ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

inf | Informatik
Computer Science

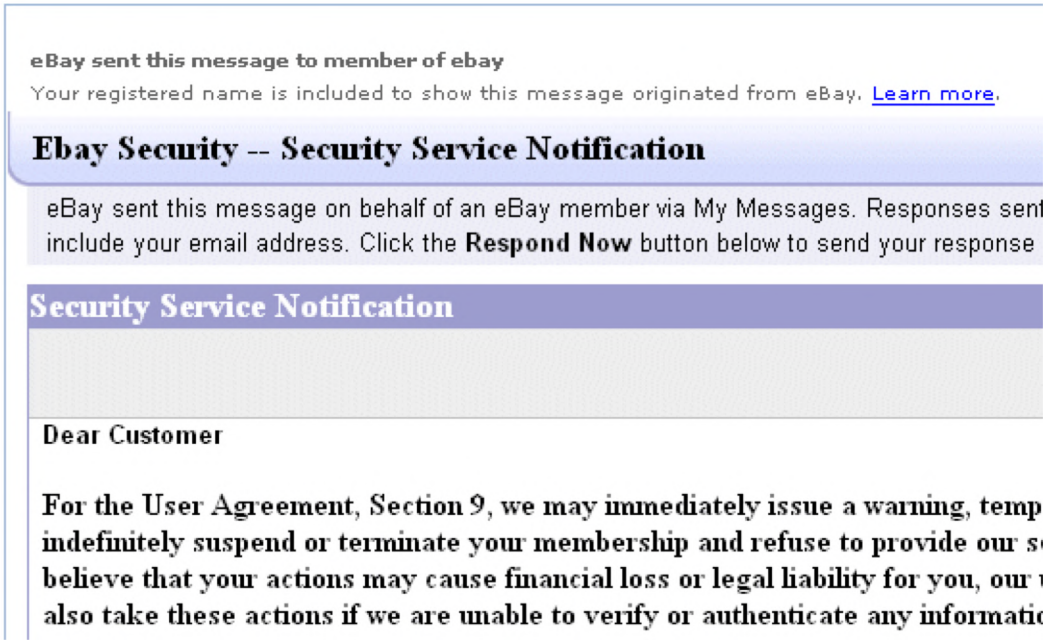
Introduction to Machine Learning

Introduction

Prof. Andreas Krause
Institute for Machine Learning
(las.ethz.ch)

What is Machine Learning I: An example

Classify email messages as “Spam” or “Non Spam”


eBay sent this message to member of ebay

Your registered name is included to show this message originated from eBay. Learn more.

Ebay Security -- Security Service Notification

eBay sent this message on behalf of an eBay member via My Messages. Responses sent
include your email address. Click the **Respond Now** button below to send your response

Security Service Notification

Dear Customer

For the User Agreement, Section 9, we may immediately issue a warning, temp
indefinitely suspend or terminate your membership and refuse to provide our s
believe that your actions may cause financial loss or legal liability for you, our
also take these actions if we are unable to verify or authenticate any informatic

Classical Approach: manual rules

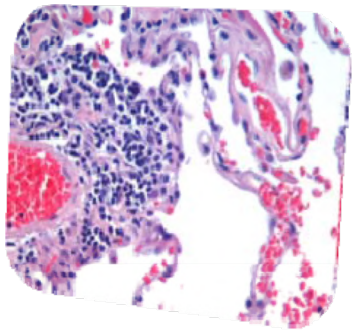
IF text body contains “Please login here”
THEN classify as “spam” ELSE “non-spam”

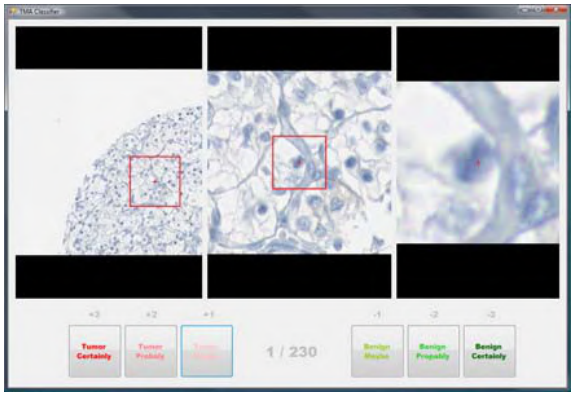
Machine Learning: Automatic identification of rules from training data (examples)

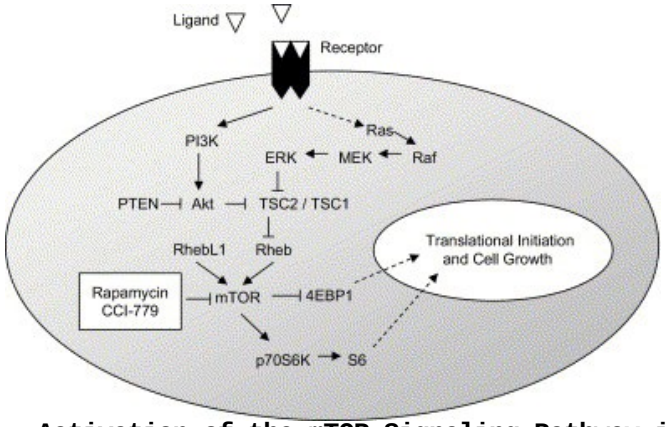
What is ML II: One Definition [Tom Mitchell]

„A computer program is said to learn from **experience E** with respect to some class of **tasks T** and **performance measure P**, if its performance at tasks in T, as measured by P, improves with experience E“

Our Digital Society and the Information Technology value chain







Activation of the mTOR Signaling Pathway in Renal Clear Cell Carcinoma. Robb et al., J Urology 177:346 (2007)

Data → **Information** → **Knowledge** → **Value**

happy (alive) patients

Machine Learning plays a core role in this value chain

Related disciplines

information
theory

philosophy
epistemiology
causality

statistics

machine learning

algorithms
& optimization

neuro-
informatics

Overview

- Introductory course
- Preparation for M.Sc. Level ML courses
- Two main topics
  - Supervised learning
  - Unsupervised learning
- Algorithms, models & applications
- Handouts etc. on course webpage
  - https://las.inf.ethz.ch/teaching/introml-s19
  - Old slides available at …/introml-s18
  - Password can be retrieved from within ETH network
- Textbooks listed on course webpage (some available online)

Prerequisites

- Basic knowledge in linear algebra, calculus and probability
- If you need a refresher:
  - Part I of ”Mathematics for Machine Learning” by Deisenroth, Faisal, Ong
  - Available online at https://mml-book.github.io
- If you plan not to complete the course, please deregister!

Syllabus

- Linear regression
- Linear classification
- Kernels and the kernel trick
- Neural networks & Deep Learning
- Unsupervised learning
- The statistical perspective
- Statistical decision theory
- Discriminative vs. generative modeling
- Bayes' classifiers
- Bayesian approaches to unsupervised learning

After participating in this course you will

- Understand basic machine learning ideas & concepts
- Be able to apply basic machine learning algorithms
- Know how to validate the output of a learning method
- Have some experience using machine learning on real data
- Learn what role machine learning plays in decision making under uncertainty

Relation to other ML Courses @ ETHZ

- Advanced Machine Learning (Fall)
  - Continuation and advanced topics
- Deep Learning (Fall)
  - Deep neural networks and their applications
- Probabilistic Foundations of AI (Fall)
  - Reasoning and decision making under uncertainty
- Computational Intelligence Lab (Spring)
  - Matrix Factorization, Recommender Systems, projects
- Statistical Learning Theory (Spring)
  - Theoretical foundations; model validation
- Computational Statistics (D-MATH, Spring)

Overview

- *Instructor*:
  Andreas Krause (krausea@ethz.ch)

- *Teaching assistants*:
  Head TA: Mojmir Mutny (mojmir.mutny@inf.ethz.ch)

  Andisheh Amrollahi, Mohammad Karimi, Prashanth Chandran, Joanna Ficek, Vincent Fortuin,Gürel Nezihe Merve, Harun Mustafa, Jingwei Tang, Kjong Lehmann, Natalie Davidson, Olga Mineeva, Laurie Prelot, Stefan Stark, Johannes Kirschner, Sebastian Curi, Max Paulus, Phillipe Wenk, Aytunc Sahin, Kfir Levy, Anastasiia Makarova, Maysam Haghdan

