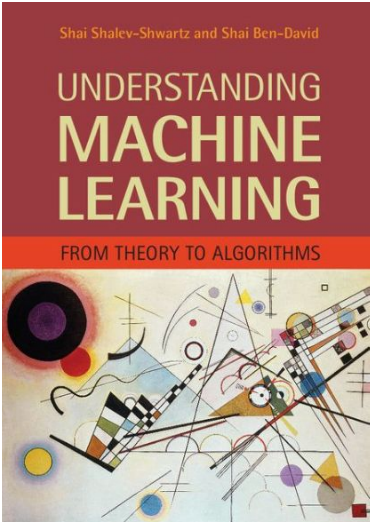
Machine Learning Theory 2024
Lecture 1

Tim van Erven

- Intro
- Statistical Decision Theory
- Empirical Risk Minimization and Overfitting
- PAC-Learnability for finite classes, realizable case

Book: Shai^2 (for First Half of the Course)

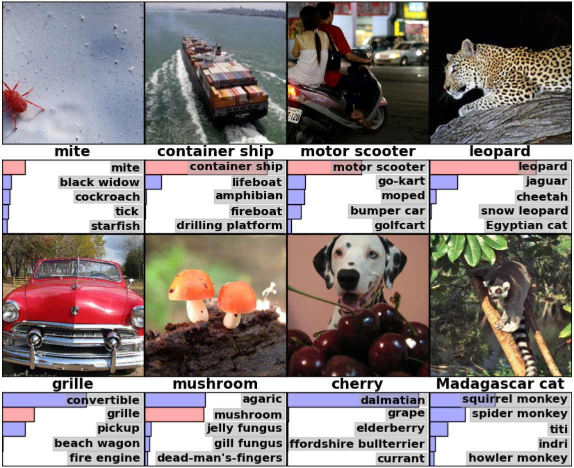


Shai Shalev-Shwartz and Shai Ben-David

UNDERSTANDING MACHINE LEARNING

FROM THEORY TO ALGORITHMS

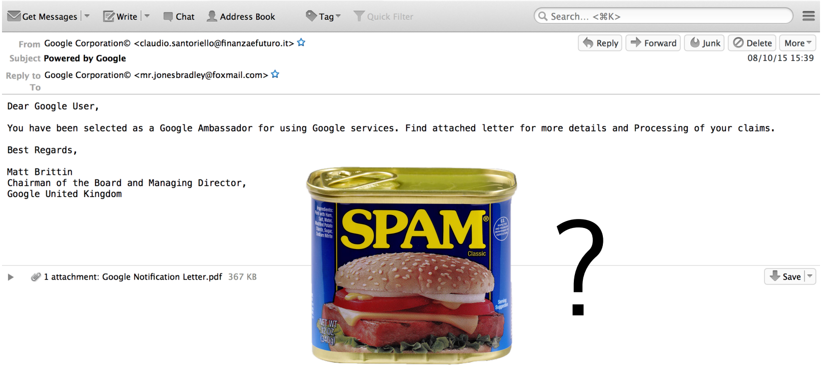
Multiclass Classification Example: Images



Y = image class, $\boldsymbol{X}$ = vector with pixel values

Krizhevsky, Sutskever, Hinton, **ImageNet Classification with Deep Convolutional Neural Networks**, NeurIPS 2012

Binary Classification Example: Spam Detection



From Google Corporation© <claudio.santoriello@finanzaefuturo.it>
Subject **Powered by Google**
Reply to Google Corporation© <mr.jonesbradley@foxmail.com>
To

08/10/15 15:39

```
Dear Google User,

You have been selected as a Google Ambassador for using Google services. Find attached letter for more details and Processing of your claims.

Best Regards,

Matt Brittin
Chairman of the Board and Managing Director,
Google United Kingdom
```

