Deep Learning Applications for collider physics Lecture 1

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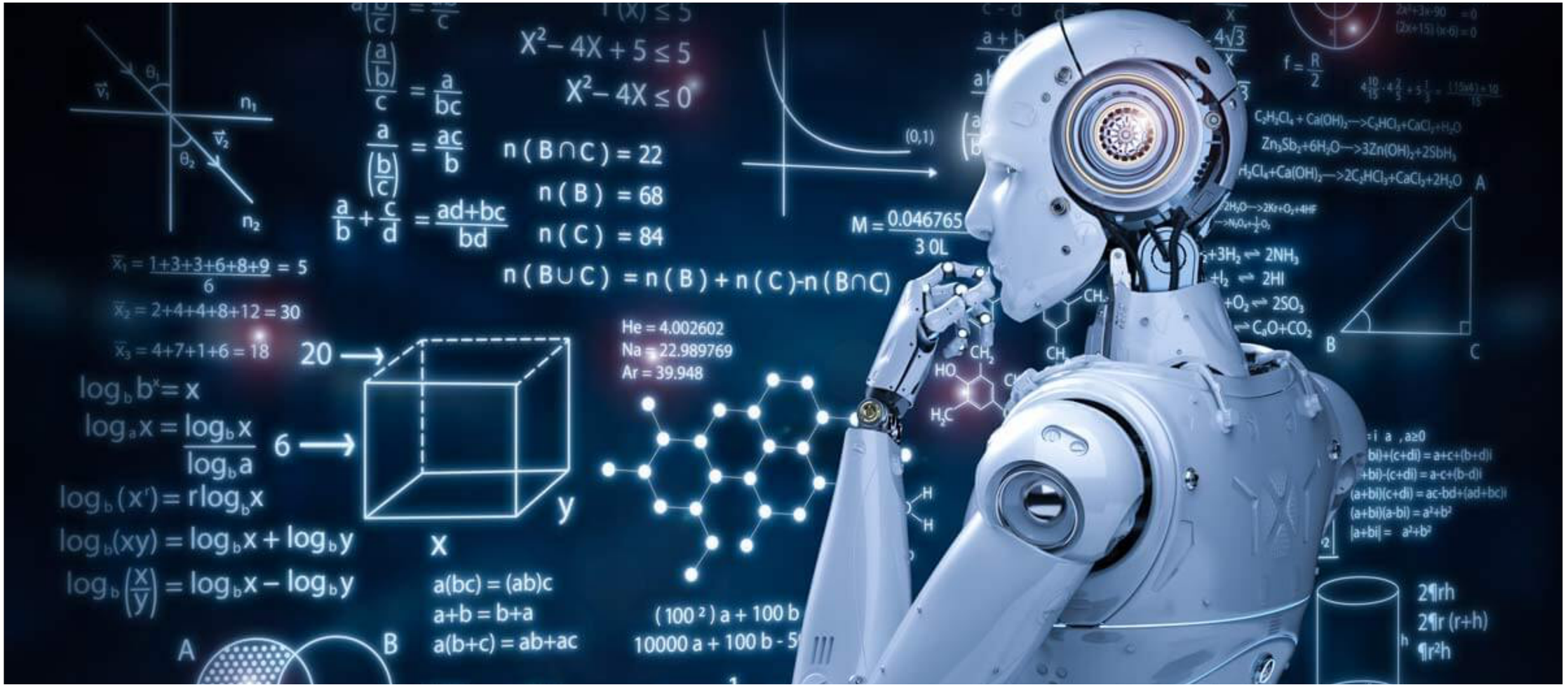
Plan for these lectures

	Day1	Day2	Day3	Day4	Day5
1st hour	Introduction	ConvNN	LHC & fast Inference	Anomaly Detection	Graphs
2nd hour	Dense NNNs	GANs	RNNs	VAEs	Graphs
Tutorial	Dense NNNs	ConvNN	RNNs	AE	Graphs

European Research Council



What is Machine Learning ?

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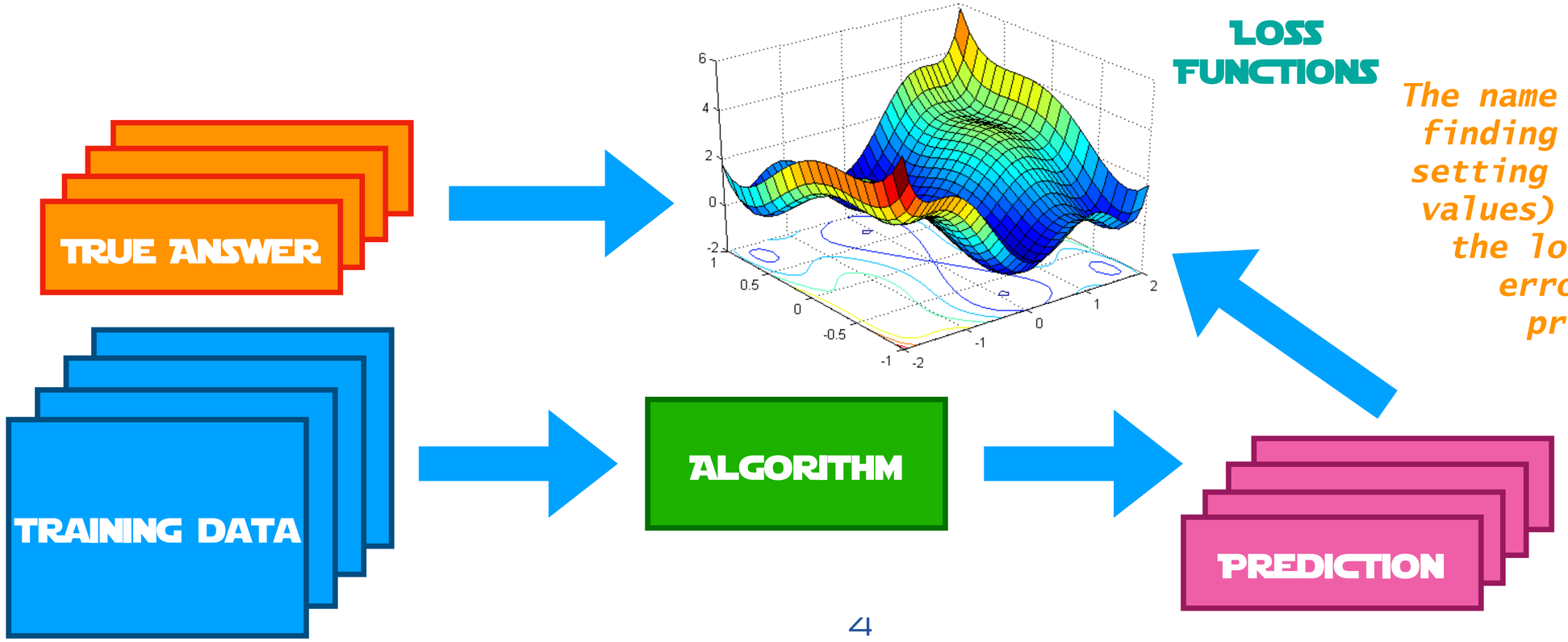
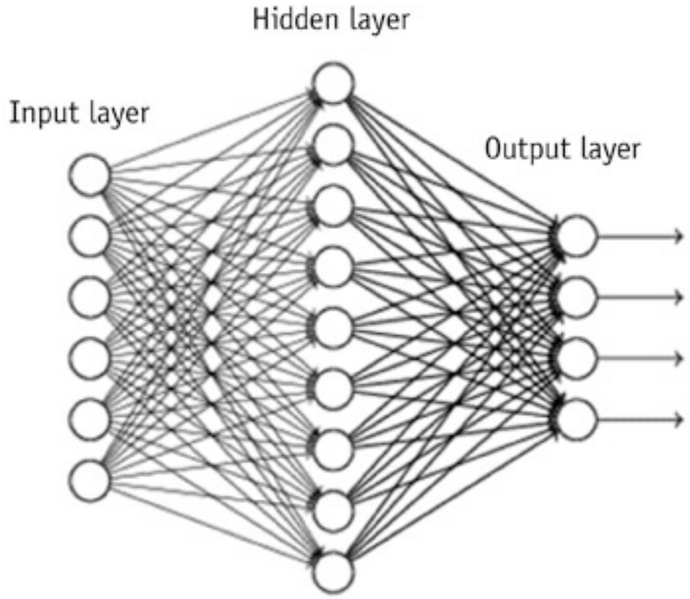
A definition (Wikipedia)

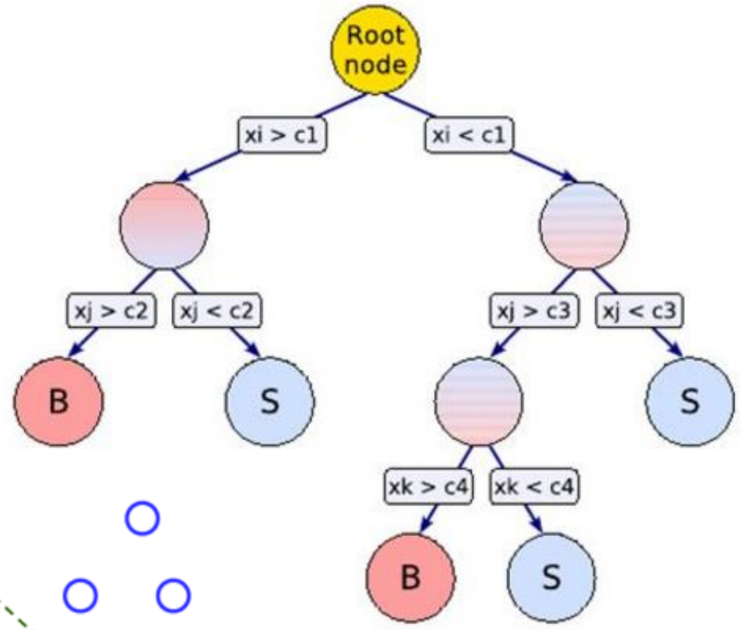
Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to progressively improve their performance on a specific task. Machine learning algorithms build a mathematical model of sample data, known as "training data", in order to make predictions or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

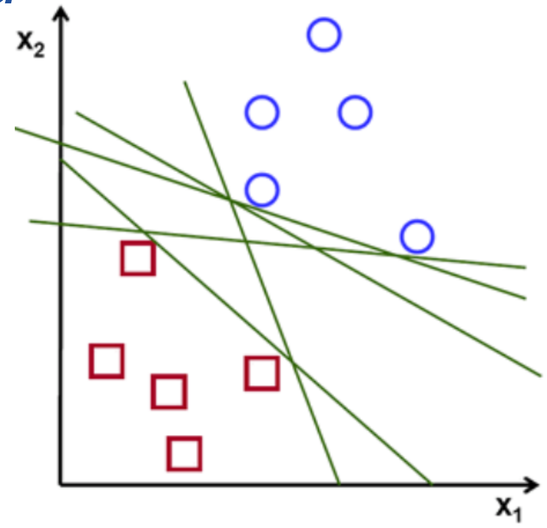


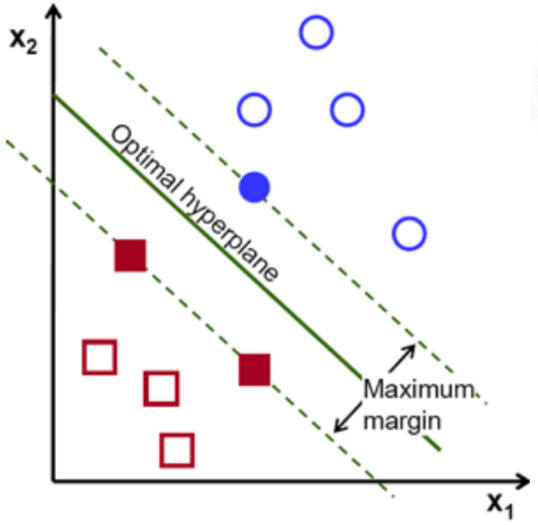
Many flavors of ML

- *Different ML algorithms had their moment of glory*
  - *(Shallow) neural networks dominated in the 80's*
  - *Alternatives emerged in the 90's*
    - *Support vector machine*
    - *Boosting of decision trees*



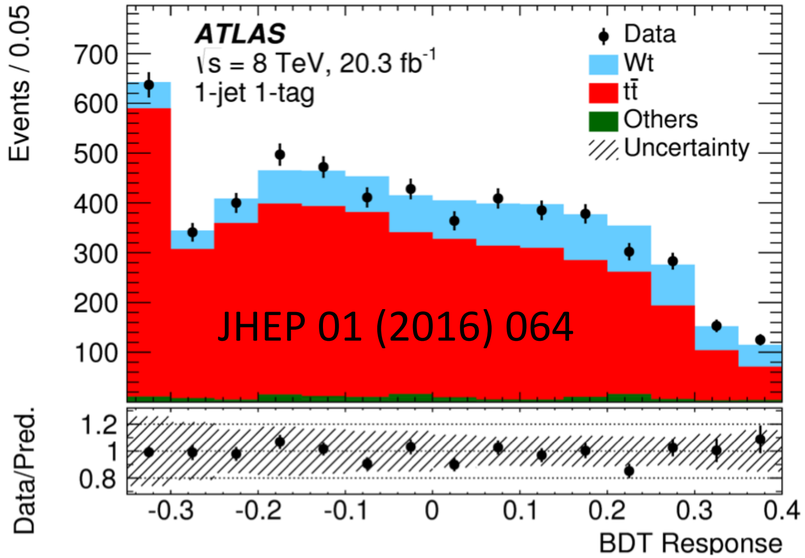


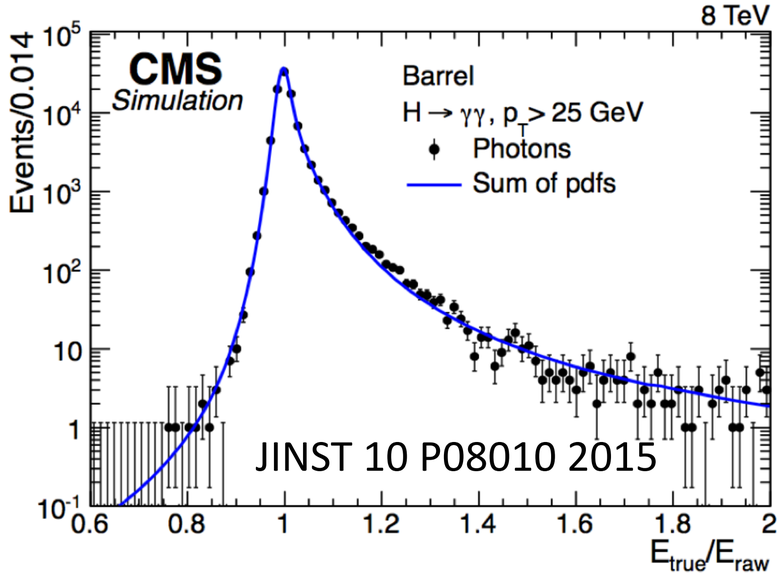




Machine Learning in HEP

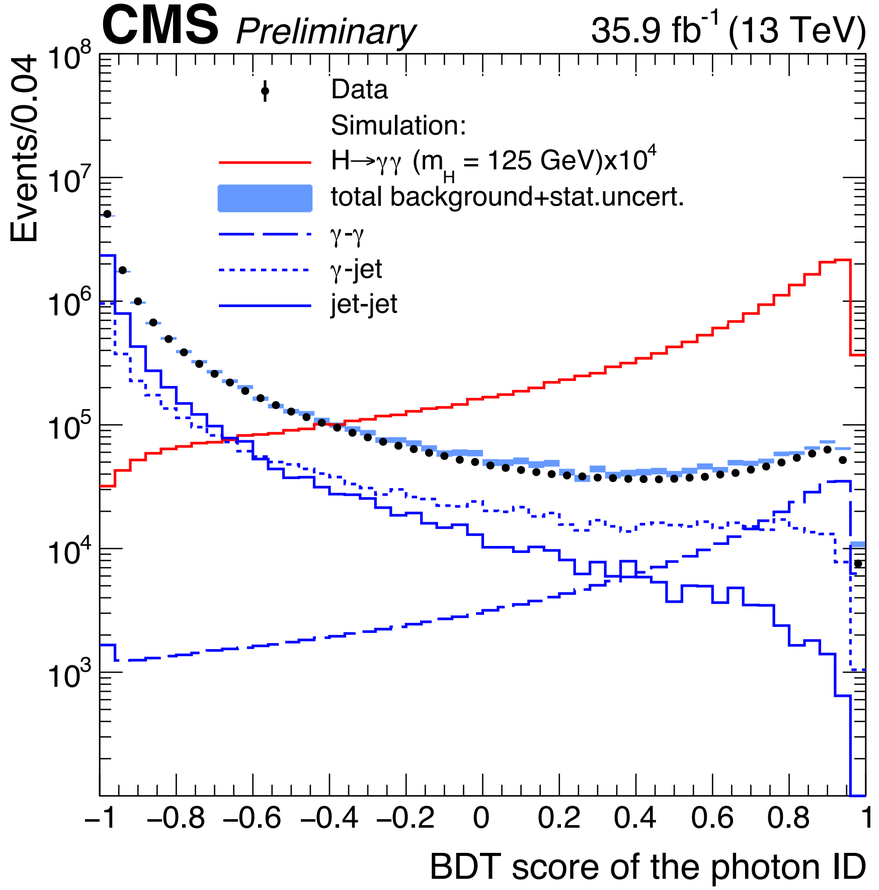
- *Classification:*
  - *given an image, identify the object represented*
  - *in particle physics, given a particle shower, identify the particle kind*
- *Regression:*
  - *given a set of quantities x, learn some function f(x)*
  - *in particle physics, given a particle shower, learn its energy*