Exercises

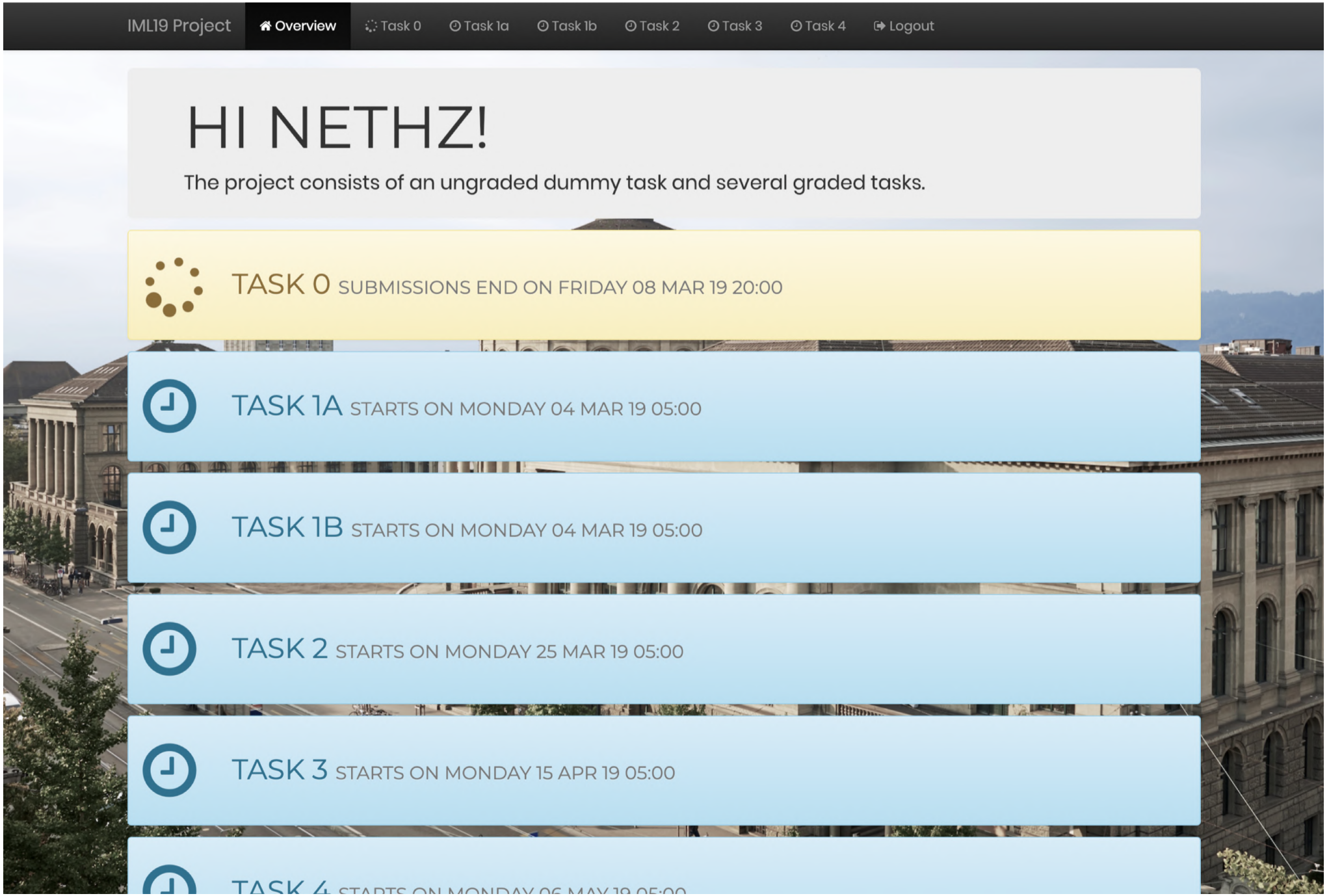
- Take them seriously if you want to pass the exam...
- Four sessions (attend according to initial of last name)
  - Mon 15-17 HG D 1.2 Last Names **A-C**
  - Tue 15-17 HG D 1.2 Last Names **D-H**
  - Wed 15-17 CAB G 11 Last Names **I-M**
  - Fri 13-15 ML D 28 Last Names **N-Z**
- This week: Optional refresher on basic linear algebra, calculus and probability

Course Project

- In a course project, you will apply basic learning methods to make predictions on real data
- Submit predictions on test data
- To do now:
  - Team up in groups of (up to) three students
  - Will send instructions on how to register by end of week
- More details to follow in the tutorials

- Contributes to 30% of final grade
- Project must be passed on its own and has a bonus/penalty function

Project server: https://project.las.ethz.ch



Some FAQs

- Distance exams
  - are possible (as exception), but need to officially request with study administration
- Doctoral students who need a “Testat”
  - need to receive a passing grade (4.0 or higher)
- Repeating the exam
  - requires repeating the project

- Will maintain an FAQ list on webpage

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Introduction to Machine Learning

A brief tour of supervised and unsupervised learning

Prof. Andreas Krause
Learning and Adaptive Systems (las.ethz.ch)

Machine Learning Tasks

Supervised Learning

- Classification
- Regression
- Structured Prediction, …

Unsupervised Learning

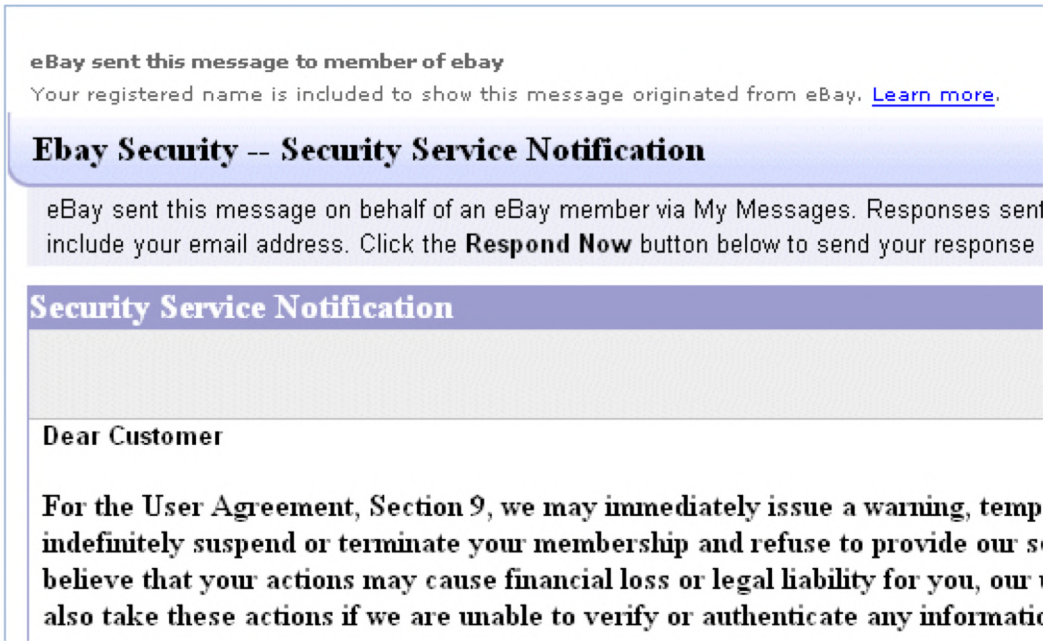
- Clustering
- Dimension reduction
- Anomaly detection, …

