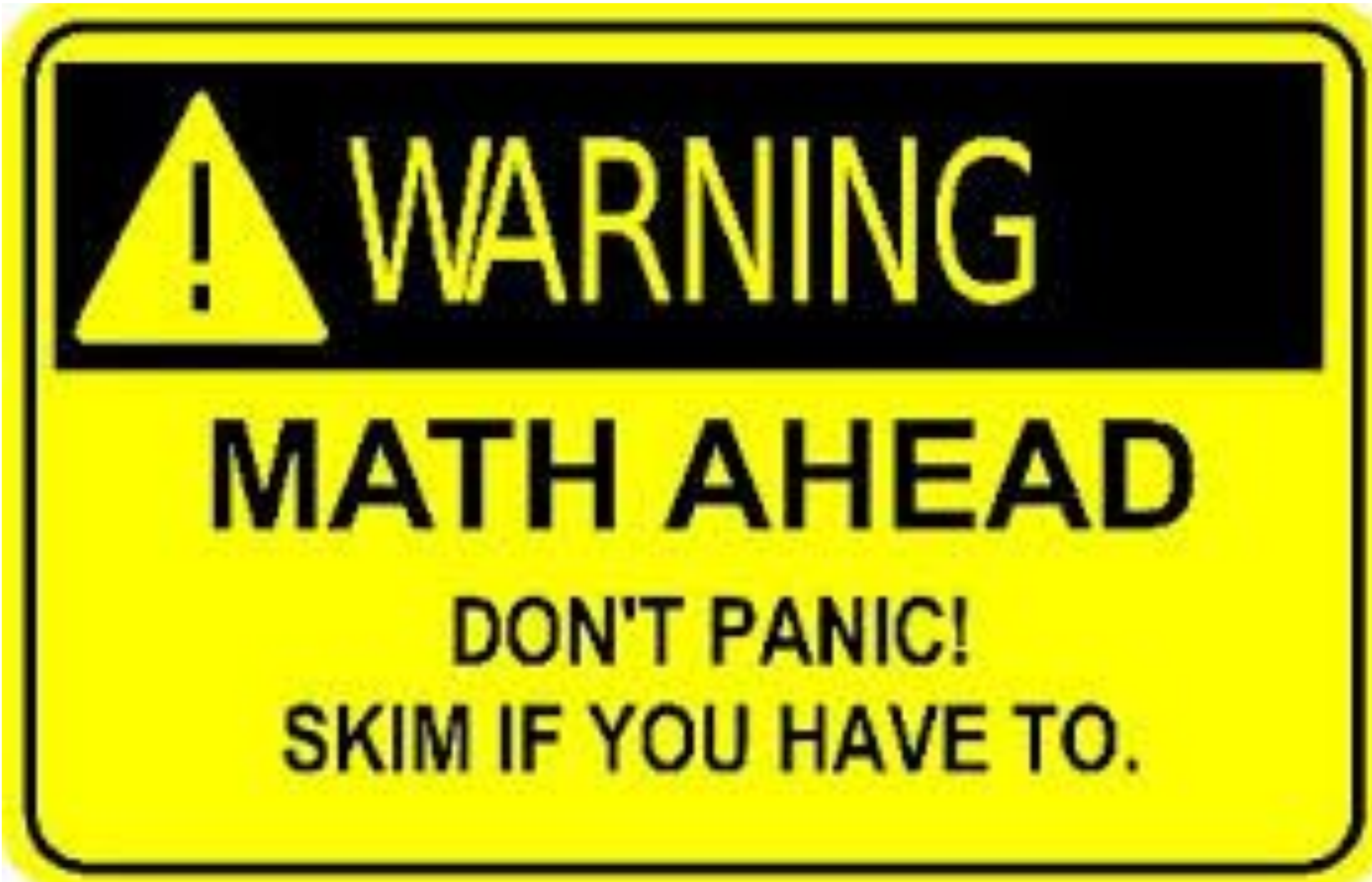
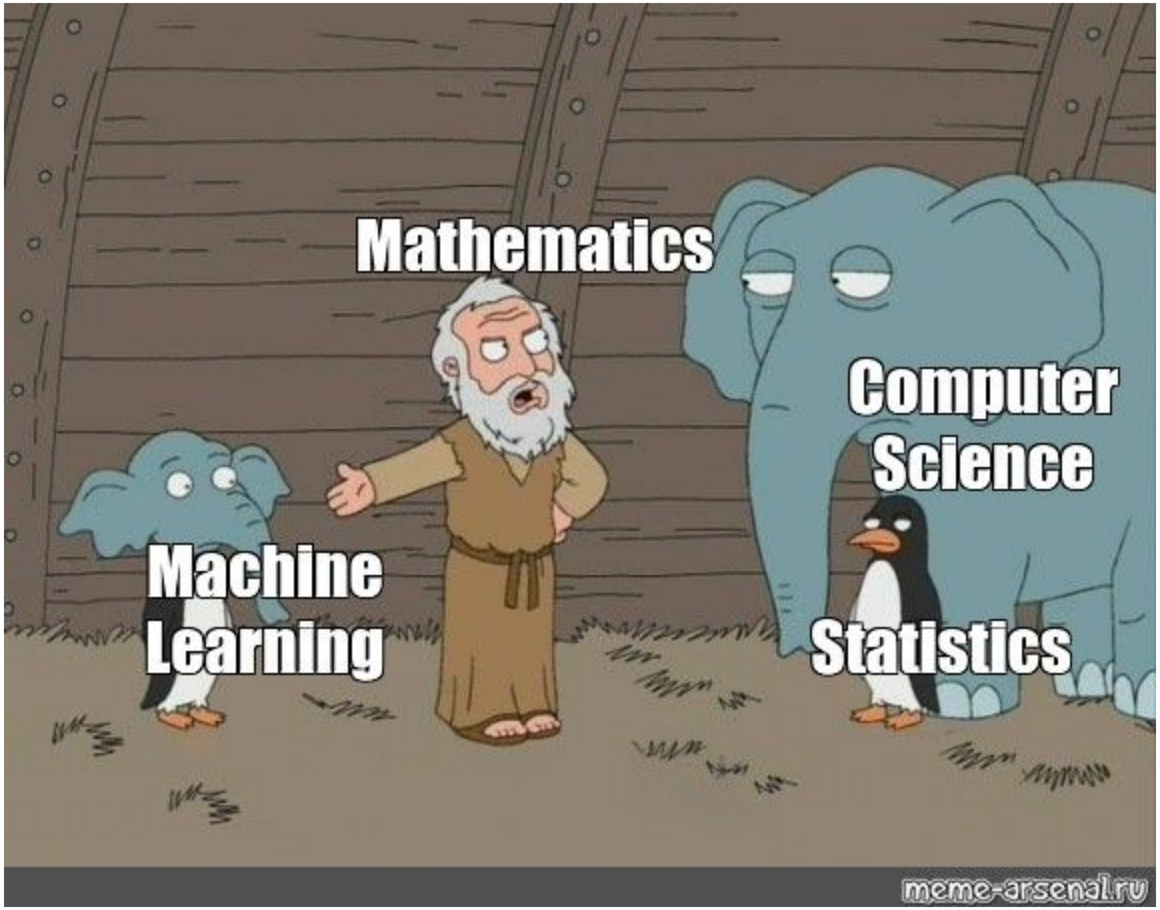


https://www.general-staff.com/wp-content/uploads/2019/03/MathWarning-300x193.jpg



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

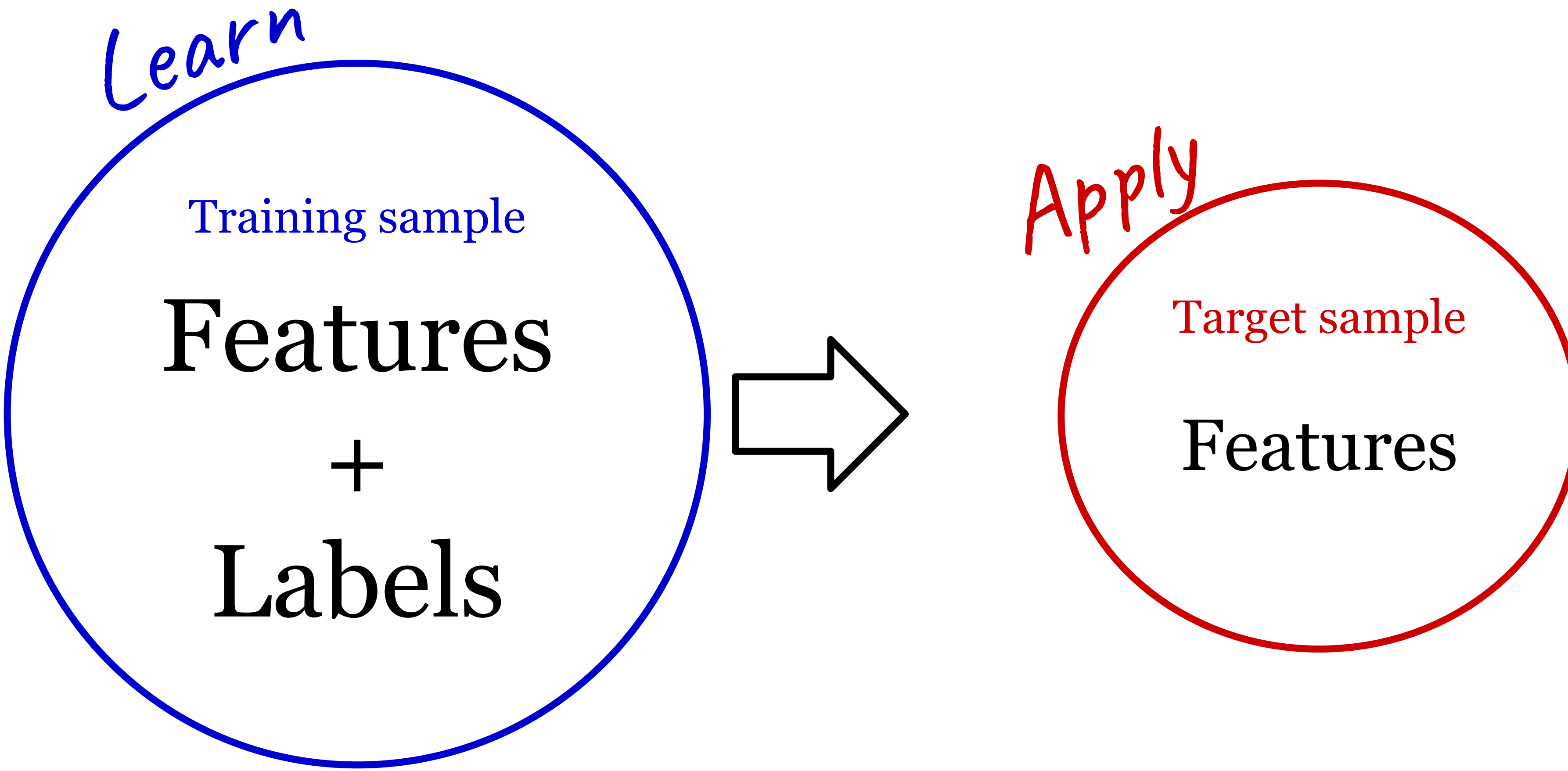
What is learning ?

“A relatively permanent change in behaviour due to past experiences.”

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

Supervised Learning

Learn by example



Question:

List 2 animals that you believe are capable of learning.

Discuss examples of their learning capabilities.