Machine Learning in HEP

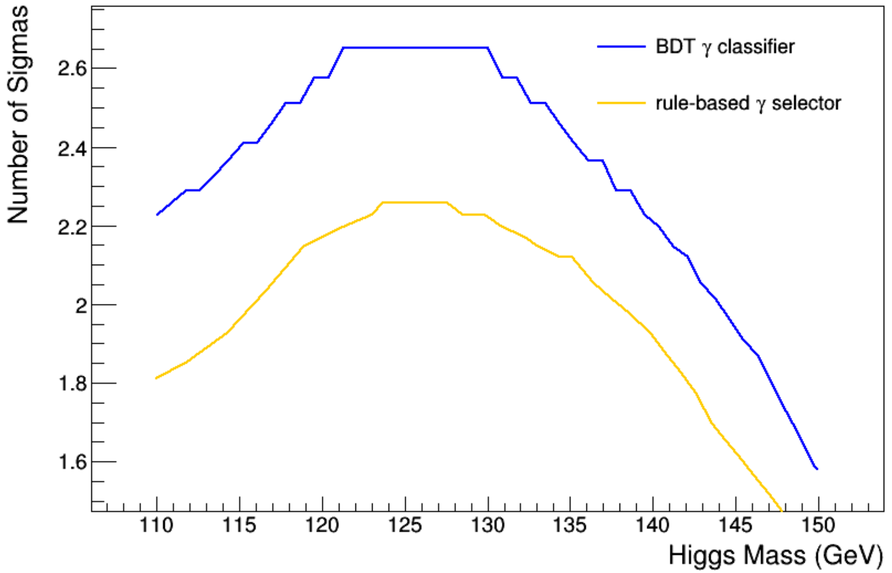
- *Classification:*
  - *identify a particle & reject fakes*
  - *identify signal events & reject background*
- *Regression:*
  - *Measure energy of a particle*
- *We typically use BDTs for these task*
  - *moved to Deep Learning for analysis-specific tasks*
  - *same will happen for centralised tasks (eventually)*

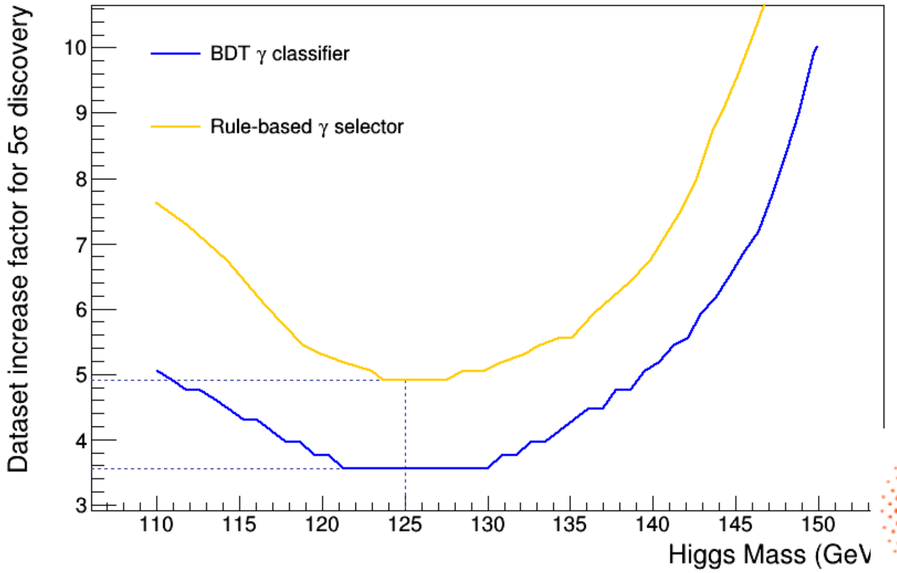


Centralised task (in online or offline reconstruction)
Analysis-specific task (by users on local computing infrastructures)

Machine Learning in HEP

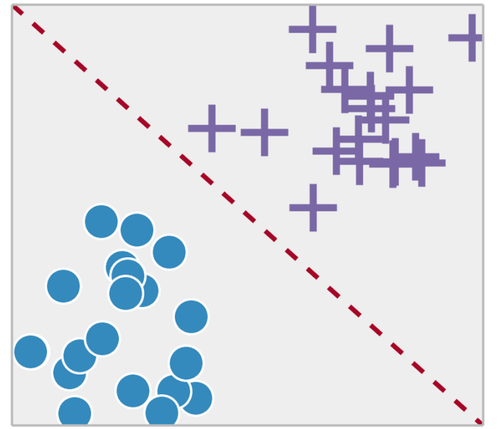
- *Long tradition*
  - *Neural networks used at LEP and the Tevatron*
  - *Boosted Decision Trees introduced by MiniNooNE and heavy used at BaBar*
  - ***BDTs ported to LHC and very useful on Higgs discovery***
  - *Now Deep Learning is opening up many new possibilities*

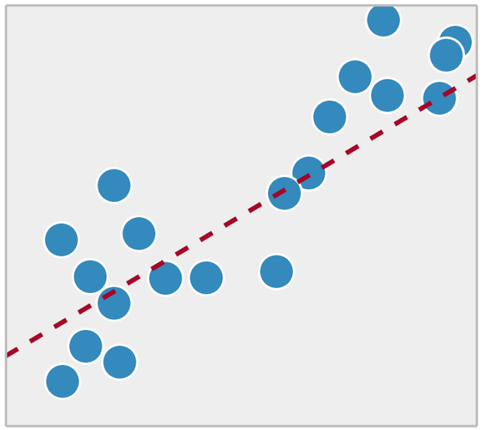


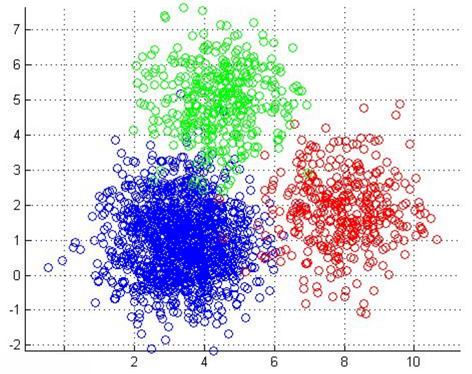


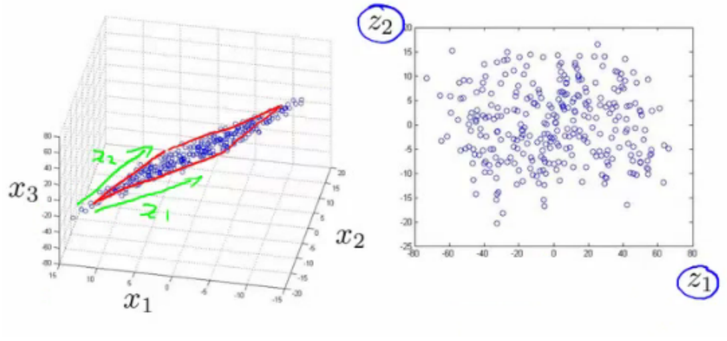
Typical problems

- ***Classification***: *associate a given element of a dataset to one of N exclusive classes*
- ***Regression***: *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)*



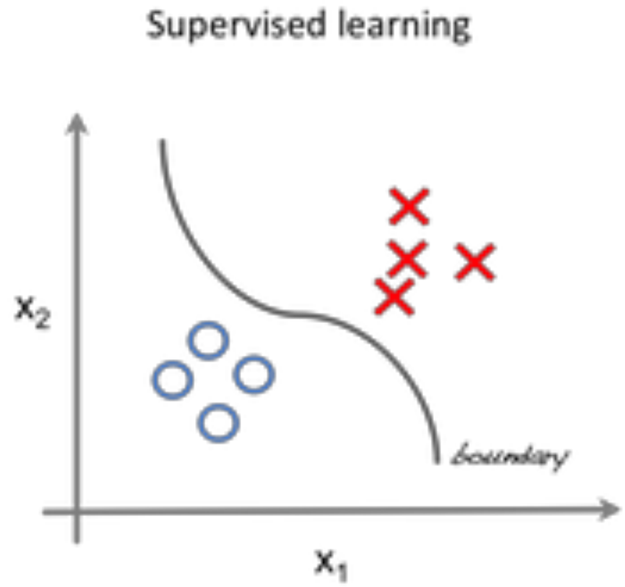


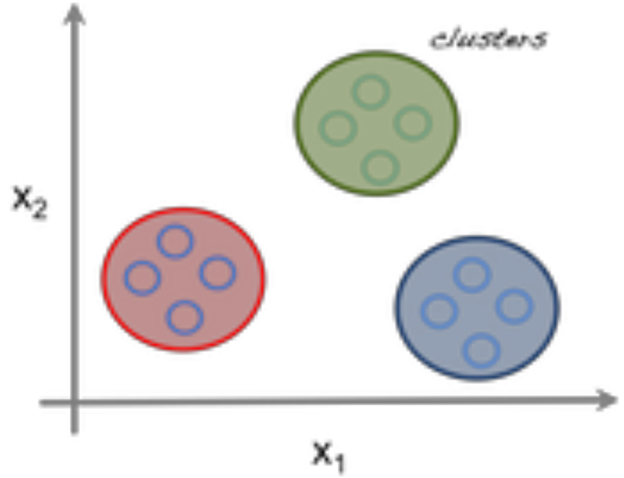




A two-steps process

- ***Learning:*** *train the algorithm on a provided dataset*
  - ***Supervised:*** *the dataset X comes with the right answer y (right class in a classification problem). The algorithm learns the function*
  - ***Unsupervised****: the dataset X comes with no label. The algorithm learns structures in the data (e.g., alike events in a clustering algorithm)*
  - ***Reinforcement:*** *learn a series of actions and develop a decision-taking algorithm, based on some action/reward model*
- ***Inference****: once trained, the model can be applied to other datasets*





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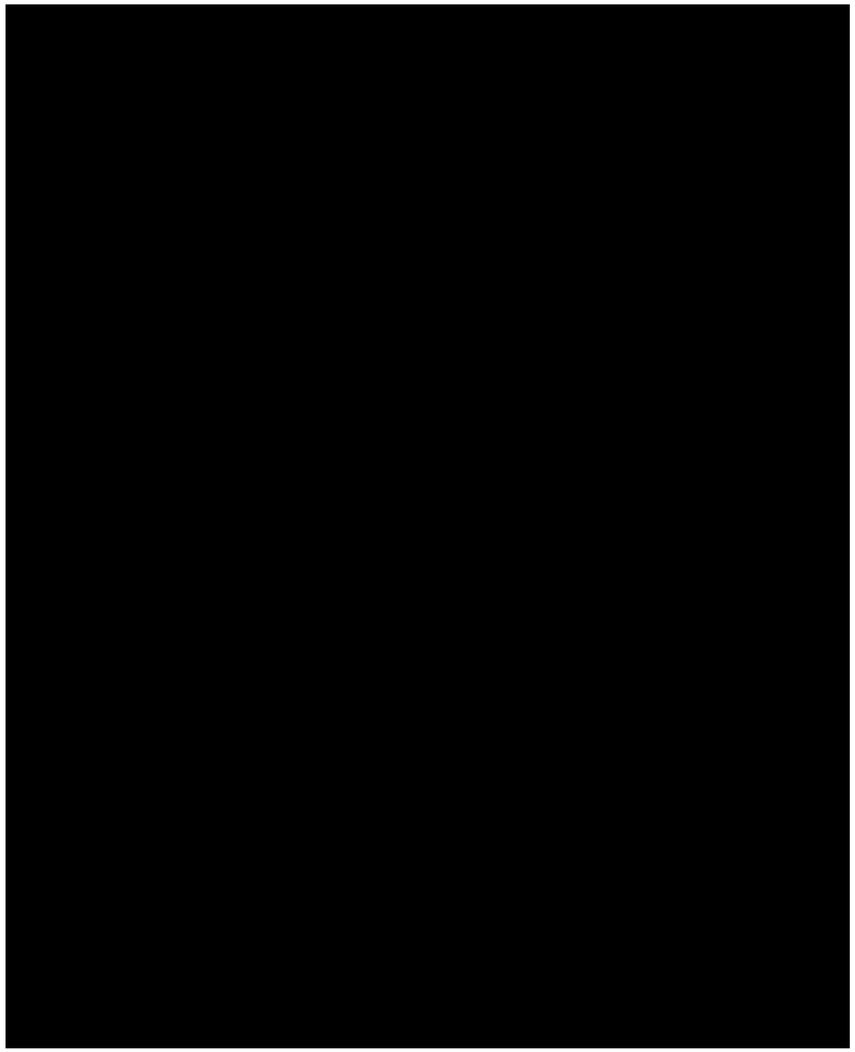
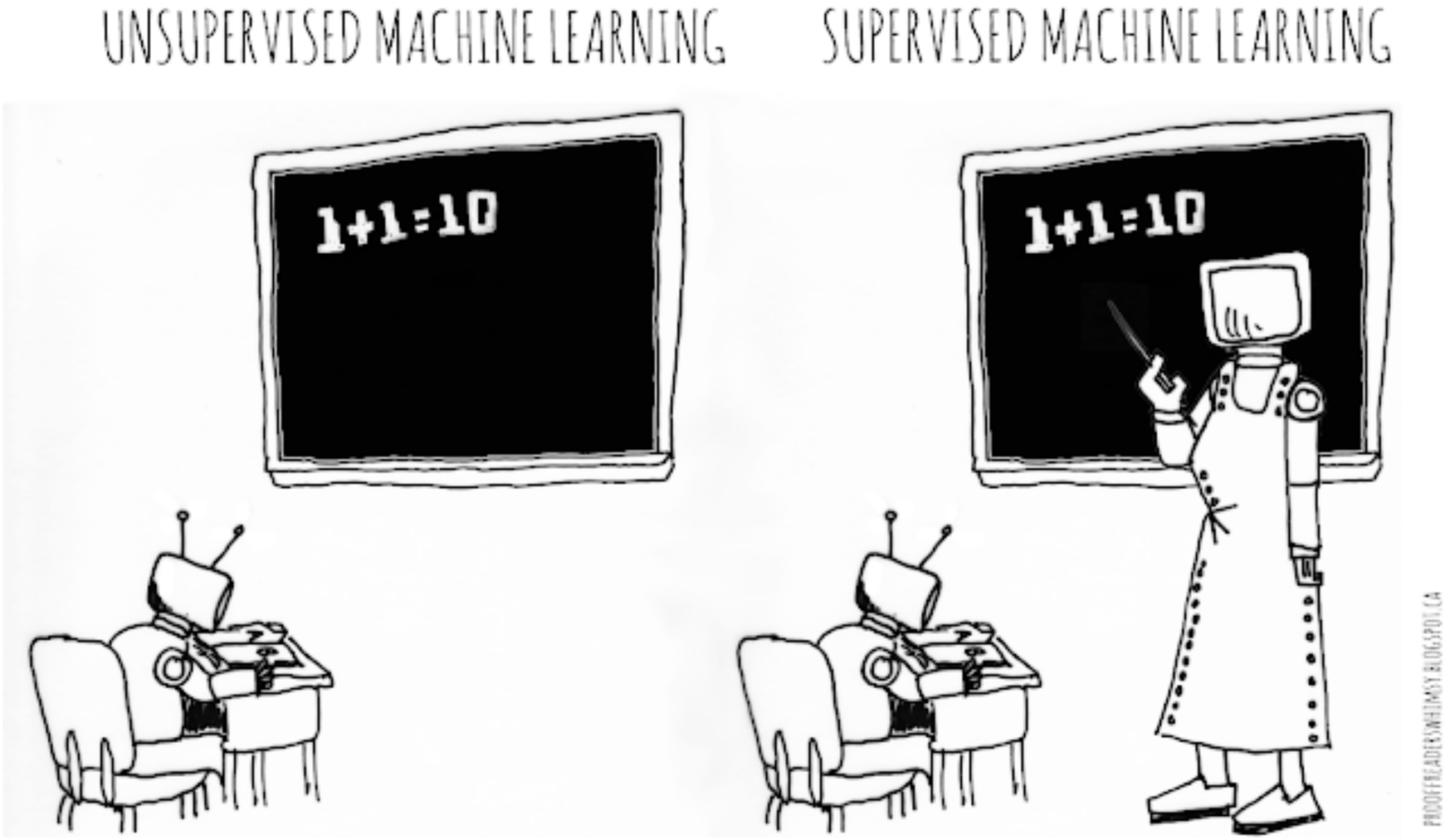
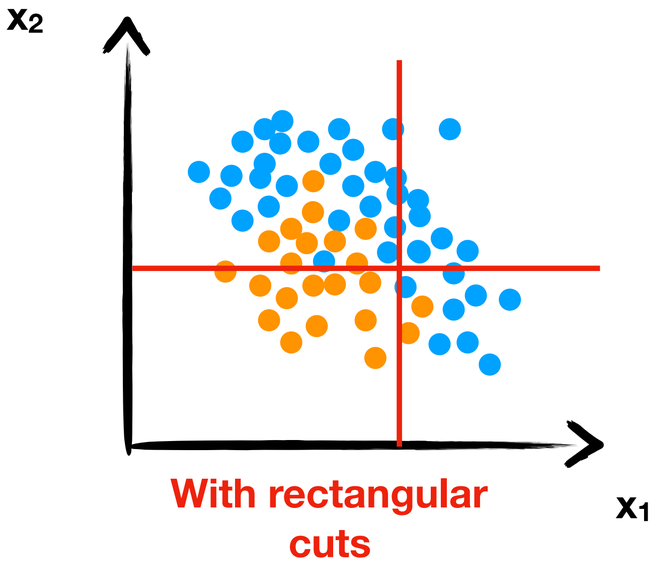


