

Lecture 2: Introduction to Machine Learning



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A definition (Ulikipedia) SMARTHER

Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to progressively improve their performance on a specific task. Machine learning algorithms build a mathematical model of sample data, known as "training data", in order to make predictions or decisions without being explicitly programmed to perform the task.











• Different ML algorithms had their moment of glory

Input layer

● (Shallow) neural networks dominated in the 80's



Support vector machine

 Boosting of
 A second seco decision trees

Hidden layer





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A two-steps process smart

• Learning: train the algorithm on a provided dataset

- <u>Supervised</u>: the dataset X comes with the right answer y (right class in a classification problem). The algorithm learns the function
- Insupervised: the dataset X comes with no label. The algorithm learns structures in the data (e.g., alike events in a clustering algorithm)

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• **Inference**: once trained, the model can be applied to other datasets









Machine Learning in HEP

• Long standing tradition

Neural networks used at LEP and the Tevatron

• Boosted Decision Trees introduced by MiniNooNE and heavy used at BaBar

BDTs ported to LHC and BDTs ported to LHC and Section Sect very useful on Higgs <u>discovery</u>

• Now Deep Learning is opening up many new possibilities













• Classification: associate a given element of a dataset to one of N exclusive classes

• <u>Regression</u>: determine a continuous value y from a set of inputs x

• Clustering: group elements of a dataset because of their similarity according to some *learned metric*

 Dimensionality reduction:
 find the k quantities of the N inputs (with k<N) that incorporate the relevant information (e.g., principal component analysis)

Tupical problems smarter and the second seco







UNSUPERVISED MACHINE LEARNING SUPERVISED MACHINE LEARNING



Supervised Learning





PRODEFREADERSWHIMSY.BLDG5PD1.CA





• Define a selection to separate the signal from the background







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A simple example: S vs B selectionsmart

• For any linear boundary, the *quantity* $h(\mathbf{x} | \mathbf{w}) = w_1 x_1 + w_2 x_2$ *is*

 $\odot = 0$ along the boundary

 $\odot > 0$ above the boundary, the larger the distance, the bigger $h(\mathbf{x} | \mathbf{w})$

• <0 below the boundary, the
</pre> larger the distance the bigger $-h(\mathbf{x} \mid \mathbf{w})$

• In other words, the larger (smaller) is $h(\mathbf{x} | \mathbf{w})$, the larger is the probability for a given point to be blue (signal) or orange (background)





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• We can model the probability of being a signal with a logistic model

• This definition has the desired properties:

- The larger (and positive) $h(\mathbf{x} | \mathbf{w})$, the closer p to 1
- The larger (and negative) $h(\mathbf{x} | \mathbf{w})$, the closer p to 0

• The optimal boundary (i.e., the optimal choice of w_1 and w_2) is such that we maximise probability for signal points and minimise that of background points

• To do so, we need

• A set of points for which we have a ground truth $x_i \in \mathbb{R}^n$ and $y_i = \{0,1\}$

• A loss function to minimise











Uhich is the unknown?

• <u>Probability</u>: When we introduced distributions, we started from known distributions (e.g., a Poissort M. Kown λ) and we tried to characterize a typical experiment outcome
 Hypothesis Testing: New Stancerted the problem: we know the experiment Outcome (e.g., we counted events above threspondent on the experiment of which of two λ values (bkg-only or sig+bkg) they come from

• Inference: we could also just ask what is the value of λ more compatible with the observation (trivial question in this case - right? - but not in general). This is a typical application of maximum likelihood fits and a regression problem in Machine Learning (not much to say about this today)

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Maximum Likelihood estimation

• We are given a likelihood model $\mathscr{L}(D|w)$ and some data D

• D is known, w are unknown

the most probable outcome of the experiment

• If we knew these \hat{w} values, the probability of known)

You can convince yourselves that $\hat{w} = \arg \max \mathcal{L}(D \mid w)$ ${\mathcal W}$

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- \bigcirc We want to find the \hat{w} values that would make our data D
 - observing D is maximal (here D is unknown and \hat{w} is









Bernoulli's process (Y/N question):

probability of a Y is p

 \bigcirc probability of a N is (1-p)

• If we assign labels (Y -> 1 and N -> 0) we can write the probability for a i-th event as $p^{x_i}(1-p)^{1-x_i}$, where x_i is the label for the i-th event

