From Field problems to Machine Learning

An introduction to the Data Science workflow and a motivation to understand Machine Learning

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ISAE SUPAERO

Schedule

1. General introduction and motivation
   How does ML fit within your business process.
   Why you should take time to understand what's under the hood in ML.
2. The importance of data pre-processing
   A practical illustration.
3. A geometrical approach to ML
   Support Vector Machines and a bit of kernel theory.
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   From mimicking the human brain to Artificial Neural Networks.
   Deep Learning.
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By the end of the class, you should be able to:

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    - SVM,
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    - Deep Learning,
    - Random Forests;
- know the existence of scikit-learn and its API.

Course material

https://github.com/erachelson/IntroML

Case studies

Let's list and discuss some cases from your experience and from the literature.

- [Your cases here!]

Case studies

Let's list and discuss some cases from your experience and from the literature.

- [Your cases here!]
- Predictive maintenance
- Market segmentation
- Demand forecast
- Preliminary design studies
- Clinical diagnosis
- Documentation management
- Satellite imaging

From tasks, to data, to ML

For all these cases, let's fill the table below, to build a common understanding of:

- the nature of data at stake
- the different tasks to automate
- the difficulties

Use case	Type of data	Properties of data	Task to automate	Difficulties	Comments

The Data Scientist perspective

Identified needs

Let's take the example of Predictive Maintenance.

We would like to build automated tools for the following tasks:

- Visualize system state
- Identify anomalies
- Predict Remaining Useful Life (RUL) / Time To Failure (TTF)
- Predict failure occurrence or probability at a given horizon

All this, in order to base our maintenance strategy on the (inferred) system state, rather than a general statistical trend.

> Can you relate this task decomposition to the other use-cases we've seen earlier?

Traditionaly, all this is based on user expertise.
Let's take a data-driven approach.

Data analysis workflow

1. Collect

- Sensors deployment
- Historical data collection
- Integrated storage (datawarehouses) and retrieval issues

→ Extract-Transform-Load (ETL) process

More on ETL: [link].

The *data engineer*'s job: data quality, management, availability.

Data analysis workflow

1. Collect
2. Analyze

- data cleaning
- feature selection / engineering
- performance criteria
- algorithm selection
- parameters tuning

The *data analyst* or *data scientist*'s job.
But can't be disconnected from field engineers on the task.

Data analysis workflow

1. Collect
2. Analyze
3. Predict

- Make predictions on new test cases
- Deploy solution in your operational process
- Make things usable

Data analysis workflow

1. Collect
2. Analyze
3. Predict
4. Decide

- Improve your decisions

End-user.
Job title depends on your professional field.

Data analysis workflow

1. Collect
2. Analyze
3. Predict
4. Decide

Need to automate as many steps as possible in this workflow
$\rightarrow$ data-driven approaches
$\rightarrow$ Machine Learning for step 2 (and 3)

A word on data quality

- amount of data: data is often abundant but crucial data is often scarce
- noise, errors, missing data, outdated data: reliability
- high-dimensional data
- class imbalance
- heterogeneous data (scalars, booleans, time series, images, text, ...)

All these will influence your algorithmic design or choices.

So let's talk about algorithms to see how we can solve the problems listed earlier.

Machines that learn?

Let's try to give a general definition.

Machine Learning

Machines that learn?
Let's try to give a general definition.

Machine learning is a field of computer science that gives computer systems the ability to "learn" (i.e. progressively improve performance on a specific task) with data, without being explicitly programmed.

(Wikipedia)

ML examples

- Given 20 years of clinical data, will this patient have a second heart attack in the next 5 years?

Image sources: Wikimedia commons

ML examples

- Given 20 years of clinical data, will this patient have a second heart attack in the next 5 years?
- What price for this stock, 6 months from now?

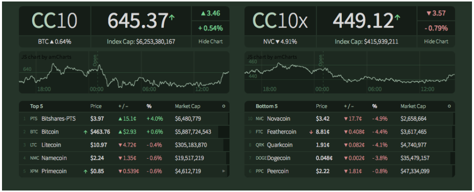

Image sources: Wikimedia commons

ML examples

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Image sources: [link]

ML examples

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- Is this e-mail a spam?

Enlarge your thesis!

Image sources: Iconfinder

ML examples

- Given 20 years of clinical data, will this patient have a second heart attack in the next 5 years?
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- Is this e-mail a spam?
- Can I cluster together customers? press articles? genes?


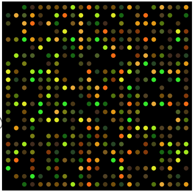

Image sources: People.jpg / Writing to Discuss: Use of a Clustering Technique / DNA microarray

ML examples

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- Is this handwritten number a 7?
- Is this e-mail a spam?
- Can I cluster together customers? press articles? genes?
- What is the best strategy when playing Counter Strike? or poker?

Image sources: CS:source / poker

ML tasks

What does ML do? 3 main tasks.