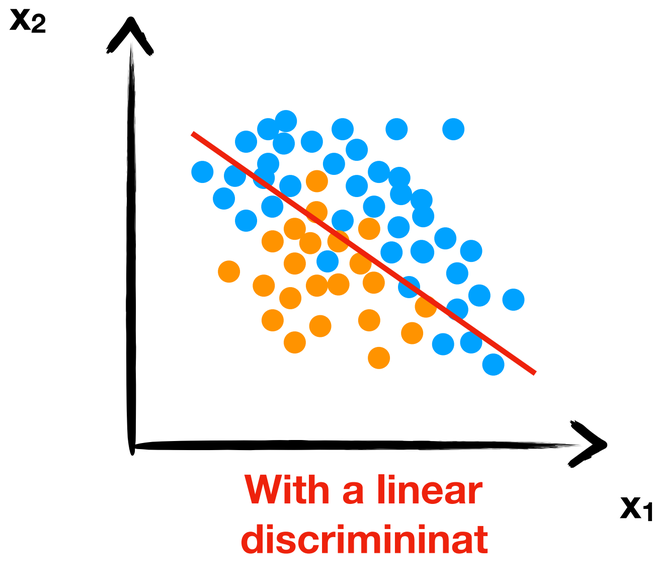


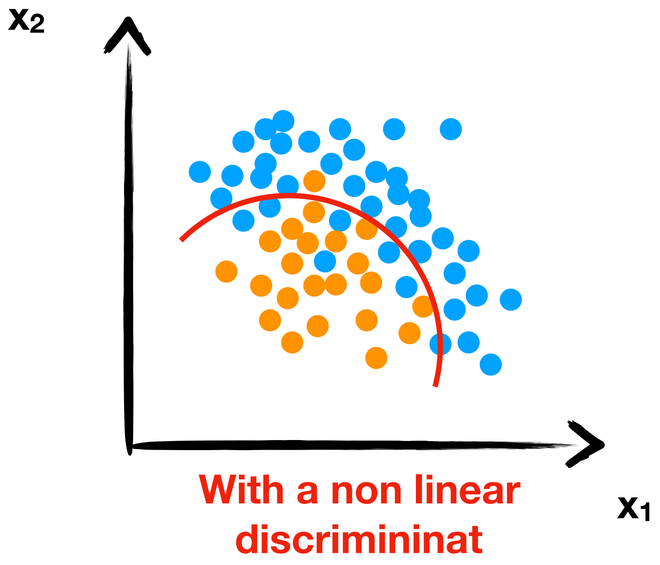
Supervised Learning

A simple example: S vs B selection

- *Define a selection to separate the signal from the background*

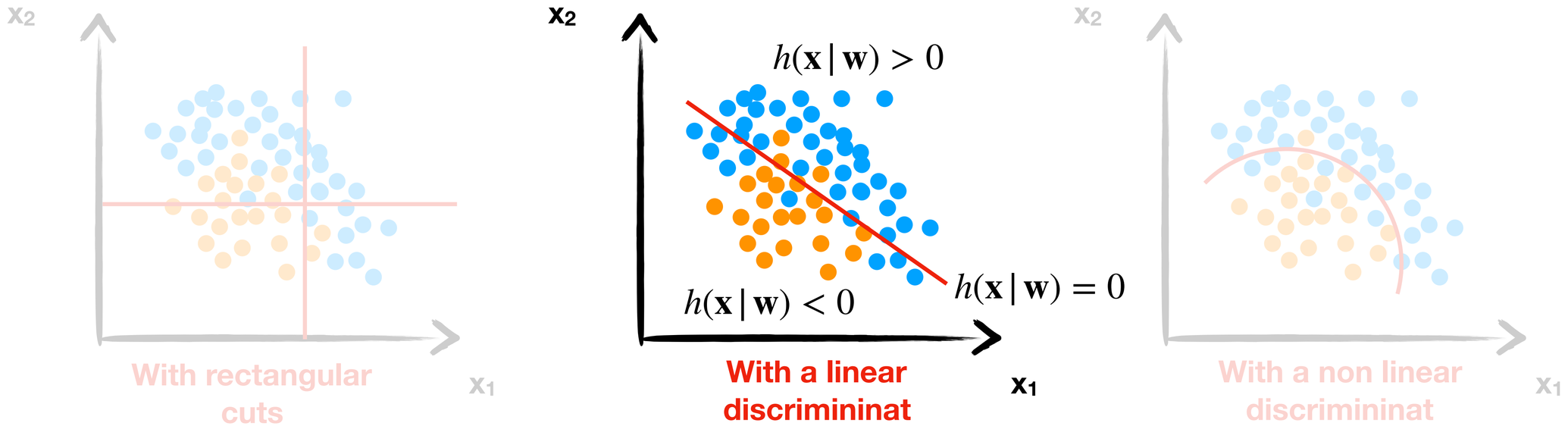






A simple example: S vs B selection

- *Define a selection to separate the signal from the background*



- *Define a decision boundary which gives optimal separation*

$$h(\mathbf{x}\,|\,\mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} = 0$$

(Signed) distance between x and the boundary plane

Logistic Regression

- Give as input pairs of inputs and outputs:

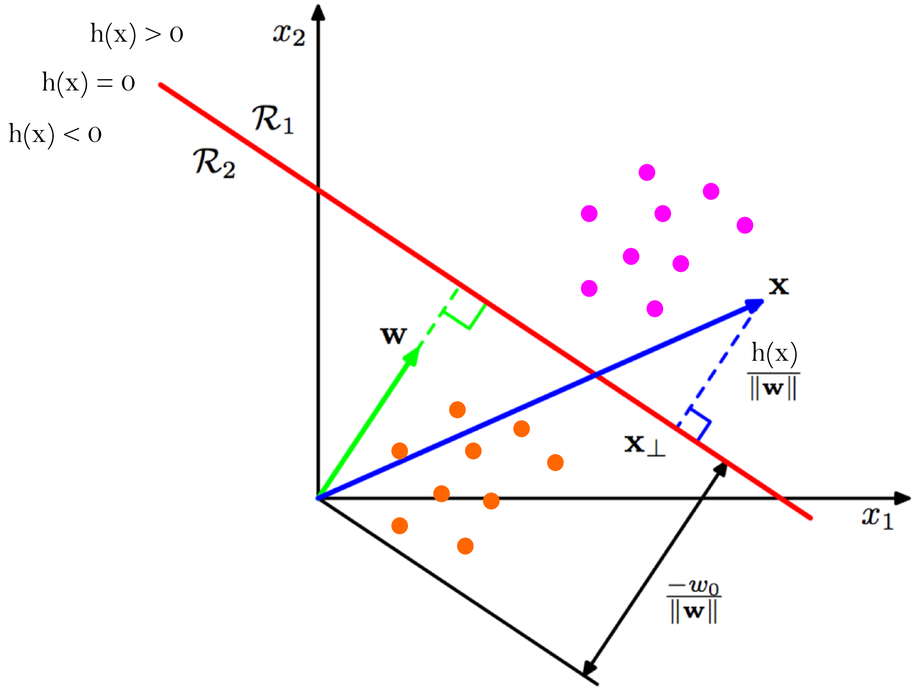
$$x_i \in \mathbb{R}^n \qquad y_i = \{0,1\}$$

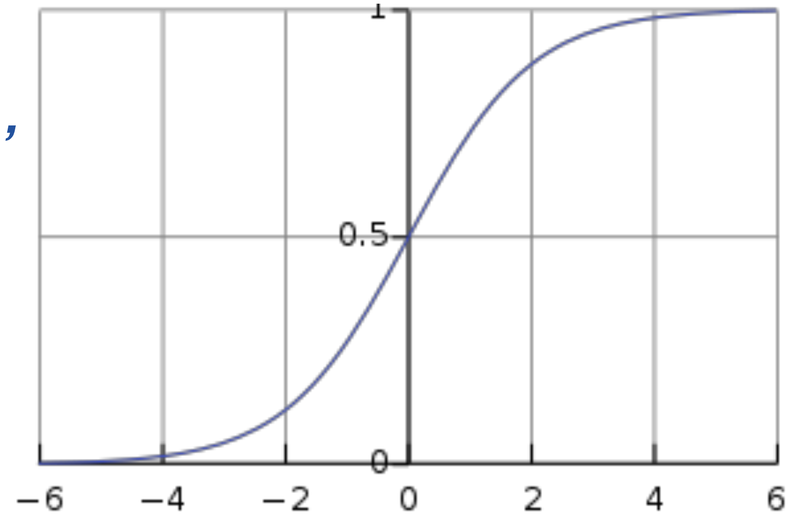
- Model the probability of x to be signal (y=1) as

$$p(y=1\,|\,x) = \frac{1}{1+e^{-\mathbf{w}^{\mathrm{T}}\mathbf{x}}}$$

  - The larger (and positive) the distance the closer p to 1
  - The larger (and negative) the distance, the closer p to 0

- We can choose the plane such that we maximise the probability of the signal and minimise that of the background





Bernoulli's problem

- *Bernoulli's problem: probability of a process that can give 1 or 0*
- *The corresponding likelihood is (as usual) the product of the probabilities across the events*
- *Maximizing the likelihood corresponds to minimizing the -logL*
- *Minimizing the -logL corresponds to minimise the binary cross entropy*
- *How do we minimise it?*

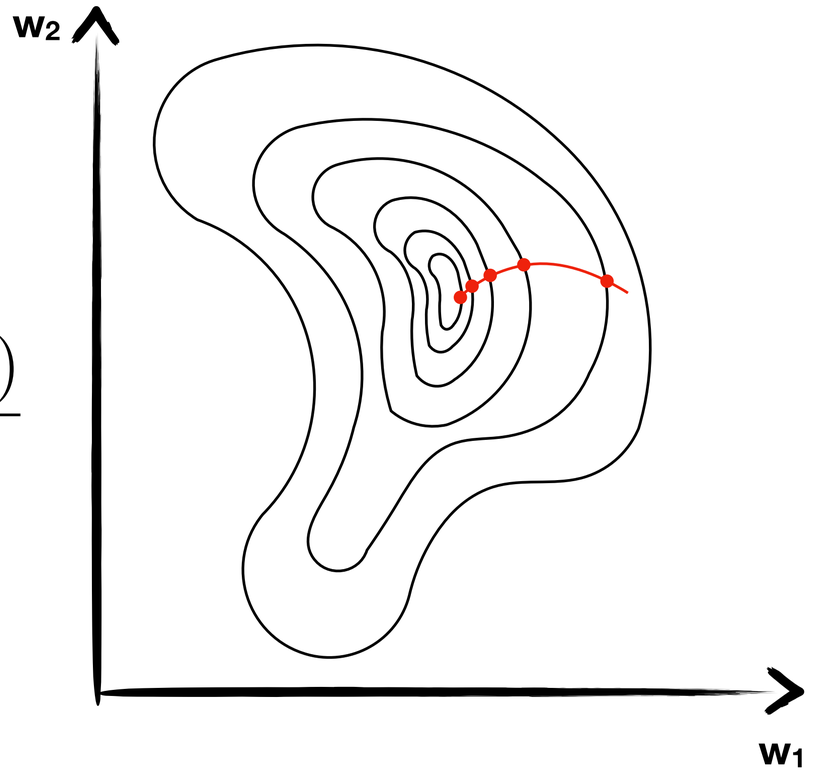
$$\mathscr{L} = \prod_i p_i^{x_i}(1-p_i)^{1-x_i}$$

$$-\log \mathscr{L} = -\log[\prod_i p_i^{x_i}(1-p_i)^{1-x_i}]$$

$$= -\sum_i \left[x_i \log p_i + (1-x_i)\log(1-p_i)\right]$$

Gradient Descent

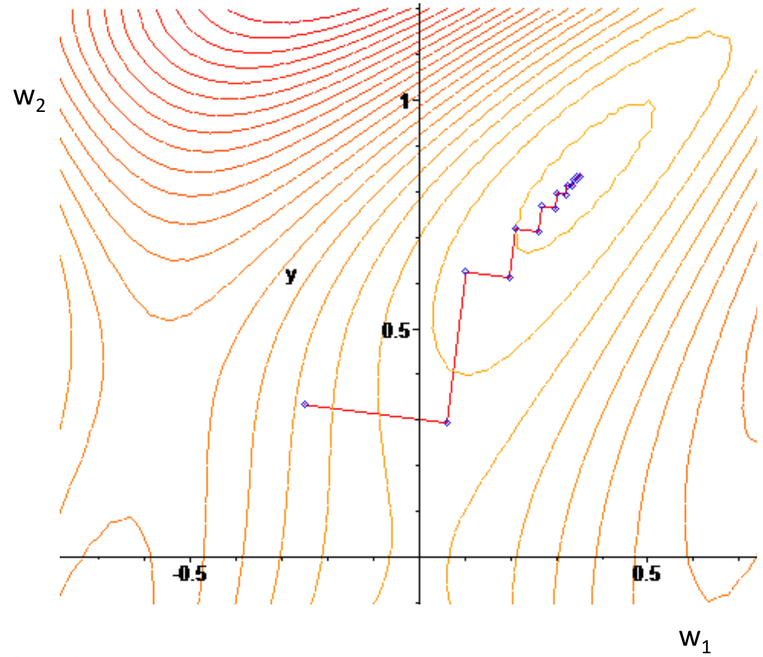
- *Gradient Descent is a popular minimisation algorithm*
  - *Start from a random point*
  - *Compute the gradient wrt the model parameters* $\frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$
  - *Make a step of size* η *(the* ***learning rate****) towards the gradient direction*
  - *Update the parameters of the mode accordingly*
  - *Effective, but computationally expensive (gradient over entire dataset)*

