MA2823: Foundations of Machine Learning

École Centrale Paris — Fall 2016

Chloé-Agathe Azencott

Centre for Computational Biology, Mines ParisTech chloe-agathe.azencott@mines-paristech.fr







• TAs:

- Benoît Playe benoit.playe@mines-paristech.fr
- Mihir Sahasrabudhe mihir.sahasrabudhe@centralesupelec.fr

Course material & contact

```
http://tinyurl.com/ma2823-2016
https://github.com/chagaz/ma2823_2016
chloe-agathe.azencott@mines-paristech.fr
```

Slides thanks to Ethem Alpaydi, Matthew Blaschko, Trevor Hastie, Rob Tibshirani and Jean-Philippe Vert.

What is (Machine) Learning?

Why Learn?

- Learning: Modifying a behavior based on experience. [F. Benureau]
- Machine learning: Programming computers to optimize a performance criterion using example data.
- There is no need to "learn" to calculate payroll.
- Learning is used when
 - Human expertise does not exist (bioinformatics);
 - Humans are unable to explain their expertise (speech recognition, computer vision);
 - Solutions change in time (routing computer networks);
 - Solutions need adapting to new cases (user biometrics).

Artificial Intelligence

Machine Learning is a subfield of **Artificial Intelligence:**

- A system that lives in a changing environment must have the ability to learn in order to adapt.
- ML algorithms are building blocks that make computers behave more intelligently by generalizing rather than merely storing and retrieving data (like a database system would do).

What we talk about when we talk about learning

- Learning general models from particular examples (data)
 - Data is (mostly) cheap and abundant;
 - Knowledge is expensive and scarce.
- Example in retail:

From customer transactions to consumer behavior

People who bought "Game of Thrones" also bought "Lord of the Rings" [amazon.com]

 Goal: Build a model that is a good and useful approximation to the data.

Data mining: Applying ML to (large) databases

- Retail: Market basket analysis, Customer relationship management (CRM).
- Finance: Credit scoring, fraud detection.
- Manufacturing: Control, optimization, troubleshooting.
- Medicine: Medical diagnosis.
- Telecommunications: Spam filters, intrusion detection, network optimization, routing.
- Science: Analyze large amounts of data in physics, astronomy, biology.
- Web: Search engines.

What is machine learning?

- Optimizing a performance criterion using example data or past experience.
- Role of Statistics:

Build mathematical models to make inference from a sample.

- Role of Computer Science: Efficient algorithms to
 - Solve the optimization problem;
 - Represent and evaluate the model for inference.

Classes of machine learning problems

- Association rule learning: Discover relations between variables
- Supervised learning: Predict outcome from features
 - Classification
 - Regression
 - Ranking
 - Ordered categories (e.g. scores)
- Unsupervised learning: Find patterns in the data
 - Dimensionality reduction
 - Clustering
- Semi-supervised learning: Predict outcome for unlabeled but known instances
- Reinforcement learning: Maximize cumulative reward

Learning associations

Market basket analysis:

```
X, Y: products/services
P ( Y | X ): probability that somebody who buys X also buys Y.
```

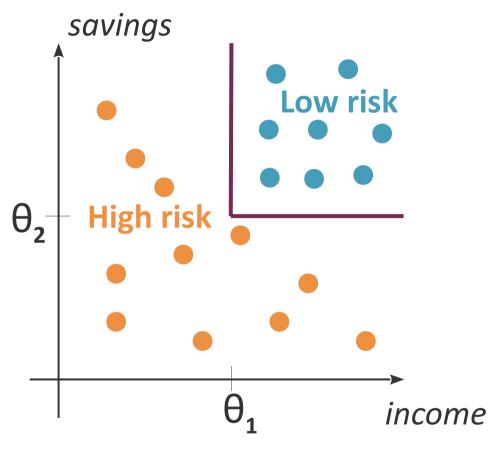
Example:

```
P (chips | beer) = 0.70
P (chips | beer, M, age < 30) = 0.85
```

Classification (or pattern recognition)

Example: Credit scoring

 Differentiate between low-risk and high-risk customers, from their income and savings



Discriminant: IF $income > \theta_1$ AND $savings > \theta_2$ THEN low-risk ELSE high-risk

Classification: Applications

- Face recognition: independently of pose, lighting, occlusion (glasses, beard), make-up, hair style.
- Character recognition: independently of different handwriting styles.
- Speech recognition: account for temporal dependency.
- Medical diagnosis: from symptoms to illnesses.
- Precision medicine: from clinical & genetic features to diagnosis, prognosis, response to treatment.
- Biometrics: recognition/authentication using physical or behavioral characteristics: Face, iris, signature...