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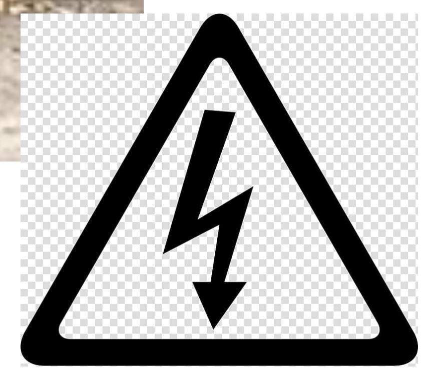
Rat bait shyness - I

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

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

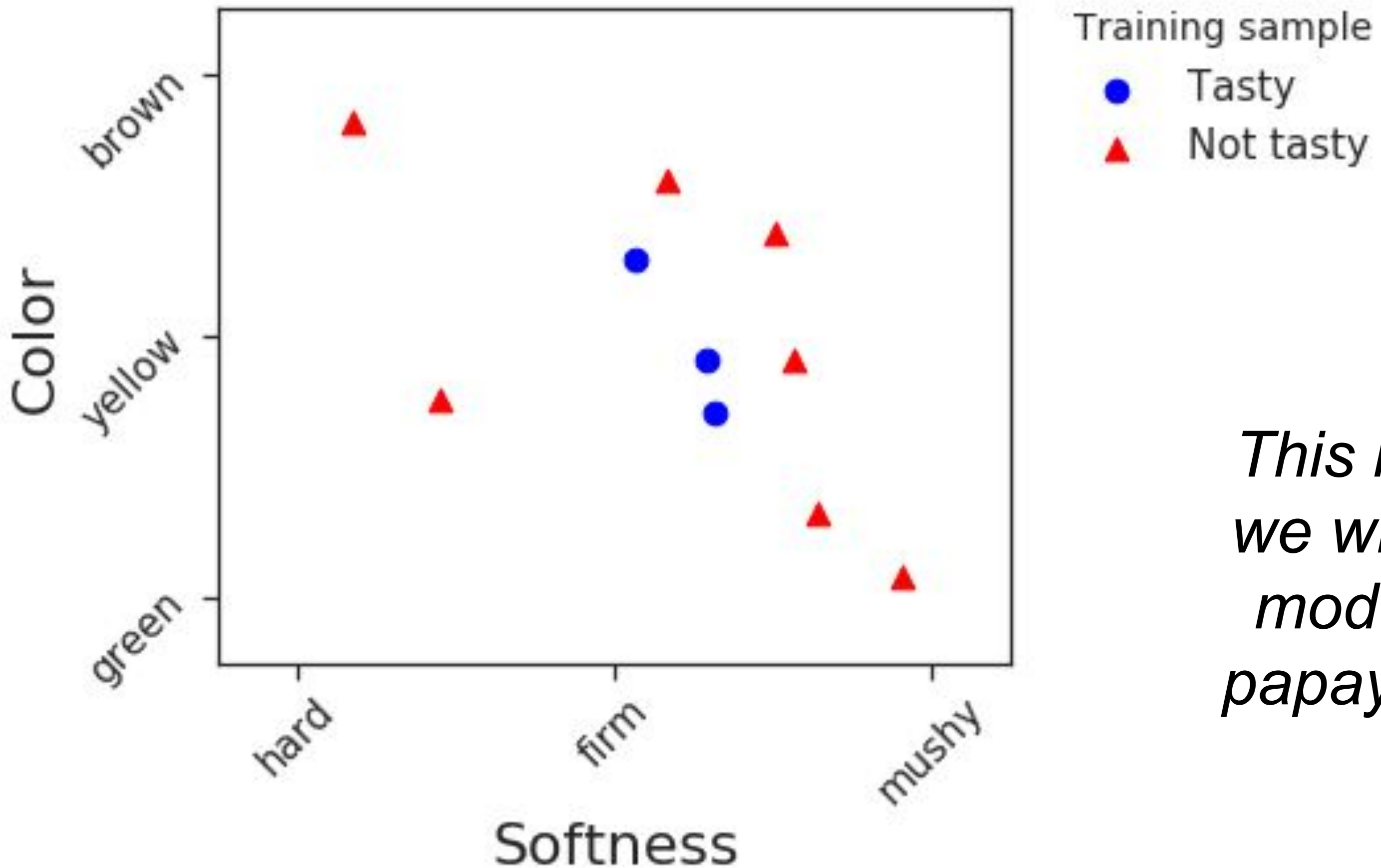
Take home message

Priors knowledge is crucial for effective learning

A controlled example:

Papaya tasting

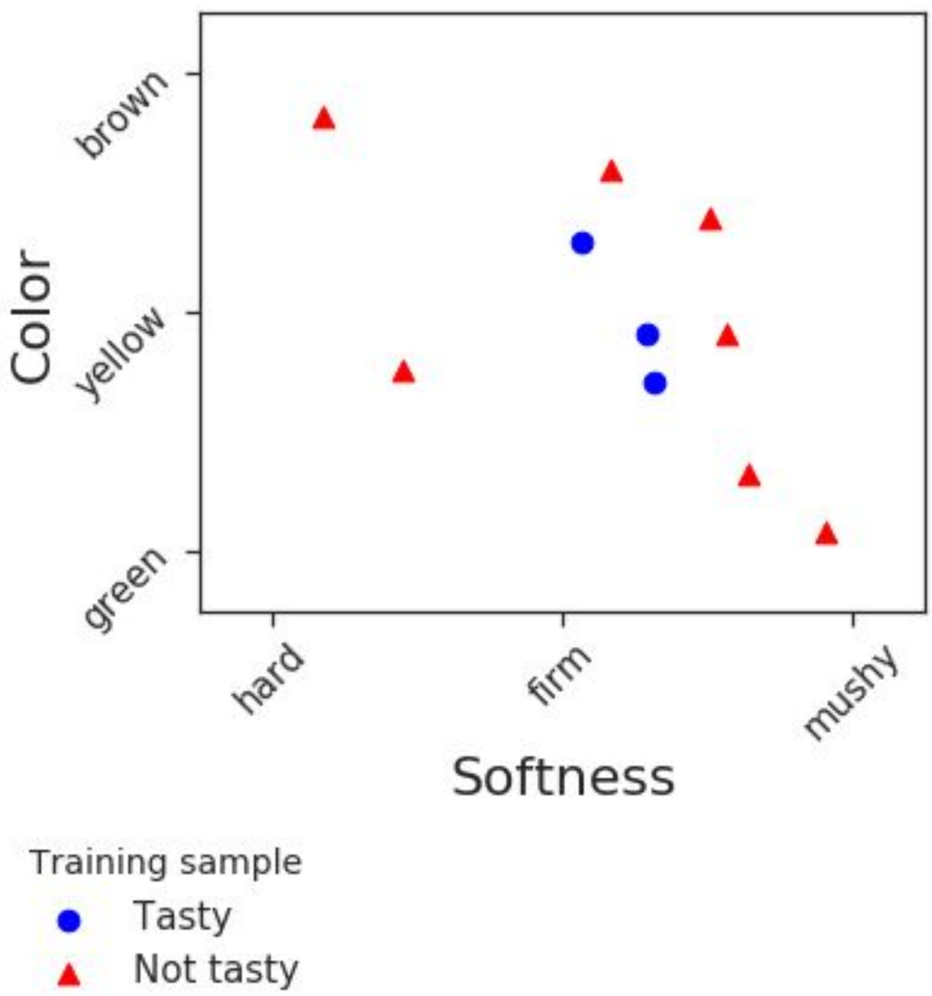
Binary classification



This is all the data we will input to the model about the papayas in the real world!

YouTube class on the papaya testing example:
https://www.youtube.com/watch?v=b5NlRg8SjZg&list=PLPW2keNyw-usgvmR7FTQ3ZRjfLs5jT4BO&index=2&t=0s

Papaya tasting



X: set of all features,

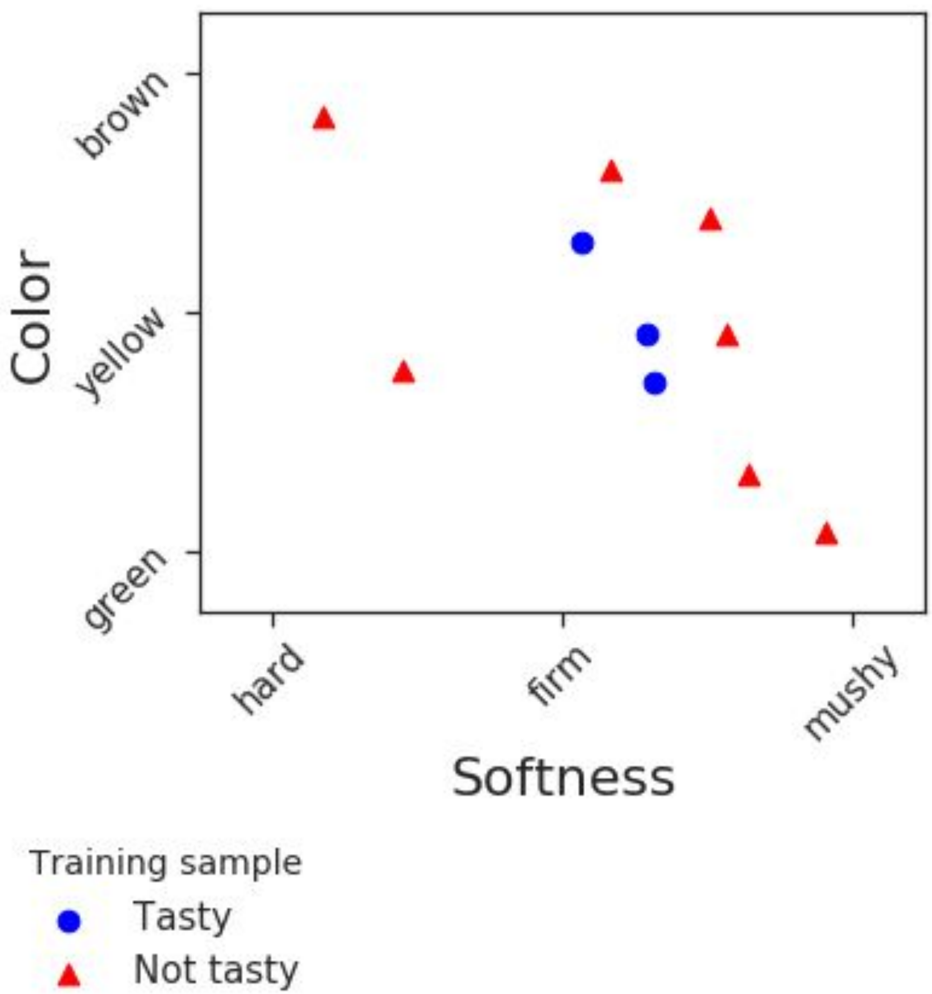
x = [softness, color]

Y: set of possible labels,

y = [tasty, not tasty]

A controlled example:

Papaya tasting



X: set of all features,

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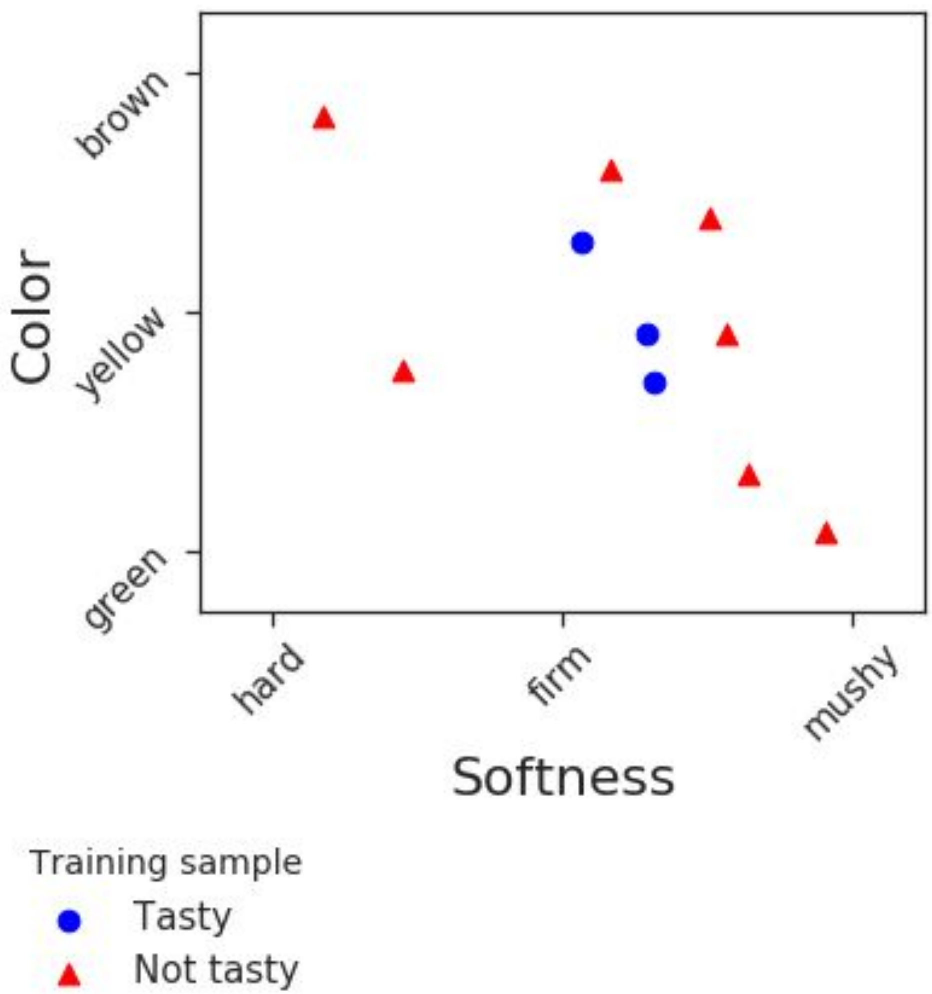
D: data generation model,

