

Brai Human S Machine Learning



Goals of today's event

Motivations:

- Scientific event with a subject transverse to the 4 departments
- Clear trend in our fields since already many years
- Already several use of ML in our researches

Goals:

- Inform about activities done @ IPHC
- Starting point to sharing expertise?
- Network ?
- Common interests Structuration ?

Morning's session

To be discussed during the round table

ML: an expanding field

[Σ)

Machine learning is not new

- First ideas already in 50's
- History of Neural Network
 - First paper (1943)
 - First algo still in use (Perceptron): 1958
 - First annual meeting :NN for computing" (1985)
 - AlphaGo (Google DeepMind) win a professional player (2015) ...

• Expansion of the ML field

- Boost from big data
- Large increase of computing resources (massive parallelisation)
- ML implementation eased by user-friendly (open source) packages
- Variety of applications (interests in tech compagnies and industry)
- Dynamic field: many ML contests, ...

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'Mark I Perceptron at the Cornell Aeronautical Laboratory', hardware implementation of the first Perceptron





Machine Learning: an e-crystal ball





Use data to "**predict**" (estimate/infer) a quantity / state / category /... on the studied object

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Machine Learning: an e-crystal ball







Children learn by experiment how to solve this problem without determining explicitly any physics law !

Machine Learning goals



ML goals:

- Learning
- Finding patterns & trends
- Improving decision making
- Generating data
- Improving/optimizing "tasks"
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Pro(*con*)fusion of keywords ...



Artificial Intelligence

Any technique which enables computers to mimic human behaviour. It uses ML but not only. Creates applications that react, adapt,

Ex: self-drive car, chatbot, ...



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Deep Learning

Subset of ML which make use of multi-layer neural networks (Artificial NN, Convolutional NN, Recurrent NN, ...)

- "deep" \rightarrow number of layers & neurons
 - ightarrow many parameters to be estimated
 - ightarrow need large datasets and long training period



Maths/Statistics

Programming

Biological inspired rules

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Big data

- Does not imply the use of ML
- ML complexity & performances depends on the size of the data used to learn

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ML is everywhere in everyday's life



APPLICATIONS OF MACHINE LEARNING



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ML algo can improve "experimental performances" Could be a cheaper/less demanding solution than building a new "apparatus"







Example in HEP:

- Used to detector anomalies •
- Attempt to use it to search for new phenomena (*example here*)



Anomaly = unexpected experimental signature (sign of new phenomena)

DETECTION



ARNING



1- Should I need to use ML?

- Algorithm complexity, dataset size, computing resources used are not guarantees that the performances will be better than what you could achieve with more "traditional methods" !
- **ML is not the solution to all problems**: If you have an analytical model (*scientifically motivated*) describing your data, why should you spend resources to approximate it with ML ? (*discussion about GAN*)
- ightarrow Useful to go beyond current knowledge in a data-driven way
- Gain vs effort
 - \rightarrow Can I expect a large improvement compare to current method ?
 - \rightarrow How much effort is needed to implement a ML solution?
 - \rightarrow Do I have enough resources to perform the training ?

| THIS IS YOUR MACHINE LEARNING SYSTEM? |
|--|
| YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE. |
| WHAT IF THE ANSWERS ARE WRONG? |
| JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT. |
| Xkcd.com |



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- Algorithm complexity, dataset size, computing resources used are not guarantees that the performances will be better than what you could achieve with more "traditional methods" !
- ML is not the solution to all problems:
- Gain vs effort

ML CANNOT be "blindly used":

ML does not replace the human knowledge / judgment

- Needs human guidance in the process of applying ML techniques
 - <u>Ex</u>: "spurious correlation in large datasets" (p-score)
- For interpretation:
 - correlation does imply not causal relation
 - Remark: hard to interpret the "ML model"

MORE IPHONES MEANS MORE PEOPLE DIE FROM FALLING DOWN STAIRS





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2- Which category of ML algorithms should I use ?

- We have presented 5 class of algorithms
- Subcategories for some of the classes
- Many algorithms are devoted to a given class of problem

3- What is the "nature" of the data to analyze ?

4 types of data:

- Numerical data
- Categorical data
- Time series (video, sound, ...)
- Text





Fig. Types of Data Structure

4- How large is our sample ?

- Choose an algorithm adapted to our sample
- Deep learning requires very large datasets

You should now have a list of algorithms that may suit our needs.



