Summer School ML

II Machine Learning Basics

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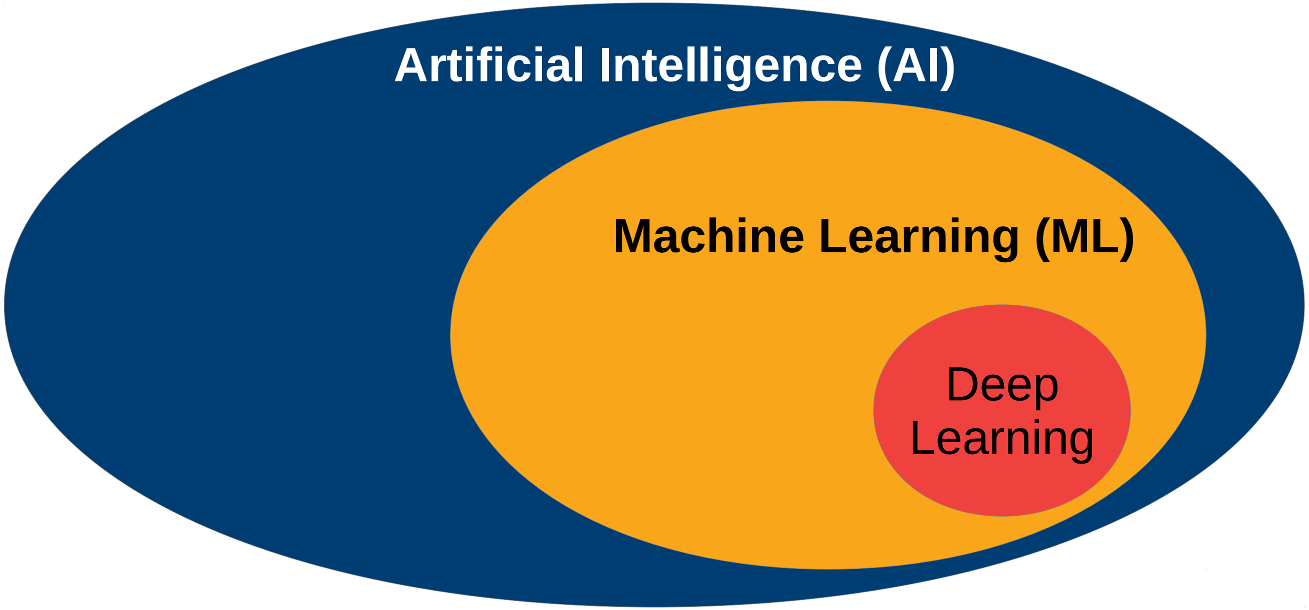
Introduction to ML

Research and Application Fields



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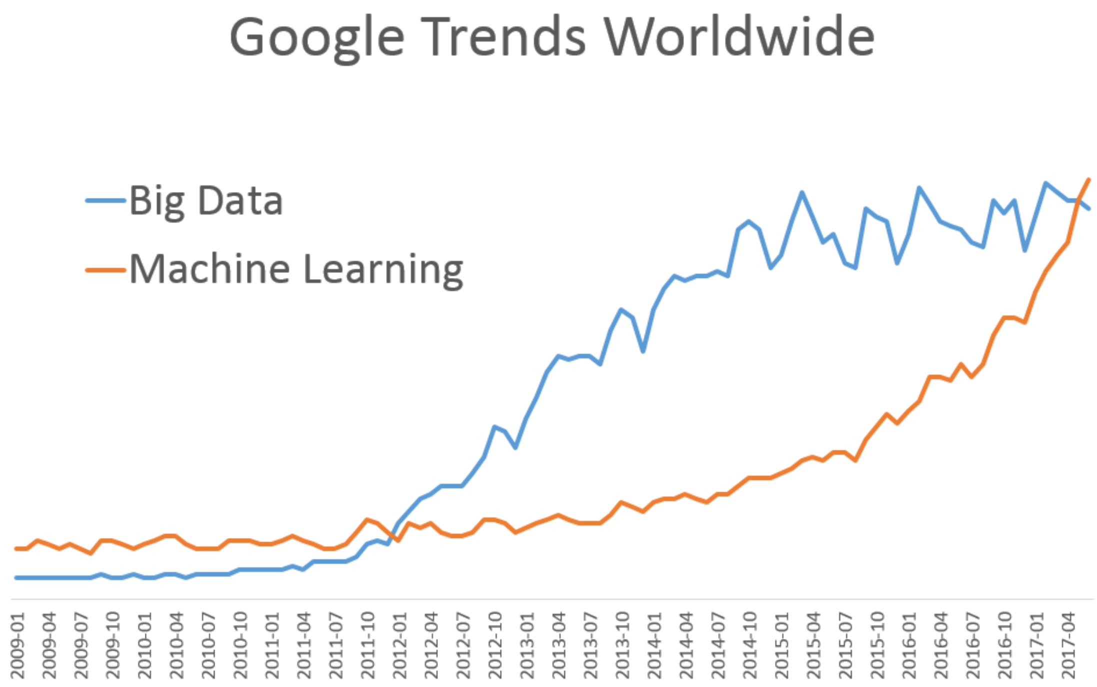
The ML Hype



Introduction to ML

Basic Types of Machine Learning Algorithms

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

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Basic Types of Machine Learning Algorithms

Supervised Learning

Unsupervised Learning

Reinforcement Learning

- Labeled data
- Direct and quantitative evaluation

- Learn model from „ground truth“ examples
- Predict unseen examples

Introduction to ML

Supervised Learning

Basic Notation:

Data is given as tuples

$$(X, Y) := \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$$

Where X is the actual **data** (sample) and y the associated **label.**

For most ML algorithms **(many Deep Learning algorithms are an exception)**

$$x_i \in \mathbb{R}^n, y_i \in \mathbb{R}$$

The data has to be represented as vectors and the labels are scalars.