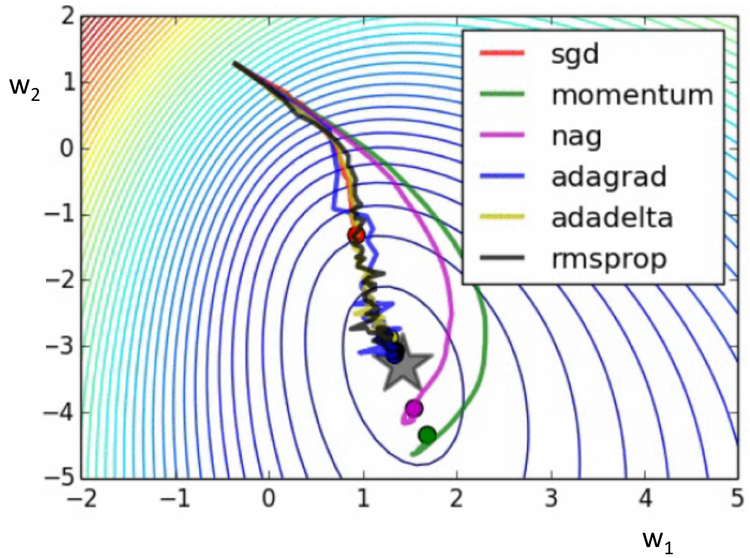


$$\mathbf{w}' \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$$

Stochastic Gradient Descent

- *Make the minimisation more computationally efficient by*
  - *Compute gradient on a small batch of events (faster & parallelisable, but noisy)*
  - *Average other the batches to reduce noise*
  - *BEWARE: better scalability come at the cost of (sometimes) not converging*
  - *Many recipes exist to prevent that, by playing with the algorithm setup (e.g., learning rate)*





Example: regression & MSE

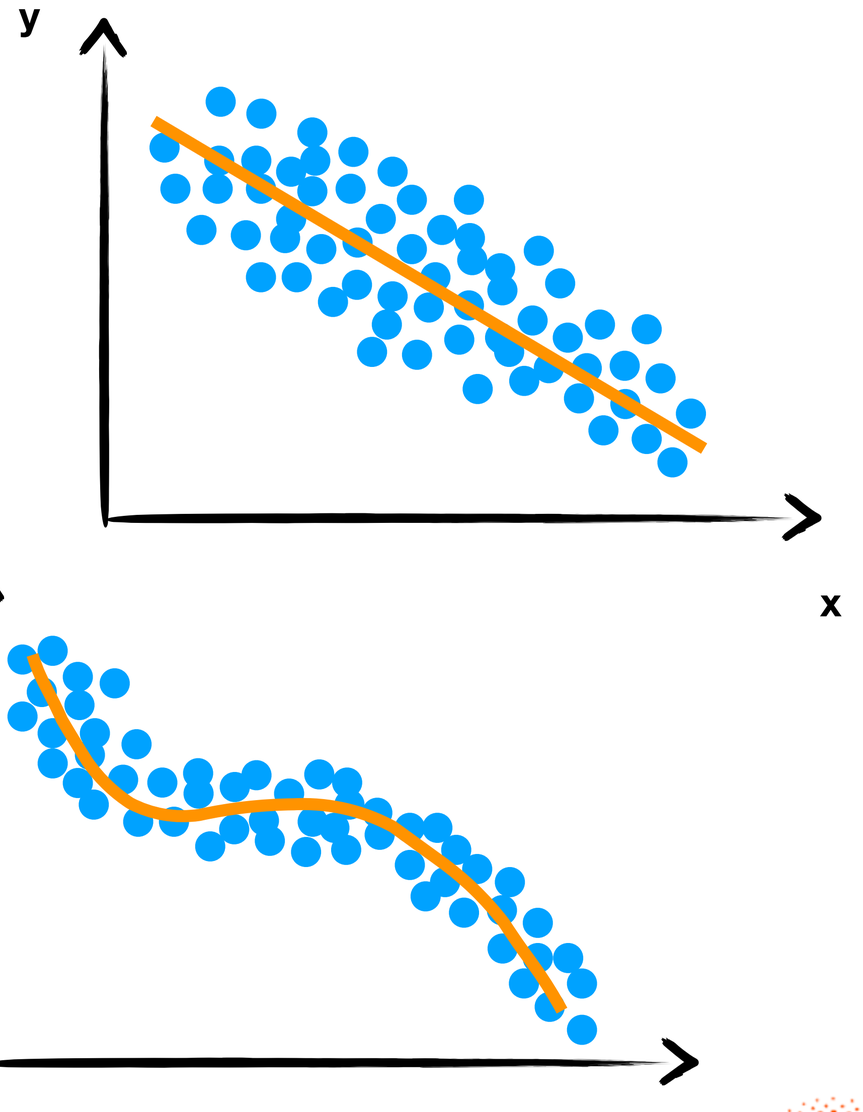
- Given a set of points, find the curve that goes through them
  - Can be a linear model

$$y_i = ax_i + b$$

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

$$y_i = a\,\phi(x_i) + b$$

New feature, “engineered” from the input features



Example: regression & MSE

- Take some model (e.g., linear)

$$h(x_i \mid a, b) = ax_i + b$$

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

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

- Assume that the resolution σ is fixed

- Write down the likelihood

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

Example: regression & MSE

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

$$argmin[-2\log\mathscr{L}] = argmin\Big[-2\log[\prod_i \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - h(x_i))^2}{2\sigma^2}}]\Big]$$

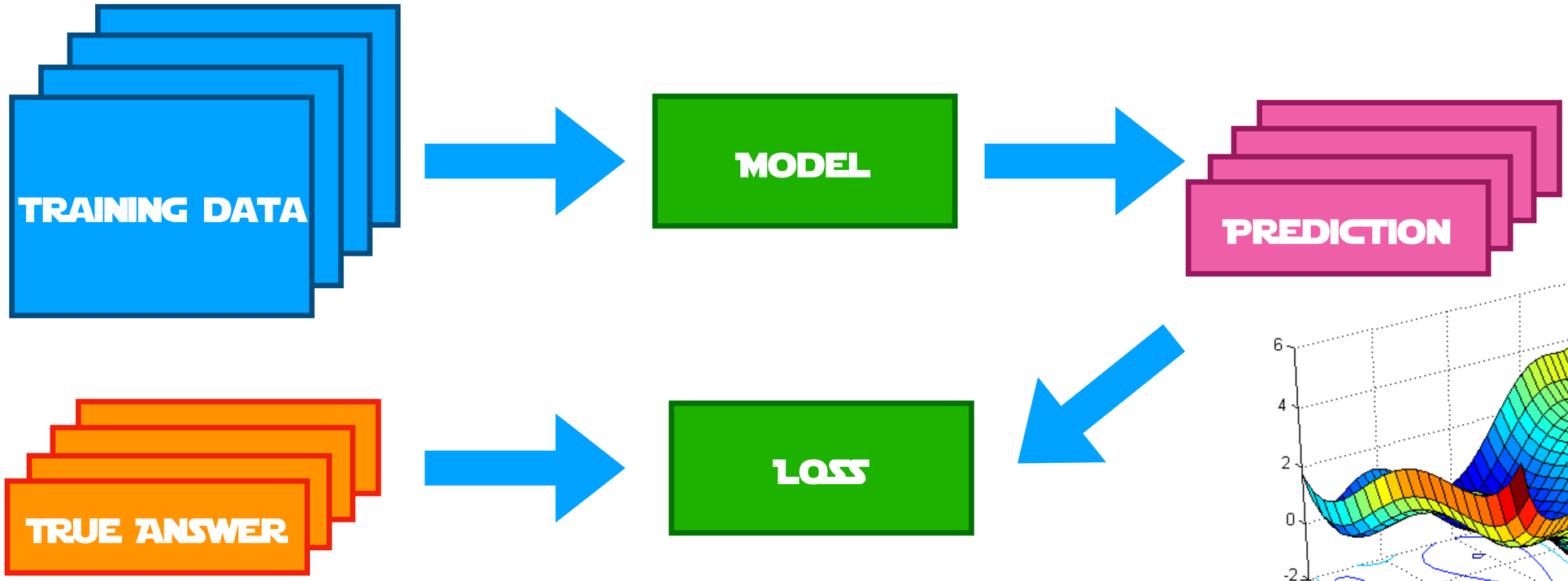
$$= argmin\Big[\sum_i \frac{(y_i - h(x_i))^2}{\sigma^2}\Big] = argmin\Big[\sum_i (y_i - h(x_i))^2\Big] = MSE$$

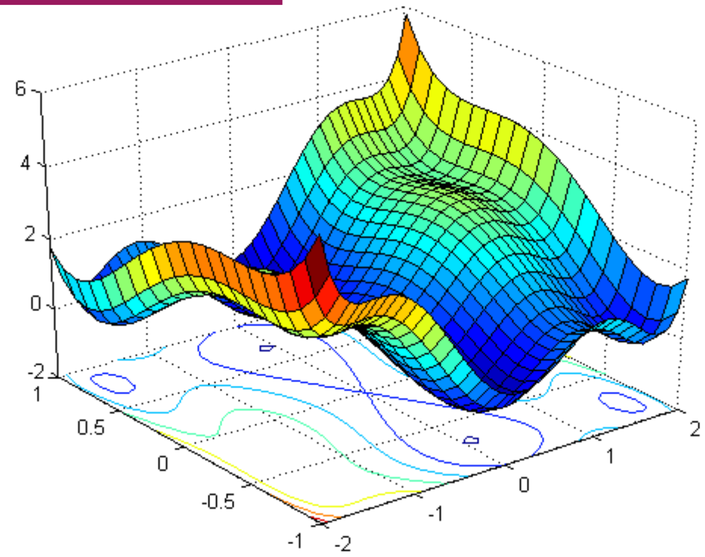
- *MSE is the most popular loss function when dealing with continuous outputs. We will use it a few times in the next days*

- ***BE AWARE OF THE UNDERLYING ASSUMPTION:*** *if you are using MSE, you are implicitly assuming that your y are Gaussian distributed, with fixed RMS*

- *What is the RMS is not a contact?*

Supervised Learning in a nutshell





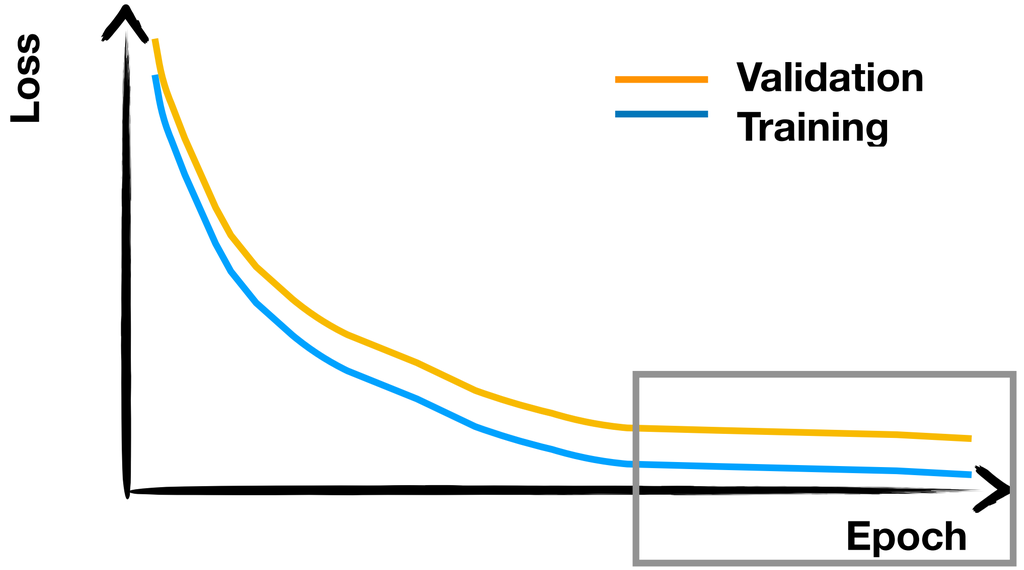
- *A training dataset* ***x***
- *A target y*
- *A model to go from* ***x*** *to y*
- *A loss function quantifying how wrong the model is*
- *A minimisation algorithm to find the model h that corresponds to the minimal loss*

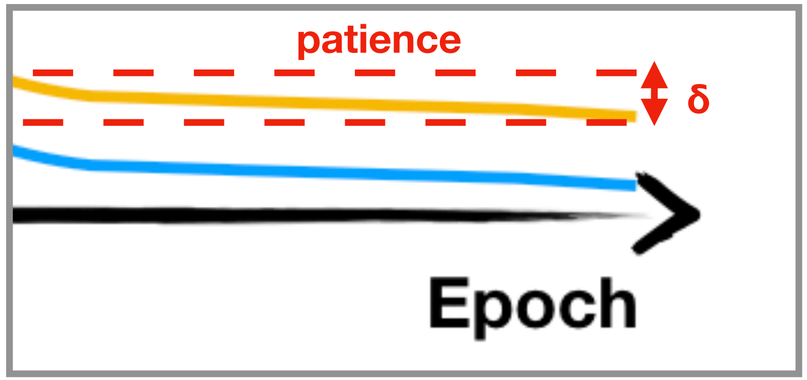
Training in practice

- *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 in practice

- Train across multiple epochs
  - 1 epoch = going once through the full dataset
- Use small batches (64, 128, etc)
- 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)