Many other specialized tasks

Supervised Learning

$$f : X \rightarrow Y$$

Example: E-Mail Classification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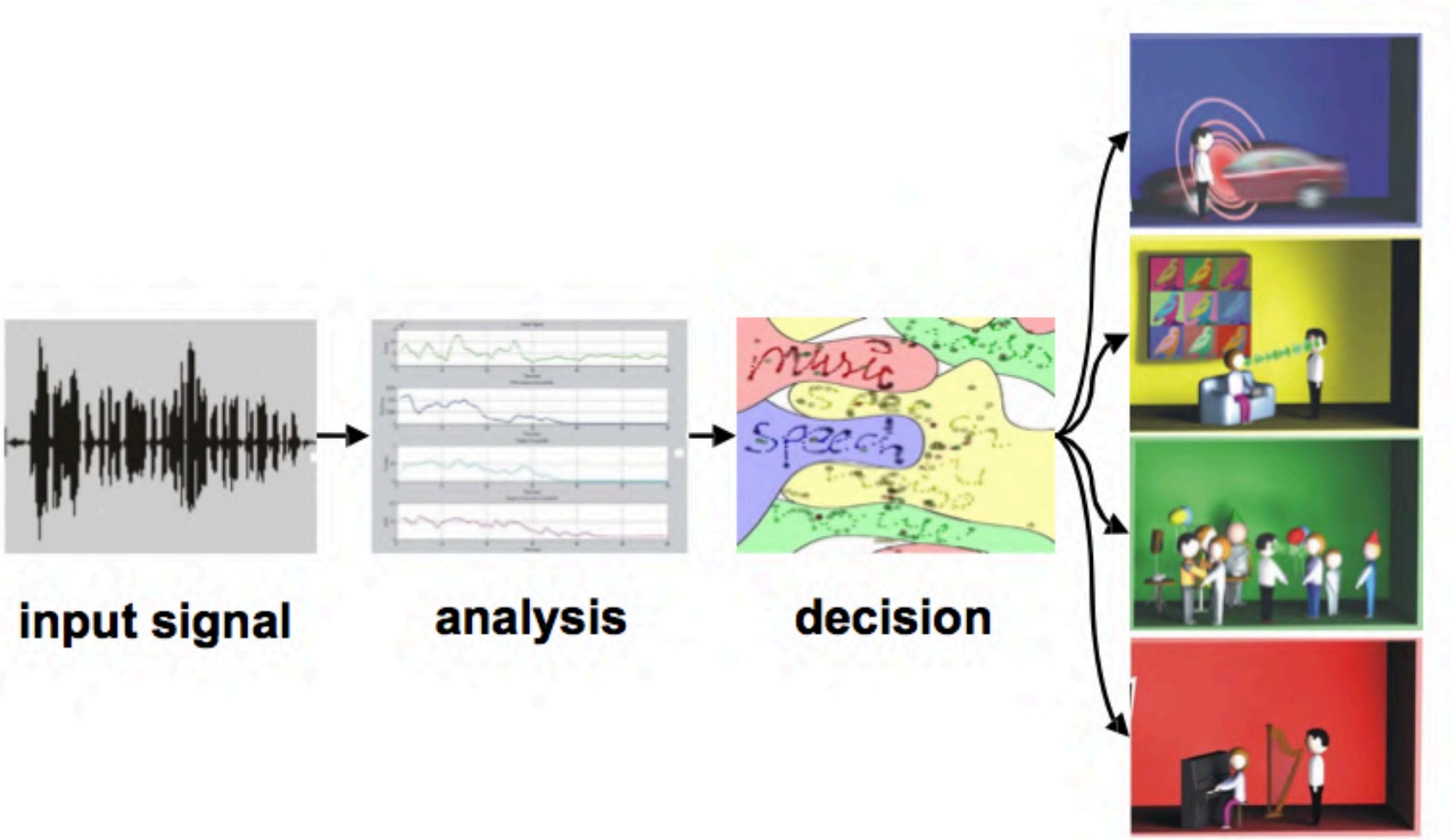
- **X:** E-Mail Messages
- **Y:** label: "*spam*" or "*non-spam*"

Example: Improving Hearing Aids

[Buhmann et al]

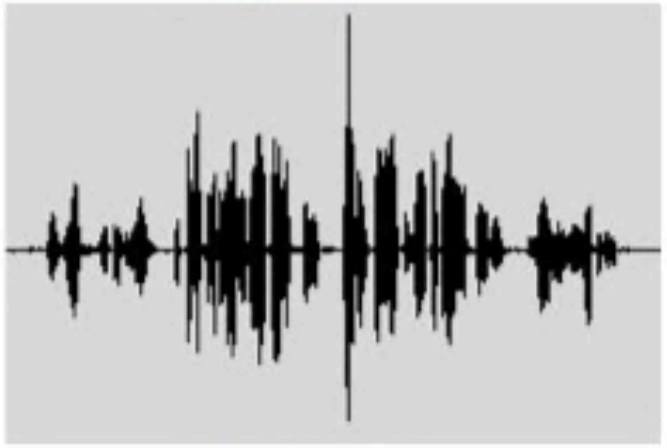


- **X**: Acoustic waveforms
- **Y**: label *speech, speech in noise, music, noise*

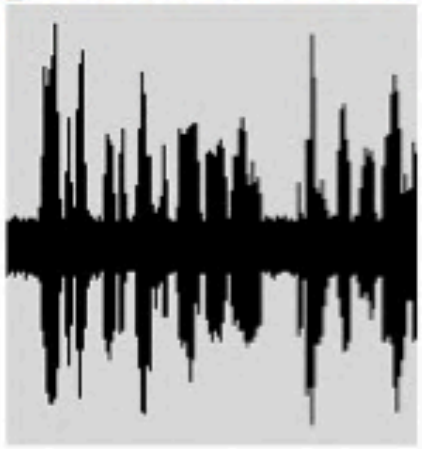
Example: Improving Hearing Aids

Music

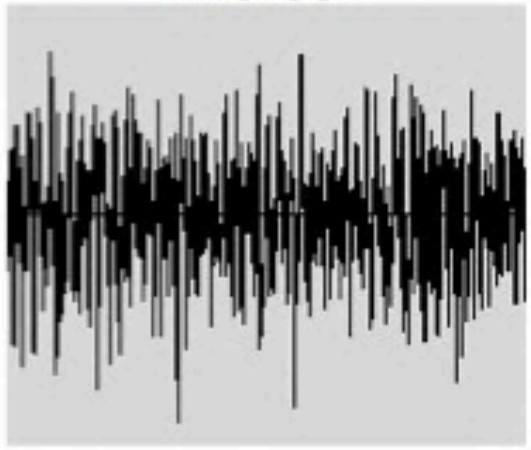
Speech



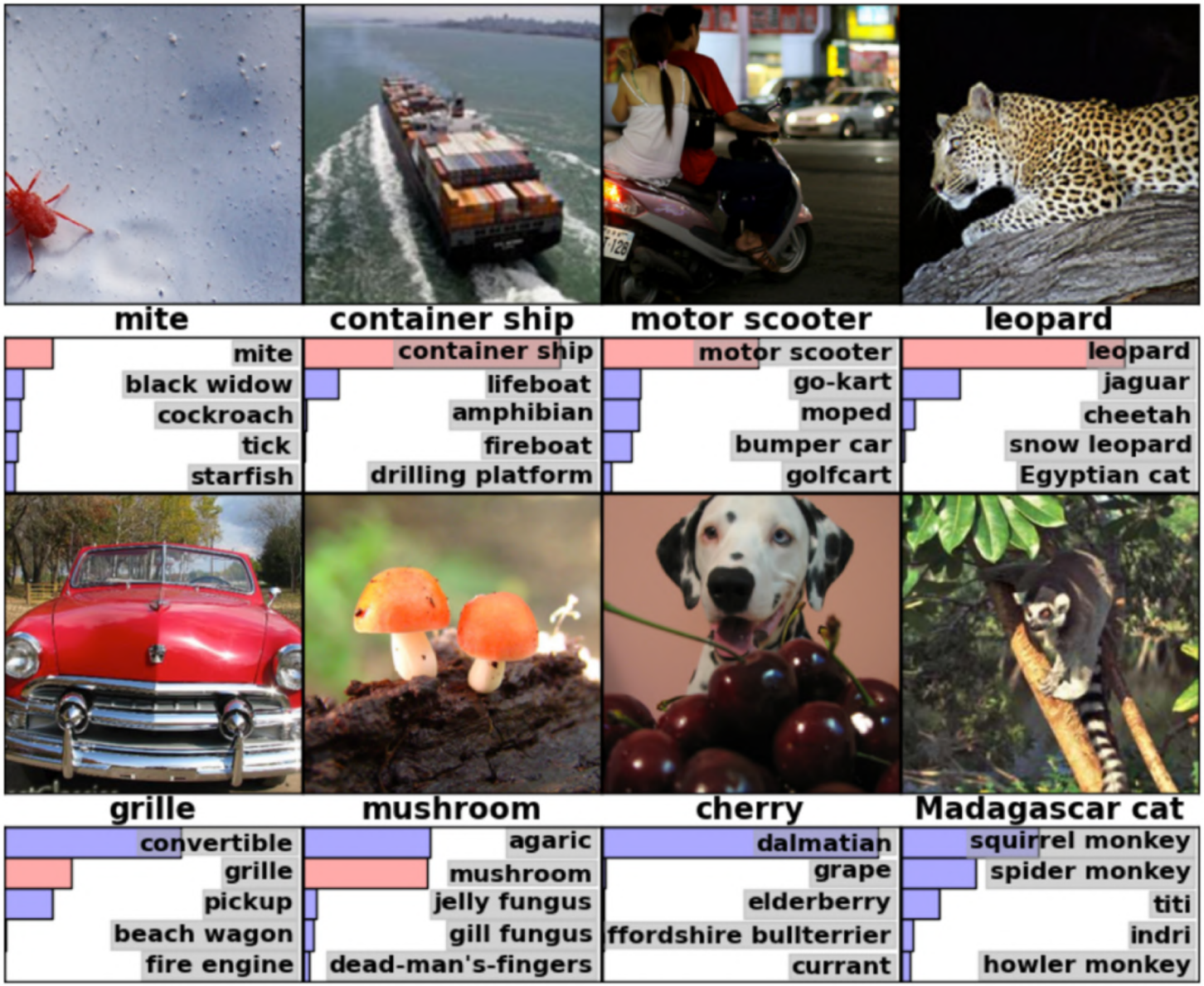
Speech in noise



Noise



Example: Image Classification



Krizhevsky et al. ImageNet Classification with Deep Convolutional Neural Networks '12