$D \Longrightarrow P(X)$

A controlled example:

Papaya tasting



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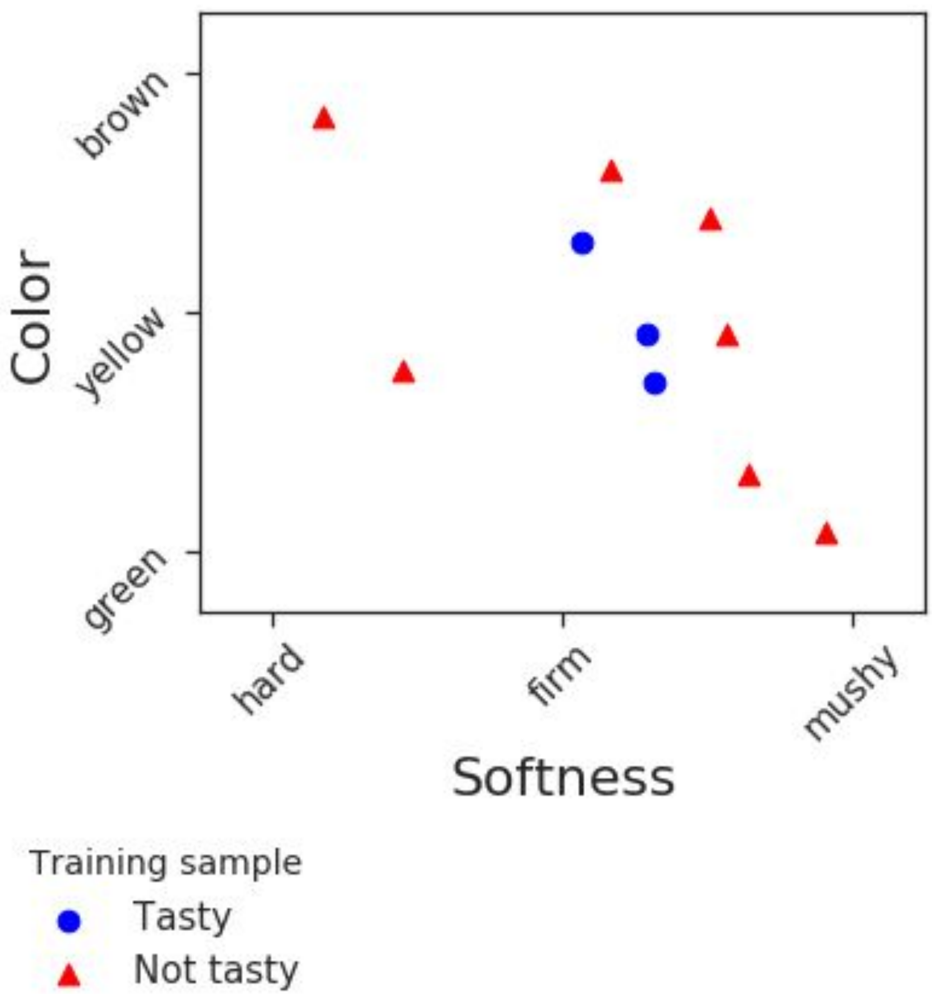
True Labelling function: y = f(x)

A controlled example:

Papaya tasting



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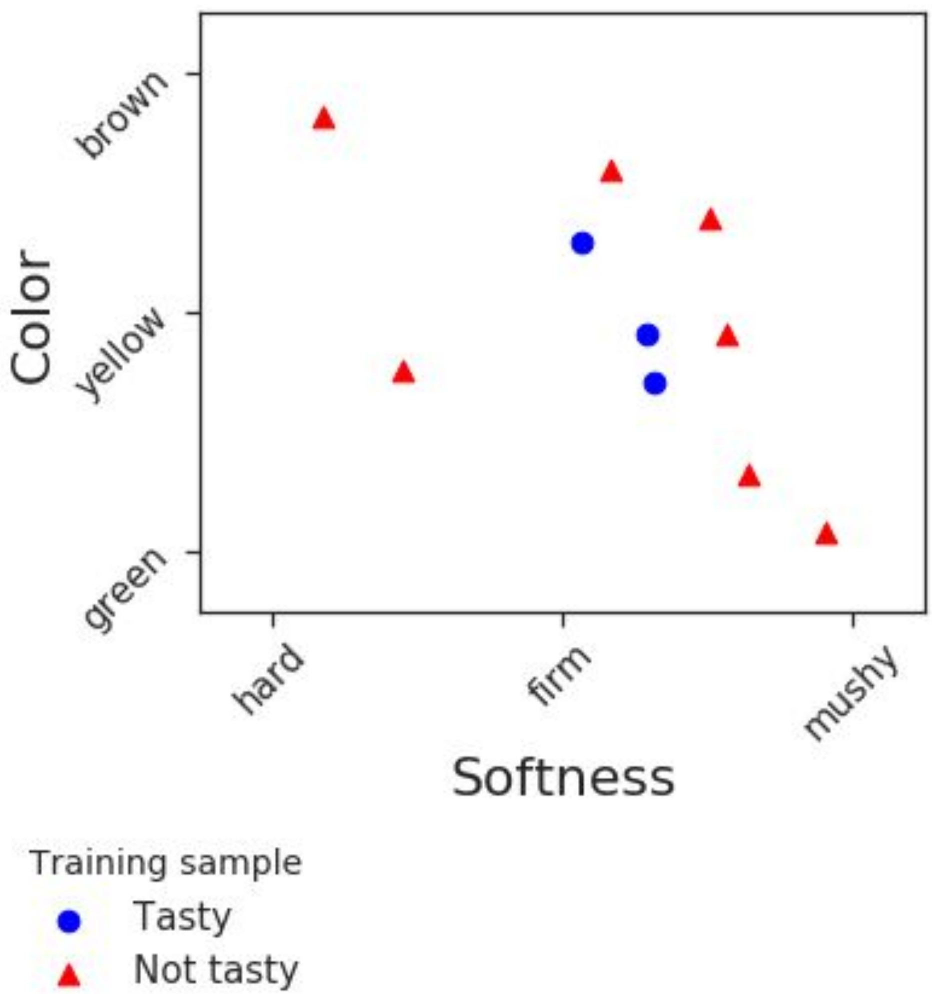
m: number of objects for training

A controlled example:

Papaya tasting



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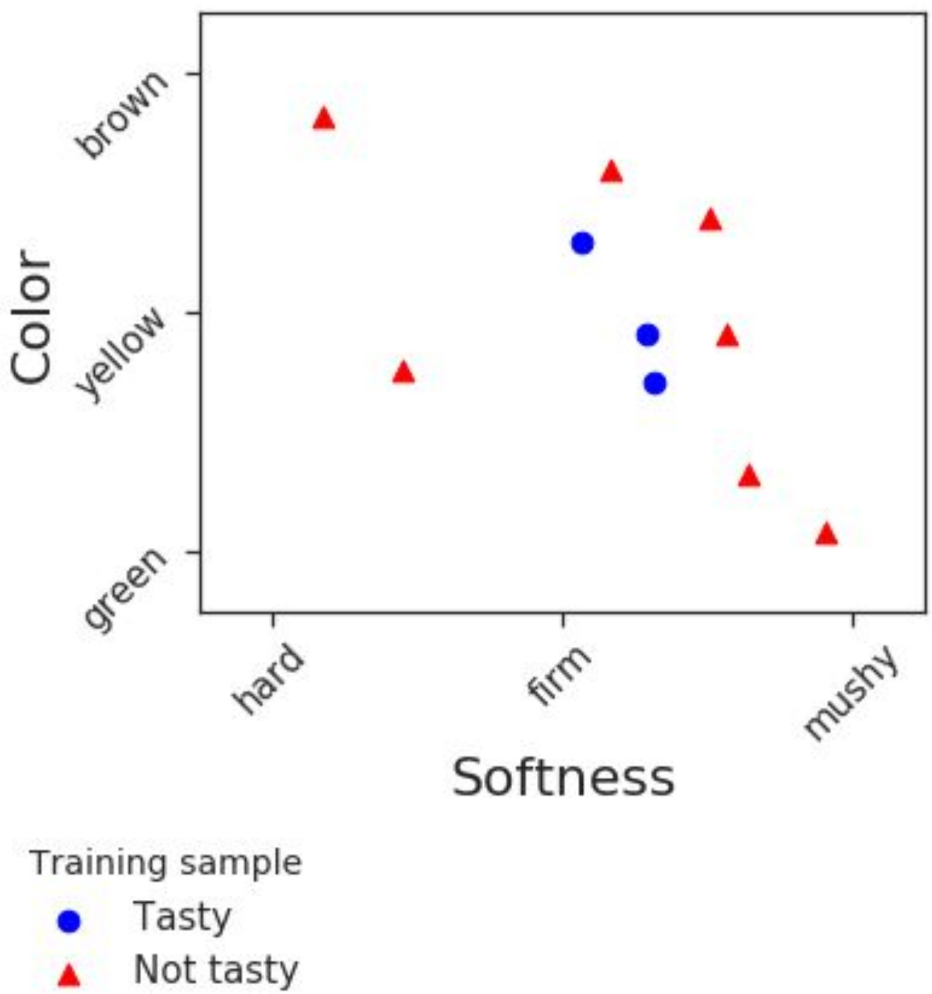
A controlled example:

Papaya tasting



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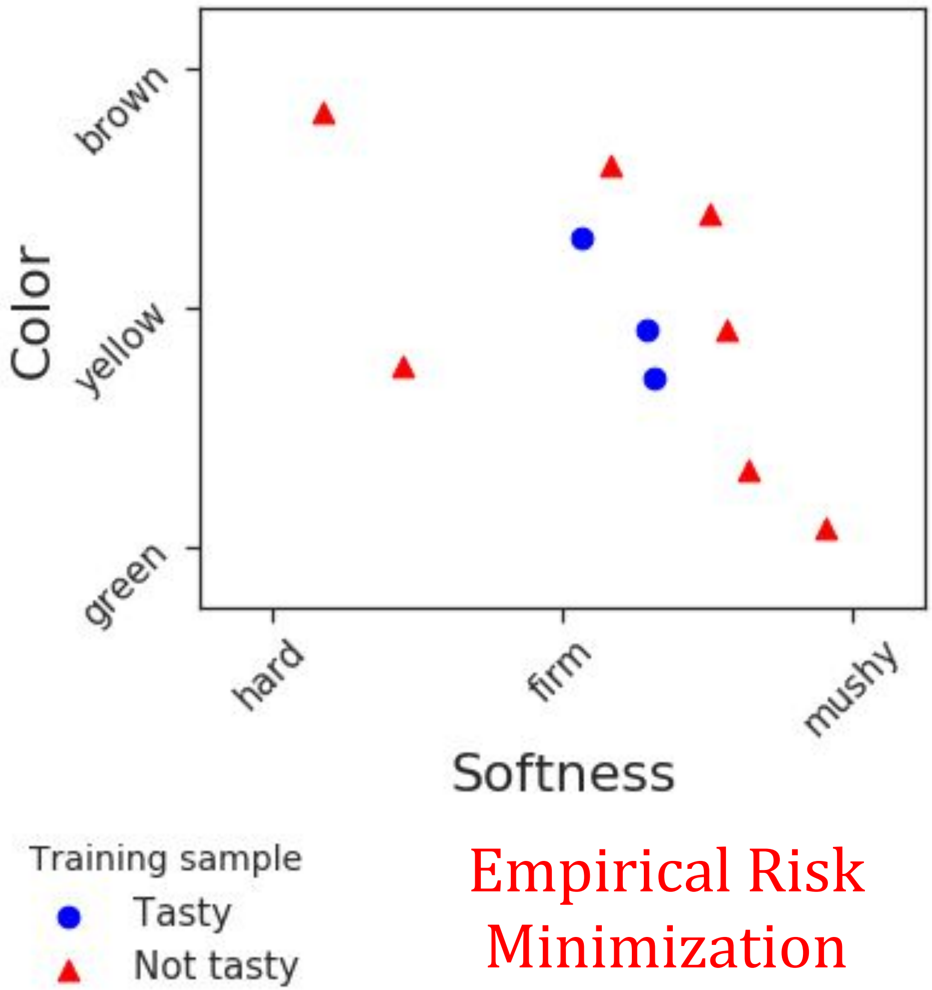
h_S learner: $y_{est;i} = h_S(x_i)$

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

A controlled example:

Papaya tasting



Empirical Risk Minimization (ERM)