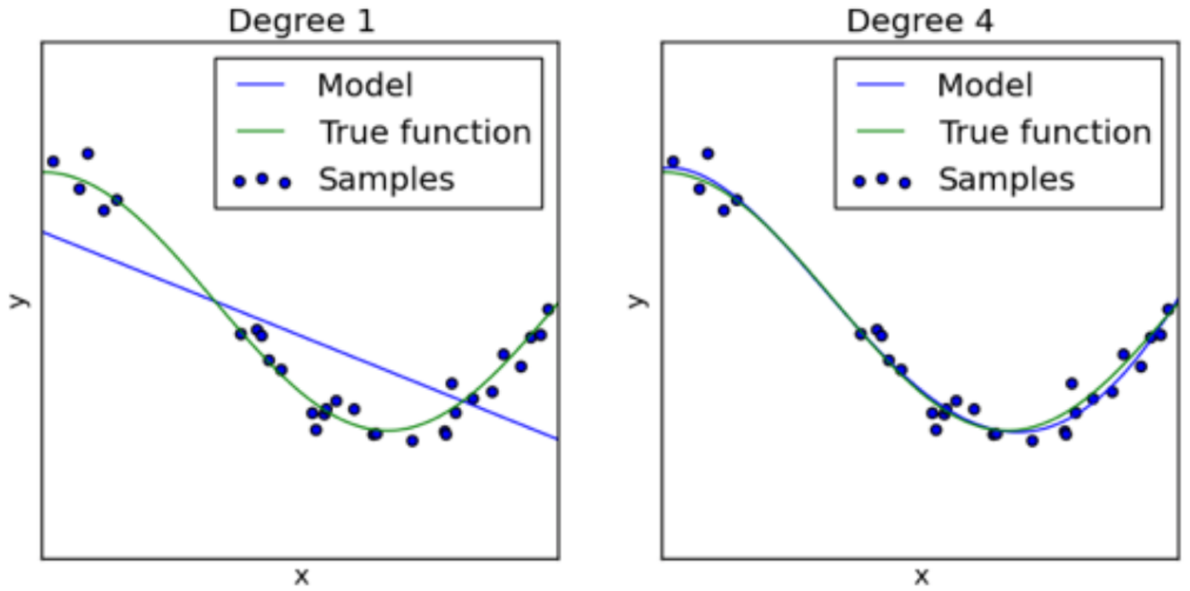


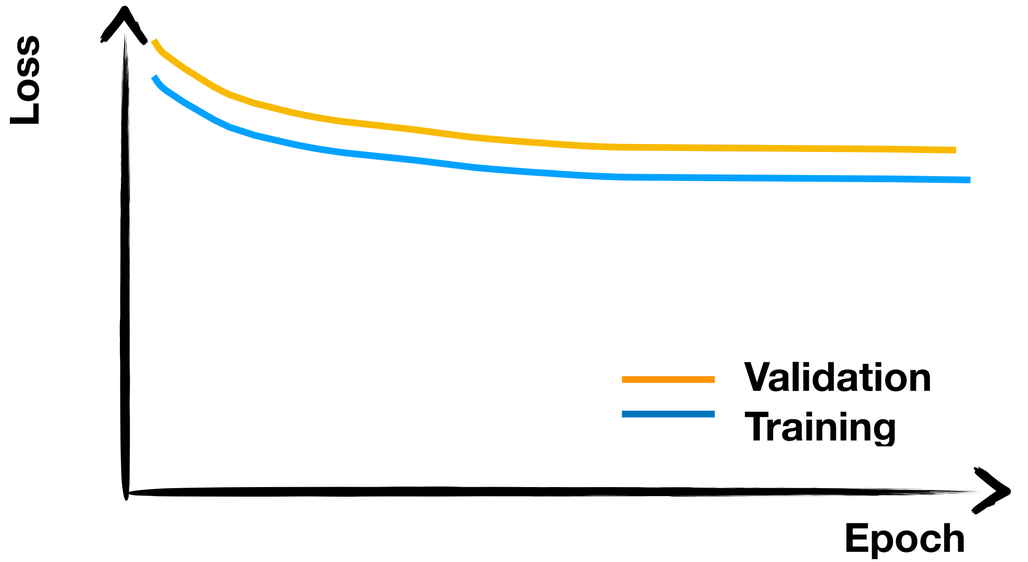


EARLY TOPPING: stop the train if the validation loss didn't change more than δ in the last n epochs (patience)

What can go wrong: underfitting

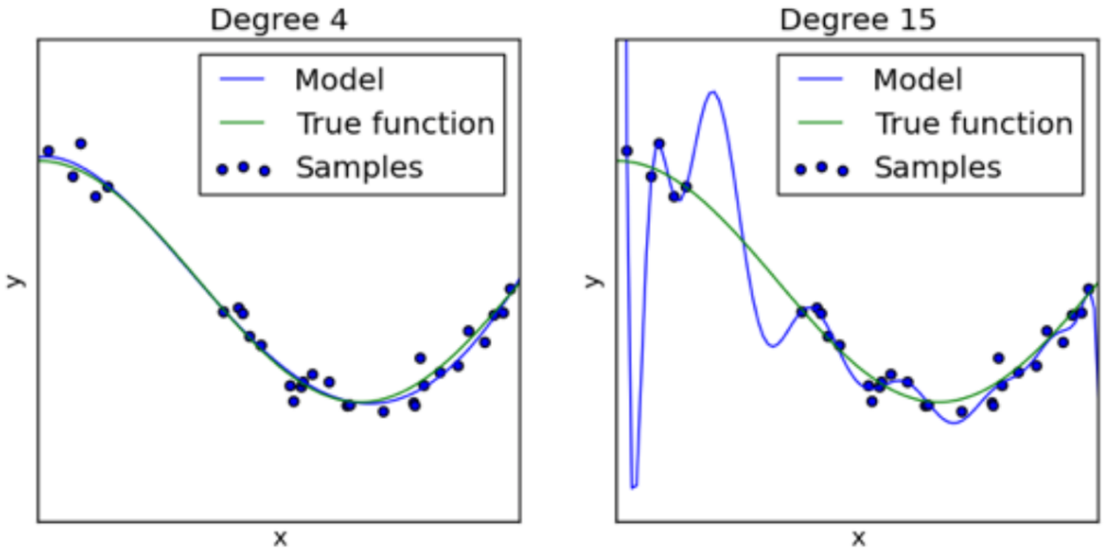
- *If your model has not enough flexibility, it will not be able to describe the data*
- *The training and validation loss will be close, but their value will not decrease*
- *The model is said to be underfitting, or being **biased***

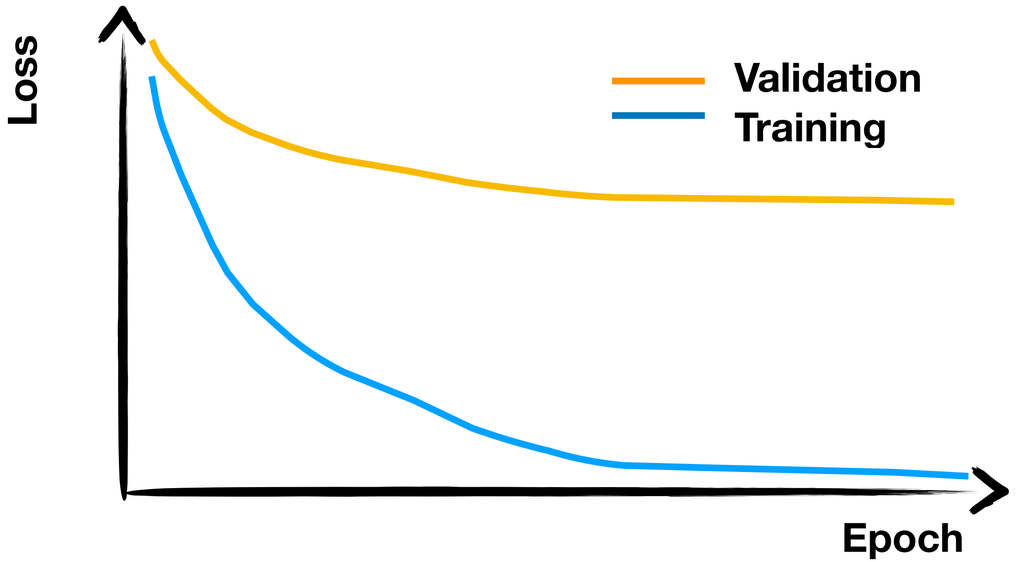




What can go wrong: overfitting

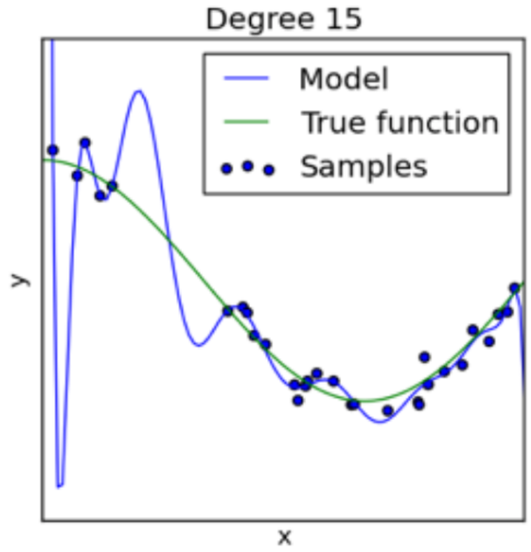
- *Your model can learn too much of your training dataset*
  - *e.g., its statistical fluctuations*
- *Such an overfitted model would not generalise*
- *So, its description of the validation dataset will be bad (i.e., **the mode doesn't generalise**)*
- *This is typically highlighted by a divergence of the training and validation loss*

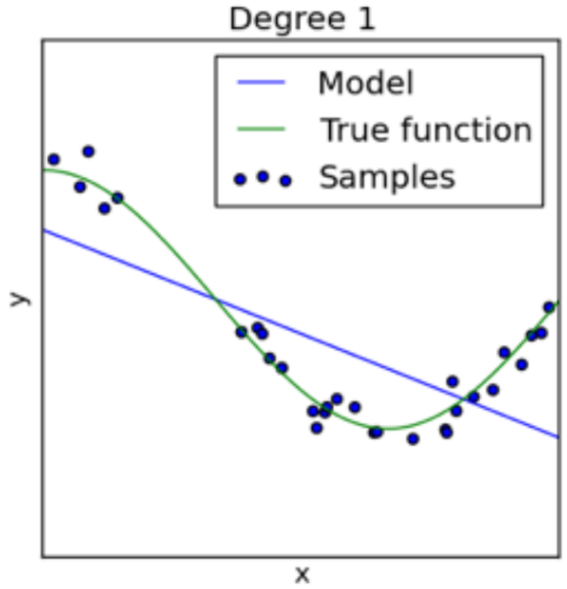




The Bias vs Variance tradeoff

- ***A model would underfoot it too simple:*** *it will not be able to model the mean value*
- ***A model would overfit it too complex:*** *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)*





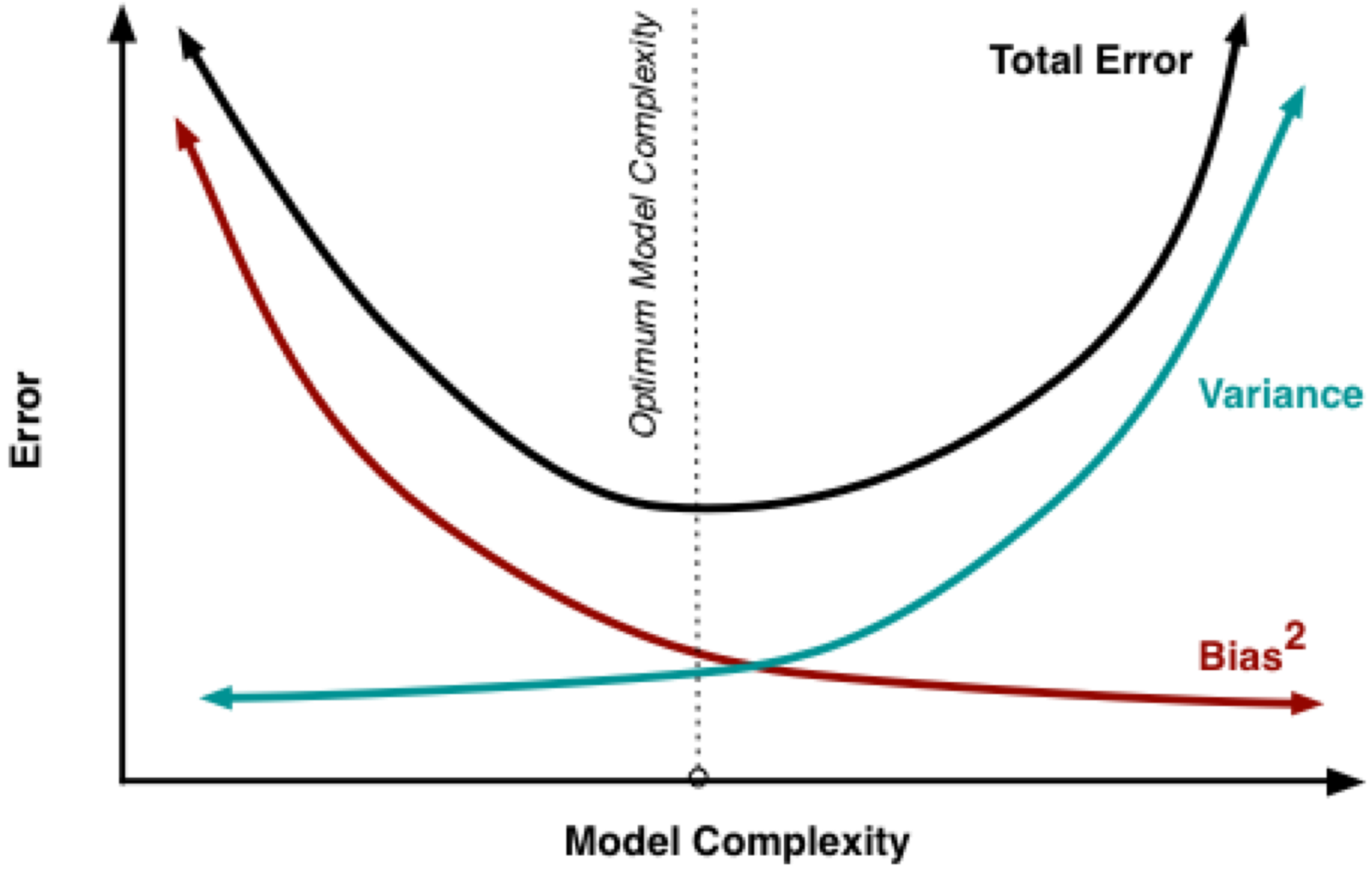
The Bias vs Variance tradeoff

- *Generalization error can be written as the sum of three terms:*
  - *The intrinsic statistical noise in the data*
  - *the systematic error (bias wrt the mean)*
  - *the variance of the prediction around the mean*

$$E[(y - h(x))^2] = E[(y - \bar{y})^2] + (\bar{y} - \bar{h}(x))^2 + E[(h(x) - \bar{h}(x))^2]$$

Noise **Bias Squared** **Variance**

The Bias vs Variance tradeoff



Regularization

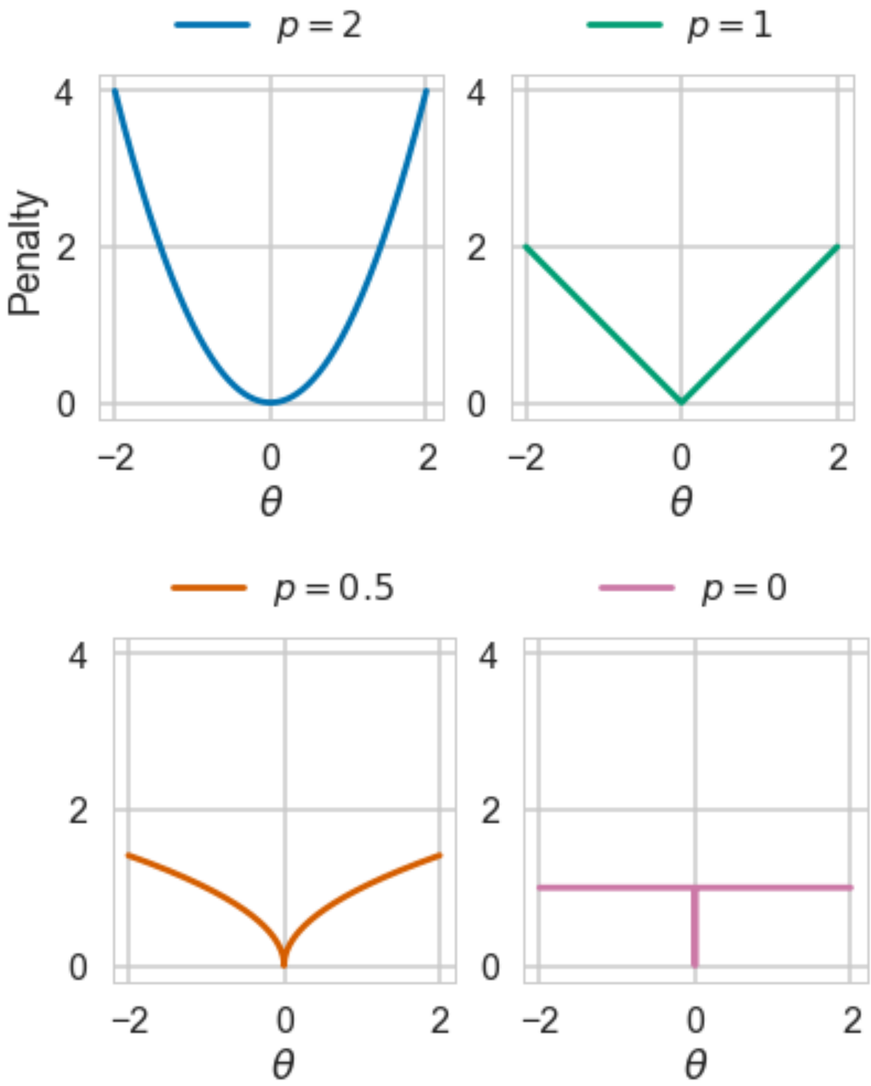
- *Model complexity can be "optimized" when minimizing the loss*
  - *A modified loss is introduced, with a penalty term attache to each model parameter*