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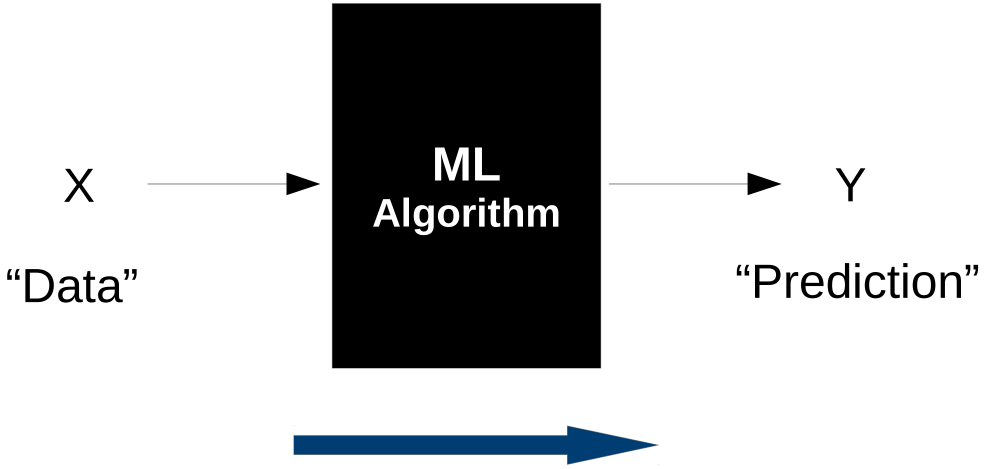
Supervised Learning as a Black Box



ML algorithms “learns” ***mapping*** from input to output by example tuples

Introduction to ML

Supervised Learning: Example: Classification

X: Image

ML

“coffee mug”

Classification: Y discrete
semantic class label

ML algorithms “learns” ***mapping*** from input to output by example tuples

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Supervised Learning: Example: Classification

X: Image

ML

“coffee mug”

Scalar

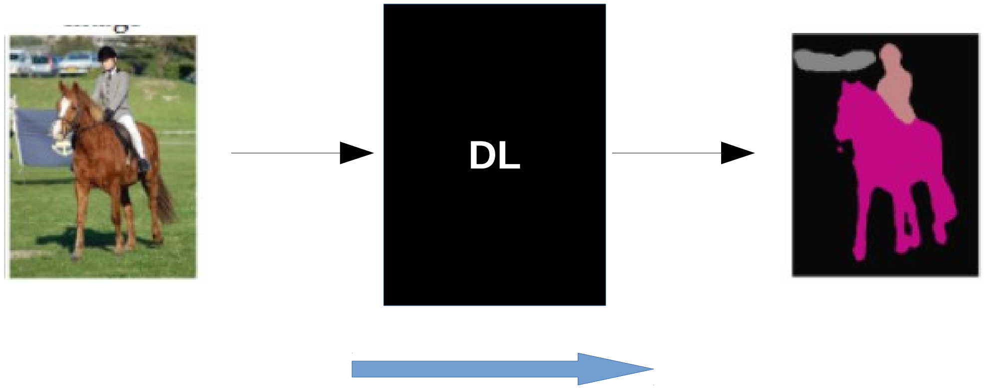
Vector

Classification: Y discrete
semantic class label

ML algorithms “learns” ***mapping*** from input to output by example tuples

Function f(x) → y

More Examples (here Deep Learning)



Example: semantic segmentation

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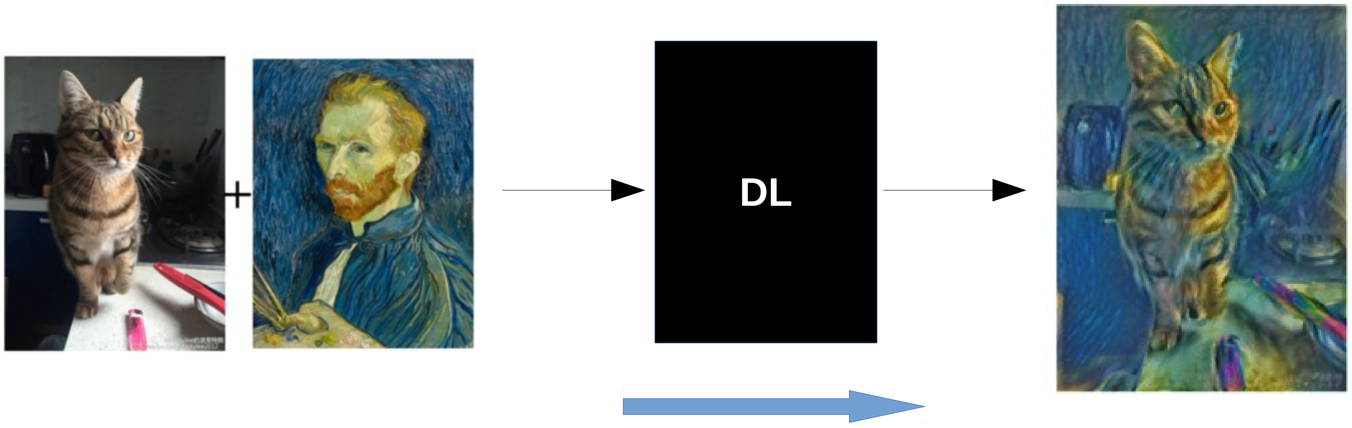
More Examples (here Deep Learning)