Task	Supervised Learning	Unsupervised Learning	Reinforcement Learning
Goal	Learn a function, $f(x) = y$	Find groups and correlations, $x \in C$	Optimal control, $f(x) = u \ / \ \max \sum r$
Data	$\{(x, y)\}$	$\{x\}$	$\{(x, u, r, x')\}$
Sub-task	Classification, Regression	Clustering, Density estimation, Dimensionnality reduction	Value estimation, Policy optimization
Algo ex.	Neural Networks, SVM, Random Forests	k-means, PCA, HCA	Q-learning

Evaluation criteria

Evaluating ML methods? What do we really want?

Ability to fit the training data:

- Regression: Mean Square Error
- Classification: Accuracy, TP, FP, ROC, AUC...
  cf. this Wikipedia article
- Clustering: similarity scores

Ability to generalize:

- Goal: filter out noise, avoid overfitting, generalize to unseen cases.
- ML Notions:
  - maximize margin
  - minimize difference btw class distributions (cross-entropy)

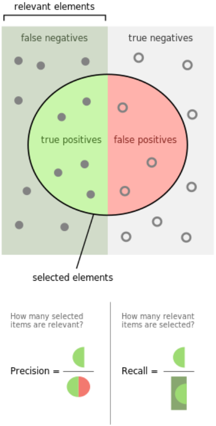


Image source: Wikimedia commons

Misconceptions and clarifications

AI ML is only a small (currently fashionable) part of Artificial Intelligence.

BD Big Data refers to working with datasets that have large Volume, Variety, Velocity (, Veracity, and Value).

DL Deep Learning is Machine Learning with Deep Neural Networks.

threat ML / Data Science / Big Data are as much of a threat (to jobs, the society, the economy…) as the combustion engine was in the XIXth century.

ethics Technical problems are not just technical problems and solutions *always* imply some tradeoff. Who bears the (moral) responsibility?


DATA

Data Scientist: The Sexiest Job of the 21st Century

by Thomas H. Davenport and D.J. Patil

FROM THE OCTOBER 2012 ISSUE

When Jonathan Goldman arrived for work in June 2006 at LinkedIn, the business networking site, the place still felt like a start-up. The company had just under 8 million accounts, and the number was growing quickly as existing members invited their friends and colleagues to join. But users weren't seeking out connections with the people who were already on the site at the rate executives had expected. Something was apparently missing in the social experience. As one LinkedIn manager put it, "It was like arriving at a conference reception and realizing you don't know anyone. So you just stand in the corner sipping your drink—and you probably leave early."

October 2012 Issue

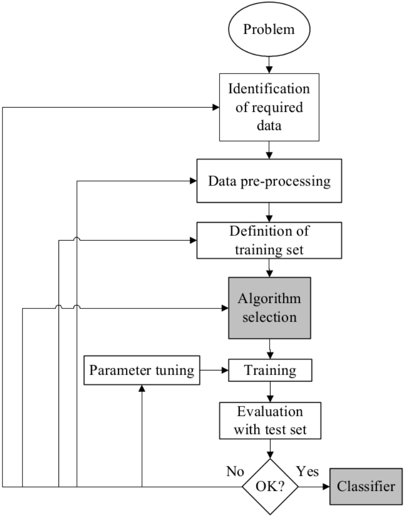
ML software

Software:

- Many free software libraries: scikit-learn, tensorflow, pytorch…check `www.mloss.org` if you're curious.
- Free environments: Weka, RStudio…
- Commercial embedded solutions (more or less specialized): Matlab, IBM, Microsoft…

Short "time to market" and high innovation pace.

The process of (Un)Supervised Learning



From **Supervised Machine Learning: A Review of Classification Techniques**, S. B. Kotsiantis, *Informatica*, 31:249–268, 2007.

Relating your needs and ML

Back to the example of Predictive Maintenance tasks.

- Visualizing system state
  $\rightarrow$ Dimensionnality reduction (Unsupervised learning)
- Detecting anomalies
  $\rightarrow$ Density estimation (Unsupervised learning)
- Predicting RUL or TTF
  $\rightarrow$ Regression (Supervised learning)
- Predicting failure in N cycles
  $\rightarrow$ Classification (Supervised learning)

Relating your needs and ML

Back to the example of Predictive Maintenance tasks.

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  $\rightarrow$ Classification (Supervised learning)

Thinking like a Maintenance Engineer:
How can I monitor my system to manage my maintenance operations?
Thinking like a Data Scientist:
Is this a supervised or an unsupervised problem? What available data?

Relate this example to your own field.
Now you can start discussing with data scientists to design together the most appropriate method for your data and your problem.

A word on scikit-learn

Scikit-learn = Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license
- Well documented, with lots of examples

`http://scikit-learn.org`

Let's take a look at the documentation's table of contents to grasp a few more keywords.

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- know the existence of scikit-learn and its API.