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

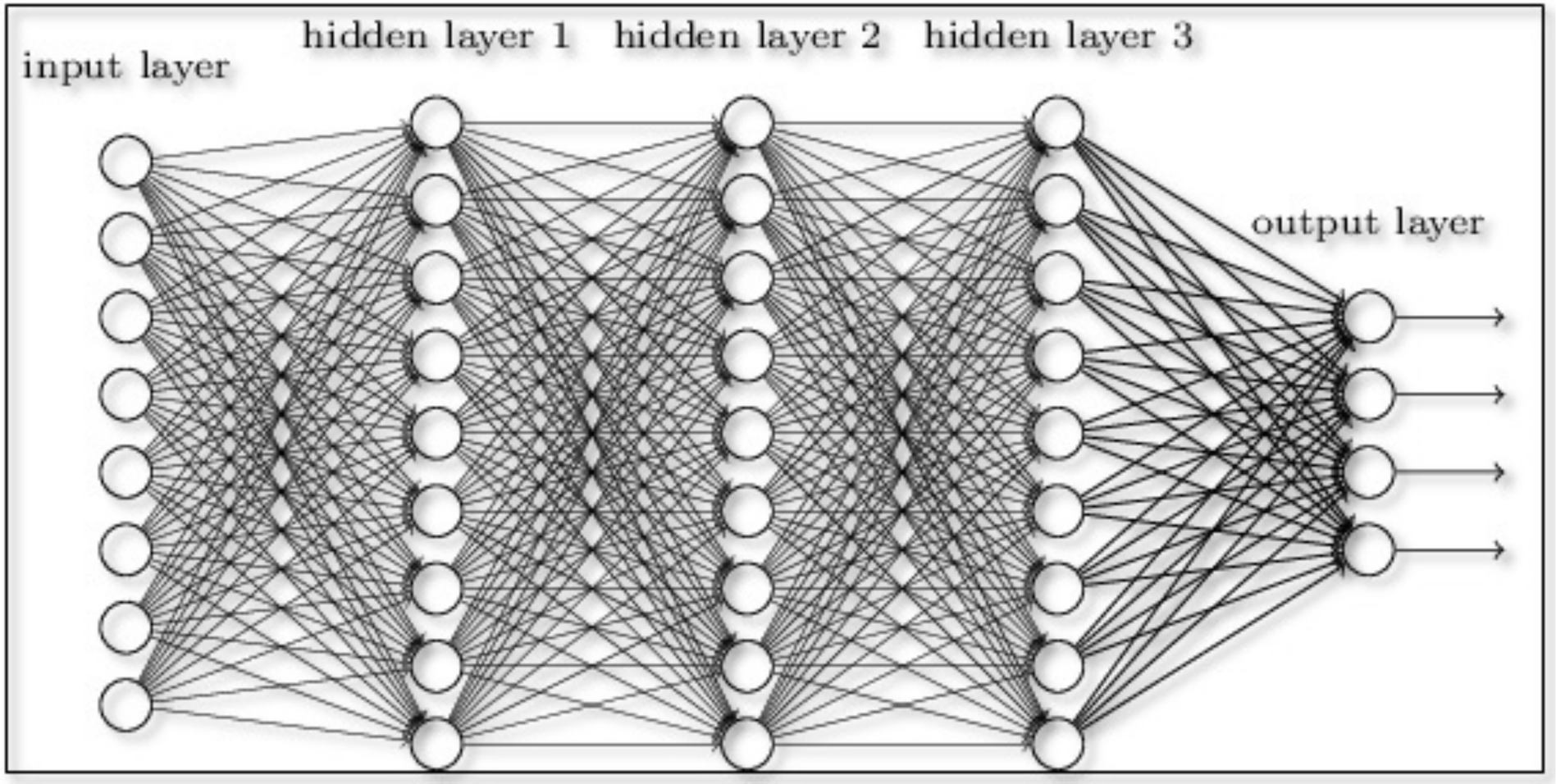
- *For instance, Lp regularisation*

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

- *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*



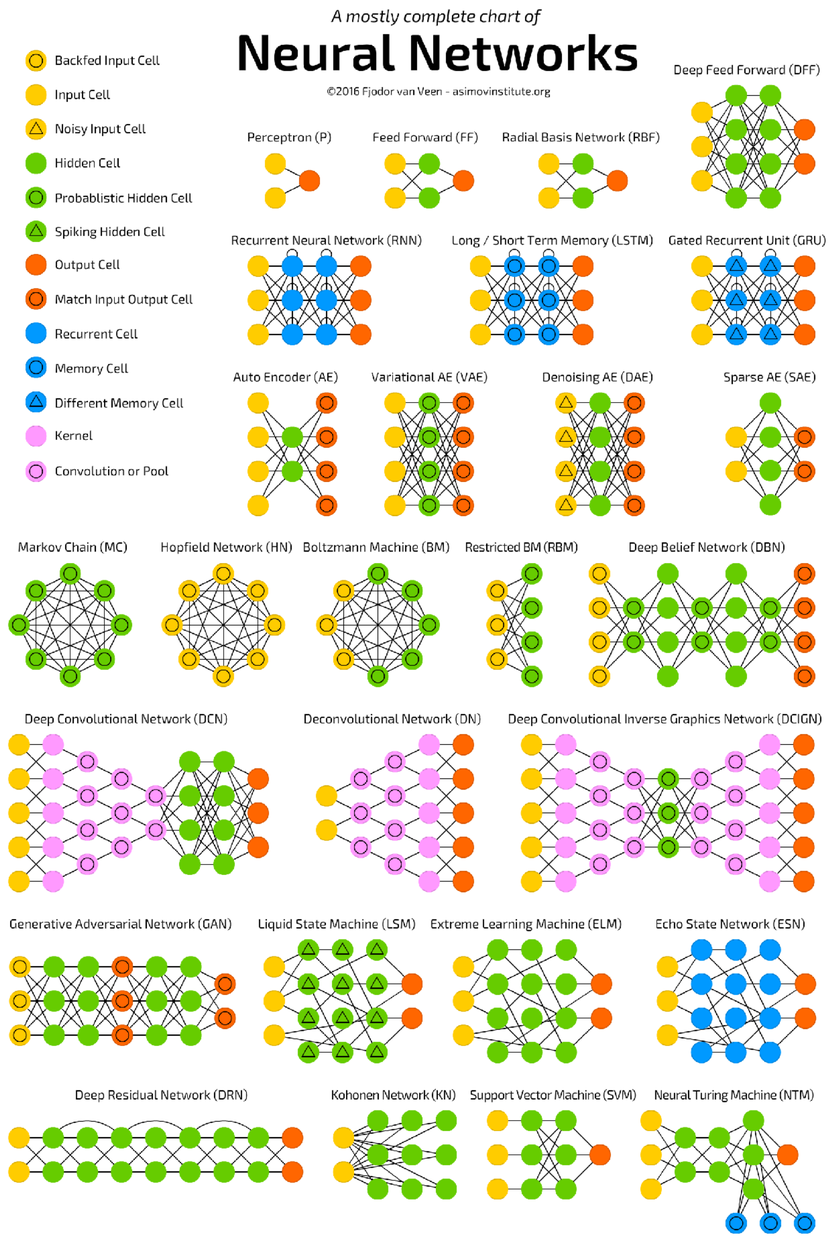
https://openreview.net/pdf?id=H1Y8hhg0b



Deep Learning

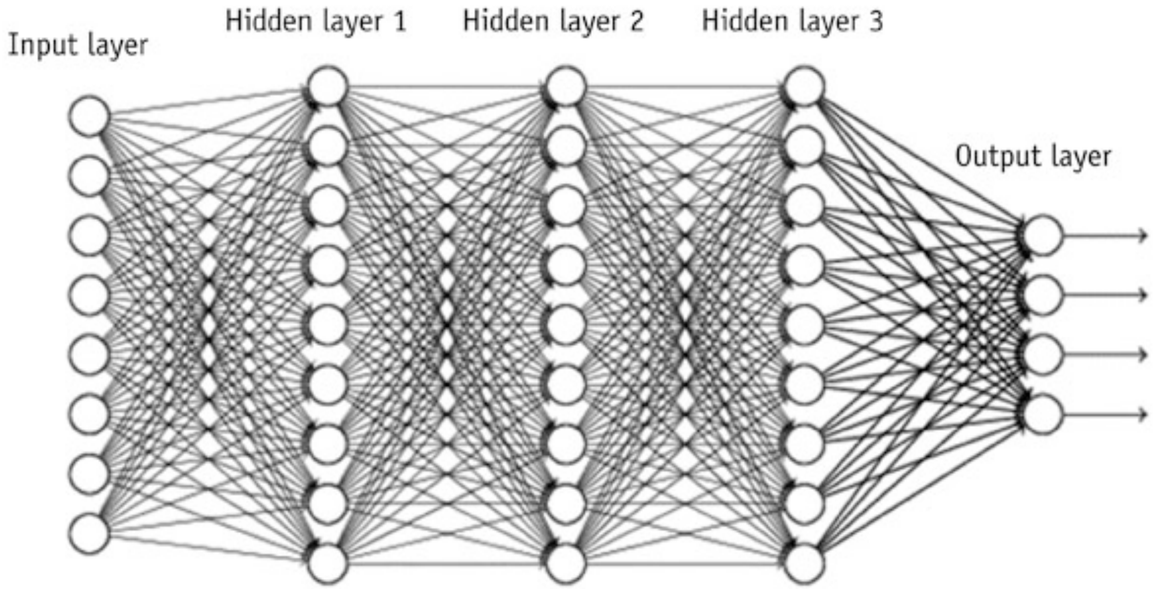
Neural Networks in a nutshell

- 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



Deep Neural Networks

- *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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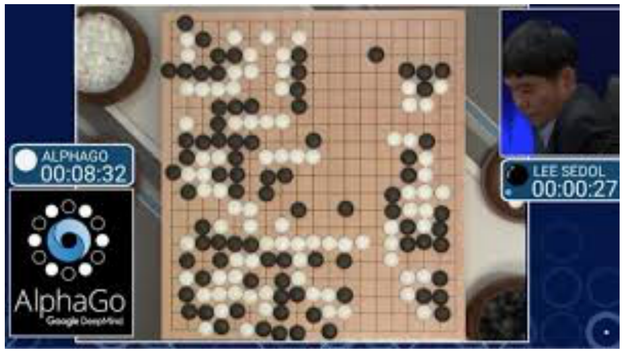
What is DL used for

Image processing

text/sound processing



Reinforcement Learning

Everything is a Recommendation

Over 75% of what people watch comes from our recommendations

Recommendations are driven by **Machine Learning**

NETFLIX

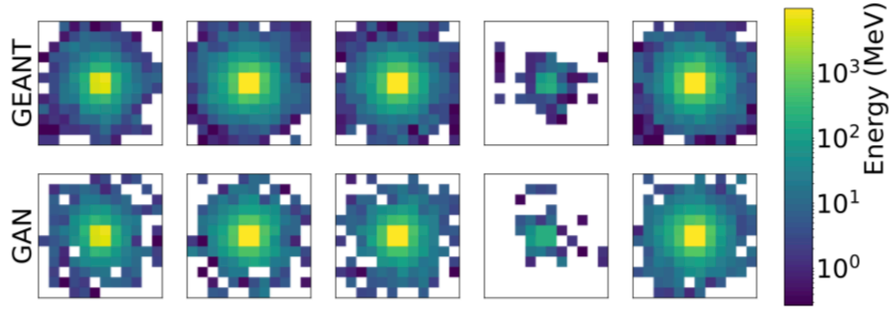
6

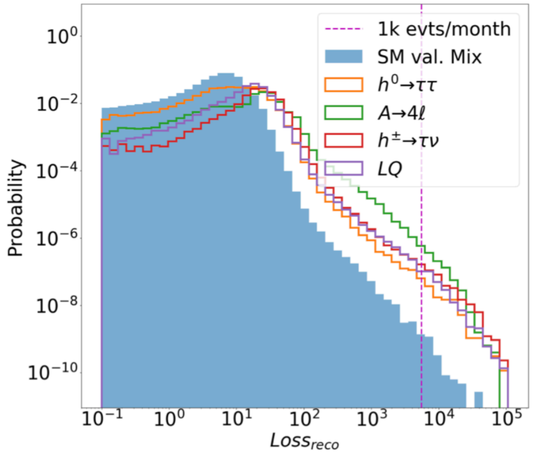
Clustering

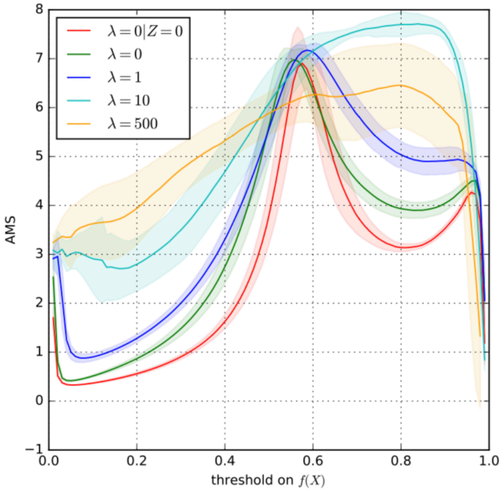
European Research Council

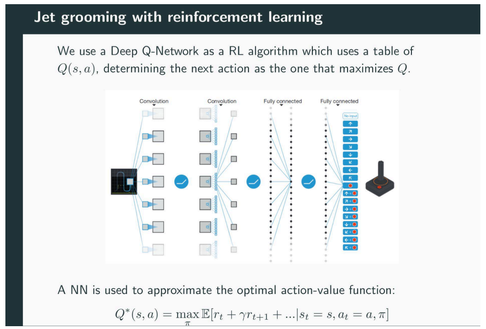
DL, HEP, and new opportunities

- *Event Generation with generative models*
- *Anomaly Detection to search for new Physics*
- *Adversarial training for systematics*
- *Reinforcement learning for jet grooming*
- …