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D: data generation model,

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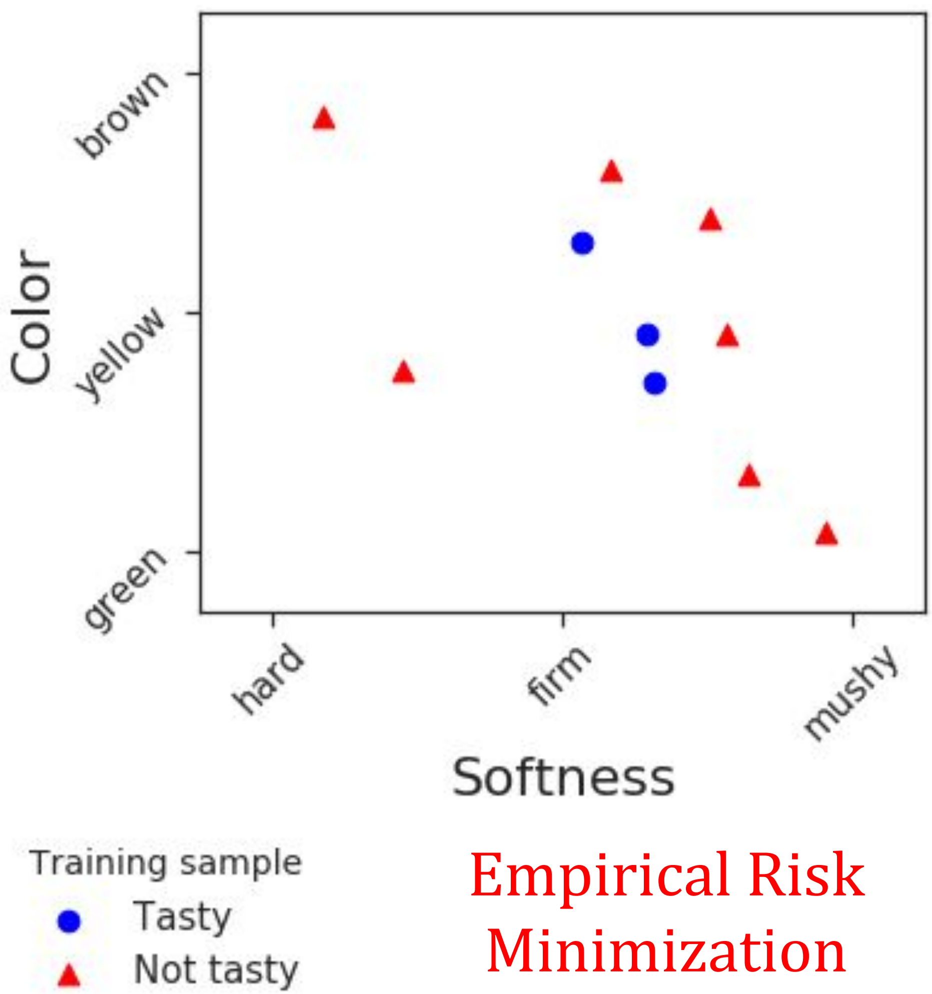
h_S learner: $y_{est;i} = h_S(x_i)$

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

$L \longrightarrow$ *fraction of incorrect predictions*

A controlled example:

Papaya tasting



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

Empirical Risk Minimization (ERM)

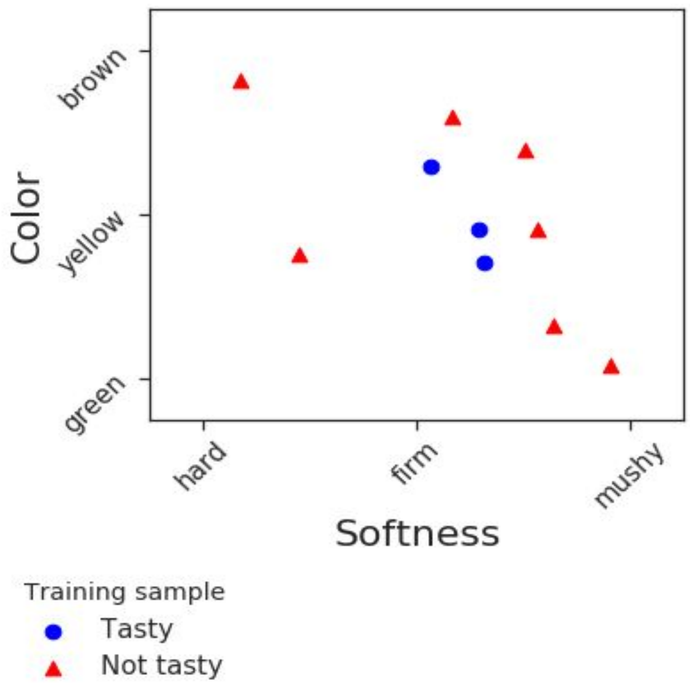
$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$

A controlled example:

Papaya tasting

Proposed learner:

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



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D ⇒ P(X)

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Papaya tasting

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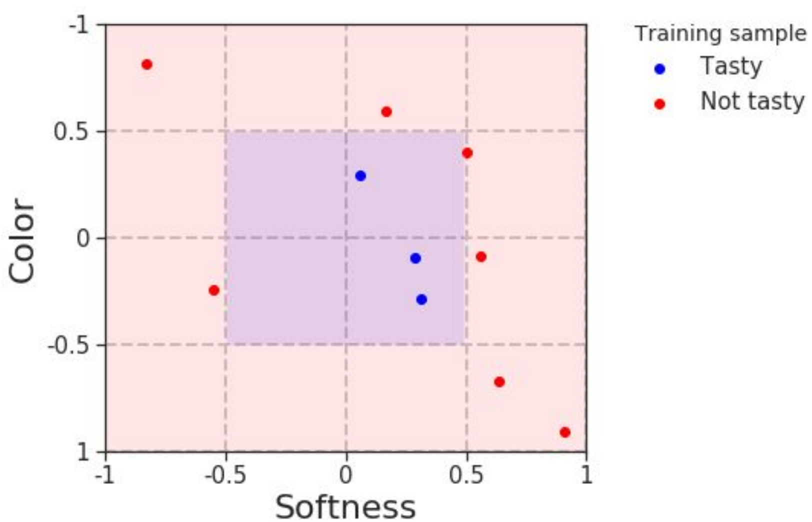
Toy model …



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D: data generation model,

D ⟹ P(X)

True Labelling function: y = f(x)

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m: number of objects for training

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

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

A controlled example:

Question:

Proposed learner:

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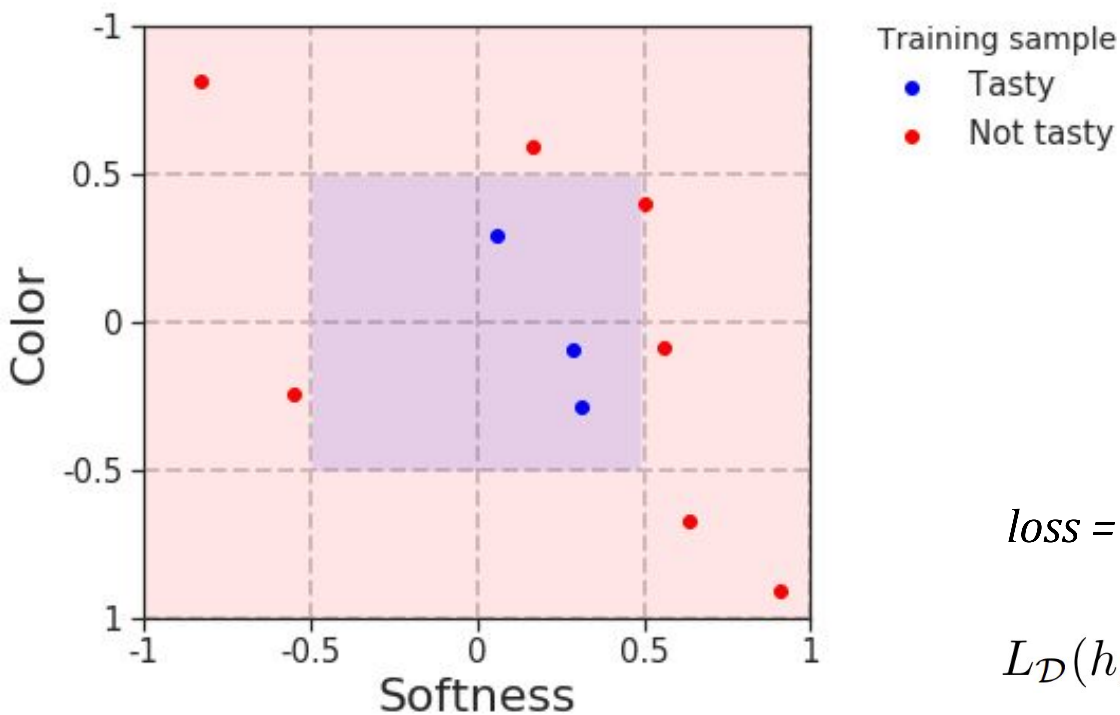

[tasty, not tasty] = [1, 0]

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

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loss = fraction of incorrect predictions

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

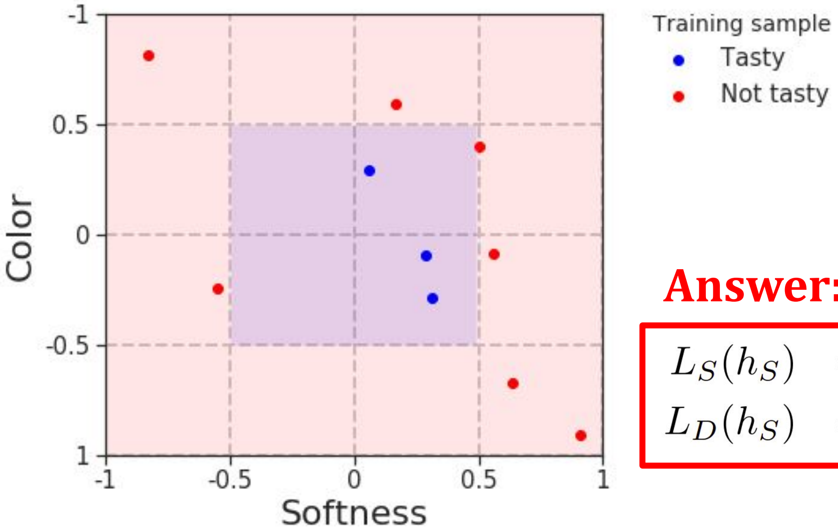
A controlled example:

Papaya tasting

Proposed learner:

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

Answer:



Answer:

$$\begin{aligned} L_S(h_S) &= 0.0 \\ L_D(h_S) &= 0.25 \end{aligned}$$

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

D: data generation model,

D ⟹ 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

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

A controlled example:

Papaya tasting

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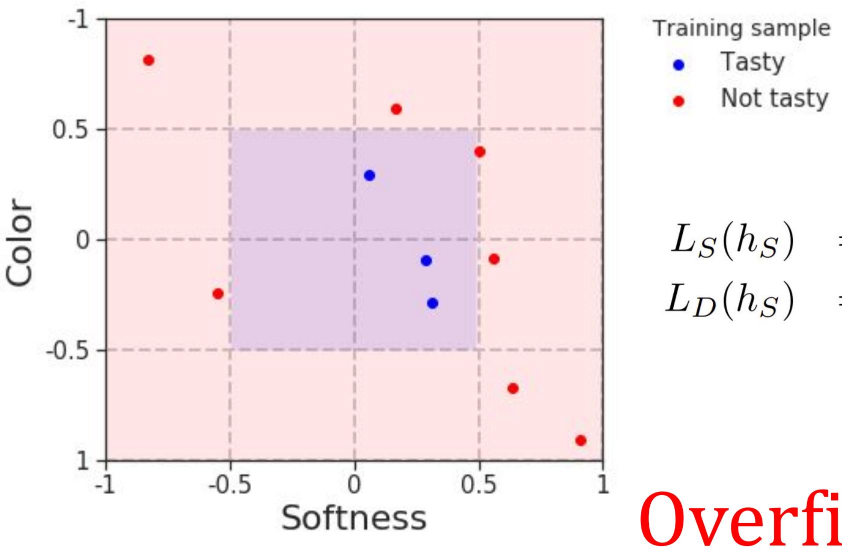
Answer:



$$L_S(h_S) = 0.0$$
$$L_D(h_S) = 0.25$$

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True Labelling function: y = f(x)

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h_S learner: $y_{est;i} = h_S x_i$
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$$L_{\mathcal{D}}(h_S) = \frac{|\{x \in \mathcal{D} : h_S(x) \neq f(x)\}|}{m}$$

Overfitting! 😨

Question:

- How can we avoid overfitting?