Example: contend generation, e.g. style transfer learning

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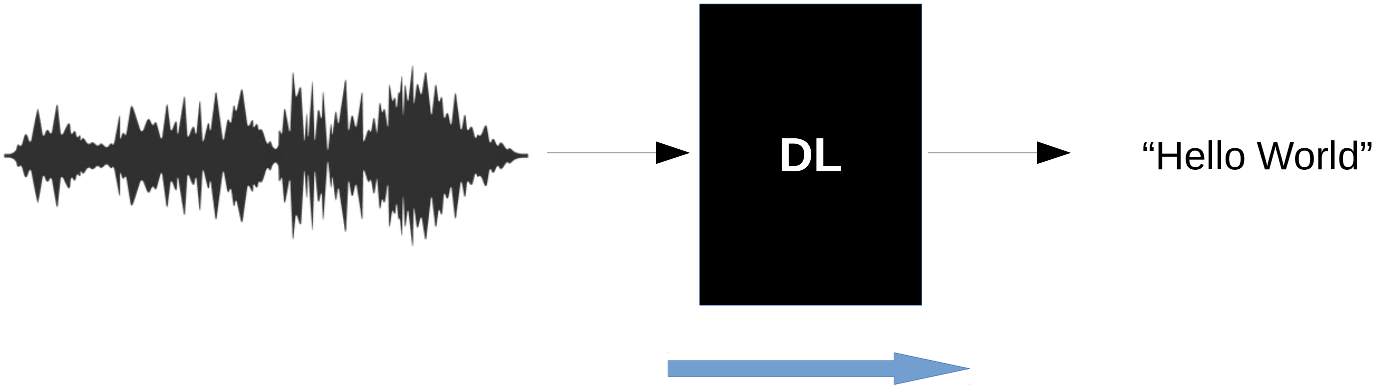
More Examples (here Deep Learning)



Example: Speech recognition

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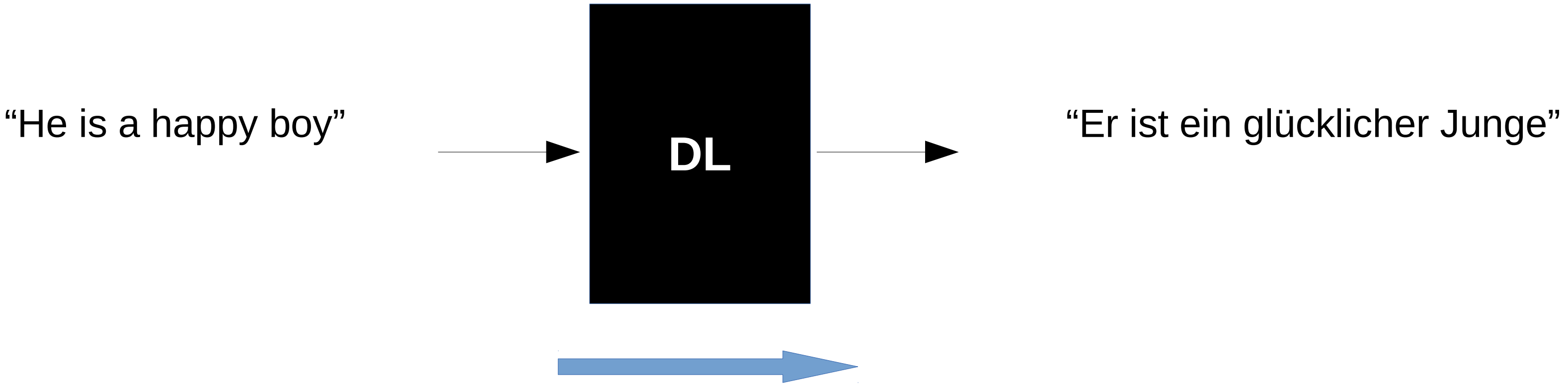
More Examples (here Deep Learning)



Example: Text understanding, e.g. translations

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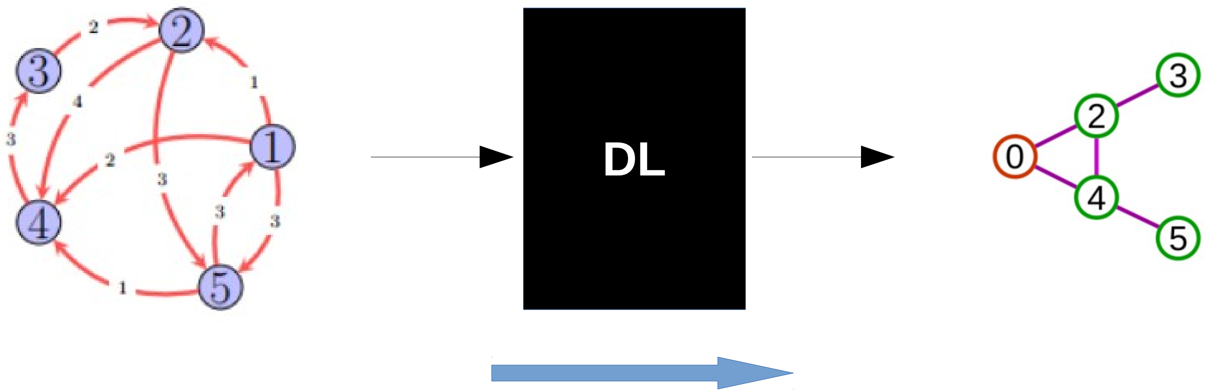
More Examples (here Deep Learning)



Example: Graph analysis

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More Examples (here Deep Learning)

→ **DL** → “move right”

Video sequence → action

Example: game playing

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Supervised Learning: Example: Classification

X: Image

$\longrightarrow$ **ML** $\longrightarrow$ Y: {“coffee mug”, “non coffee mug}

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Supervised Learning: Example: Classification

X: Image

pixel by pixel

$$\begin{pmatrix} 5 \\ 8 \\ 15 \\ 23 \\ 21 \\ 30 \\ 28 \\ \dots \\ 5 \end{pmatrix}$$