Regression

- **Goal**: Predict real valued labels (possibly vectors)
- Examples:

X	Y
Flight route	Delay (minutes)
Real estate objects	Price
Patient & drug	Treatment effectiveness
….	…

Example: Recommender systems

- **X**: User & article / product features
- **Y**: Ranking of articles / products to display

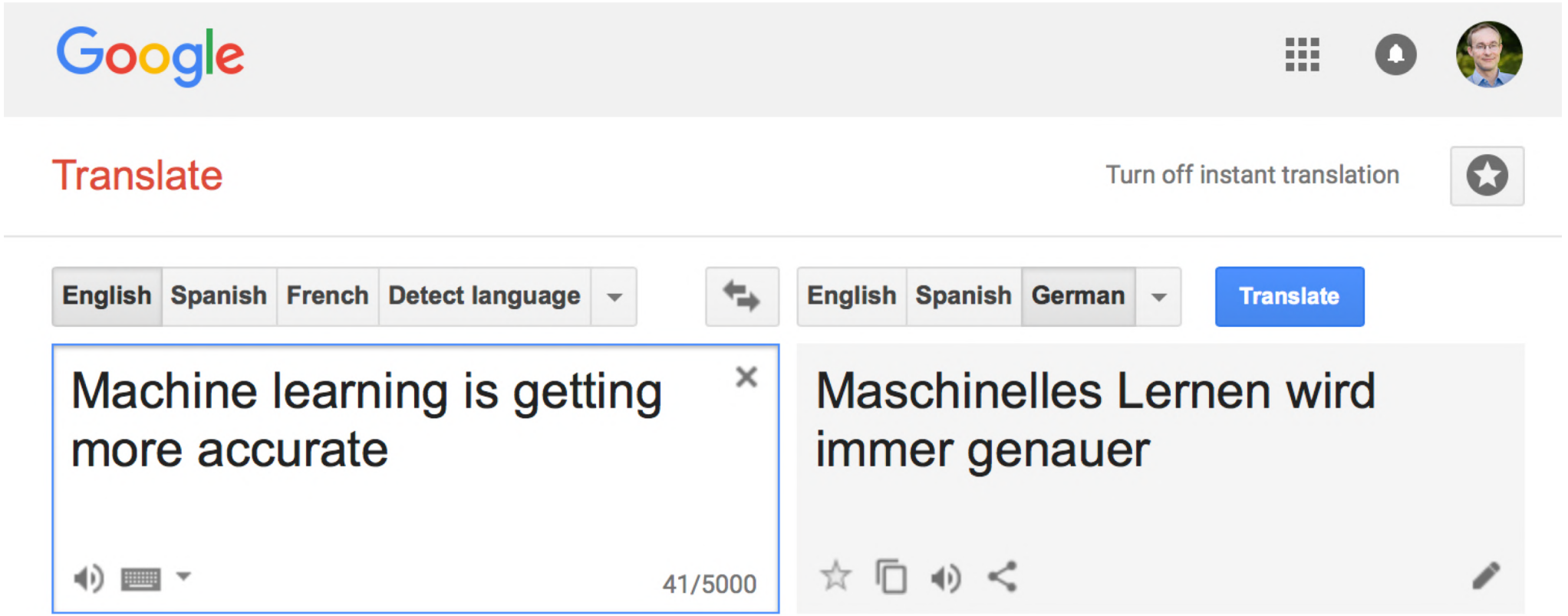
Example: Image captioning

Y

X

Vinyals et al. *Show and Tell: A Neural Image Caption Generator* '14

Example: Translation

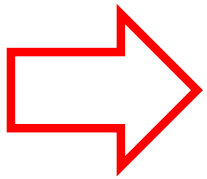


X **Y**

Example: Predicting program properties

[Raychev, Vechev, Krause POPL '15]

```
function chunkData(e, t) {
  var n = [];
  var r = e.length;
  var i = 0;
  for (; i < r; i += t) {
    if (i + t < r) {
      n.push(e.substring(i, i + t));
    } else {
      n.push(e.substring(i, r));
    }
  }
  return n;
}
```



```
/* str: string, step: number, return: Array */
function chunkData(str, step) {
  var colNames = []; /* colNames: Array */
  var len = str.length;
  var i = 0; /* i: number */
  for (; i < len; i += step) {
    if (i + step < len) {
      colNames.push(str.substring(i, i + step))
    } else {
      colNames.push(str.substring(i, len));
    }
  }
  return colNames;
}
```

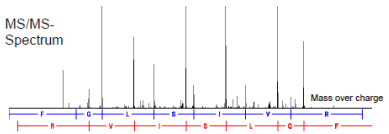
X **Y**

jsnice.org

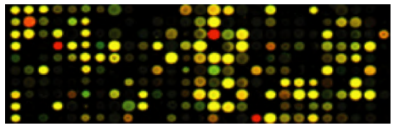
Example: Computational Pathology

[Buhmann, Fuchs et al.]