The likelihood is then written as



 $\mathscr{L}(y|p) = \prod_{i=1}^{y} p_i^{y} (1-p)^{(1-y_i)}$









Cross Entropy as a MLE SM

• We can make our probability model more *complicated*

• p could be a function of a set of quantities x that we know about our data

• for instance, this could be our logistic regression problem

Minimizing the -logL corresponds to minimizing the binary cross entropy

$$p_i = p(y_i = 1 | x_i) = \frac{1}{1 + e^{-h(x_i | w)}}$$









• Given a set of points, find the curve that goes through them

• Can be a linear model

$$y_i = ax_i + b$$

• Can be a linear function of non-linear kernel of the x. For instance, a polynomial basis

- 0

New feature, "engineered" from the input features









Take some model (e.g., linear)

• Consider the case of a Gaussian dispersion of y around the expected value

• Assume that the resolution σ is fixed and write down the likelihood



 $h(x_i | a, b) = ax_i + b$

 $y_i = h(x_i) + e_i$ $p(e_i) = \frac{1}{\sqrt{2\pi\sigma}}e^{-\frac{1}{\sqrt{2\pi\sigma}}}$

 $\mathscr{L} = \prod_{i} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{e_i^2}{2\sigma^2}} = \prod_{i} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(y_i - h(x_i))^2}{2\sigma^2}}$













• The maximisation of this likelihood corresponds to the minimisation of the mean square error (MSE)

 $\arg\min[-2\log\mathscr{L}] = \arg\max$

$$= \arg\min\left[\sum_{i} \frac{(y_i - h(x_i))^2}{\sigma^2}\right] = \arg\min\left[\sum_{i} (y_i - h(x_i))^2\right] = MSE$$

you are implicitly assuming that your y are Gaussian distributed, with fixed RMS

• What if the RMS is not a constant?

$$\min\left[-2\log\left[\prod_{i}\frac{1}{\sqrt{2\pi\sigma}}e^{-\frac{(y_i-h(x_i))^2}{2\sigma^2}}\right]\right]$$

• MSE is the most popular loss function when dealing with continuous outputs. We will use it a few times in the next days

• **BE AWARE OF THE UNDERLYING ASSUMPTION:** if you are using MSE,







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• Split your sample in three:

• Training: the biggest chunk, where you learn from

• Validation: an auxiliary dataset to verify generalization and prevent overtraining

• Test: the dataset for the final independent check

Training











• Gradient Descent is a popular minimisation algorithm

- Start from a random point
- ullet Compute the gradient wrt the model $\partial L(\mathbf{w})$ parameters
- Make a step of size η (the <u>learning</u>) <u>rate</u>) towards the gradient dimection
- Update the parameters of the mode accordingly
- Effective, but computationally expensive (gradient over entire dataset)











Stochastic Gradient Descent SMARTHER

Make the minimisation more computationally efficient

• Compute gradient on a small bate of events (faster & parallelizable, but noisy)

Average over the batches to reduce noise

• BEWARE: better scalability come at the cost of (sometimes) not converging

Many recipes exist to help convergence, by playing with the algorithm setup (e.g., adapting *learning rate)*









• Train across multiple epochs

 $\odot 1$ epoch = going once through the full dataset

• Check your training history

• on the training data (training loss)

• and the validation ones (validation loss)

• Use an objective algorithm to stop (e.g., early stopping)



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EARLY TOPPING: stop the train if the validation loss didn't change more than δ in the last n epochs (patience)







Uhat can go wrong: underfitting smarther

• If your model has not enough flexibility, it will not be able to describe the data

• The training and validation loss will be close, but their value will not decrease

• The model is said to be underfitting, or being **biased**









Uhat can go wrong: overfitting smarther

• Your model can learn too much of your training dataset

• e.g., its statistical fluctuations

• Such an overfitted model would not generalise

• So, its description of the validation dataset will be bad (i.e., <u>the mode doesn't</u> <u>generalise</u>)

This is typically highlighted by a divergence of the training and validation loss









A model would underfit if too simple: it will not be able to model the mean value

A model would overfit if too <u>complex:</u> it will reproduce the mean value, but it will underestimate the variance of the data

• The generalization error is the error made going from the training sample to another sample (e.g., the test sample)

The Bias vs Variance tradeoff smarther













• Generalization error can be written as the sum of three terms:

• The intrinsic statistical noise in the data • the bias wrt the mean • the variance of the prediction around the mean

 $E[(y - h(x))^{2}] = E[(y - \bar{y})^{2}] + (\bar{y} - \bar{h}(x))^{2} + E[(h(x) - \bar{h}(x))^{2}]$ **/ariance** Bias Squared













Model Complexity

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Model complexity can be "optimized" when minimizing the loss