$$X \in \mathbb{R}^n$$

ML

Y': {-1,1} $Y' \in \mathbb{R}$

1: “coffee mug”,
-1: “non coffee mug

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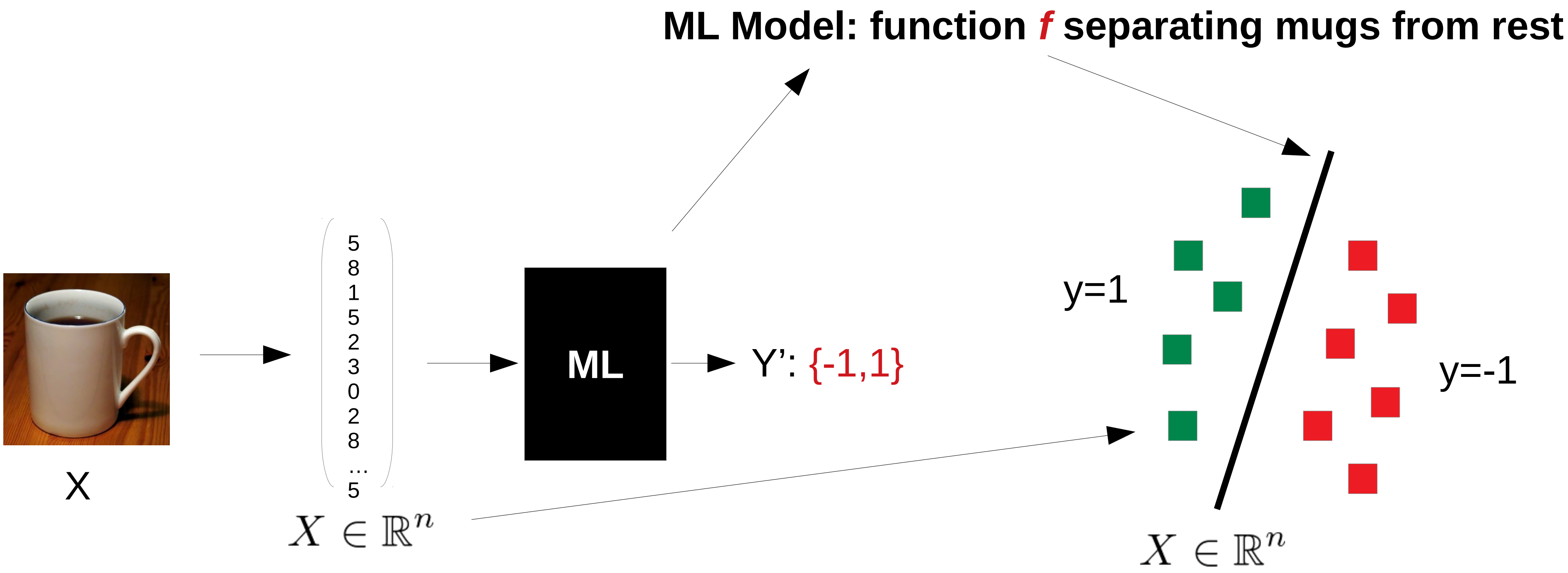
Supervised Learning: Example: Classification



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Supervised Learning: Example: Classification

LEARNING: approximate „best“ *f* for the given data

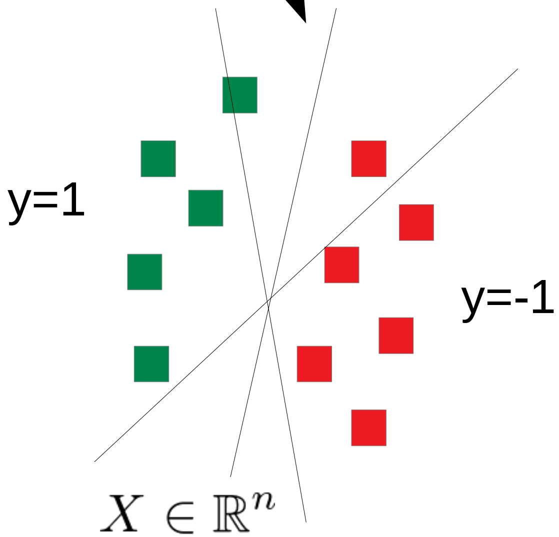
X

$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \dots \\ 5 \end{pmatrix}$$

$X \in \mathbb{R}^n$

ML

Y': {-1,1}



Supervised Learning: Example: Classification

LEARNING: optimization problem:

$$min(\|f(X,Y),Y'\|)$$

X

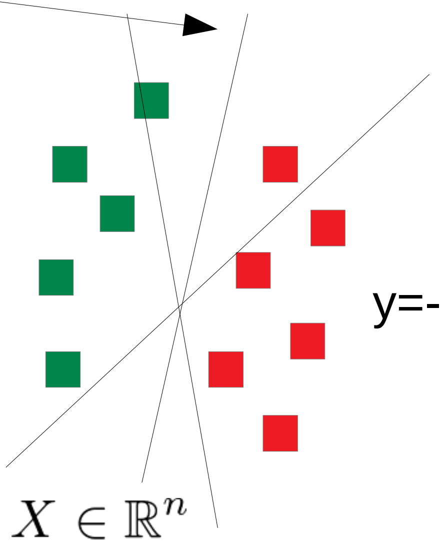
$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \dots \\ 5 \end{pmatrix}$$

$X \in \mathbb{R}^n$

ML

Y’: {-1,1}

y=1



y=-1

$X \in \mathbb{R}^n$

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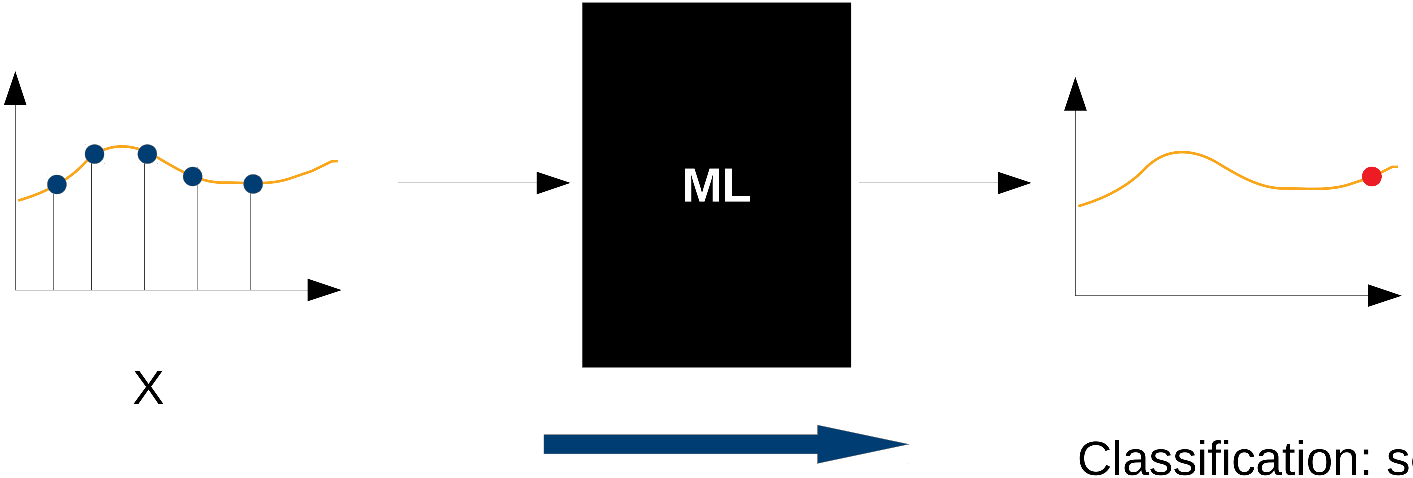
Supervised Learning: Example: Regression