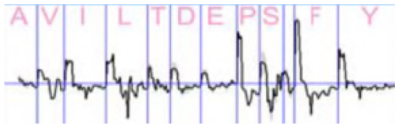
Proteomics

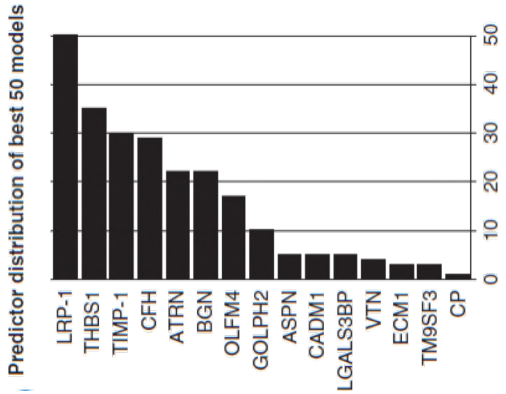


Transcriptomics

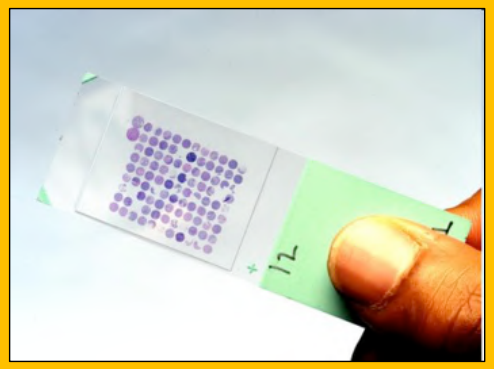


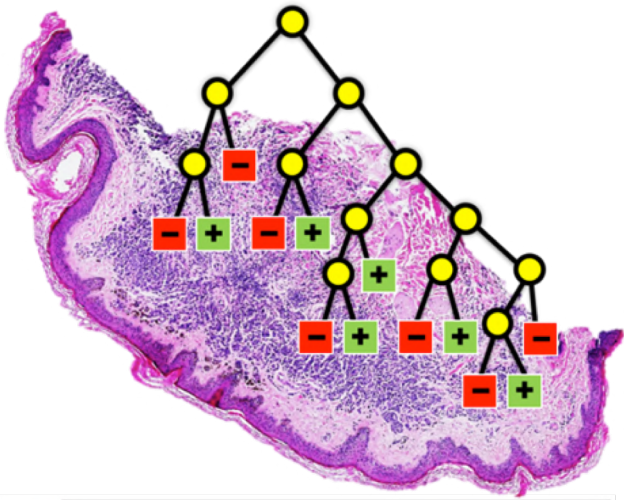
Metabolomics

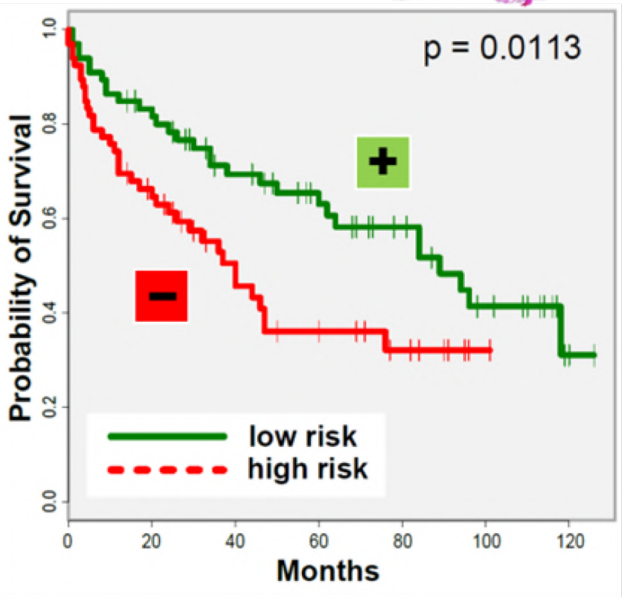




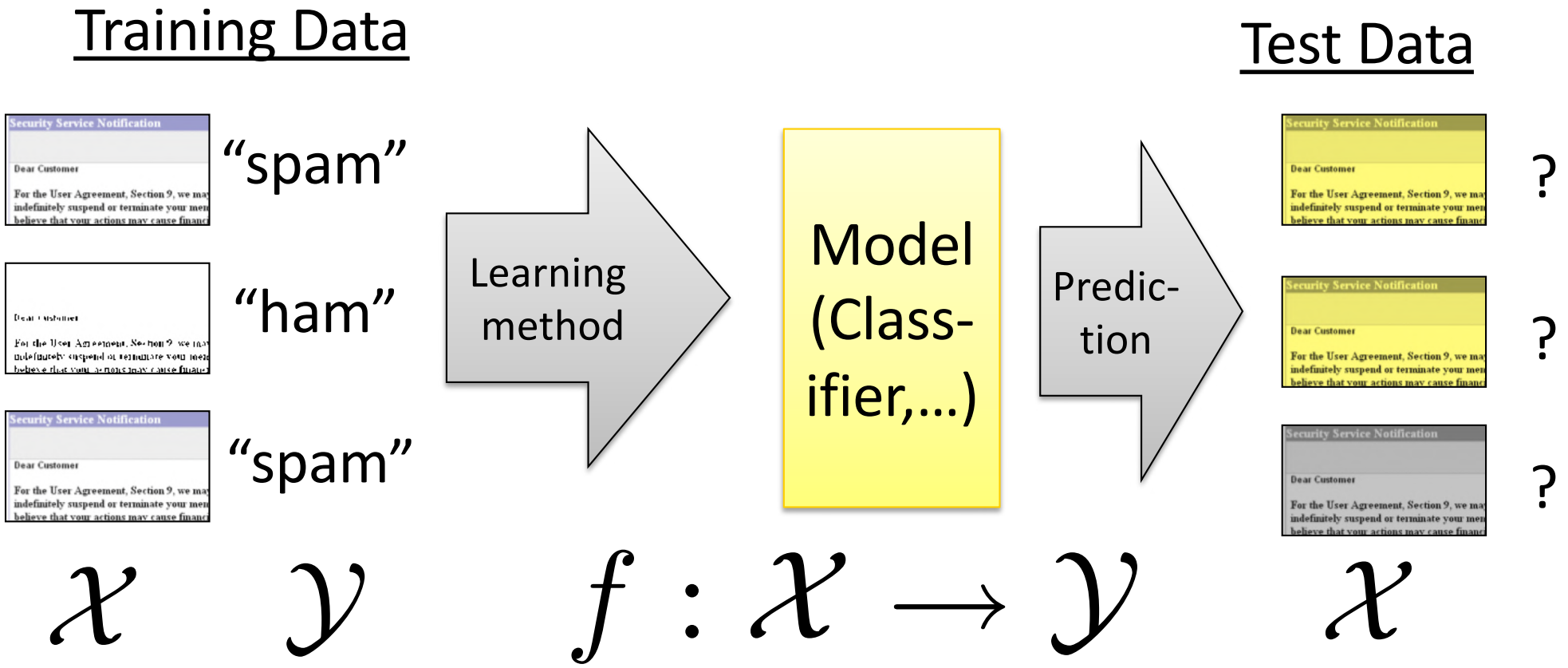
Human Tissue
TMA







Basic Supervised Learning Pipeline



Representing Data

- Learning methods expect standardized representation of data (e.g., Points in vector spaces, nodes in a graph, similarity matrices ...)

The quick brown fox jumps over the lazy dog …

[0 1 0 0 0 3 2 0 1 0 0 0]

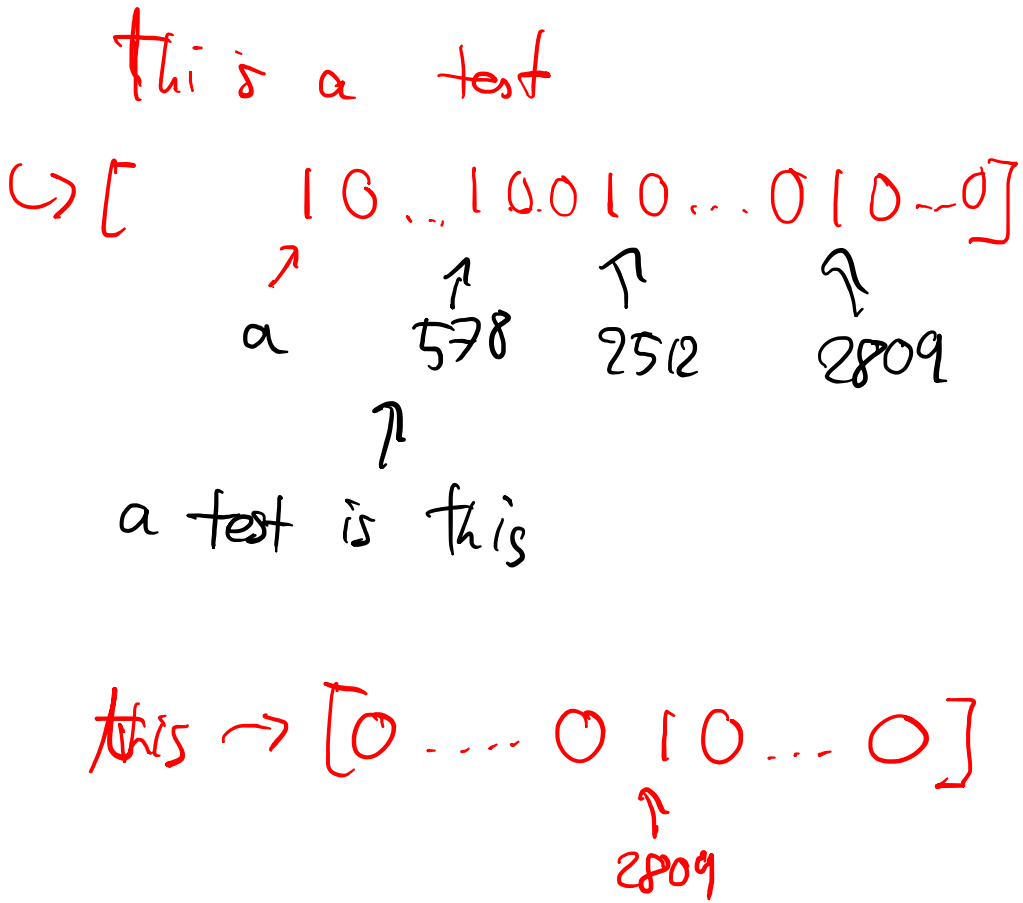
[.3 .01 .1 2.3 0 0 1.1 …]

- Concrete choice of representation („features“) is crucial for successful learning
- This class (typically): feature vectors in $\mathbb{R}^d$

Example: Bag-of-words

- Suppose language contains at most *d=100000* words
- Represent each document as a vector ***x*** in $\mathbb{R}^d$
  - *i*-th component x_i counts occurrence of *i*-th word