Answer: finding a (free / open source /maintained) implementation !

- (Google) Tensorflow (2015)/Keras
 - Fast-growing easy-to-use python lib (but also in C++, ...)
 - Allows applications of deep-learning models
 - Interface to Tensorflow, Theano backends \rightarrow GPU support
- <u>Scikit-learn</u> (2007)
 - Python lib that implements many (non-deep) techniques
 - A lot of data preprocessing & statistics tools
- **TMVA** (used in subatomic physics ROOT based)

But also:

- <u>Torch</u> / <u>PyTorch</u>
- <u>Caffee</u> (C++/python)
- <u>Accord.net</u> (C++)
- <u>R</u>

...

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Hardware

Answer: where to run the ML training ?

• Use our laptop:

several ML-analyses can be done on (from few min to few hours)

- Multi-threading
- Use dedicated GPU(s)

reasonable dataset - large computing time

- Several algorithms profit a lot from GPU parallelization
- From few 100's to few 1000's euros
- Use server/computing center large data / complex models
 - Tier2
 - Mesocentre
 - CC-in2p3
 - CERN
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What's next ?



ML workflow



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- N "samples".
- M "features" per sample [dimension]
- (predicator variables)



N "observations"

- Predictive function: y = f(x)
- Depends on the choice of the algo
- Configuration (ex: NN: #layers, #nodes, ...)
- Have **many** parameters to be determined





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- One (or few) response (*target*) variable
- Can be discrete or continuous

Requirements:

Step 1: Define the objective
→ choice of algo/implementation
→ choice of hardware chosen
Step 2: Data gathering



Step 3: Data preparation

data cleaning, filtering, binning, transformation ...

Step 4: Exploratory Data Analysis (EDA)



Understand patterns, trends, correlations, ...

<u>Goal</u>: Selection input variables (features) & "samples" Advices:

- \rightarrow Avoid variables too sensitive to noise, uncertainties, ...
- ightarrow Avoid variable badly described by our simulation if the dataset is simulation based
- \rightarrow Use a representative "samples"







Step 5: Building a Machine Learning Model == Model training

- Define a (large) subset of data == training sample
- Most CPU/GPU demanding task
- **Goal**: determining the parameters of the model
- <u>Advices</u>:
- \rightarrow sample should be large enough (depends on model complexity)
- → Computation time can be speed-up depending on both the hardware architecture chosen & the model
 - \rightarrow <u>Remark</u>: processing does not necessarily linearly scale with #threads !
- \rightarrow Check that there is no **overtraining**











Step 6: Model Evaluation

- Define a (small / independent) subset of data == test sample
- Evaluate the performances
 - True vs False Positive Rage
 - ROC: Receiver Operating Characteristic
 - AUC: Area under the curve
- Cross-validation
 - \rightarrow Avoid overtraining





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Step 7: Model optimization (refinement)

- (Hyper-)parameter tuning (ex with NN: #layers, #nodes, ..)
- Test/Optimize feature selection (ex: change/add input var)
- Imply retraining (CPU/GPU demanding)

 \rightarrow This **loop** can be done several times ...

Step 8: Predictions ... !

 \rightarrow algo deployment/integration/maintenance

<u>Remark</u>: Retraining can be needed (even if inputs/parameters are fixed)

if the model is applied on data collected in new conditions (new sensors/calibration/alignment etc ...)

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Machine Learning Development Lifecycle



jeremyjordan.me

Networks & training

<u>Networks</u>

- ML collaborations @ IN2P3
- IML (LHC ML working group)
- ...

Training

- Master "Big data and ML" @ unistra
- IN2P3 school of statistics
- Ecole doctorale (ED 182)
- MOOC
- ...



GAN: Generative Adversarial Network

Technique used to generate "realistic human face"

Can have application in HEP to **speed-up simulation**

Source A: gender, age, hair length, glasses, pose

- Simulation of proton-proton collision @ LHC
- Simulation of detector response

Source B:

everything else



Dominated by : calorimeter simulation and tracking

Result of combining A and B



Beyond activities presented this morning, additional are done

Non exhaustive list:

- Clustering in CMOS pixels with NN (DRHIM, Finck & al)
- Use of AI to improve detector performances in the context of PET (tomography) (*DRHIM*, *Brasse & aI*)
- Automatic ML-based localisation of radioactive contamination zone with an autonomous drone (learning based on MC) (*DRS, Arbor & al*)



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