Regression

Y is **continuous**

Classification: separation function

Regression: continuous mapping
→ harder problem

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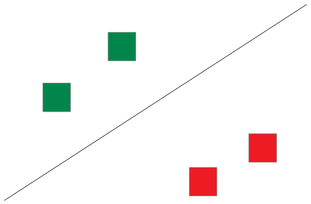
Challenges of Supervised Learning

- Not only need data – also need to have $Y \rightarrow$ human annotation
  - Getting “enough” labeled data is expensive
  - Sometimes impossible

UNDERFITTING

$$min(\|f(X,Y),Y'\|)$$



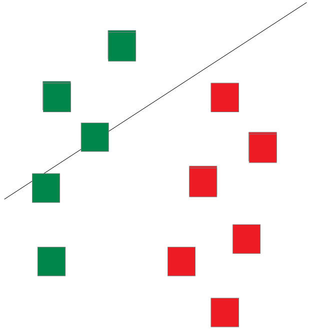
Training model
On little data

Challenges of Supervised Learning

- Not only need data – also need to have $Y \rightarrow$ human annotation
  - Getting “enough” labeled data is expensive
  - Sometimes impossible

UNDERFITTING

$$min(\|f(X,Y),Y'\|)$$



$\rightarrow$ bad sampling
Of the data distribution

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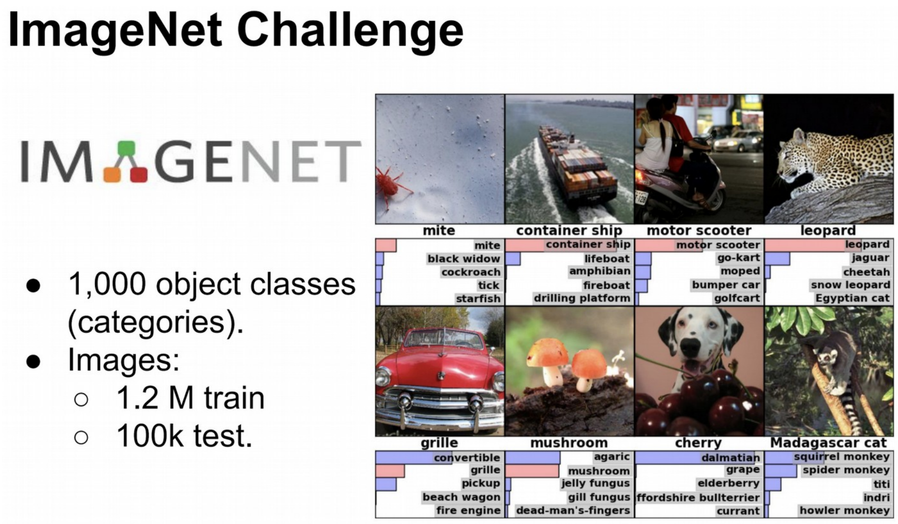
Challenges of Supervised Learning

- Not only need data – also need to have Y → human annotation
  - Getting “enough” labeled data is expensive
  - Sometimes impossible

Example:



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Challenges of Supervised Learning

- Not only need data – also need to have *Y* → human annotation
  - Getting “enough” labeled data is expensive
  - Sometimes impossible

Example:

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Challenges of Supervised Learning

- Not only need data – also need to have Y → human annotation
  - Getting “enough” labeled data is expensive
  - Sometimes impossible

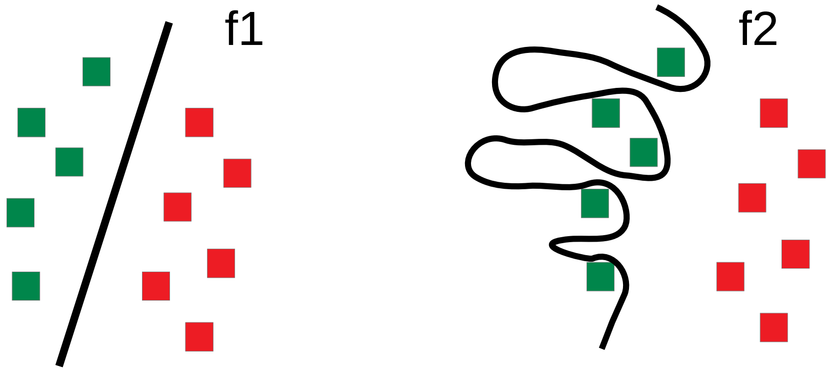
- Training data is **only a sample:** prediction must work on **all data** → **generalization**

Challenges of Supervised Learning

- Training data is **only a sample:** prediction must work on **all data** → **generalization**

Which model is better?