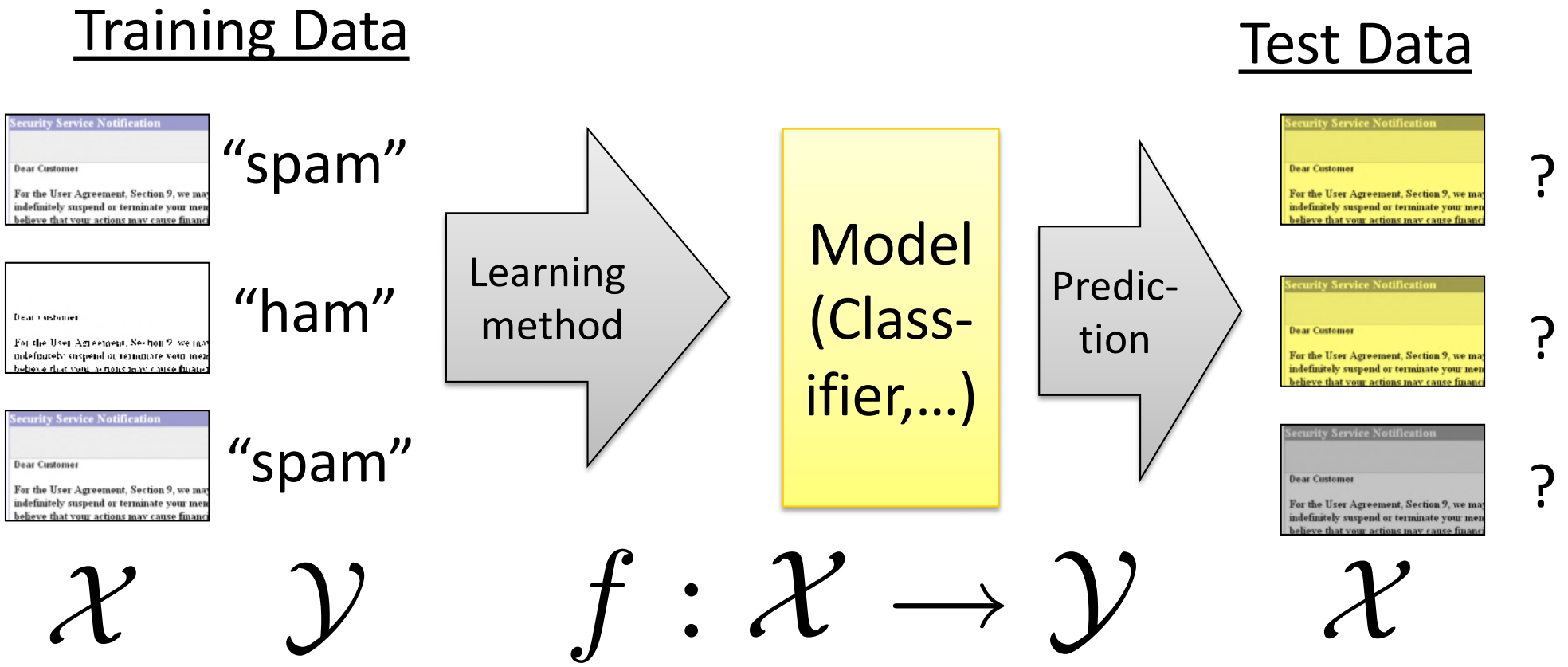
Word	Index
a	1
abandon	2
ability	3
…	
is	578
…	
test	2512
…	
this	2809
….	



Bag-of-words: Improvements

- Length of the document should not matter
  - Replace counts by binary indicator (yes/no)
  - Normalize to unit length
- Some words more „important“ than others
  - Remove „stopwords“ (the, a, is, ...)
  - Stemming (learning, learner, learns -> learn)
  - Discount frequent words (tf-idf)
- Bag-of-words ignores order
  - Consider pairs (n-grams) of consecutive words
- Does not differentiate between similar and dissimilar words (ignores semantics)
  - Word embeddings (e.g., word2vec, GloVe)

Basic Supervised Learning Pipeline

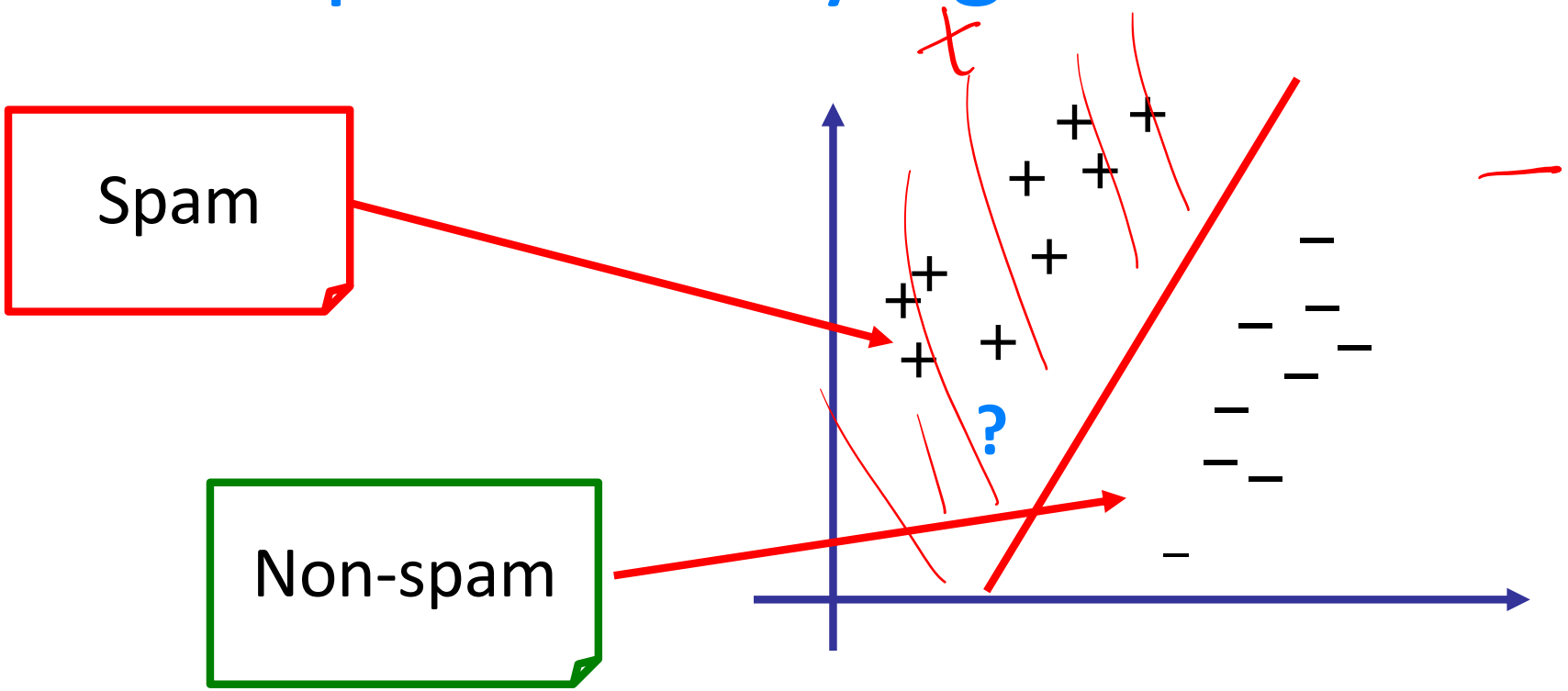


Representation

Model fitting

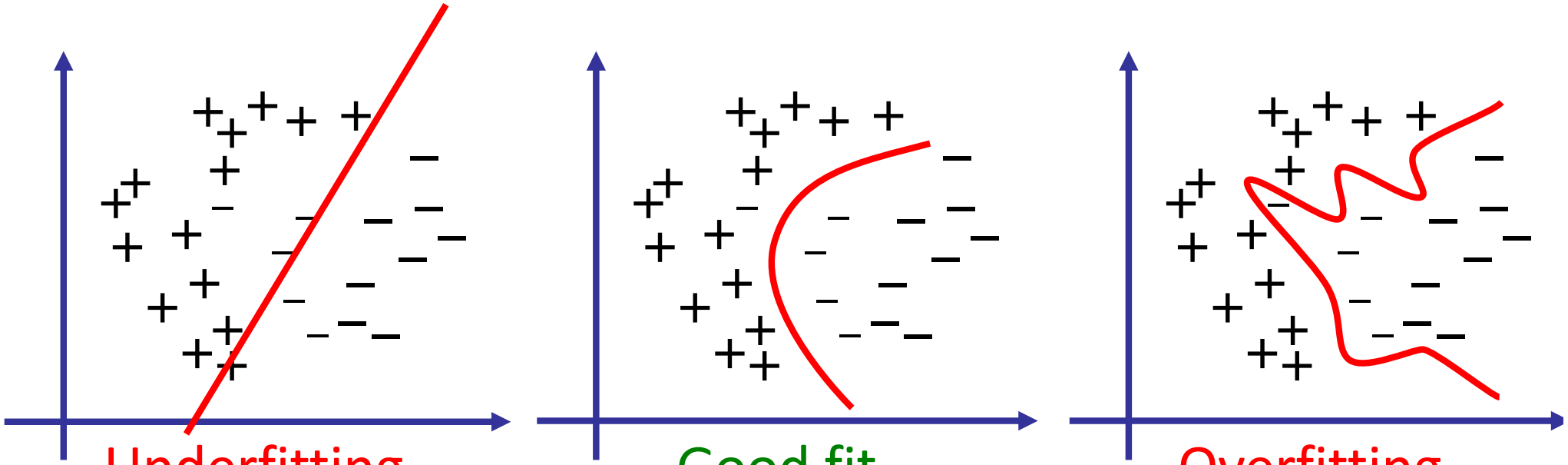
Prediction and Generalization

Example: Classifying Documents



- **Input**: Training examples (e.g., "bag-of-words") with positive (+) and negative (-) labels
- **Goal**: Decision rule (aka hypothesis, e.g., linear, decision tree, random forests, graphical models, deep neural networks…)

Model selection and validation



Underfitting
(too simple)

Good fit

Overfitting
(too complex)

- Automatic model-selection and validation of crucial importance (➔ statistical learning theory)
- **Goal**: Balance of "Goodness of Fit" and complexity
- Ideal models are simultaneously statistically and computationally efficient

Machine Learning Tasks

Supervised Learning

- Classification
- Regression
- Structured Prediction, …

Unsupervised Learning

- Clustering
- Dimension reduction
- Anomaly detection, …

Many other specialized tasks

Basic Unsupervised Learning Pipeline

Training Data

Learning method

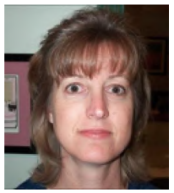
Model

Predic-tion

Test Data

?