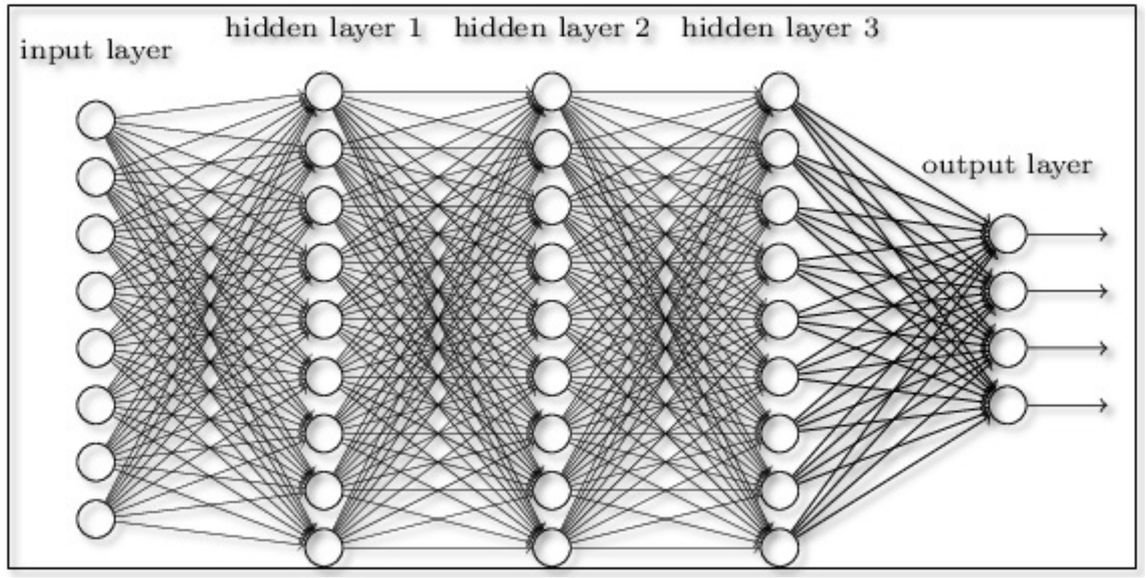






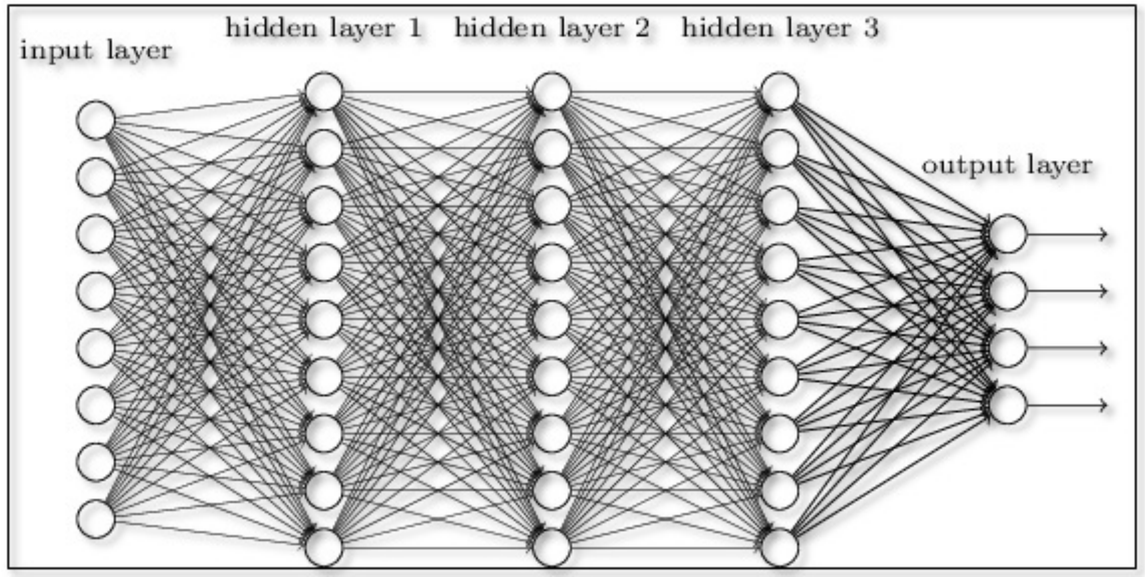
Feed-Forward NNs

- 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



The role of a network node

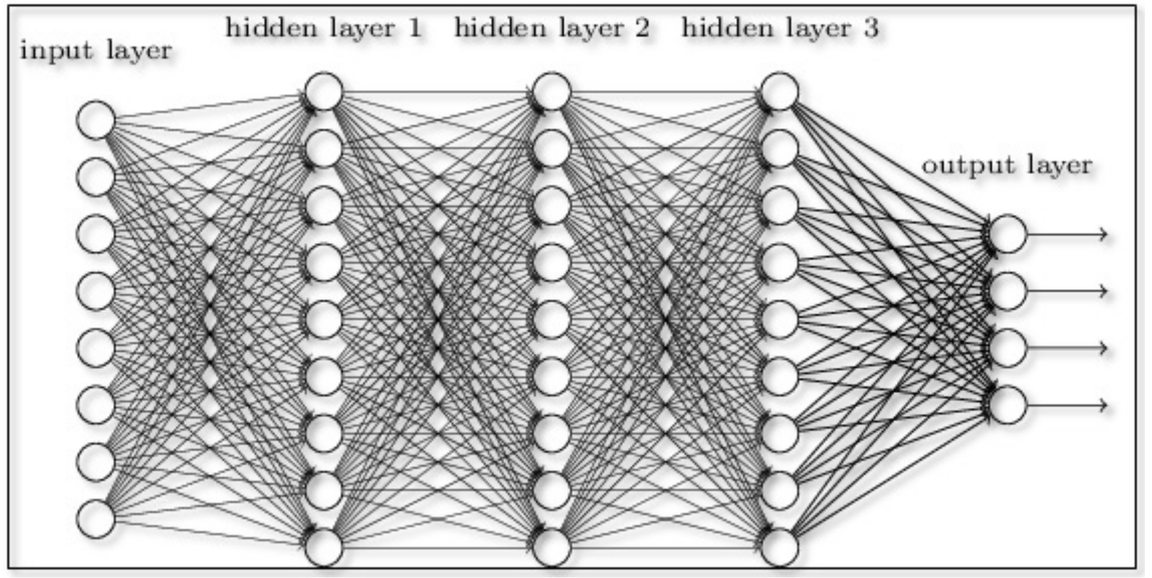
- **Each input is multiplied by a weight**
- The weighted values are summed
- A bias is added
- The result is passed to an activation function



$$w_{ij}x_j$$

The role of a network node

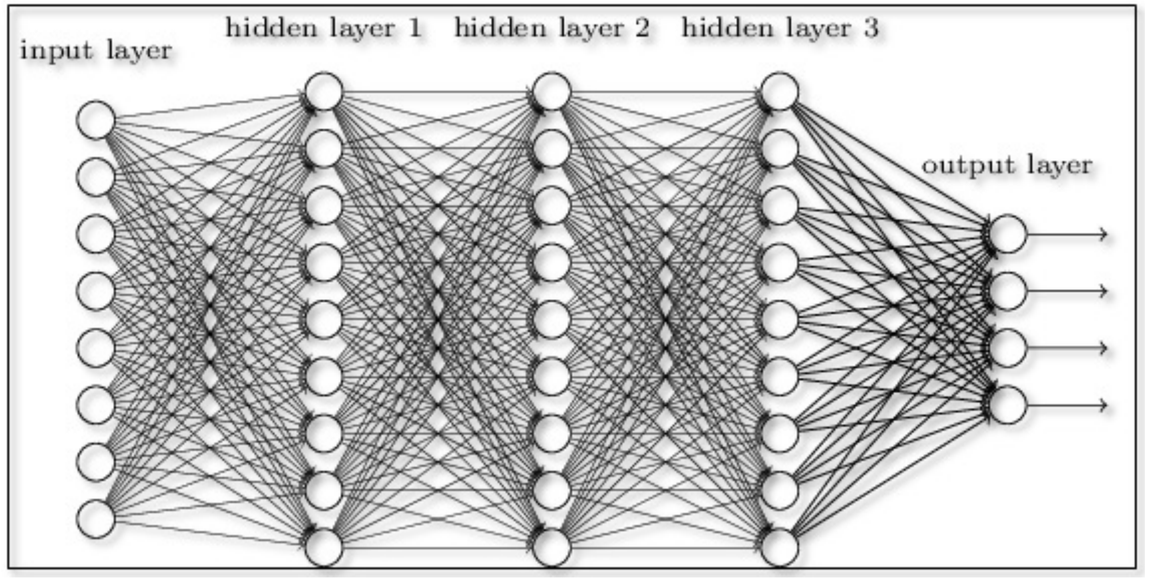
- Each input is multiplied by a weight
- **The weighted values are summed**
- A bias is added
- The result is passed to an activation function



$$\Sigma_j w_{ij} x_j$$

The role of a network node

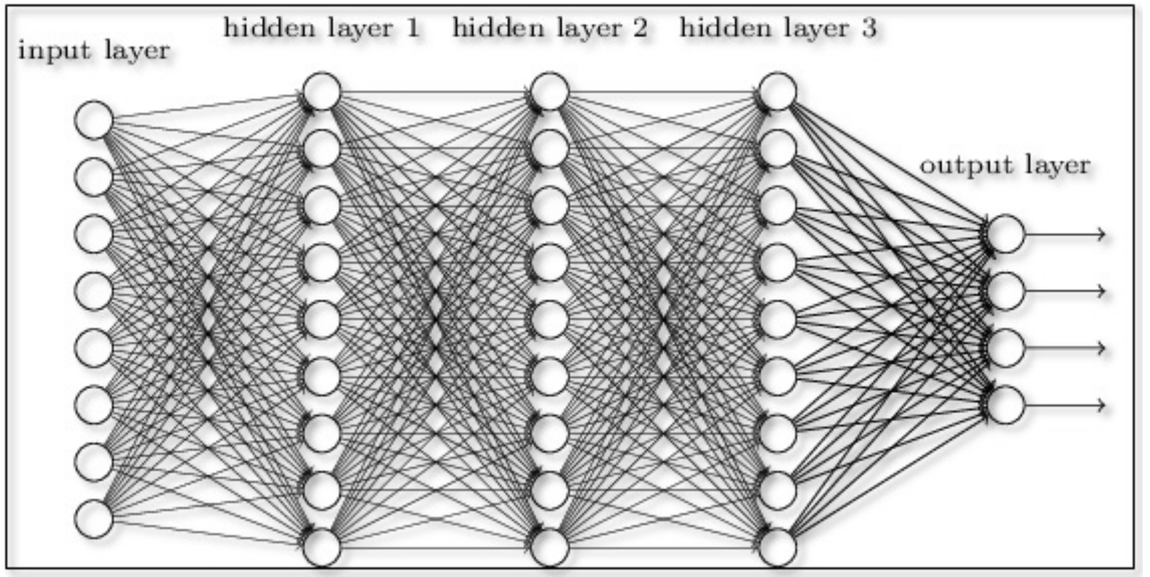
- Each input is multiplied by a weight
- The weighted values are summed
- **A bias is added**
- The result is passed to an activation function



$$\Sigma_j w_{ij} x_j + b_i$$

The role of a network node

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

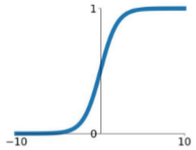


$$y_i = f(\Sigma_j w_{ij} x_j + b_i)$$

Activation Functions

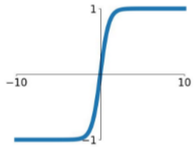
Sigmoid

$\sigma(x) = \frac{1}{1+e^{-x}}$



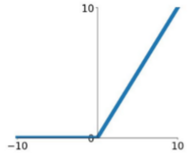
tanh

$\tanh(x)$



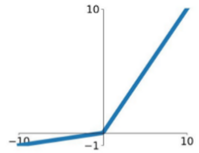
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

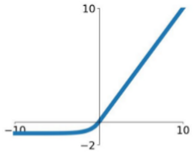


Maxout

$\max(w_1^T x + b_1, w_2^T x + b_2)$

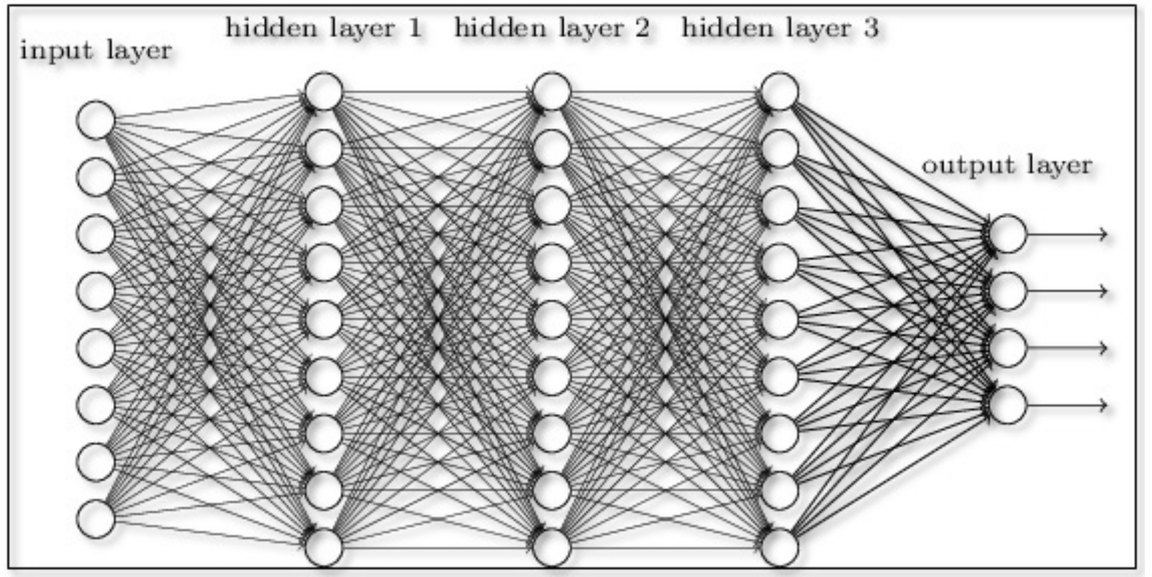
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



The full picture

- *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*

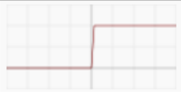
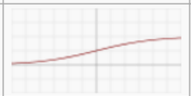
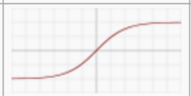
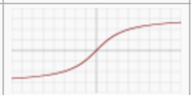
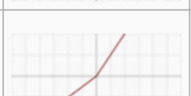


$$y_j = f^{(3)}(\Sigma_l w_{jl}^{(3)} f^{(2)}(\Sigma_k w_{lk}^{(2)} f^{(1)}(\Sigma_i w_{ki}^{(1)} x_i + b_k^{(k)}) + b_l^{(2)}) + b_j^{(3)})$$

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

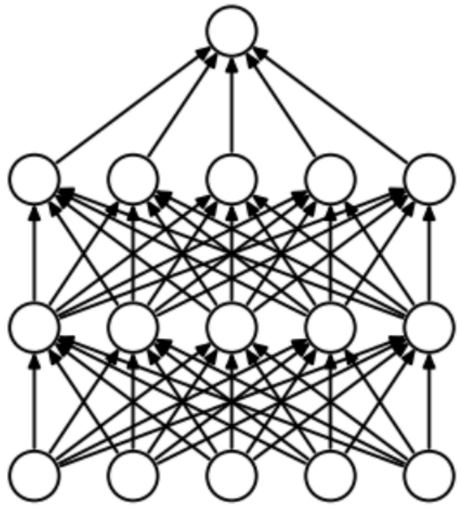
Activation Functions

- *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.)*

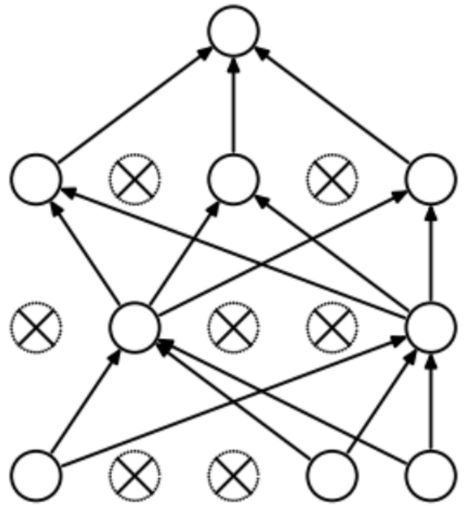
Name	Plot	Equation	Derivative
Identity		$f(x) = x$	$f'(x) = 1$
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ 1 & \text{for } x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$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

Dropout Layer

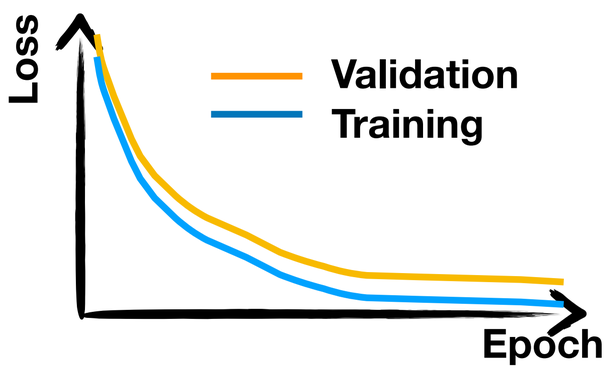
- *A special kind of layer, introduced for regularisation purpose*
- *Randomly drop links between neurons, with probability p*
- *The connections are re-established during the validation and inference steps*
- *Typical sign of it: invert hierarchy between training and validation loss*

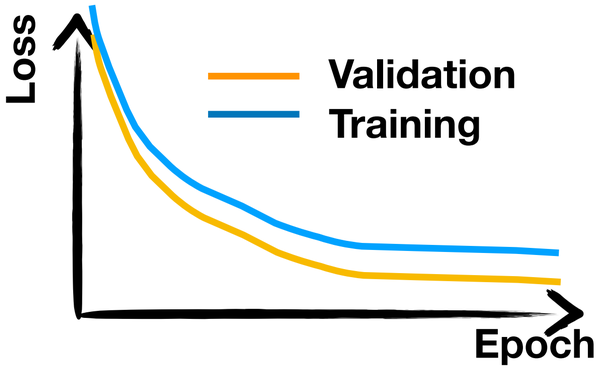


(a) Standard Neural Net



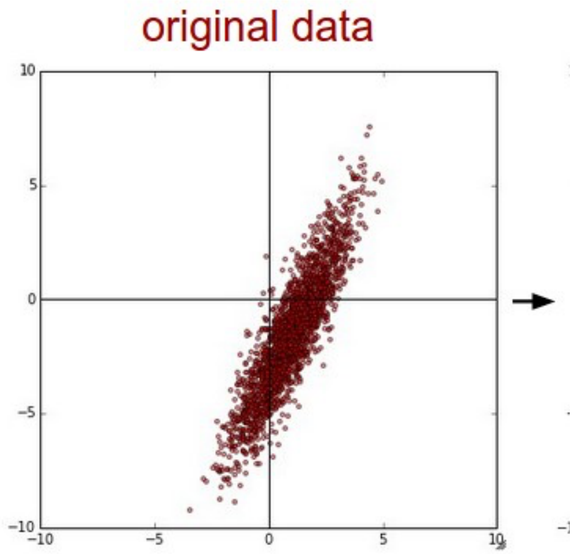
(b) After applying dropout.