Face recognition example

Training examples (one person)









Test images





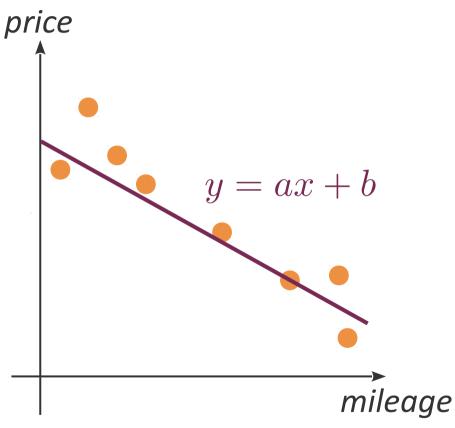




Regression

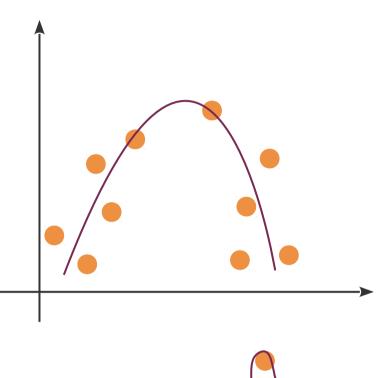
Example: Price of a used car

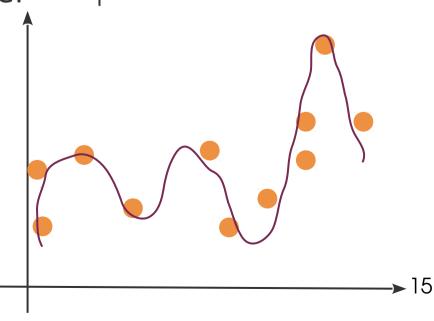
- x: milage
- y: price
- $y = f(x | \theta)$
 - f = model
 - $-\theta$ = parameters
 - $-\theta = (a, b)$



Regression: Applications

- Car navigation: angle of steering
- Kinematics of a robot arm
- Binding affinities between molecules
- Age of onset of a disease
- Solubility of a chemical in water
- Yield of a crop
- Direction of a forest fire





Ranking

- Find a function that orders a given list of items of X
- As a classification problem: pairwise approach
 - Is {x1, x2} correctly ordered?
- As a regression problem: pointwise approach
 - -f(x) such that $x_1 \prec x_2 \Leftrightarrow f(x_1) \prec f(x_2)$
- Listwise approach: directly optimize for the best list.

Ranking: applications

Chemoinformatics:

- virtual screening
- scoring 3D structures.

Recommander systems:

- rank movies according to how likely a user is to view them.
- rank items according to how likely a consumer is to buy them.

Information retrieval:

- document retrieval
- web search.

Uses of supervised learning

- Prediction of future cases:
 - Use the rule to predict the output for new inputs.
- Knowledge extraction:
 - Interpret the rule.
 - Assumes the rule is easy to understand.
- Compression:
 - The rule is simpler than the data it explains.
- Outlier detection:
 - Find exceptions that are not covered by the rule (they might be fraud, intrusion, errors).

Unsupervised learning

- No output
- Learn "what normally happens"

- Density estimation: Find the structure (regularities) in the data
- Clustering
- Dimensionality reduction.

Clustering

- Goal: Group objects into clusters, i.e. classes that were unknown beforehand.
- Objects in the same cluster are "more similar" to each other than to objects in a different cluster.
- Motivation:
 - Understanding general characteristics of the data;
 - Visualization;
 - Infering some properties of an object based on how it relates to other objects.

Clustering: applications

- Customer relationship management: Customer segmentation
- Image compression: Color quantization
- Document clustering: Group documents by topics (bagof-words)
- Bioinformatics: Learning motifs.

Dimensionality reduction

Goal: Reduce the number of input variables

– Feature selection:

Only keep the **features** (= variables) that are relevant

– Feature extraction:

Transform the data into a space of lower dimension.

Goals:

- Reduce storage space & computational time
- Remove colinearities
- Visualization (in 2 or 3 dimensions) and interpretability.

Reinforcement learning

- Output = sequence of actions
- Learn a policy: sequence of correct actions to reach the goal
- No supervised output but delayed reward
- Examples
 - Game playing
 - Robot in a maze
- Issues: multiple agents, partial observability, ...

Artificial intelligence

Electrical engineering

Signal processing

Pattern recognition

Engineering

Optimization

Knowledge discovery in databases

Computer science

Inference

Discriminant analysis

Statistics

Data mining

Big data Business

Data science

Induction

Learning objectives

After this course, you should be able to

- Identify problems that can be solved by machine learning;
- Given such a problem, identify and apply the most appropriate classical algorithm(s);
- Implement some of these algorithms yourself;
- Evaluate and compare machine learning algorithms for a particular task.