$$min(\|f(X,Y),Y'\|)$$



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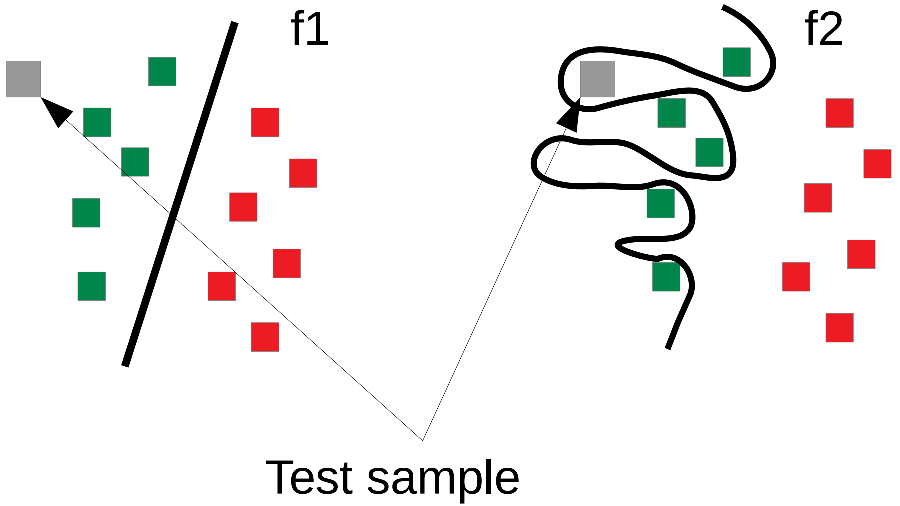
Challenges of Supervised Learning

- Training data is **only a sample:** prediction must work on **all data** → **generalization**

Which model is better?

$$min(\|f(X,Y),Y'\|)$$



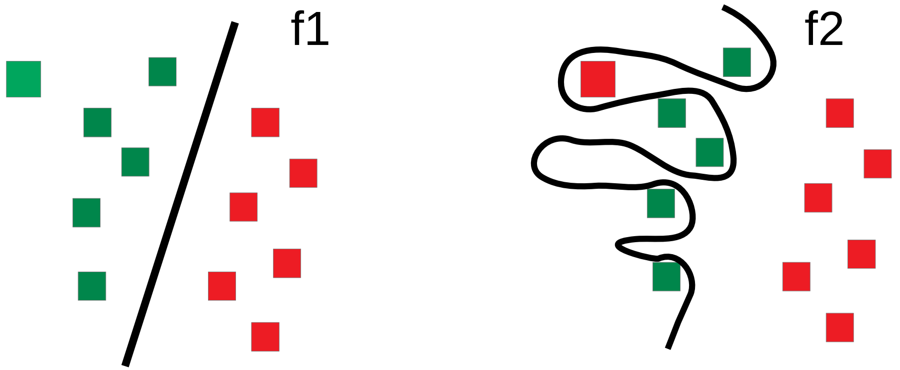
Challenges of Supervised Learning

- Training data is **only a sample:** prediction must work on **all data** → **generalization**

OVERFITTING

Model “to close” to train data

Very likely to happen in practice.
→ we need to work against this...



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Data Preparation: Split into Train, Test, and Validate

A basic technique (we will learn more later) to at least detect overfitting is to split the available data into two or three subsets:

- Use unbiased **test set** for final evaluation of a model
- Use **train set** for model training
- **Validation set** (part of train set) can be used to optimize hyper parameters of the model

Caution: sets must be unbiased! (→ random sampling)
In practice it can be hard to guarantee clean train/test sets:
e.g. how to treat possible variance different data sources?
→ statistical analysis needed!

Basic Types of Machine Learning Algorithms

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

- NO Labeled data
- NO Direct and quantitative evaluation

- Explore structure of data

Introduction to ML

Unsupervised Learning

Data without “labels” $(x_1, x_2, \ldots, x_n)$

- **Clustering**
- **Outlier Detection (e.g. Defect or Intrusion detection)**

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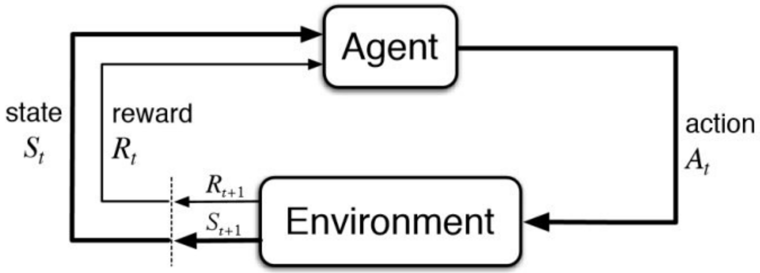
Basic Types of Machine Learning Algorithms

Supervised Learning

Unsupervised Learning

Reinforcement Learning



- Learning decisions in an interactive environment
- State ↔ Action learning
- Game playing and robotics
- Hardly use in Data Science

Recall Classification

Supervised Learning: Annotated Training Data

Vector representation

(X,Y)

$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \dots \\ 5 \end{pmatrix} \rightarrow \boxed{\textbf{ML}} \rightarrow Y': \{-1,1\}$$

$X \in \mathbb{R}^n$

Recall Classification

Supervised Learning: Annotated Training Data

Vector representation

(X,Y)

$$\begin{pmatrix} 5 \\ 8 \\ 1 \\ 5 \\ 2 \\ 3 \\ 0 \\ 2 \\ 8 \\ \vdots \\ 5 \end{pmatrix}$$

$X \in \mathbb{R}^n$

ML

Y': {-1,1}

(feature extraction / engineering)

Recall Classification

Supervised Learning: Annotated Training Data

Vector representation

Feature vector representation
Defines the learning problem!

(X,Y)

5
8
1
5
2
3
0
2
8
...
5

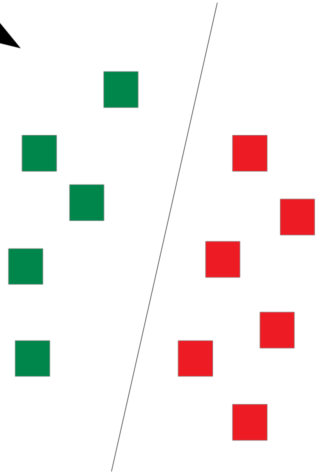
$X \in \mathbb{R}^n$

ML

Y': {-1,1}

(feature extraction / engineering)

y=1



y=-1

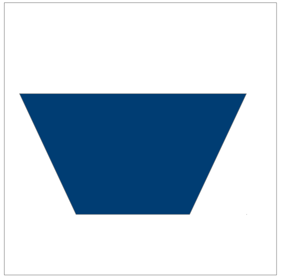
$X \in \mathbb{R}^n$

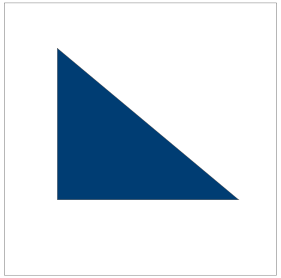
Feature Extraction

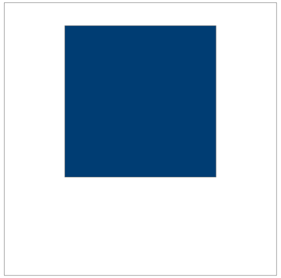
A Simple Example

A algorithm that can classify three different shape in an image:

- How to vectorize the data samples?