Question:

- How can we avoid overfitting?

by adding prior knowledge ...

Choosing the learner

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

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

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

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

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

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

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

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

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- $\mathcal{H}$ is finite, $N_{\mathcal{H}}$ = number of hypothesis
- The true labelling function is part of $\mathcal{H}$:

$$f \in \mathcal{H}$$

Choosing the learner

χ: set of all features,
x = [softness, color]

Y: set of possible labels,
y = [tasty, not tasty]

D: data generation model,
D ⟹ P(χ)

True Labelling function: y = f(x)

S: training sample: $[x_i, y_i]$, $i \in$ *training*

h_S learner: $y_{est;i} = h_S(x_i)$

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- *S* is identically independently distributed (*i.i.d.*) from *D*

Choosing the learner

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Machine Learning:

(a personal favorite)

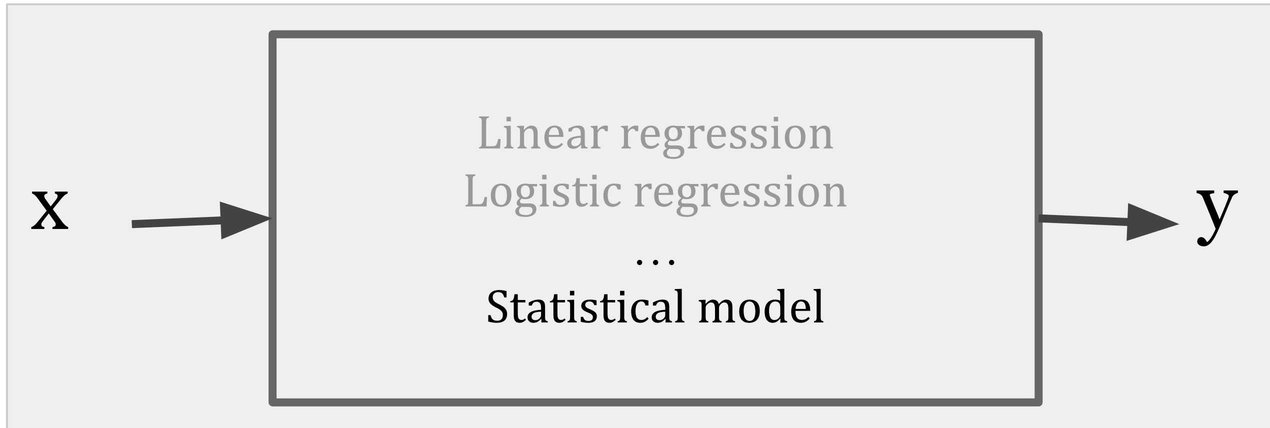
Supervised definition

Hypothesis:

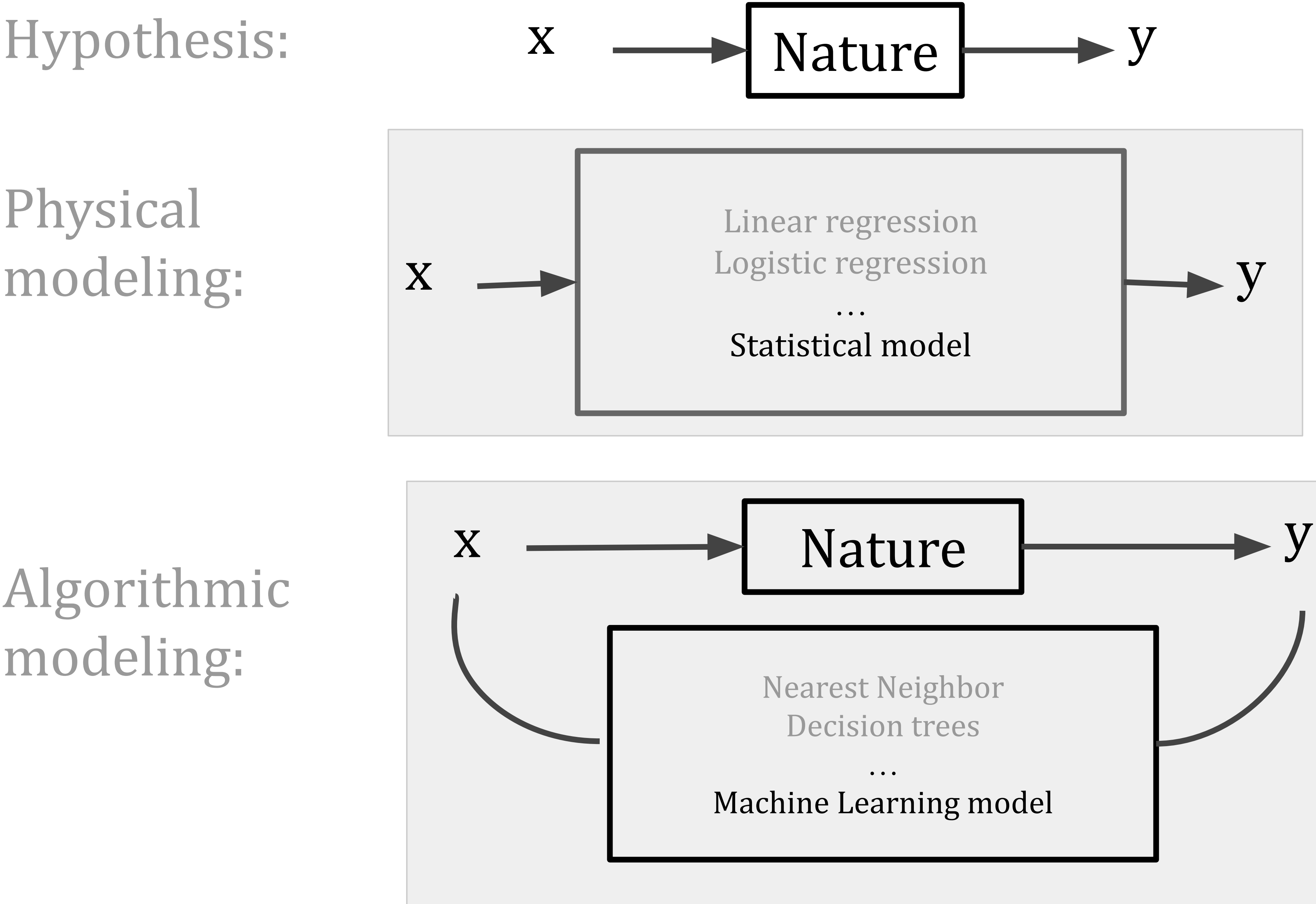
Breiman, L., Statistical Modeling: The Two Cultures, Stat. Sci, Volume 16 (2001)

Hypothesis:

Physical modeling:



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



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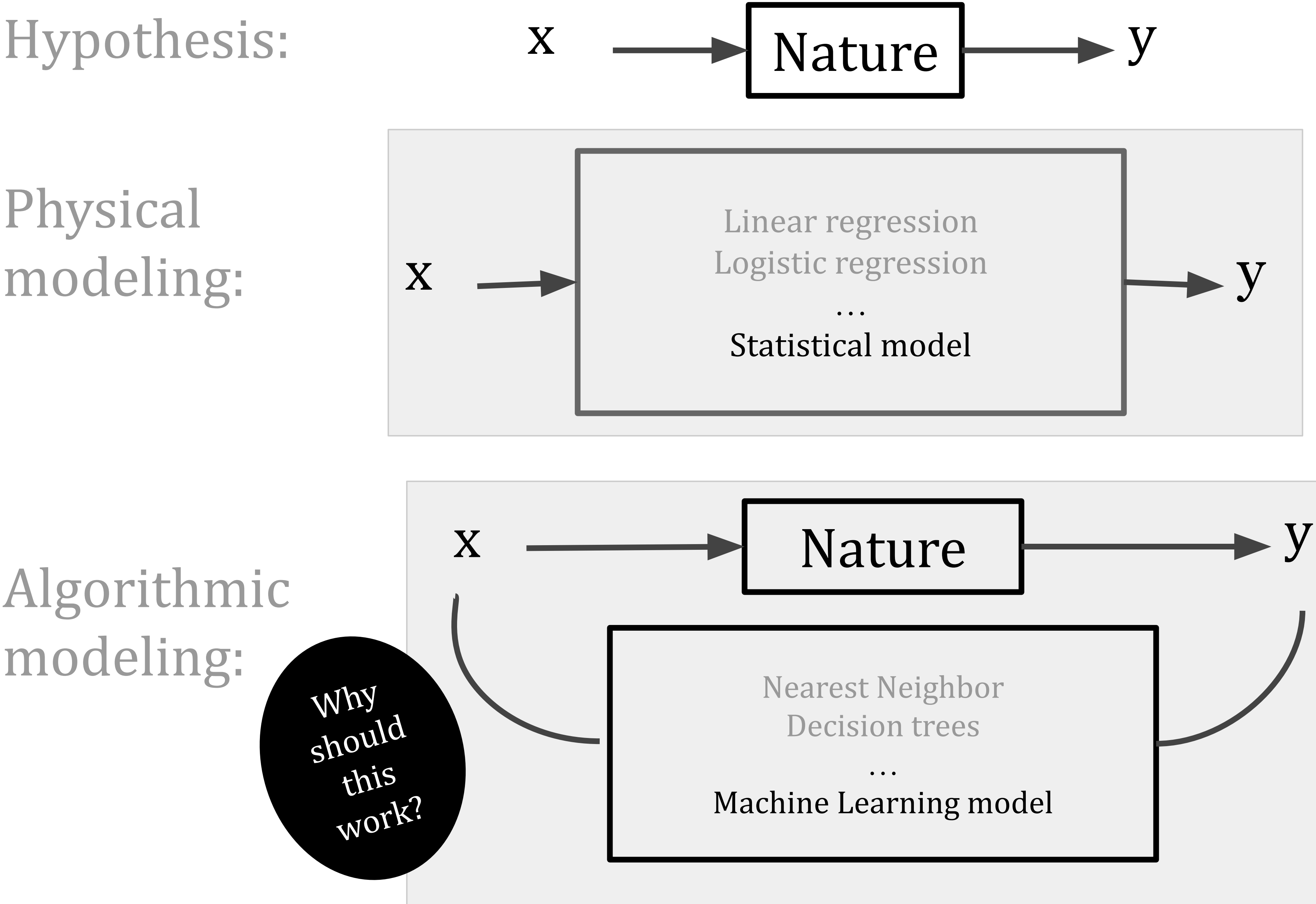

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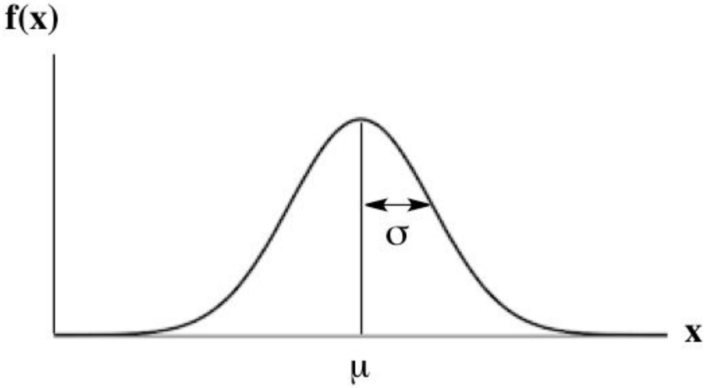
Representativeness

Probability distribution, *P*



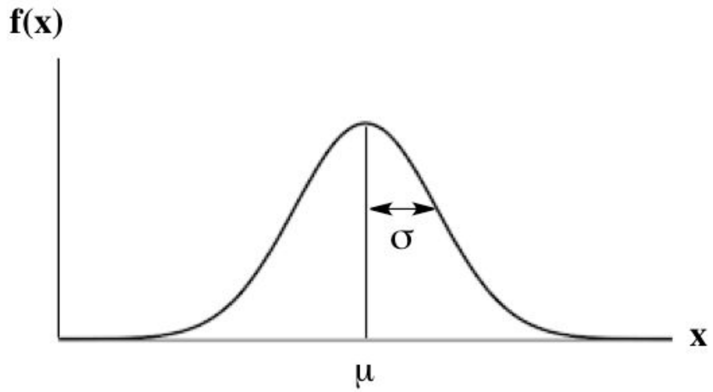
$$(\mu_P, \sigma_P)$$

Sample, S1

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

Representativeness

Probability distribution, *P*



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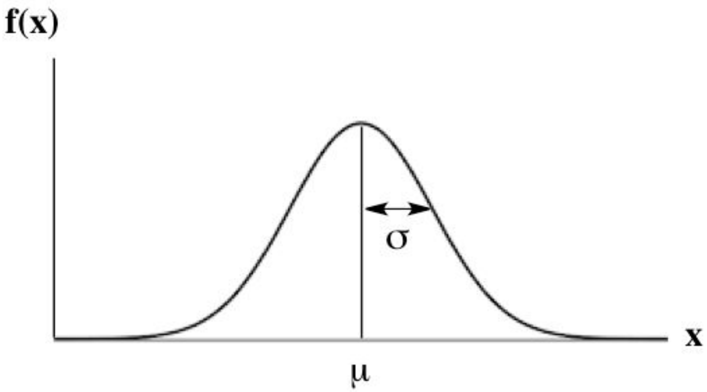
Representativeness