?



?

x ~~y~~ $f : \mathcal{X} \rightarrow \mathcal{Y}$

Representation Model fitting Prediction

Unsupervised learning

- „Learning without labels“
- Examples:
  - Clustering (e.g., unsupervised classification)
  - Dimension reduction (e.g., unsupervised regression)
  - Generative modeling (topic models, autoencoders, GANs etc.)
- Common goals:
  - Compact representation / compression of data sets
  - Identification of latent variables
- Use-cases:
  - Exploratory data analysis
  - Feature learning / embedding
  - Anomaly detection of„unusual“ data points

Example: Clustering

- **Input**: Data set without labels
- **Goal**: Assignment to clusters (infer labels)

Example: Dimension Reduction

[Saul & Roweis]

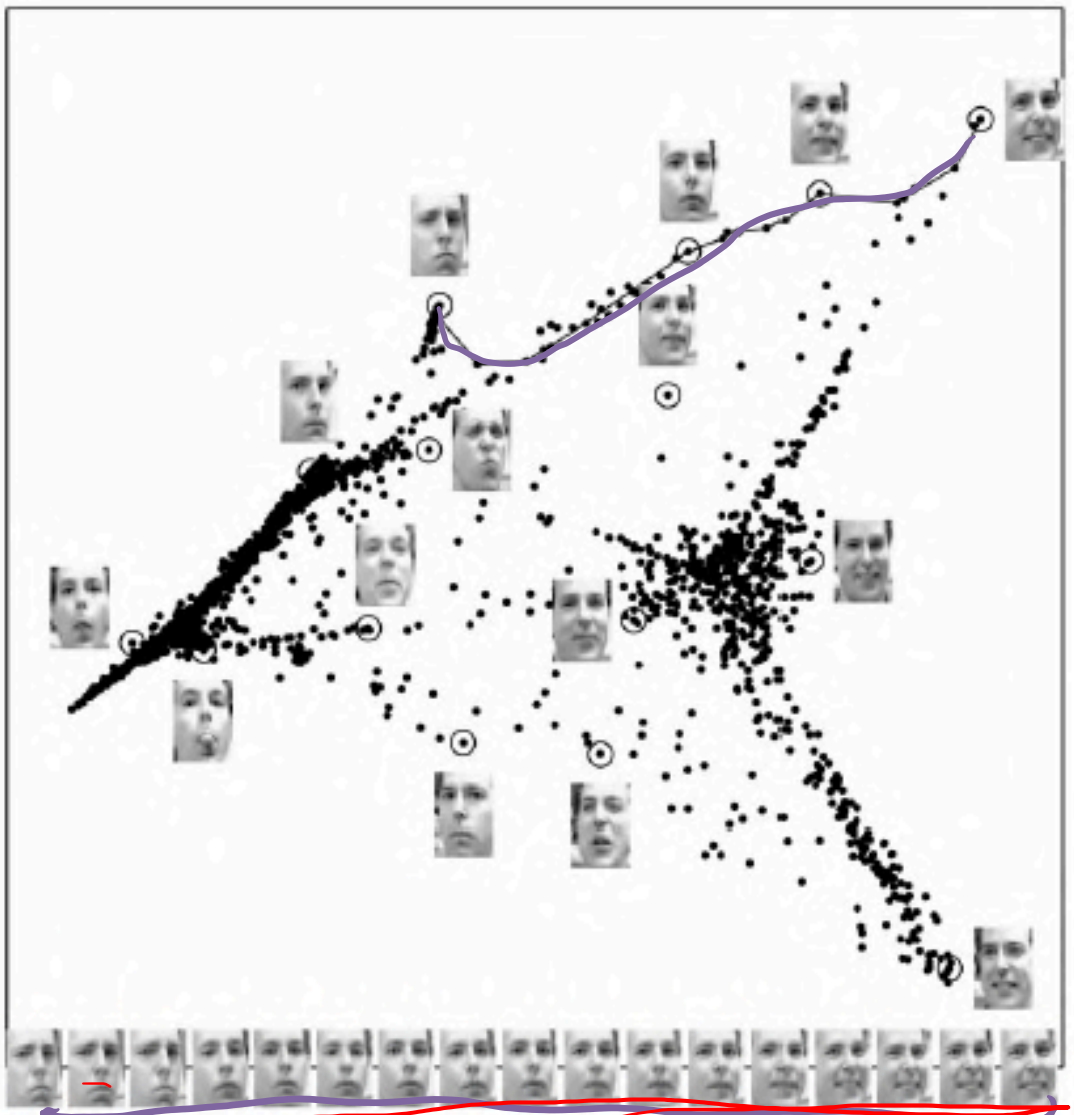
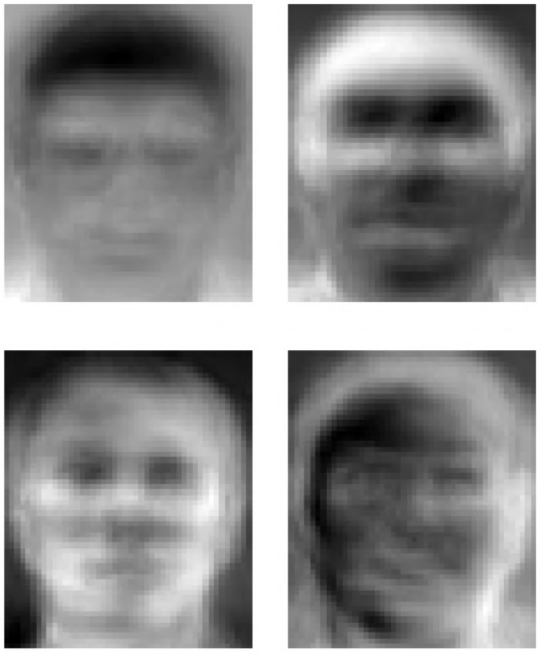


Fig. 3. Images of faces (*11*) mapped into the embedding space described by the first two coordinates of LLE. Representative faces are shown next to circled points in different parts of the space. The bottom images correspond to points along the top-right path (linked by solid line), illustrating one particular mode of variability in pose and expression.