What you should expect in the remainder of this class

- As many intuitive notions as possible,
- ...but also quite a bit of (hopefully painless) math,
- ...and a fair amount of hands-on manipulations and demos.

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The importance of data pre-processing

Images, text, video, sound, measurement time series, continuous or discrete variables, missing data...

$\rightarrow$ filtering out noise and irrelevant data.
scaling, filtering, reducing...

$\rightarrow$ data- and application-specific procedures.
domain knowledge leverages non-representative datasets.

$\rightarrow$ source of potential harm.
keep goals in mind, to make informed tradeoffs that might induce bias.

$\Rightarrow$ Crucial elements for a good start.

Never neglect the pre-processing.

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A geometrical approach to ML

1. Draw a line that sits as far as possible from the data points $\rightarrow$ Support Vector Machines
2. Send all data points in a higher dimension space where they are linearly separable $\rightarrow$ kernel trick

$\Rightarrow$ SVM + kernel trick = Find the optimal separating hyperplane in this higher dimension space, without ever computing the mapping.

- SVM try to separate data by maximizing a geometrical margin
- They are computed offline
- They offer a sparse, robust to class imbalance, and easy to evaluate predictor
- Kernels are a way of enriching (lifting) the data representation so that it becomes linearly separable
- SVMs + kernels offer a versatile method for classification, regression and density estimation
- Link to documentation in scikit-learn

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A probabilistic approach to ML

Bayesian approach: find y that maximizes $\mathbb{P}(Y = y|\mathrm{data}, X = x)$

This problem of Bayesian inference is hard to solve without additional hypothesis.

A probabilistic approach to ML

Naive Bayes classifiers

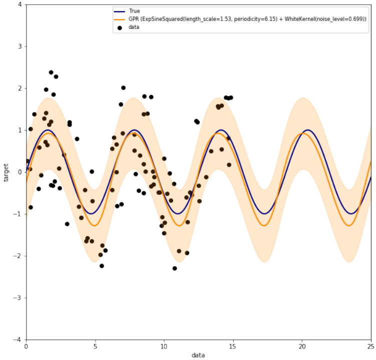
- Make a naive, counter-intuitive hypothesis of conditional independence of the feature variables;
- Compute each class' probability for a new example using this hypothesis and picks the most probable one;
- Are a simple, scalable, online method;
- Despite their simplicity, perform surprisingly well and are competitive in many applications.

A probabilistic approach to ML

Gaussian Processes

- Compute the most probable function that passes through the data points, given a priori information about how related two data points are (through a covariance kernel);
- Also provide a measure of prediction uncertainty in each point;
- Are computed offline and require an $N \times N$ matrix inversion for N data points in the training set (computationnally costly);
- Careful engineering of covariance kernels can help incorporate priori knowledge into Gaussian Processes;
- Are suitable both for regression and classification.

Note that Gaussian Processes are widely used in preliminary design phases, especially as surrogate models that replace physics computations.



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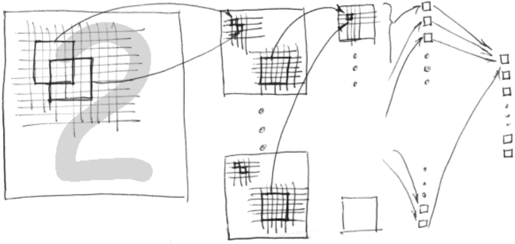
Artificial Neural Networks

Keywords:

- Computation graph $f_\theta(x)$
- Forward pass and gradient backpropagation
- Online training
- Minibatches
- The vanishing gradient problem
- Keras, Tensorflow, Caffe, Pytorch, Theano
- Avoiding overfitting: dropout, regularization, data augmentation
- Convolutional neural networks

Artificial Neural Networks

- Versatile, online training
- State-of-the-art performance on many benchmarks
- But fragile and hard to tune
- Lots of "recipes" still today
- Hard to guarantee convergence or performance
- CNNs = method of choice for structured data (images, sound, time series. . .)



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Decision trees

- Easy to interpret and to explain
- Poor representative power
- Greedy growth procedure $\Rightarrow$ suboptimal resulting tree
- Offline training
- Very sensitive to noise in the input data

Random Forests

- RF = decision trees + random feature selection + Bagging
- Robust, scalable, out-of-the-box classifier

$\Rightarrow$ excellent multi-purpose benchmarking algorithm!

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Extra things

- Installing anaconda, jupyter, etc.
- ML research: arXiv, JMLR, MLJ, IEEE PAMI, NeurIPS, ICML, ICLR...
- datasets: Kaggle, UCI, ImageNet, CIFAR...
- Other algorithms? (scikit-learn documentation or other notebooks)
- Dataviz: upstream methods (PCA...) and storytelling (Tableau...)
- What should I look for in a data scientist's CV?
- The price to pay for AI: individual responsibility, collective literacy, guiding principles.

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