 A modified loss is introduced, with
 a penalty term attache to each model parameter

$$L_{reg} = L + \Omega(w)$$

• For instance, Lp regularisation

$$L_p = \|\mathbf{w}\|^p = \sum_{i} |w_i|^p$$

• The minimisation is a tradeoff between:

• pushing down the 1st term by taking advantage of the parameters

• pushing down the 2nd term by switching off the parameters

Regularization



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• NNs are (as of today) the best ML solution on the market

• NNs are usually structured in nodes connected by edges

each node performs a math operation on the input

• edges determine the flow of neuron's inputs & outputs

Neural Metworks in a nutshell SMARTHER



Deep Meural Metuorks SMARTHER SCIENCE AND INDUSTRY

Deep neural networks are those with >1 inner layer

• Thanks to GPUs, it is now possible to train them efficiently, which boosted the revival of neural networks in the years 2000

• In addition, new architectures emerged, which better exploit the new computing power

Large-scale Deep Unsupervised Learning using Graphics Processors

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Image processing

Reinforcement Learning

text/sound processing

Everything is a Recommendation

Over 75% of what people watch comes from our recommendations

Recommendations are driven by Machine Learning

erc

NETFLIX

Clustering

• Event Generation with generative models

Anomaly Detection to search for new Physics

Adversarial training for systematics

 Reinforcement learning for
 jet grooming

DL, HEP, and new opportunities SMARTH

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- Feed-forward neural networks have hierarchical structures:
 - inputs enter from the left and flow to the right
 - no closed loops or circularities
- Deep neural networks are FF-NN with more than one hidden layer
- Out of this "classic idea, new architectures emerge, optimised for computing vision, language processing, etc

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Feed-Foruard Mms smarther

- Each input is multiplied by a weight
- The weighted values are summed
- A bias is added
- The result is passed to an activation function

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The role of a network node smarther science and industry

- Each input is multiplied by a weight
- The weighted values are summed
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- The result is passed to an activation function

 $\sum_{i} W_{ii} X_{i}$

The role of a network node smarther science and industry

- Each input is multiplied by a weight
- The weighted values are summed

• A bias is added

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 $\sum_{i} w_{ii} x_i + b_i$ J

The role of a network node smarther science and industry

- Each input is multiplied by a weight
- The weighted values are summed
- A bias is added

• The result is passed to an activation function

Activation Functions

 $y_i = f(\sum_i w_{ii} x_i + b_i)$

• In a feed-forward chain, each node processes what comes from the previous layer

• The final result (depending on the network geometry) is K outputs, given N inputs

• One can show that such a mechanism allows to learn generic $\mathbb{R}^{N} \rightarrow \mathbb{R}^{K}$ functions

ull picture

$y_j = f^{(3)}(\Sigma_l w_{il}^{(3)} f^{(2)}(\Sigma_k w_{lk}^{(2)} f^{(1)}(\Sigma_i w_{ki}^{(1)} x_i + b_k^{(1)}) + b_l^{(2)}) + b_i^{(3)})$

Activation Functions SM

• Activation functions are an example of network hyper parameters

• they come from architecture choice, rather than from the training itself

• Activation output of the
output layer play a special
role:

• it needs to return the output in the right domain

• it needs to preserve the wanted features of the output (e.g., periodic, positive defined, etc.)

Name	Plot	Equation	Derivative
Identity		f(x) = x	f'(x) = 1
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \ge 0 \end{cases}$	$f'(x) \bigotimes \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$	f'(x) = f(x)(1 - f(x))
TanH		$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU)		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) ^[2]		$f(x) = \begin{cases} \alpha x & \text{for } x < 0 \\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Exponential Linear Unit (ELU) ^[3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0 \\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

• A special kind of layer, introduced for regularisation purpose

 Randomly drop links
 between neurons, with probability p

• The connections are re-established during the validation and *inference steps*

• Typical sign of it: invert hierarchy between training and validation loss

(a) Standard Neural Net


```
(b) After applying dropout.
```


- It is good practice to give normalized inputs to a layer
 - With all inputs having the same order of magnitude, all weights are equal important in the gradient
 - Prevents explosion of the loss function
- This can be done automatically with BatchNormalization
 - non-learnable shift and scale parameters, adjusted batch by batch

• Dense NN architectures can be made
more complex

Multiple inputs

Multiple outputs

Different networks branches

This is possible thanks to layermanipulation layers

Add, Subtract, etc.