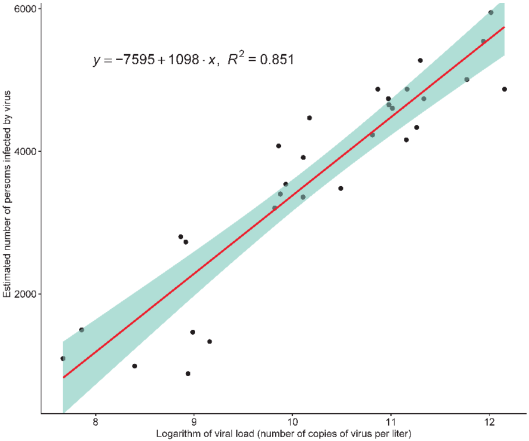
1 attachment: Google Notification Letter.pdf 367 KB

Y = ham/spam
$\boldsymbol{X} = (X_1, \ldots, X_{50\,000})$: X_i is word count for i-th word from dictionary

Spam image by Qwertyxp2000 from `https://commons.wikimedia.org/wiki/File:Spam_can.png`

Regression Example: Covid Cases from Wastewater

Y = Active number of Covid-19 cases



$\boldsymbol{X} = X_1$ = Log-viral load in wastewater

Vallejo et al., **Highly predictive regression model of active cases of COVID-19 in a population by screening wastewater viral load**, medRxiv preprint, 2020

Regression Example: Prostate Cancer

Goal: Predict level of prostate specific antigen (PSA) for men with prostate cancer

Y = log of PSA
$\boldsymbol{X} = (X_1, \ldots, X_{97})$: 97 clinical measures, including

- log cancer volume
- log prostate weight
- Gleason score
- . . .

Example from Hastie, Tibshirani, Freedman, **Elements of Statistical Learning**, 2nd edition, 2009

Scope of the Course I: Supervised vs Unsupervised

In the Course:
Supervised Machine Learning: Learn to predict response Y for input $\boldsymbol{X}$ based on examples of desired responses. E.g.

- Image classification: $\boldsymbol{X} = \text{image}$, $Y = \text{class}$
- Spam classification: $\boldsymbol{X} = \text{e-mail}$, $Y = \text{ham/spam}$
- Covid regression: $\boldsymbol{X} = \text{viral load}$, Y is nr. of active cases
- Cancer regression: $\boldsymbol{X} = \text{clinical measures}$, $Y = \text{antigen amount}$

Not in the Course:
Unsupervised Machine Learning: Identify structure in inputs $\boldsymbol{X}$. E.g.

- Group data into clusters
- Dimensionality reduction

Scope of the Course II: Batch and Online

We cover two learning models:

Part I, **Batch Learning:**

- Data is obtained as one big batch
- Then learn a predictor
- Deploy predictor once, to be used unchanged on new data

Part II, **Online Learning:**

- Data arrives sequentially over time
- Continuously make predictions for incoming data
- Use new data to keep improving predictor

Scope of this Course III: Foundations vs Practice

What is Missing:

- Not: programming, real data, getting rich and famous quickly...
- By itself this course is **too theoretical**!

...But We Make Up for It:

- Deep understanding via **beautiful concepts and proofs**
- When is learning possible and what are the fundamental limitations?
- Close connections to statistics, game theory, information theory, optimization, ...

Supervised Learning

Sample of **training data**: $S = \begin{pmatrix} Y_1 \\ \boldsymbol{X}_1 \end{pmatrix}, \cdots, \begin{pmatrix} Y_m \\ \boldsymbol{X}_m \end{pmatrix}$

(teacher shows us desired response Y_i for input $\boldsymbol{X}_i$)

Y_i: class/response variable
$\boldsymbol{X}_i \in \mathbb{R}^d$: feature vectors

Goal: Learn function $h_S : \mathcal{X} \to \mathcal{Y}$ from **hypothesis class** $\mathcal{H}$ = some set of functions

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Evaluate h_S on **test data**:

- New $\boldsymbol{X}$ from same source
- Predict corresponding Y by $\hat{Y} = h_S(\boldsymbol{X})$

Assume $\begin{pmatrix} Y_i \\ \boldsymbol{X}_i \end{pmatrix}$ independent samples from same probability distribution $\mathcal{D}$

Avoid further assumptions on $\mathcal{D}$!
(So $\mathcal{D}$ can be very complicated)

Supervised Learning: Regression

$$S = \begin{pmatrix} Y_1 \\ \boldsymbol{X}_1 \end{pmatrix}, \cdots, \begin{pmatrix} Y_m \\ \boldsymbol{X}_m \end{pmatrix}$$

$Y \in \mathbb{R}$ is a **continuous variable**. E.g.