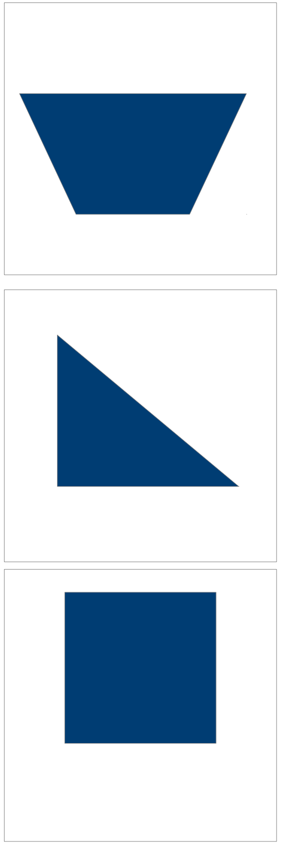
Feature Extraction

A Simple Example

A algorithm that can classify three different shape in an image:

- How to vectorize the data samples?

Naive solution: dump (raw) pixel data row by row into vector.



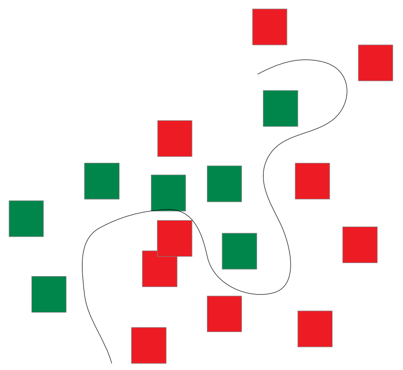
Feature Extraction

A Simple Example

A algorithm that can classify three different shape in an image:

- How to vectorize the data samples?

Example feature space



Naive solution: dump (raw) pixel data row by row into vector.

→ possible. BUT can become very difficult problem if we have high Variance in the data, e.g. shapes can **translate**, **scale** or even **rotate**.

→ results in the need for much data (to cover the variance) and the high dimensional space. Also needs complex models (danger to overfit).

Feature Extraction

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A Simple Example

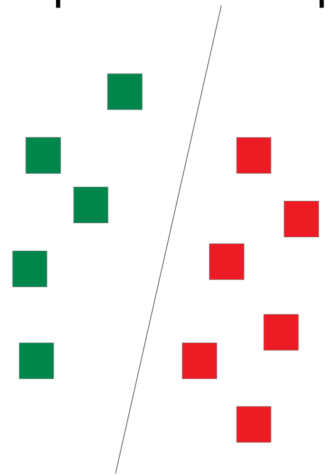
A algorithm that can classify three different shape in an image:

- How to vectorize the data samples?

Alternative: find Features T(X) that **encode separable properties** of the data.

- computed by some function T(X)
- Compact representation of X (low dimension)
- Robust against data variance (detailed definition coming up)
- **Allows much simpler model!**

Example feature space

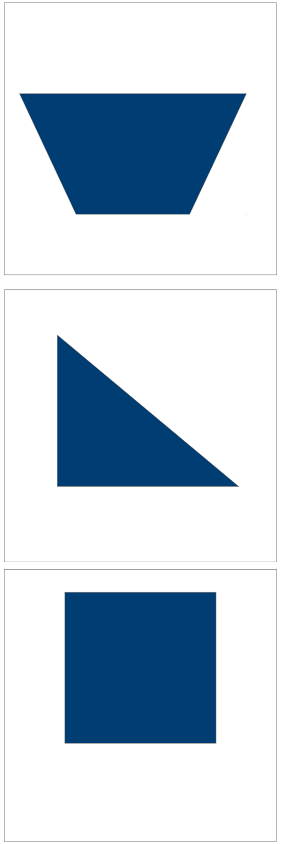


Feature Extraction

A Simple Example

Possible features for our problem?

- **Number of corners**
  → requires a corner detector (standard computer vision algorithm)
  → does not change under scaling, rotation and translation
  (but occlusion)
  → separates triangle from other two shapes

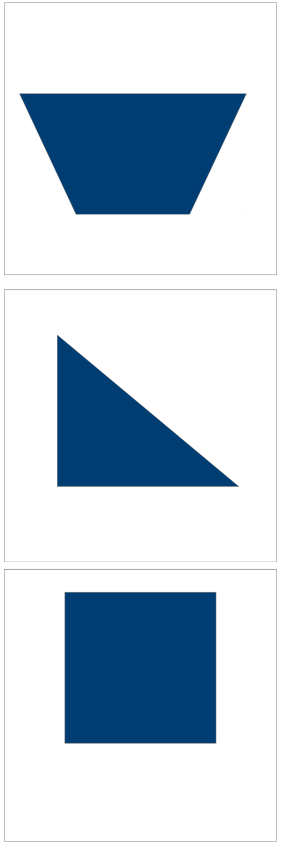


Feature Extraction

A Simple Example

Possible features for our problem?