• Concatenation

• Flattening

All these operations are usually
 provided with NN training libraries

804768079465268345534 *Concatenation*804768083455347946526

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TensorFlow

Many solutions exist. Most popular softwares live in a python ecosystem

• Google's TensorFlow

• Facebook's Pytorch

Apache MXnet

 All of them integrated in a data
 science ecosystem

• with numpy, scikit, etc.

 Convenient libraries built on top, with pre-coded ingredients

• Keras for TF (this is what we will be using) 45

O PyTorch

mxnet

NumPy

ecikit becym

● All codes come with GPU support, through CUDA

• They work on nVidia GPUs

• GPUs are very suitable to train neural networks

- dedicated VRAM provides large memory to load datasets
- architecture ideal to run vectorised operations on tensors
- can also paralyse training tasks (e.g., processing in parallel multiple batches)
- A single-precision gaming card is good enough for standalone studies (200-1000 \$, depending on mode1)
- Large tasks require access to clusters (with *libraries for distributed training)*
- Dedicated architectures (e.g., Google TPU) now
 emerging. Essentially, Deep Learning ASICs

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• You have a jet at LHC: spray of hadrons coming from a "shower" initiated by a fundamental particle of some kind (quark, gluon, W/Z/H bosons, top quark)

• You have a set of jet features whose distribution depends on the nature of the initial particle

• You can train a network to start from the values of these quantities and guess the nature of your jet

To do this you need a sample for which you know the answer

Example: jet tagging sr

• You have a jet at LHC: spray of hadrons coming from a "shower" initiated by a fundamental particle of some kind (quark, gluon, W/Z/H bosons, top quark)

• You have a set of jet features nature of the initial particle

• You can train a network to start from the values of these quantities and guess the nature of your jet

To do this you need a sample for which you know the answer

• A given threefold defines the following qualities True-positives: Class-1 events above the threshold • True-negatives: Class-0 events below the threshold • False-positives: Class-0 events above the threshold • False-negatives: Class-1 events below the threshold

Classifier metrics SM

• A given threefold defines the following qualities True-positives: Class-1 events above the threshold True-negatives: Class-0 events below the threshold • False-positives: Class-0 events above the threshold • False-negatives: Class-1 events below the threshold

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Classifier metrics SM

• A given threefold defines the following qualities True-positives: Class-1 events above the threshold • True-negatives: Class-0 events below the threshold • False-positives: Class-0 events above the threshold • False-negatives: Class-1 events below the threshold

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Classifier metrics SM

• A given threefold defines the following qualities True-positives: Class-1 events above the threshold True-negatives: Class-0 events below the threshold • False-positives: Class-0 events above the threshold • False-negatives: Class-1 events below the threshold

Classifier metrics SM

• Consider a binary classifier

- Its output ŷ is a number in [0, 1]
- If well trained, value should be close to 0 (1) for class-0 (class-1) examples

• One usually defines a threshold yt such that:

 $) \hat{y} > y_t \rightarrow Class 1$

• $\hat{y} < y_t \rightarrow Class 0$

negative (TN) rates • Accuracy: (TP+TN)/Total • The fraction of events correctly classified • Sensitivity: TP/(Total positive) • AKA signal efficiency in HEP • Specificity: TN/(Total negative) • AKA mistag rate in HEP

• Starting ingredients are true positive (TP) and true

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Receiver operating characteristic smarther

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(and not programmed) to accomplish a task

given sample

• The loss function has a direct connection to the statistical properties of the problem

• Deep Learning is the most powerful class of ML algorithms nowadays

- ML models are adaptable algorithms that are trained
- The training happens minimizing a loss function on a

It could be relevant to the future of HEP, e.g., to face the big-data challenge of the High-Luminosity LHC

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• Michael Kagan, <u>CERN OpenLab classes on Machine Learning</u> • Source of inspiration for this first lesson • Pattern Recognition and Machine learning (Bishop)

Main reference for tutorial exercise: <u>https://arxiv.org/abs/1908.05318</u>

• All notebooks and classes are/will be on GitHub: https://github.com/ pierinim/tutorials/tree/master/SMARTHEP

• Full dataset available at: <u>https://zenodo.org/record/3602260</u>

- I. Goodfellow and Y. Bengio and A. Courville, <u>"Deep Learning" MIT press</u>

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Running Tutorial Notebooks in Colab

Maurizio Pierini

Step1: Open Notebook on Colab

• Go to <u>https://colab.research.google.com</u>

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Step2: import the Tutorial from gitlab

• Click on the GITHUB tab

• Specify the repository pierinim/tutorials/SMARTHEP

• Click on the notebook

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Set your resources to use GPUs

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