- Y = Covid-19 cases
  $\boldsymbol{X} = (X_1, X_2)$: X_1 = viral load, X_2 = population size

Linear Regression ($\mathcal{H}$ = affine functions):

$$h_{\boldsymbol{w},b}(\boldsymbol{X}) = b + \langle \boldsymbol{w}, \boldsymbol{X} \rangle = b + \sum_{i=1}^{d} w_i X_i$$

Can assume $b = 0$ w.l.o.g. to simplify notation, because:

$$\boldsymbol{w}' = (b, w_1, \ldots, w_d) \qquad \boldsymbol{X}' = (1, X_1, \ldots, X_d)$$

$$h_{\boldsymbol{w}'}(\boldsymbol{X}') = \langle \boldsymbol{w}', \boldsymbol{X}' \rangle = h_{\boldsymbol{w},b}(\boldsymbol{X})$$

Supervised Learning: Classification

$$S = \begin{pmatrix} Y_1 \\ \boldsymbol{X}_1 \end{pmatrix}, \cdots, \begin{pmatrix} Y_m \\ \boldsymbol{X}_m \end{pmatrix}$$

Y is a **categorical variable**

- E.g. $Y \in \{\text{Ham}, \text{Spam}\}$ or $Y \in \{\text{Mite}, \text{Leopard}, \text{Mushroom}\}$

Binary Classification (with two classes):

- Can e.g. map "Ham" $\mapsto -1$, "Spam" $\mapsto +1$
- So assume $Y \in \{-1, +1\}$ or sometimes $Y \in \{0, 1\}$ without loss of generality (w.l.o.g.)

Halfspaces ($\mathcal{H}$ = Linear Predictors):

$$h_{\boldsymbol{w},b}(\boldsymbol{X}) = \text{sign}(b + \langle \boldsymbol{w}, \boldsymbol{X} \rangle) \in \{-1, +1\}$$

Overfitting

(why machine learning is non-trivial)

The #1 Beginner's Mistake:

- Try many machine learning methods and fine-tune their settings until the number of mistakes on the training data S is small
- What can go wrong?

Poll:

1. Trying many methods and settings can take a very long time.
2. Few mistakes on S does not guarantee good learning.
3. You should only use methods taught in this course.

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(why machine learning is non-trivial)

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Overfitting
(why machine learning is non-trivial)

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- Try many machine learning methods and fine-tune their settings until the number of mistakes on the training data S is small
- What can go wrong?

- Suppose $\boldsymbol{X}$ is uniformly distributed in $[-1,+1]^2$
- $Y=+1$ if $X_1 \geq 0$; $Y=-1$ otherwise.

$$h_S(\boldsymbol{X}) = \begin{cases} Y_i & \text{for smallest } i \in \{1,\ldots,m\} \text{ such that } \boldsymbol{X} = \boldsymbol{X}_i \\ -1 & \text{if no such } i \text{ exists} \end{cases}$$

Perfect on training data S,
but probability of mistake $= 1/2$ on new $(\boldsymbol{X}, Y)$ from $\mathcal{D}$!
No better than random guessing!

Statistical Decision Theory I: Loss

Measure error by **loss function**: $\ell(h, \boldsymbol{X}, Y)$

Classification (0/1-loss counts mistakes):

$$\ell(h, \boldsymbol{X}, Y) = \begin{cases} 0 & \text{if } h(\boldsymbol{X}) = Y \\ 1 & \text{if } h(\boldsymbol{X}) \neq Y \end{cases}$$

Regression (Squared Error):

$$\ell(h, \boldsymbol{X}, Y) = (Y - h(\boldsymbol{X}))^2$$

Other choices possible!
(Depends on what is important in your application)