- **Number of corners**
- **Area**

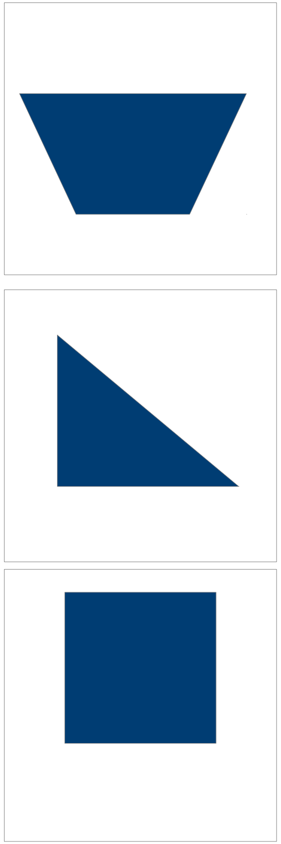


Feature Extraction

A Simple Example

Possible features for our problem?

- **Number of corners**
- **Area**
- **Area to circumference relation**
- **Max to min side length relation**
- **...**

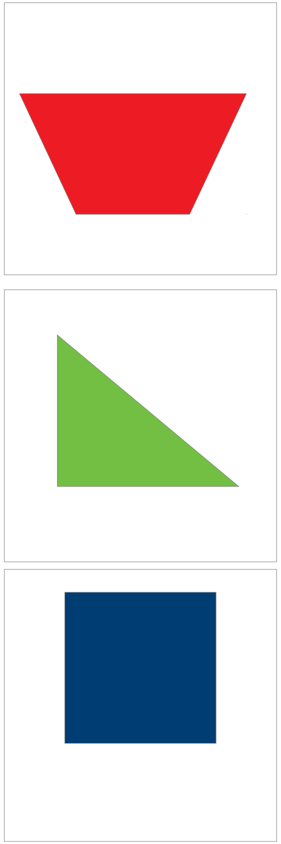


Feature Extraction

A Simple Example

Possible features for our problem?

- **Number of corners**
- **Area**
- **Area to circumference relation**
- **Max to min side length relation**
- **…**
- **Color !**



Invariant Theory

Example for invariant features – A classic inspection problem:

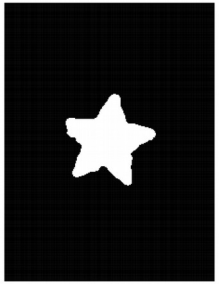
sample data

arbitrary rotations and translations

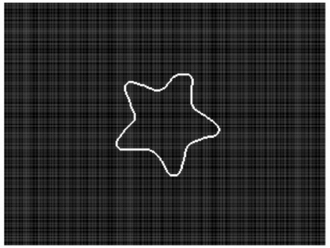
„Defect“

Invariant Theory

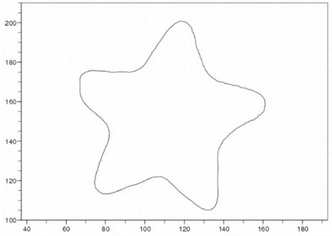
possible solution: invariant features



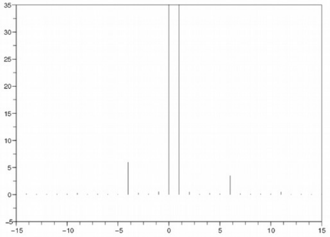
threshold



contour



polygon



Fourier spectrum

classify

Feature Extraction

Discussion:

Feature extraction vs learning algorithms

I. if we had perfect features, learning would be trivial

II. if we had perfect classifiers, we would not need features

Features are usually used to introduce prior knowledge about the Structure of the data and variances to the learning algorithm.

Feature Extraction

Discussion:

In practice:

- Good features are hard to find
- Often based on complex mathematical functions
- Depend on the application (domain knowledge needed!)

Generic Approaches:

- **Invariance by differentiation**: set properties into relation / normalization
- **Invaraince by integration**: compute average properties

Feature Reduction

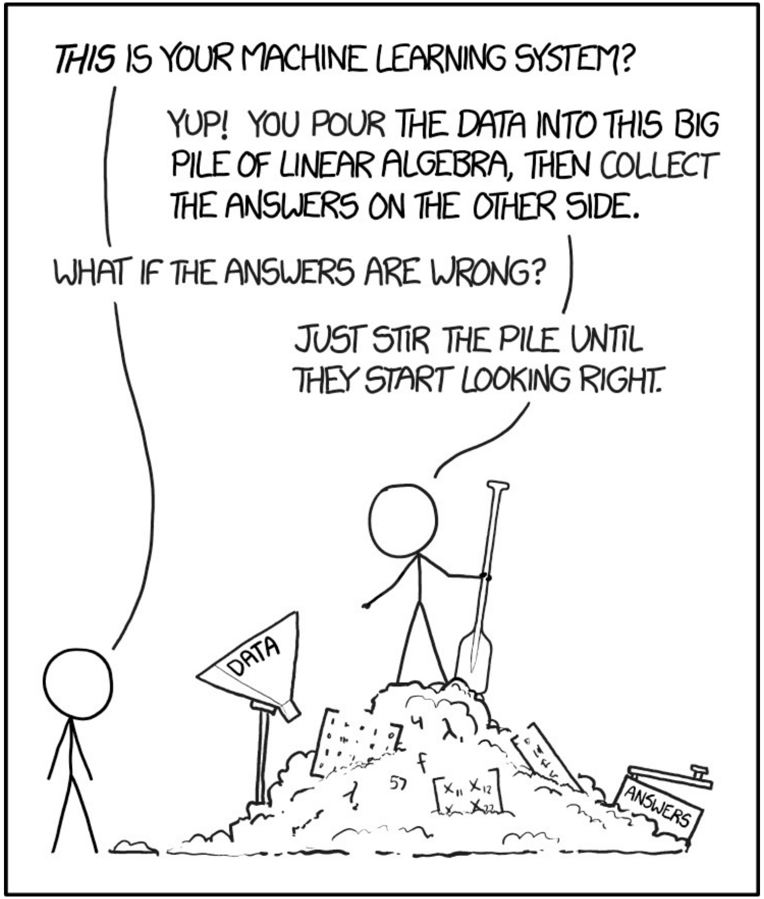
Motivation

- Very high dimensional representations require a lot of data to fill this huge space (curse of dimensionality)

- Danger of overfitting is higher if space is only sparsely sampled

  → **We would like to "compress" our data (with steerable loss) to a lower dimensional representation**

Discussion



https://xkcd.com/1838/