Course Syllabus

- Sep 7
 - 1. Introduction
 - 2. Supervised learning
- Sep 14
 - 3. Model evaluation & selection

Lab: scientific Python

- Sep 21
 - 4. Bayesian decision theory

Lab: scikit-learn

- Sep 30
 - 5. Linear and logistic regression

Lab: Intro to Kaggle challenge

- Oct 7
 - 6. Regularized linear regression

Lab: Regularized linear regression

Parametric methods

• Oct 14

7. Nearest neighbor methods

Lab: Nearest neighbor methods

Nov 4

8. Tree-based methods

Lab: Tree-based methods

• Nov 18

9. Support vector machines

Guest talk: Beyrem Khalfaoui

Nov 25

10. Neural networks

Lab: Support vector machines

Dec 04

11. Dimensionality reduction

Lab: Dimensionality reduction

• Dec 11

12. Clustering

Lab: Kaggle challenge

Non-parametric methods

Unsupervised Learning

kaggle challenge project

How Many Bikes? Challenge



https://www.kaggle.com/c/how-many-bikes

- Predict the number of shared bikes that are rented in an American city
 - Regression
 - From weather, holiday, date & time.
- Evaluation on
 - Insights learned
 - Prediction performance.



Evaluation

Final exam (60 pts)

December 16, 2016

- Pen and paper
- Closed book
- Kaggle project (30 pts)
 - Written report (25 pts)
 - Position in the leaderboard (5pts)
 - Introduction: September 30, 2016
- Homework (10 pts)
 - To get the points: turn it in!
- Scribe extra credit (5 pts)
 - Write and share lecture notes.

December 16, 2016

1 problem each week

once in the course

Scribes

- What are scribes?
 - 2-4 students / week
 - Create & share written notes from the lecture of that week.
- Why be a scribe?
 - Learn by focusing on one chapter
 - Common good: benefit from the notes taken by others
 - Experience using LaTeX and github
 - Extra credit.
- Github repository https://github.com/chagaz/ma2823_2016
 - See example of Chap. 2
- When? https://framadate.org/omVzzIPfaHHgm881
 - Sign up at least the day before class
 - Turn in notes at most the day before class.

Homeworks

One problem per week

- Similar to the questions you'll be asked at the exam
- Turn it in at the beginning of the lecture
- Solution will be posted after the lecture
- Worth 1pt if you turn it in.

Resources

Course website

```
http://tinyurl.com/ma2823-2016
```

- Syllabus
- 2 days before the lecture: printable lecture handout
- Shortly after the lecture:
 - HW Problem n+1
 - Lecture slides
 - HW Solution n.

GitHub repository

```
https://github.com/chagaz/ma2823_2016
```

- Lab notebooks
- Lecture notes.

Resources: Datasets

- UCI Repository:
 http://www.ics.uci.edu/~mlearn/MLRepository.html
- KDnuggets Datasets:
 http://www.kdnuggets.com/datasets/index.html
- lmageNet: http://www.image-net.org/
- Enron Email Dataset: http://www.cs.cmu.edu/~enron/
- Million Song Dataset: http://labrosa.ee.columbia.edu/millionsong/
- IMDB Data: http://www.imdb.com/interfaces
- Données publiques françaises: https://www.data.gouv.fr/
- TunedIT: http://www.tunedit.org/
- **Knoema:** https://knoema.com/

Resources: Journals

- Journal of Machine Learning Research http://jmlr.csail.mit.edu/
- IEEE Transactions on Pattern Analysis and Machine Intelligence https://www.computer.org/portal/web/tpami
- Annals of Statistics http://imstat.org/aos/
- Journal of the American Statistical Association http://www.tandfonline.com/toc/uasa20/current
- Machine Learning http://link.springer.com/journal/10994
- Neural Computation http://www.mitpressjournals.org/loi/neco
- Neural Networks http://www.journals.elsevier.com/neuralnetworks
- IEEE Transactions on Neural Networks and Learning Systems
 http://cis.ieee.org/ieee-transactions-on-neural-networks-and-learning-systems.html

Resources: Conferences

- International Conference on Machine Learning (ICML) http://www.icml.cc/
- Neural Information Processing Systems (NIPS) http://www.nips.cc/
- International Conference on Learning Representations (ICLR)
 http://www.iclr.cc/
- European Conference on Machine Learning (ECML)
 http://www.ecmlpkdd.org/
- International Conference on AI & Statistics (AISTATS)
 http://www.aistats.org/
- Uncertainty in Artificial Intelligence (UAI) http://www.auai.org/
- Computational Learning Theory (COLT)
 http://www.learningtheory.org/past-conferences-2/
- Knowledge Discovery and Data Mining (KDD) http://www.kdd.org/
- International Conference on Pattern Recognition (ICPR) http://www.icpr2016.org/