Example: Dimension reduction

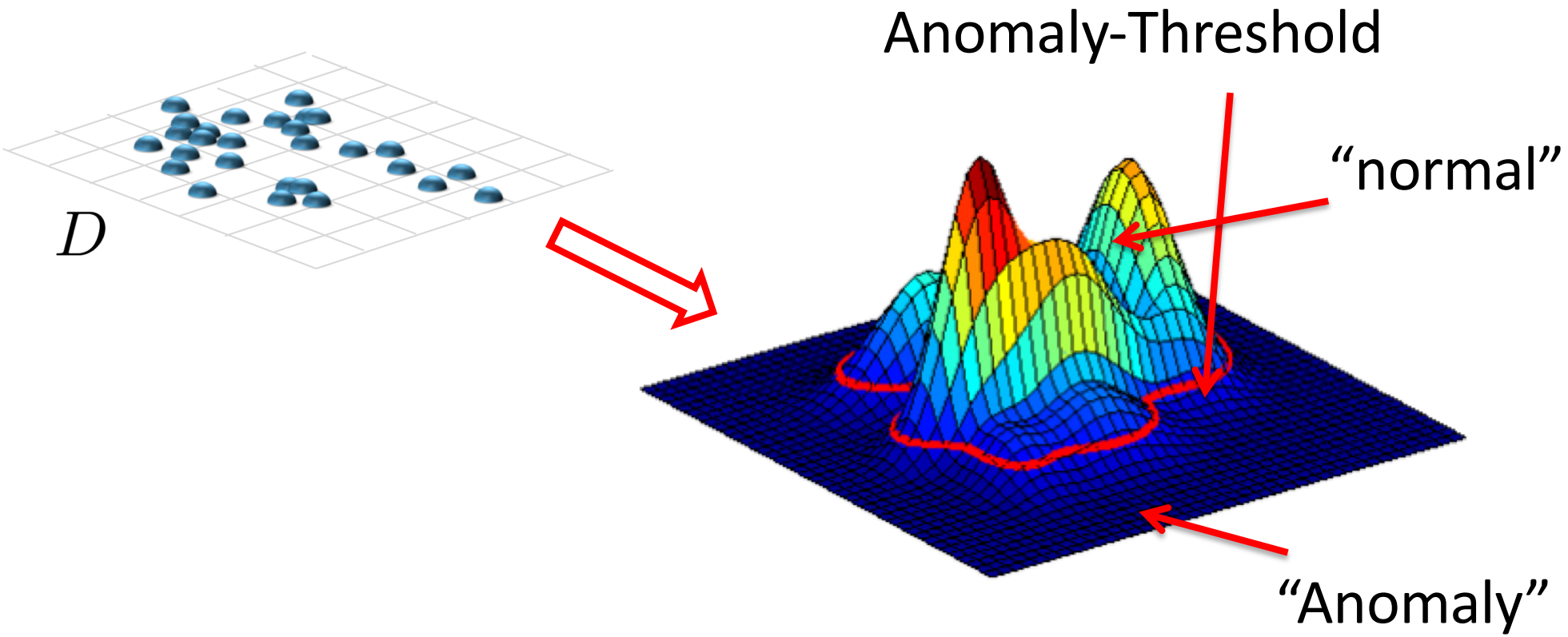
- Often, high-dimensional data can be well approximated in low dimensions
- Very useful for visualization!



Eigenfaces
[AT&T Labs Cambridge]

- Many methods available, e.g.,
  - *Linear* (Principal Component Analysis, Linear Discriminant Analysis, ...)
  - *Non-linear* (ISOMAP, Kernel-PCA, Max. variance unfolding, t-SNE, autoencoders based on neural networks, ...)
  - *Sparse modeling / inference*

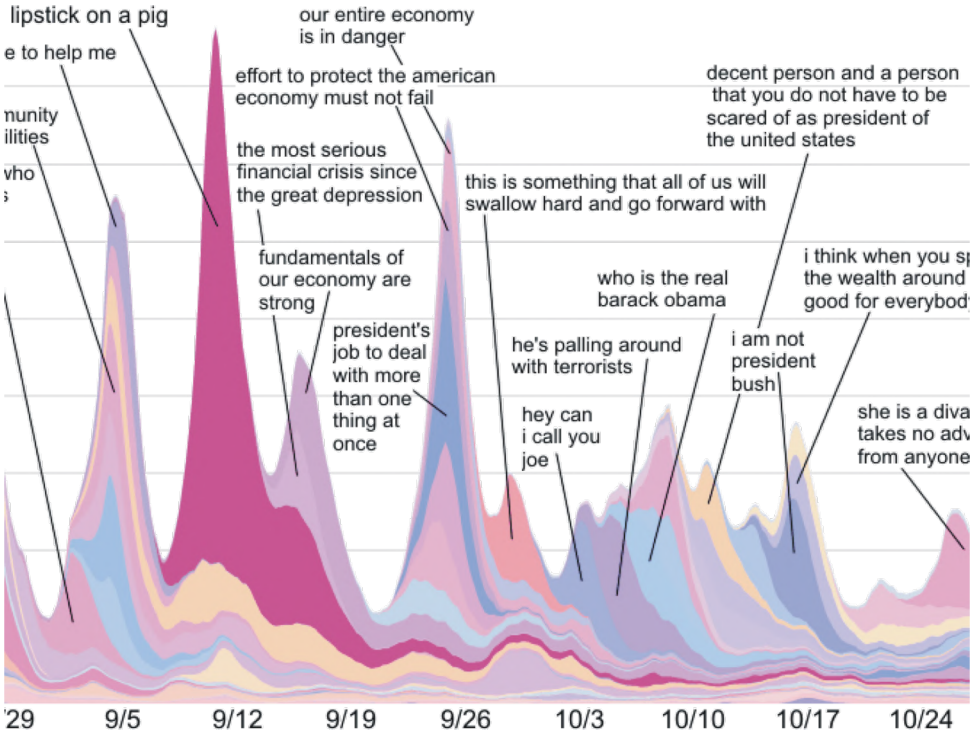
Example: Anomaly detection

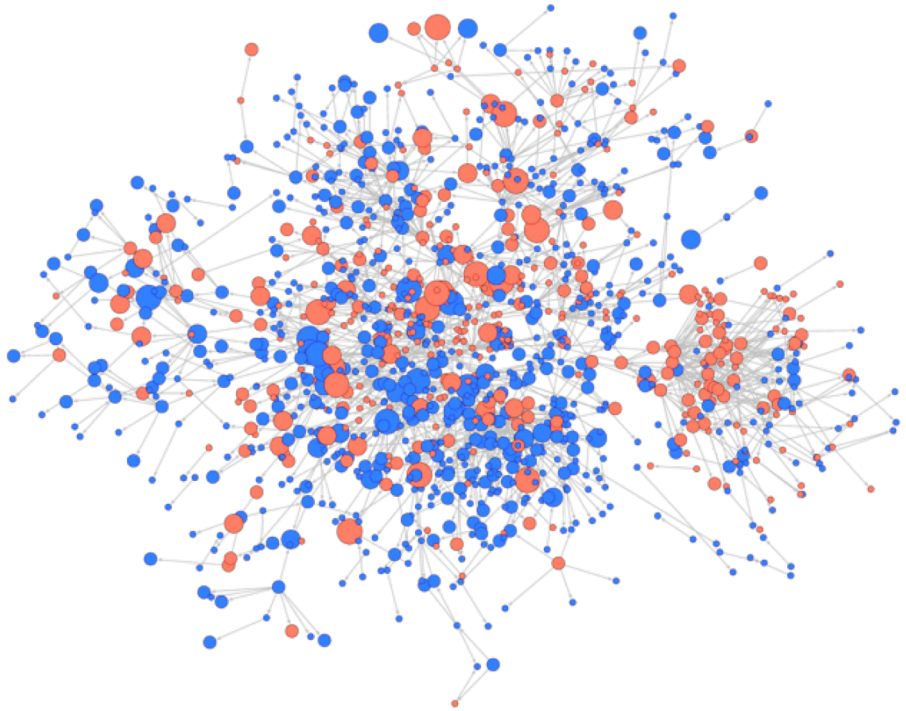


- **Application**: Quality control, fraud detection, …
- Fit statistical model of "normal" data
- Declare "unusual" (low prob.) data as anomaly

Example: Network inference

[Gomez Rodriguez, Leskovec, Krause ACM TKDE 2012]





- Estimate flow of information and influence in the „blogosphere“ (ecosystem of blogs and social media)

Example: Never Ending Language Learning

[Mitchell et al.]

(Mostly) unsupervised acquisition of facts by „reading“ the internet

Recently-Learned Facts twitter Refresh

instance	iteration	date learned	confidence
gold_coast_casino is a visualizable attribute	896	24-jan-2015	94.4
stranger_software is a tool	896	24-jan-2015	99.1
regent_beach_resort is a trail	896	24-jan-2015	100.0
squitieri_studio_theatre is a stadium or event venue	896	24-jan-2015	100.0
fish_river_seaplane_base is an airport	896	24-jan-2015	100.0
john_lucas plays the athletic team position player	901	14-feb-2015	93.8
european_architects is a generalization of walter_gropius	901	14-feb-2015	100.0
young is a person who moved to the state california	901	14-feb-2015	100.0
justine_henin is an athlete who beat svetlana_kuznetsova	901	14-feb-2015	100.0
public_administration is an academic program at the university louisiana_state_university	899	05-feb-2015	96.9

[rtw.ml.cmu.edu]

Example: GANs

[Goodfellow et al'14, Salimans et al'16]

BigGAN

[Brock, Donahue, Simonyan 09/2018]

Machine Learning Tasks

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- Structured Prediction, …

Unsupervised Learning

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Other models of learning

- Semi-supervised learning
  - Learning from both labeled and unlabeled data
- Transfer learning
  - Learn on one domain and test on another
- Active learning
  - Acquiring most informative data for learning
- Online learning
  - Learning from examples as they arrive over time
- Reinforcement learning
  - Learning by interacting with an unknown environment
- ...

Summary so far

- Two basic forms of learning:
  - Supervised vs. Unsupervised learning
- Key challenge in ML
  - Trading goodness of fit and model complexity
- Representation of data is of key importance