Probability distribution, *P*



$$(\mu_P, \sigma_P)$$

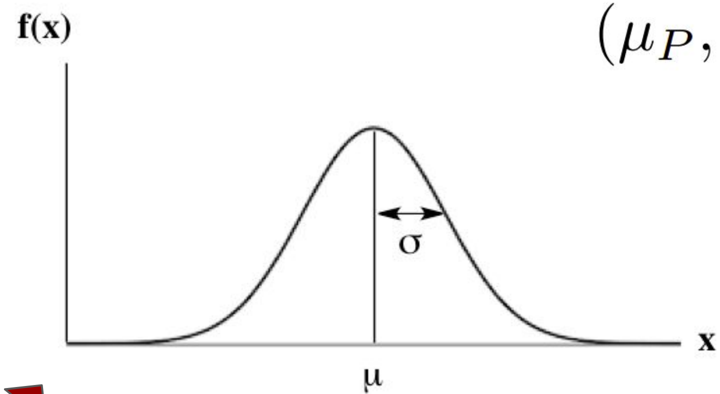
S_1 is *representative* of *P*

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

Sample, S1

Representativeness

Probability distribution, *P*



(μ_P, σ_P)

Sample, S_1

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

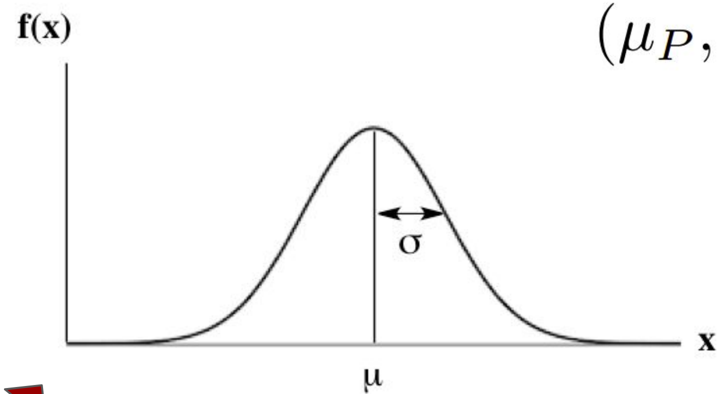
Sample, S_2

$(\mu_{S_2}, \sigma_{S_2})$

Representativeness

Probability distribution, *P*

(μ_P, σ_P)



Sample, S_1

Sample, S_2

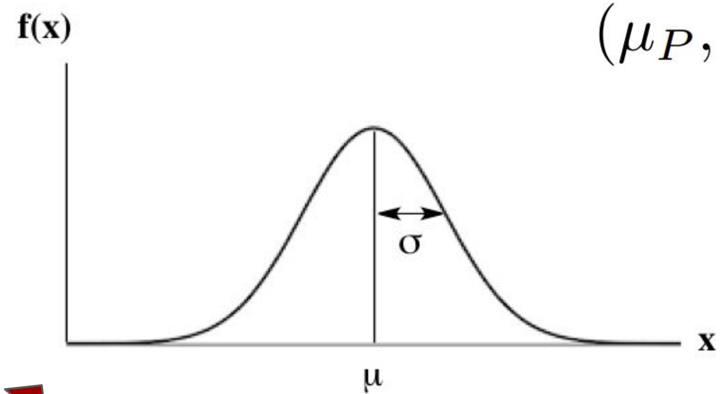
$(\mu_{S_1}, \sigma_{S_1})$

$(\mu_{S_2}, \sigma_{S_2})$

Representativeness

Probability distribution, *P*

(μ_P, σ_P)



This is why it works!

Training

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

Test

$(\mu_{S_2}, \sigma_{S_2})$

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

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- If two samples S1 and S2 are representative of P, S1 and S2 are representative in relation to each other

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?

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Model assumptions

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

S: training sample: $[x_i, y_i]$, $i \in training$
h_S 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: *loss*: $L(y_{true;i} - y_{est;i})$, $i \in training$

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

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

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

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

- $\mathcal{H}$ is finite, $N_{\mathcal{H}}$ = number of hypothesis
- The true labelling function is part of $\mathcal{H}$:

  $$f \in \mathcal{H}$$

- *S* is identically independently distributed (*i.i.d.*) from *D*

Not enough!

Break

Bad samples and hypothesis

Bad samples and hypothesis

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

Bad hypothesis and samples

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$1 - \delta \longrightarrow$ confidence parameter

Bad hypothesis and samples

δ ⟶ probability of non-representative (bad) samples

1 - δ ⟶ confidence parameter

ε ⟶ contamination. A failure will occur when $L_D(h_S) \geq \epsilon$

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

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

Bad hypothesis and samples

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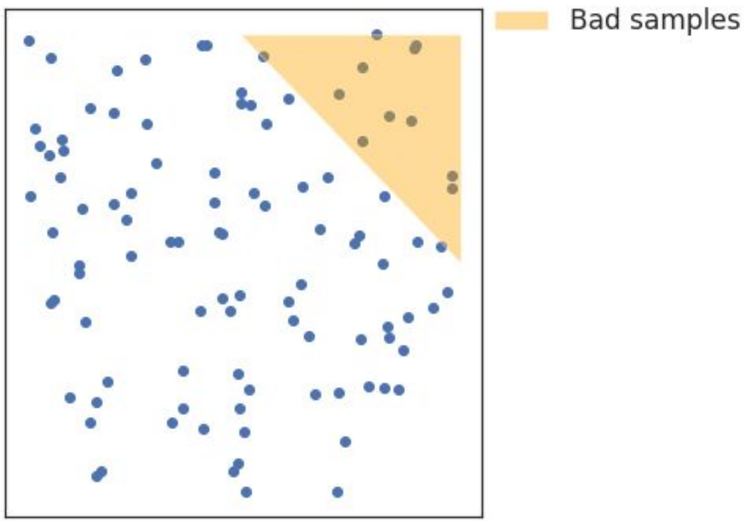
Realizability assumption, $f \in \mathcal{H}$

Constructing misleading samples

The world

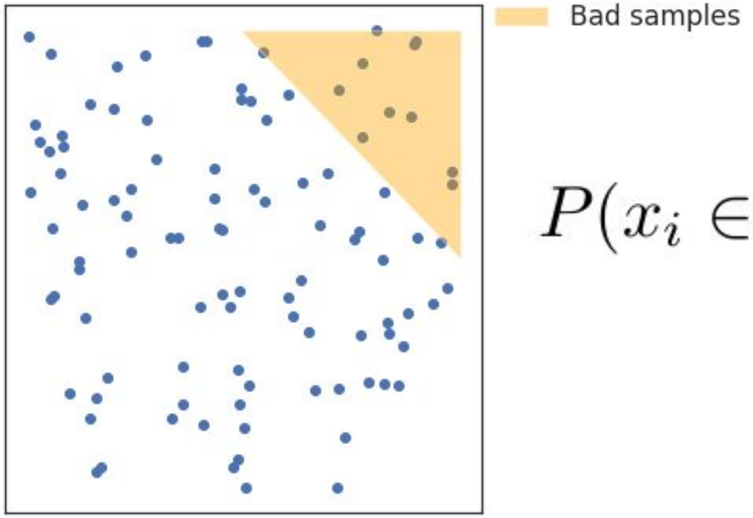


For 1 element in the training sample

$$x_i \quad | \quad h(x_i) \quad = \quad y_i$$

Constructing misleading samples

The world



For 1 element in the training sample

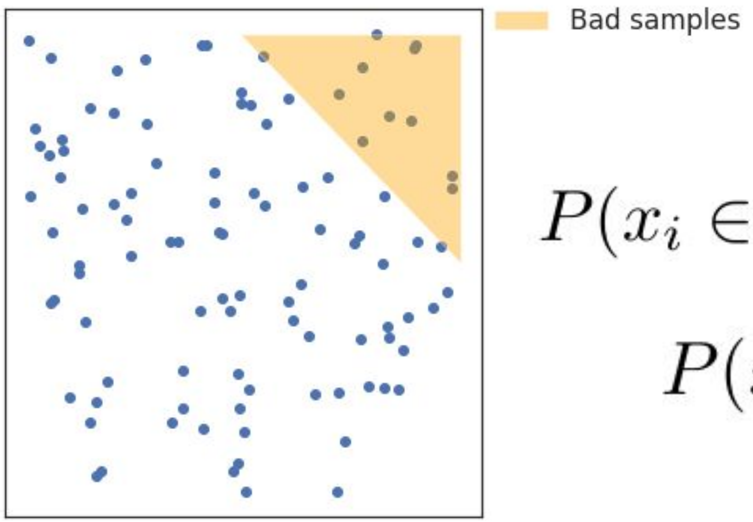
$$x_i \quad | \quad h(x_i) \quad = \quad y_i$$

$$P(x_i \in \mathcal{D} : h(x_i) \quad = \quad y_i) = 1 - L_{\mathcal{D},f}(h)$$

...

Constructing misleading samples

The world



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Constructing misleading samples

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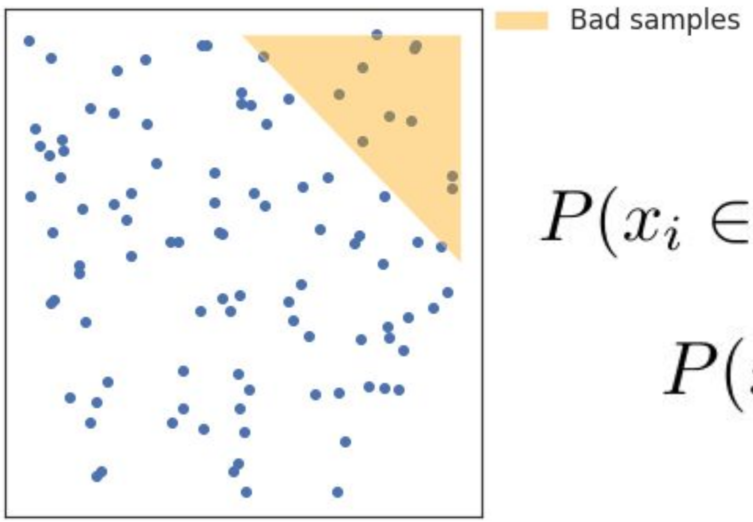

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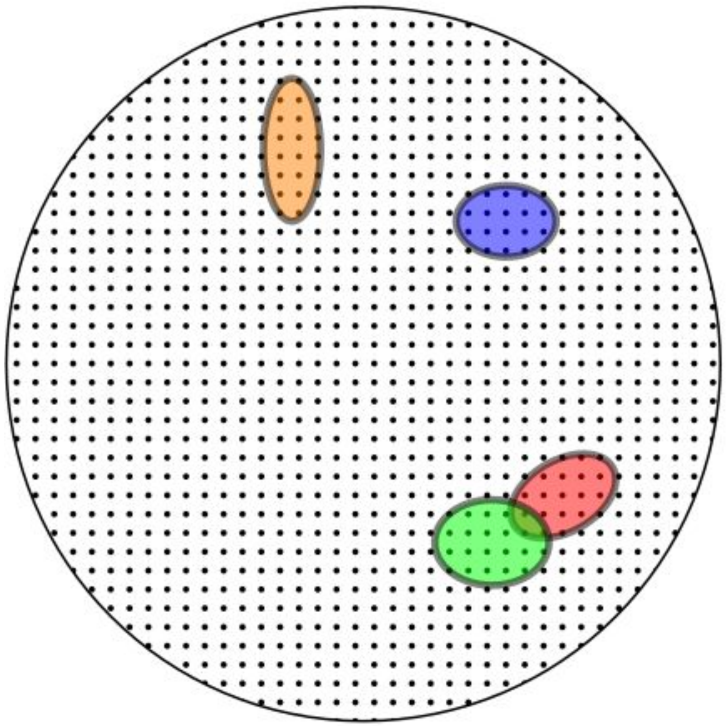
$$P(x_i \in \mathcal{D} : h(x_i) \quad = \quad y_i) \leq 1 - \epsilon$$