Statistical Decision Theory II: Risk

Risk: $$L_{\mathcal{D}}(h) = \mathbb{E}[\ell(h, \boldsymbol{X}, Y)] \qquad \text{for } (\boldsymbol{X}, Y) \sim \mathcal{D}$$

Empirical Risk: $$L_S(h) = \frac{1}{m}\sum_{i=1}^{m} \ell(h, \boldsymbol{X}_i, Y_i)$$

Bayes Optimal Predictor: $f_{\mathcal{D}} \in \arg\min_f L_{\mathcal{D}}(f)$

- Unknown, because risk depends on $\mathcal{D}$
- No learning alg can do better (by definition)

Examples for Classification:

- $L_{\mathcal{D}}(h) = \Pr(h(\boldsymbol{X}) \neq Y)$
- $L_S(h) =$ proportion of mistakes on the training data S
- $f_{\mathcal{D}}(\boldsymbol{X}) = \arg\max_y \Pr(Y = y \mid \boldsymbol{X})$ is most likely class

Statistical Decision Theory II: Risk

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Empirical Risk Minimization (ERM): $f_s \in \arg\min_{h \in \mathcal{H}} L_S(h)$

- Minimize **empirical risk** (known) instead of risk (unknown)
- Restrict to **hypothesis class** $\mathcal{H}$ to prevent overfitting

Choice of $\mathcal{H}$ is a **modeling decision**,
made before seeing the data!

No Overfitting for (Multiclass) Classification

Definition (**Realizability assumption**)

Exists $h^* \in \mathcal{H}$ that perfectly predicts Y (with probability 1):
$\Pr(h^*(\boldsymbol{X}) = Y) = 1$.

Huge simplification:

- $Y = h^*(\boldsymbol{X})$ without any noise
- We were lucky enough to include h^* in $\mathcal{H}$

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Theorem (First Example of PAC-Learning)

Assume $\mathcal{H}$ is **finite**, **realizability** *holds. Choose any $\delta \in (0,1)$, $\epsilon > 0$. Then, for all $m \geq \frac{\ln(|\mathcal{H}|/\delta)}{\epsilon}$, ERM over $\mathcal{H}$ guarantees*

$$L_{\mathcal{D}}(h_S) \leq \epsilon$$

with probability at least $1 - \delta$.

NB Lower bound on m does not depend on $\mathcal{D}$ or on h^*!

PAC learning: probably approximately correct

Proof (handwritten)

Recall that $L_D(h) = \Pr(h(\boldsymbol{X}) \neq Y)$
'Bad" hypotheses: $\mathcal{H}_B = \{h \in \mathcal{H} : \Pr(h(\boldsymbol{X}) \neq Y) > \epsilon\}$
ERM only selects a bad hypothesis h if $L_S(h) = 0$.
So sufficient to show that

$$\Pr(\text{exists } h \in \mathcal{H}_B : L_S(h) = 0) \leq \delta.$$

Lemma (Union Bound)

For any two events A and B, $\Pr(A \text{ or } B) \leq \Pr(A) + \Pr(B)$.

Hence

$$\begin{aligned}\Pr(\text{exists } h \in \mathcal{H}_B : L_S(h) = 0) &\leq \sum_{h \in \mathcal{H}_B} \Pr(L_S(h) = 0) \\ &\leq \sum_{h \in \mathcal{H}_B} (1-\epsilon)^m \leq |\mathcal{H}|(1-\epsilon)^m \leq |\mathcal{H}|e^{-\epsilon m}\end{aligned}$$

This is guaranteed to be at most δ if $m \geq \frac{\ln(|\mathcal{H}|/\delta)}{\epsilon}$.

Close Relation to Statistics, But...

Stats:

- Estimate **true parameters**, with uncertainty quantification
- Follow rigorous procedures or results are nonsense

Machine Learning:

- Estimate parameters that **predict well**
  - Possible under weaker assumptions/more complicated models!
- Can always estimate risk on a test set, even for crazy learning algorithm → **cowboy mentality can work!**
- (Fast!) algorithms

ML vs Stats (Handwritten)