*For **m** elements in the training sample*

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

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

Considering bad hypothesis



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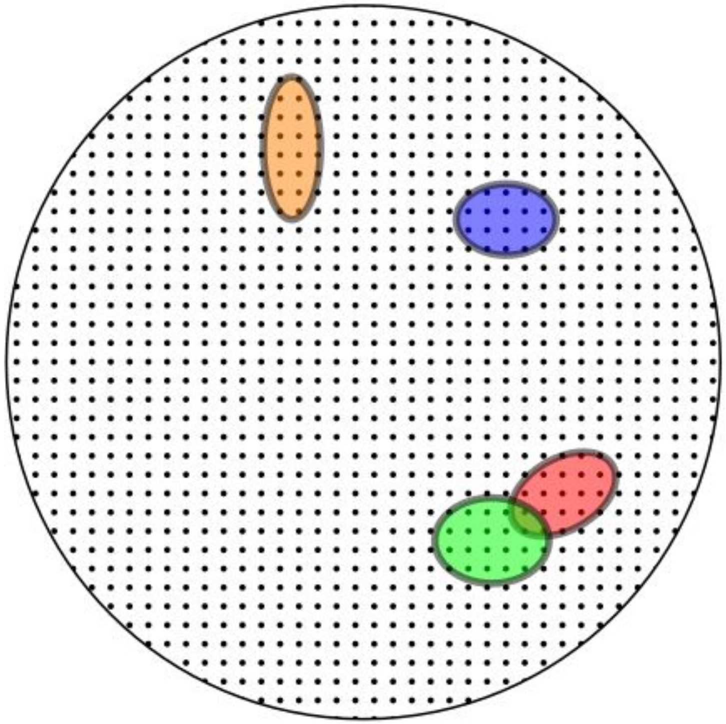


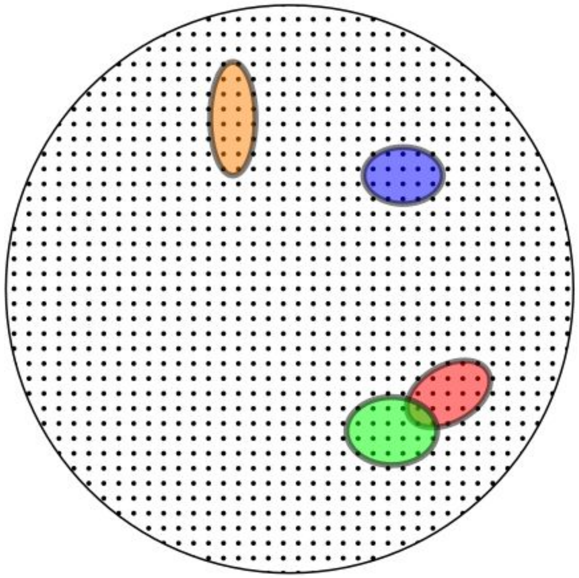
For 1 hypothesis

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

The sum rule

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

Considering bad hypothesis



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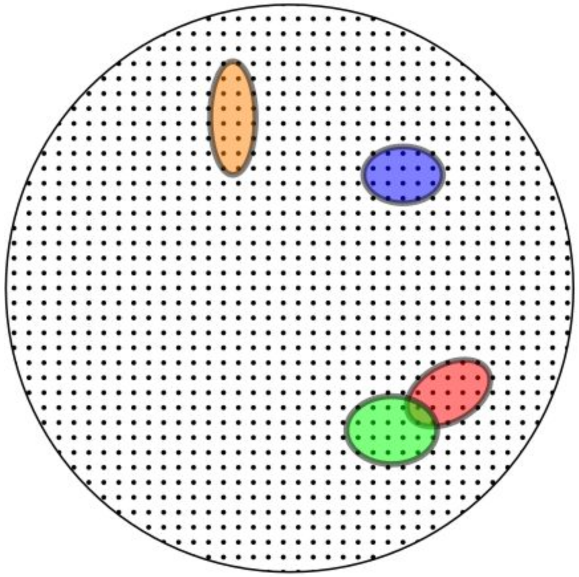
For all bad hypothesis

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

Considering bad hypothesis



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using...

$$(1-x)^y \quad \leq \quad \exp(-xy)$$

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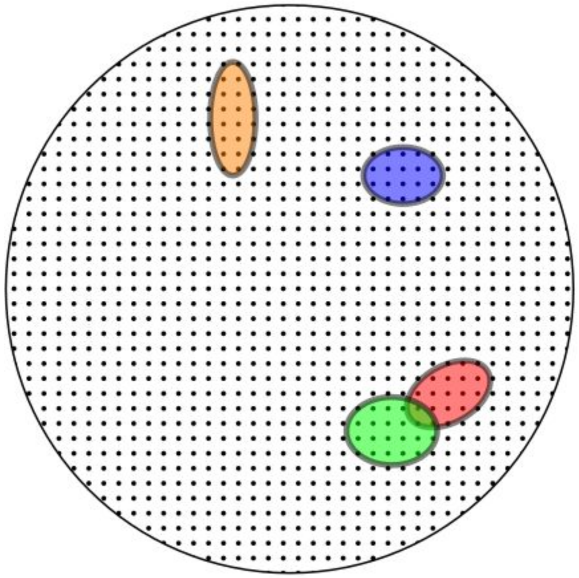

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$$\delta \leq N_{\mathcal{H}} \exp(-\epsilon m)$$

In summary …

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

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

If,

$$m_{\mathcal{H}}(\epsilon, \delta) \geq \frac{\ln(N_{\mathcal{H}}/\delta)}{\epsilon}$$

⟹ every *h* from ERM,

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PAC learning model

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⇒

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PAC learning model

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

Probably $\longrightarrow$ with confidence 1 - δ over *m* samples
Approximately $\longrightarrow$ within a contamination level ≤ ε
Correct

If, every *h* from ERM,

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

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Remember what is behind this!!

PAC Assumptions

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Y: set of possible labels,

y = [tasty, not tasty]

D: data generation model,

$D \Longrightarrow P(\chi)$

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- Representativeness

Return to a controlled example ...

Papaya tasting

χ: set of $x \in$ *[softness, color]*

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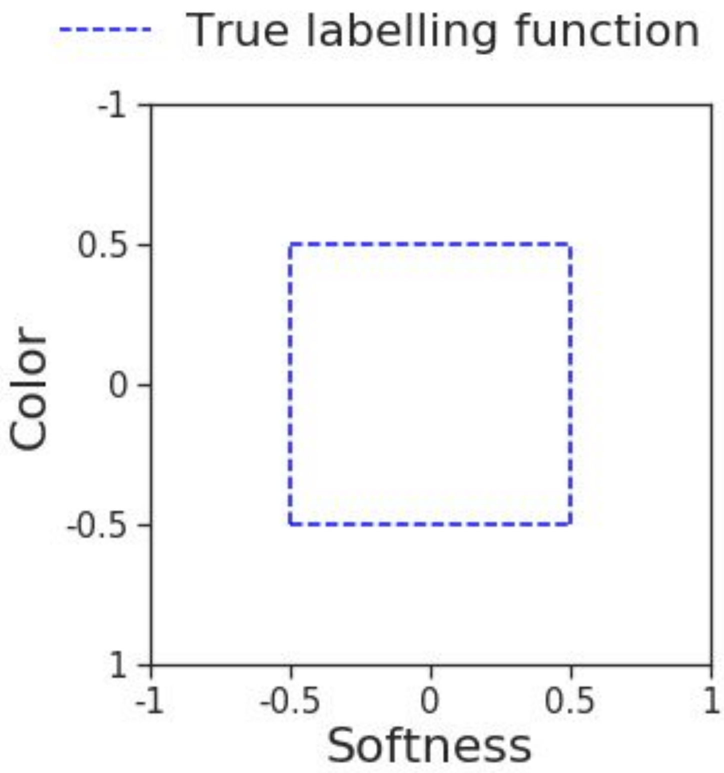

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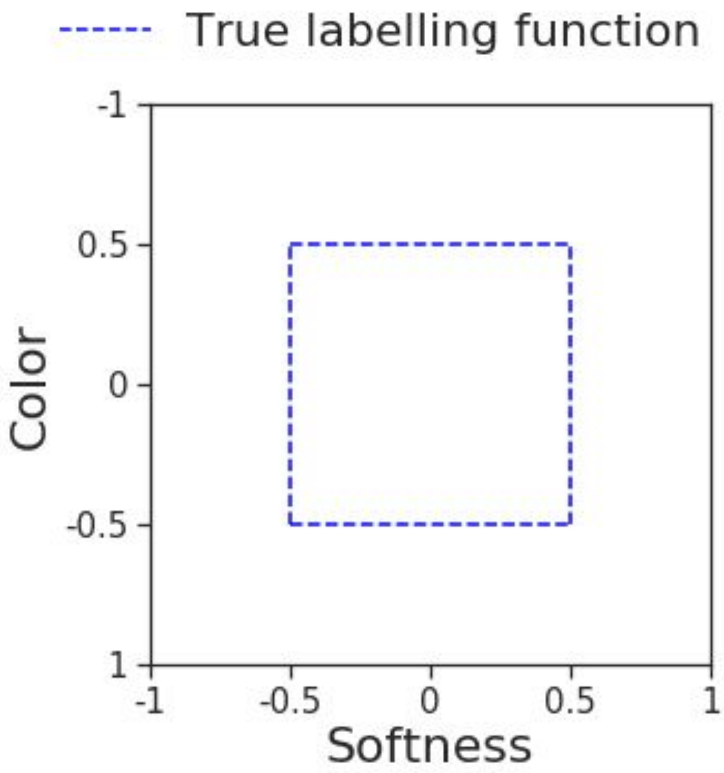

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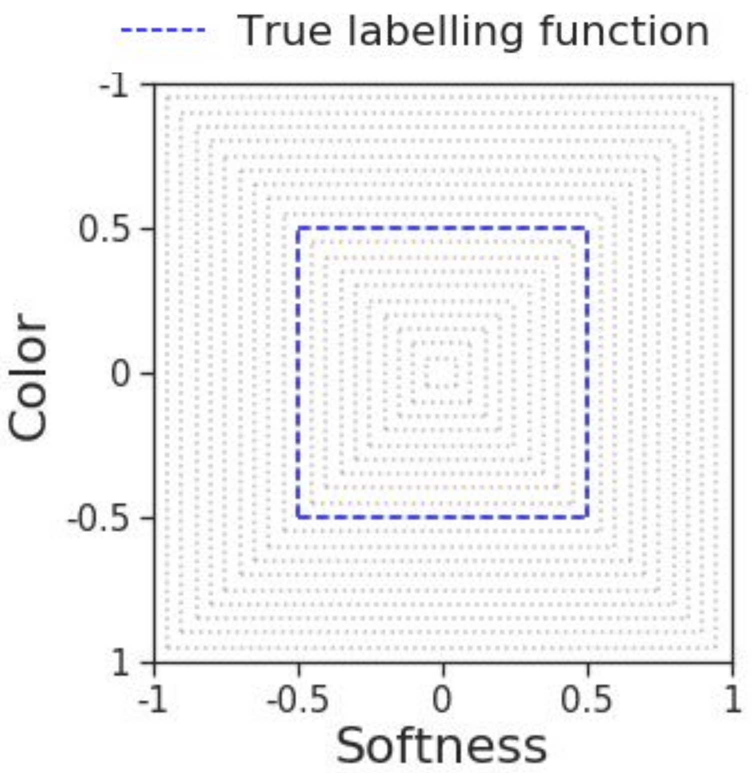
$\mathcal{H}$: *hypothesis class:*
axis aligned squares in steps of 0.05

$N_H = 20$



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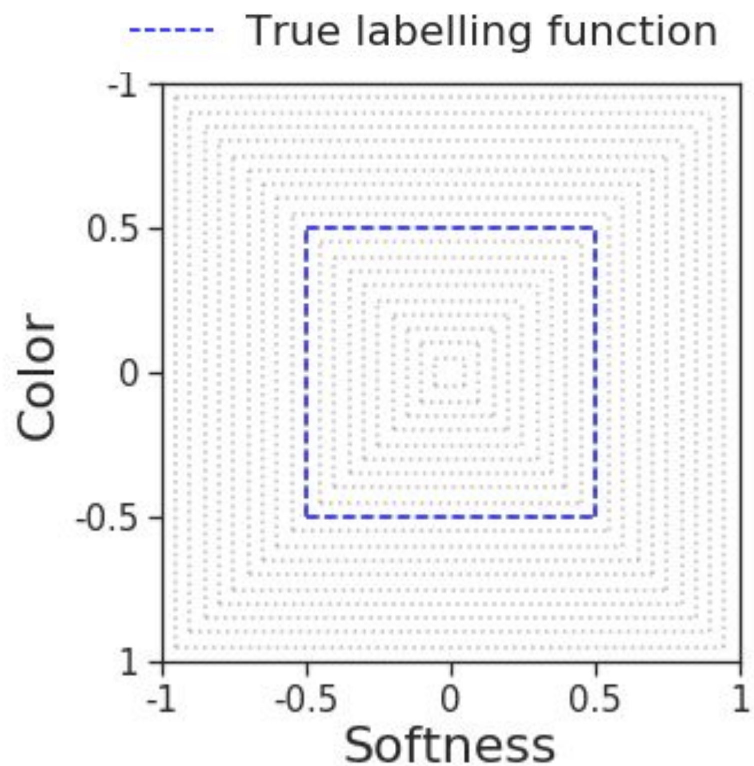


Question:

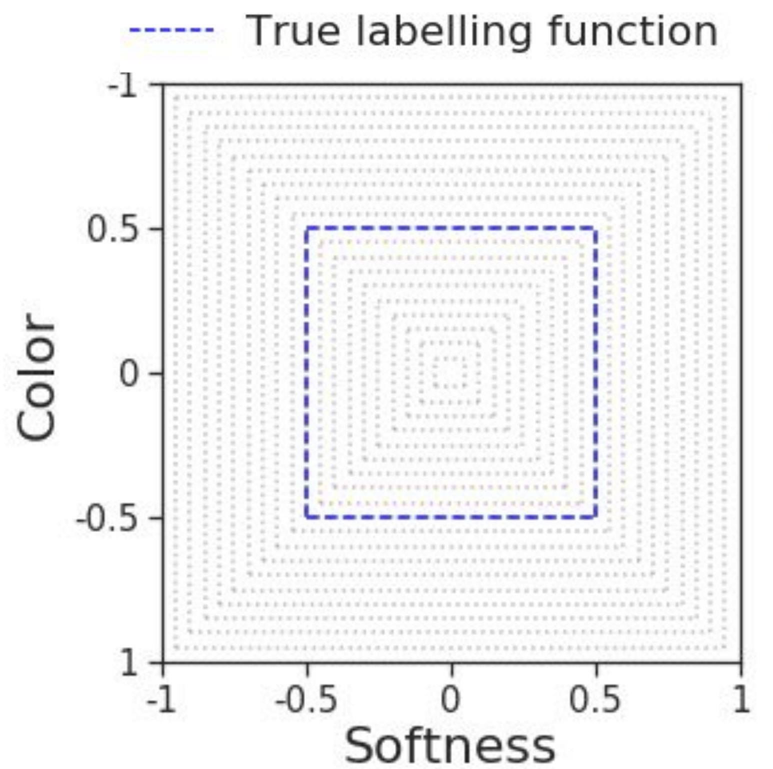
Data model: uniform distribution [-1,1] in both axis

$1 - \delta = 0.95 \leftarrow$ confidence

$\varepsilon = 0.05 \leftarrow$ contamination

$N_H = 20 \leftarrow$ number of possible squares

m = ??



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

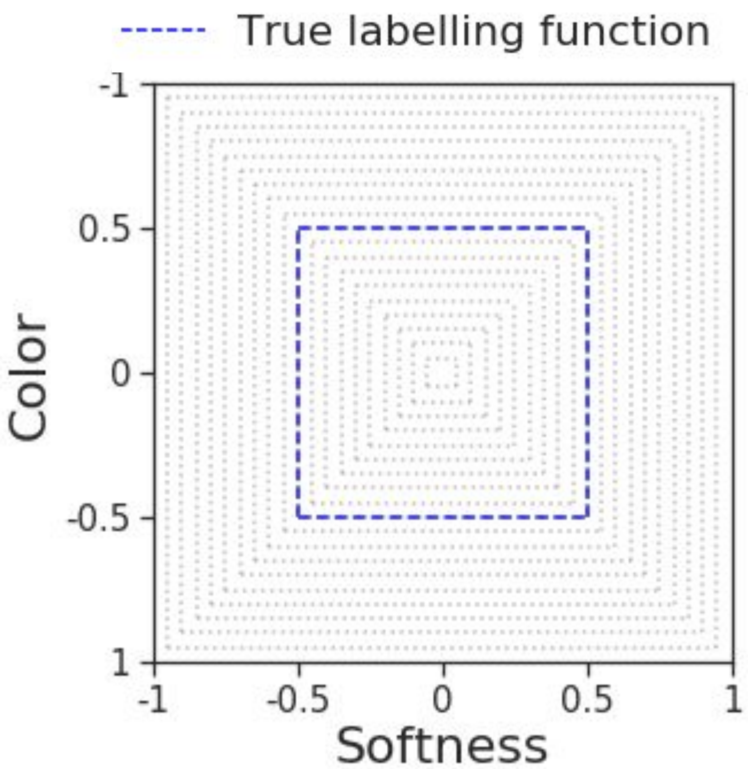
Question:

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

$1 - \delta = 0.95$ ← confidence

$\varepsilon = 0.05$ ← contamination

$N_H = 20$ ← number of possible squares



m ~ 120

Question:

Data model: uniform distribution
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$1 - \delta = 0.95$ ← confidence
$\varepsilon = 0.05$ ← contamination
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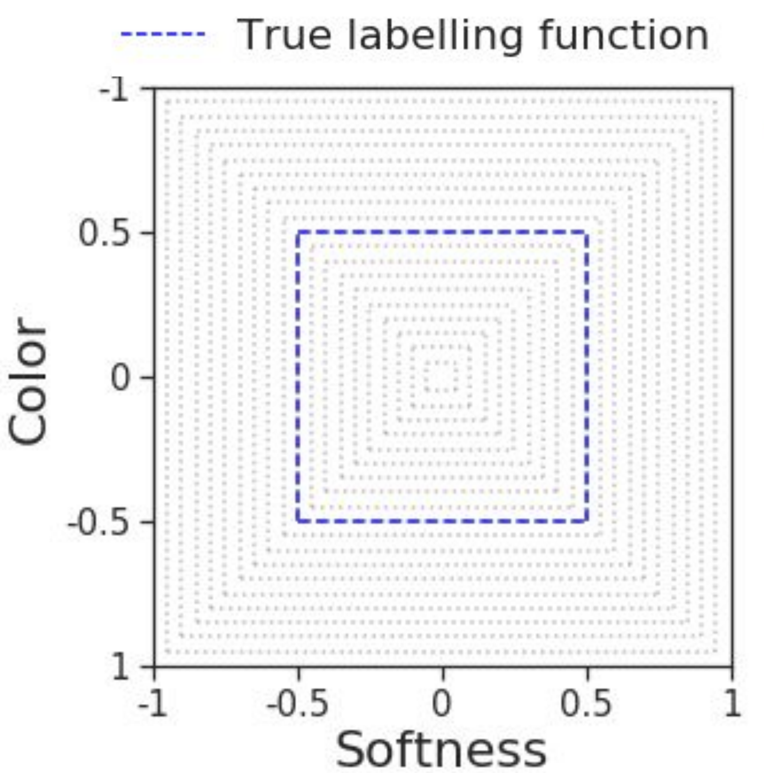

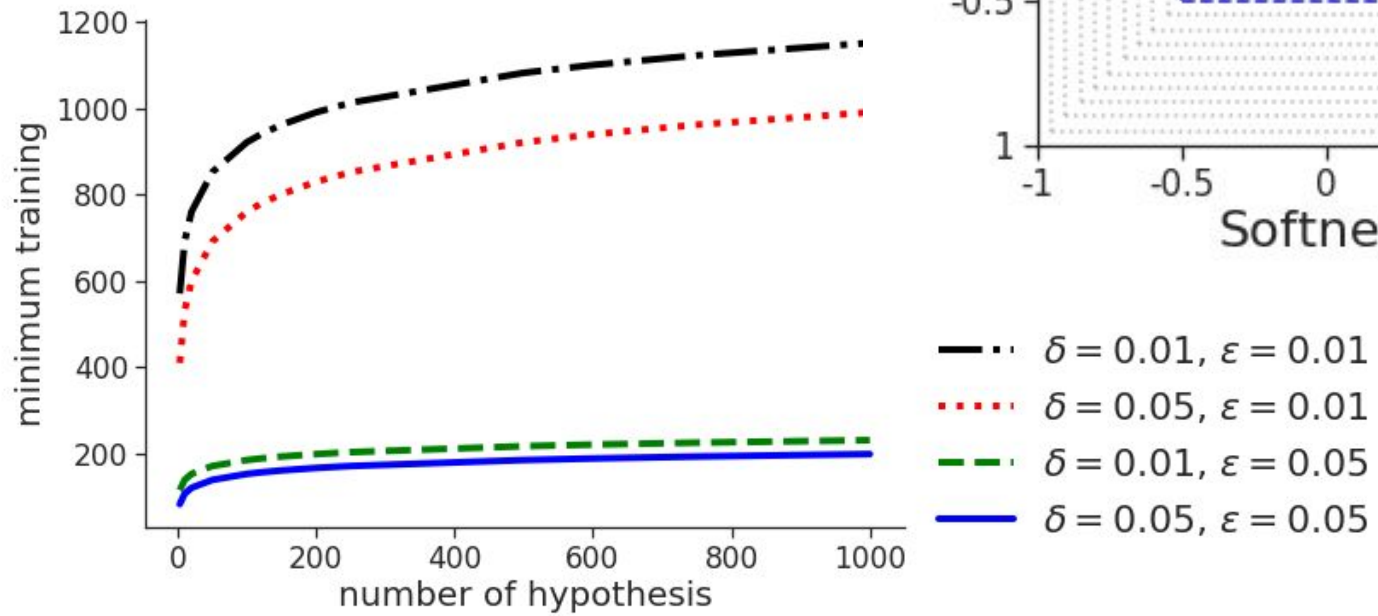

Agnostic PAC learning

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x = [softness, color]
Y: 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: training sample: $[x_i, y_i]$, $i \in training$
m: number of objects for training
h_S learner: $y_{est;i} = h_S(x_i, y_i)$

L: loss

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

Hypothesis class:

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

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

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

$$f \notin \mathcal{H}$$

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

Representativeness

in machine learning

Shalev-Shwartz, S. and Ben-David, S., *Understanding Machine Learning - from theory to algorithms*, 2014, Cambridge University Press

Representativeness

in machine learning

or

Uniform Convergence

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

Shalev-Shwartz, S. and Ben-David, S., Understanding Machine Learning - from theory to algorithms, 2014, Cambridge University Press

Representativeness

in machine learning

or

Uniform Convergence

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

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

Shalev-Shwartz, S. and Ben-David, S., Understanding Machine Learning - from theory to algorithms, 2014, Cambridge University Press

Can machine learning solve my problem?

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Can machine learning solve my problem?

- If your data satisfy all the necessary conditions;
- If you have enough training sample to fulfill your expectations;
- If the set of your hypothesis class + loss function + training data has uniform convergence (representativeness)

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

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**!*

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...*

https://www.youtube.com/watch?v=M2BJC0OyI-w

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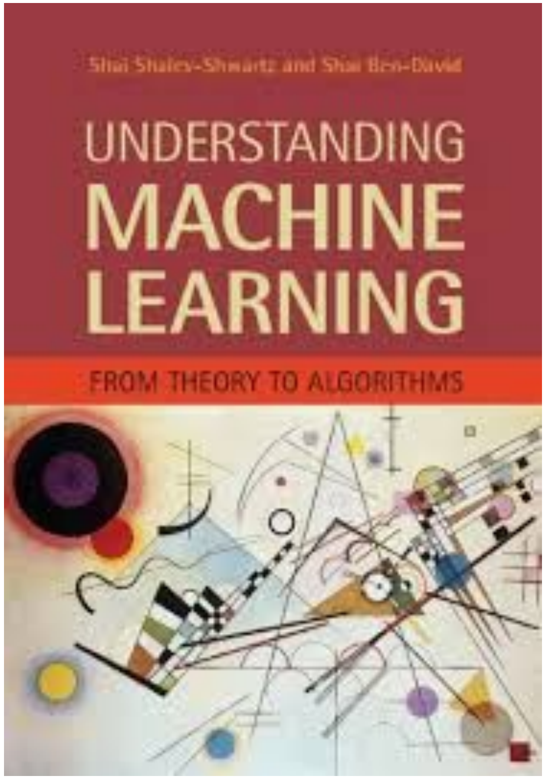
Machine learning is a wonderful field of research, which has already shown its potential in many fields! We should definitely take advantage of its results .. however ...

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



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

Enjoy!

THANK YOU