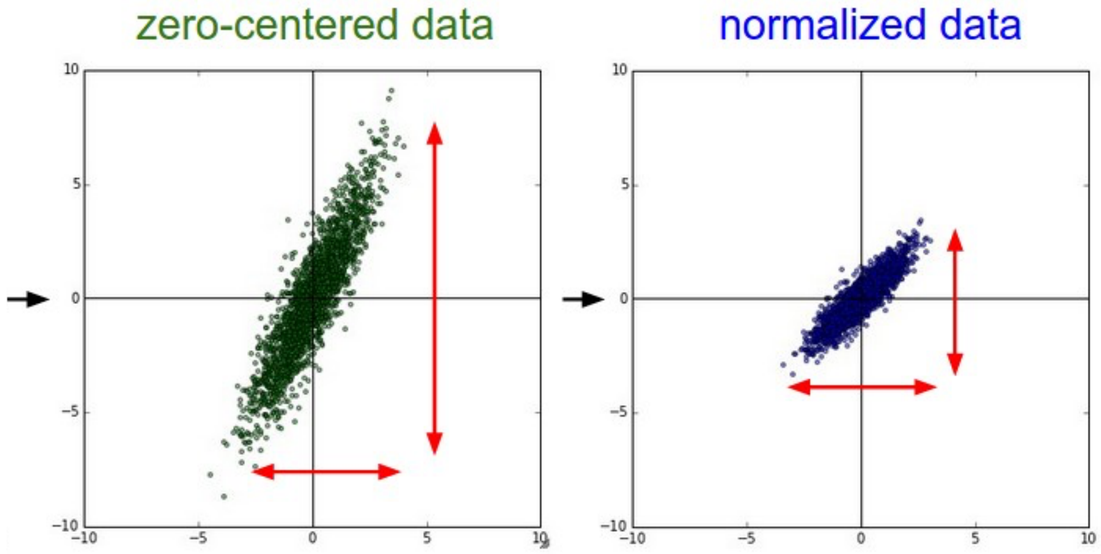




BatchNormalization Layer

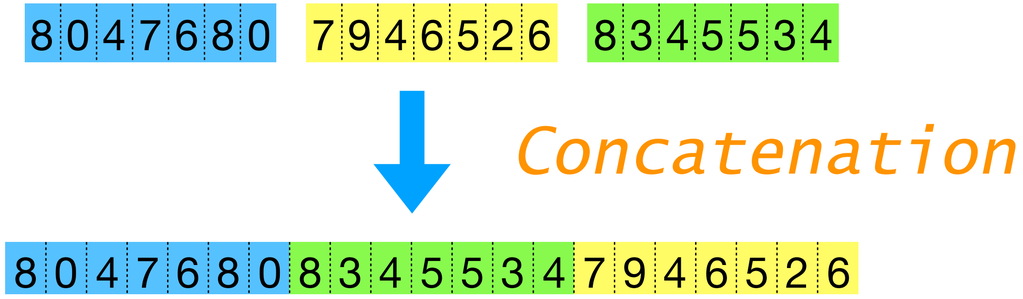
- *It is good practice to give normalized inputs to a layer*
  - *With all inputs having the same order of magnitude, all weights are equal important in the gradient*
  - *Prevents explosion of the loss function*
- *This can be done automatically with BatchNormalization*
  - *non-learnable shift and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

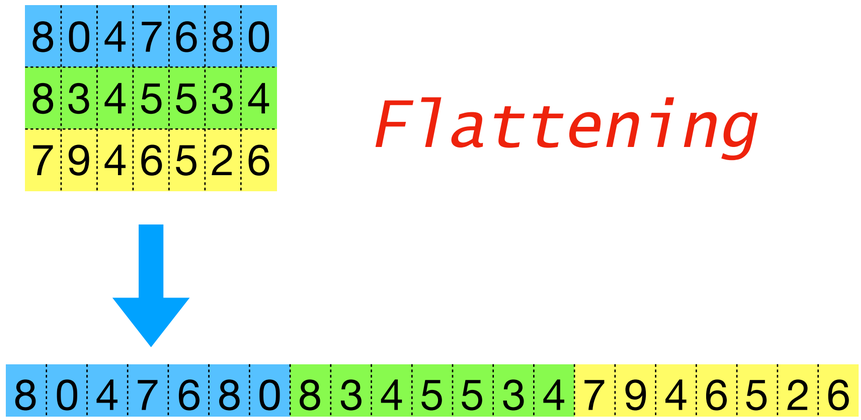




More complex structures

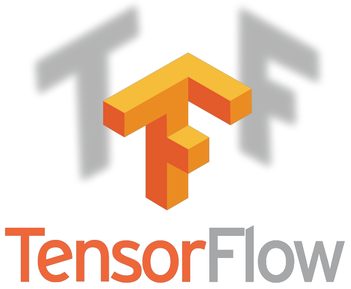
- *Dense NN architectures can be made more complex*
  - *Multiple inputs*
  - *Multiple outputs*
  - *Different networks branches*
- *This is possible thanks to layer-manipulation layers*
  - *Add, Subtract, etc.*
  - *Concatenation*
  - *Flattening*
- *All these operations are usually provided with NN training libraries*





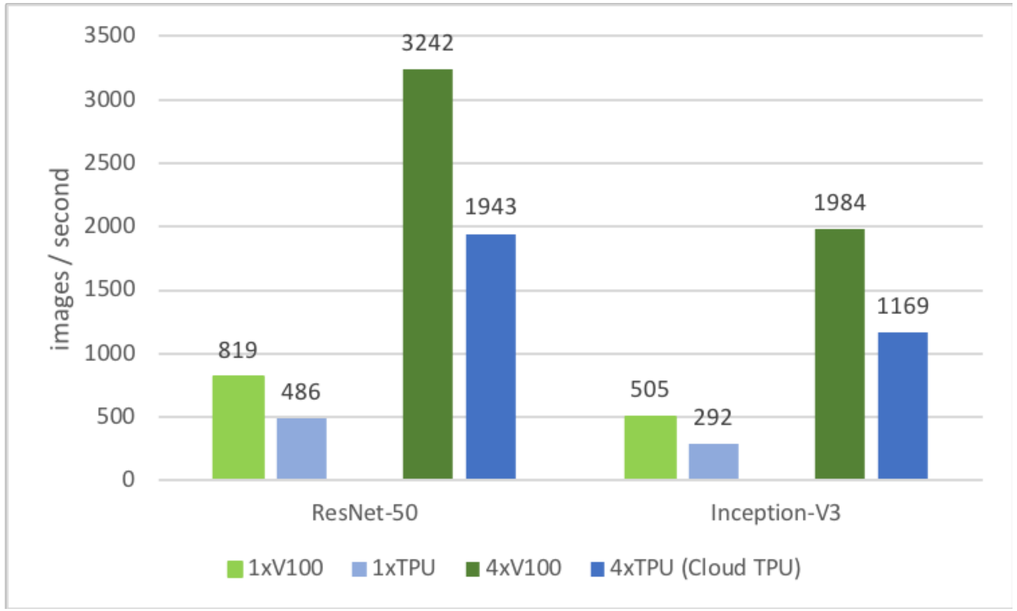
Training Libraries

- 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)



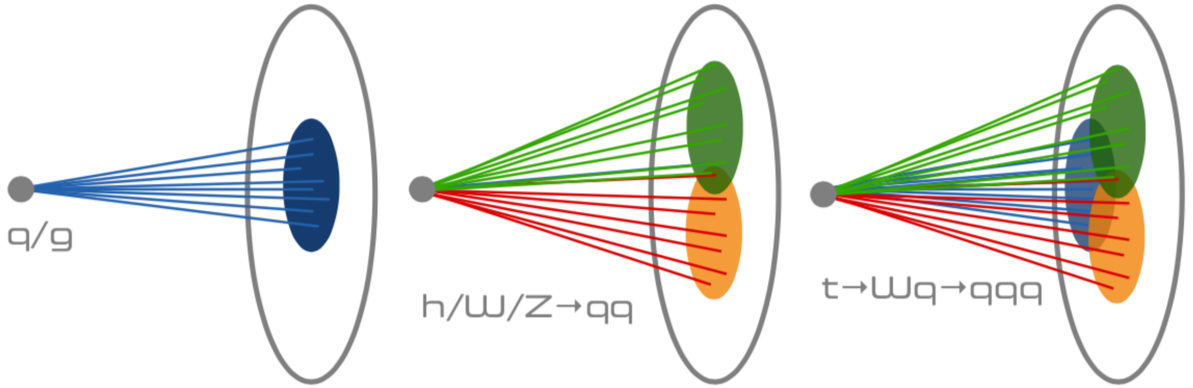
GPUs & TPUs

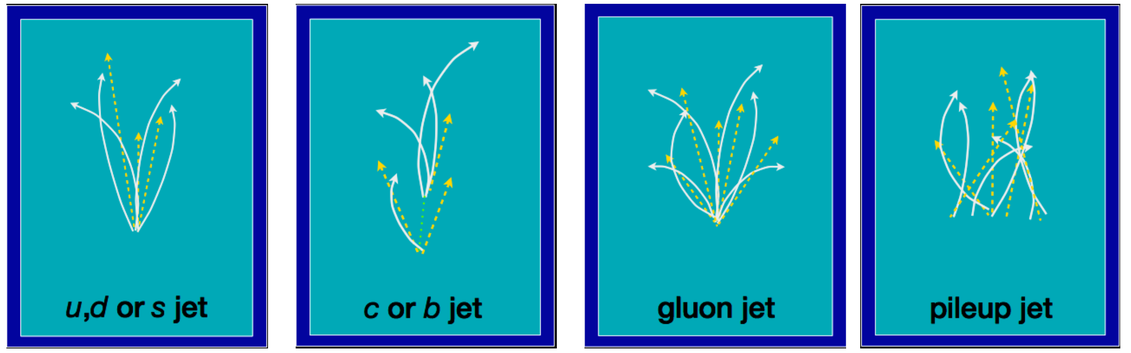
- *All codes come with GPU support, through CUDA*
  - *They work on nVidia GPUs*
- *GPUs are very suitable to train neural networks*
  - *dedicated VRAM provides large memory to load datasets*
  - *architecture ideal to run vectorised operations on tensors*
  - *can also paralyse training tasks (e.g., processing in parallel multiple batches)*
- *A single-precision gaming card is good enough for standalone studies (200-1000 $, depending on model)*
- *Large tasks require access to clusters (with libraries for distributed training)*
- *Dedicated architectures (e.g., Google TPU) now emerging. Essentially, Deep Learning ASICs*



Example: jet tagging

- *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*





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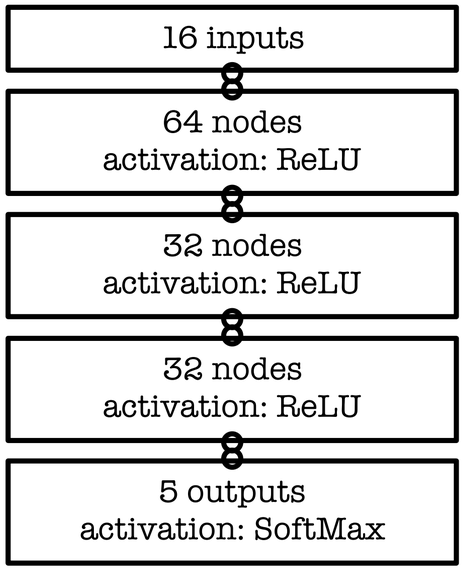

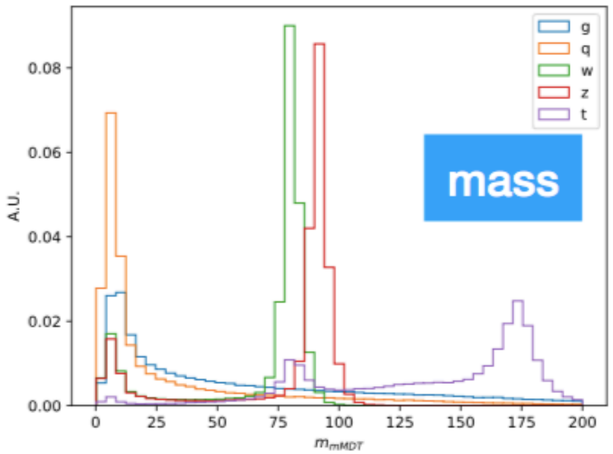

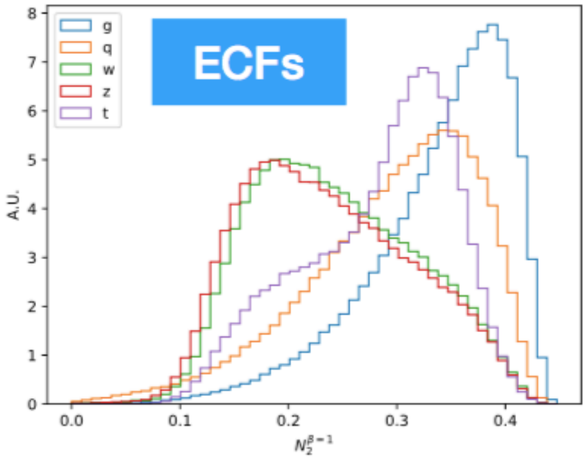

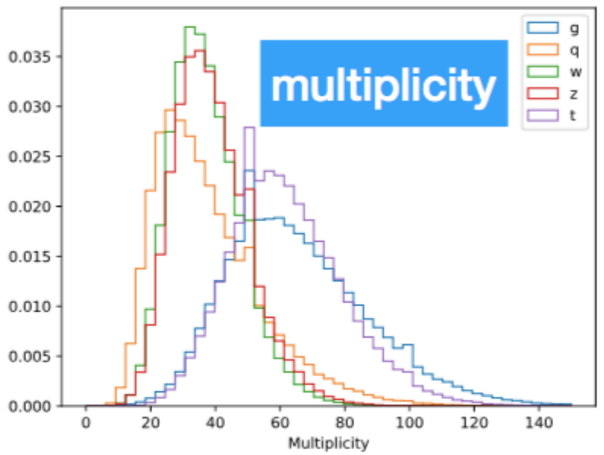

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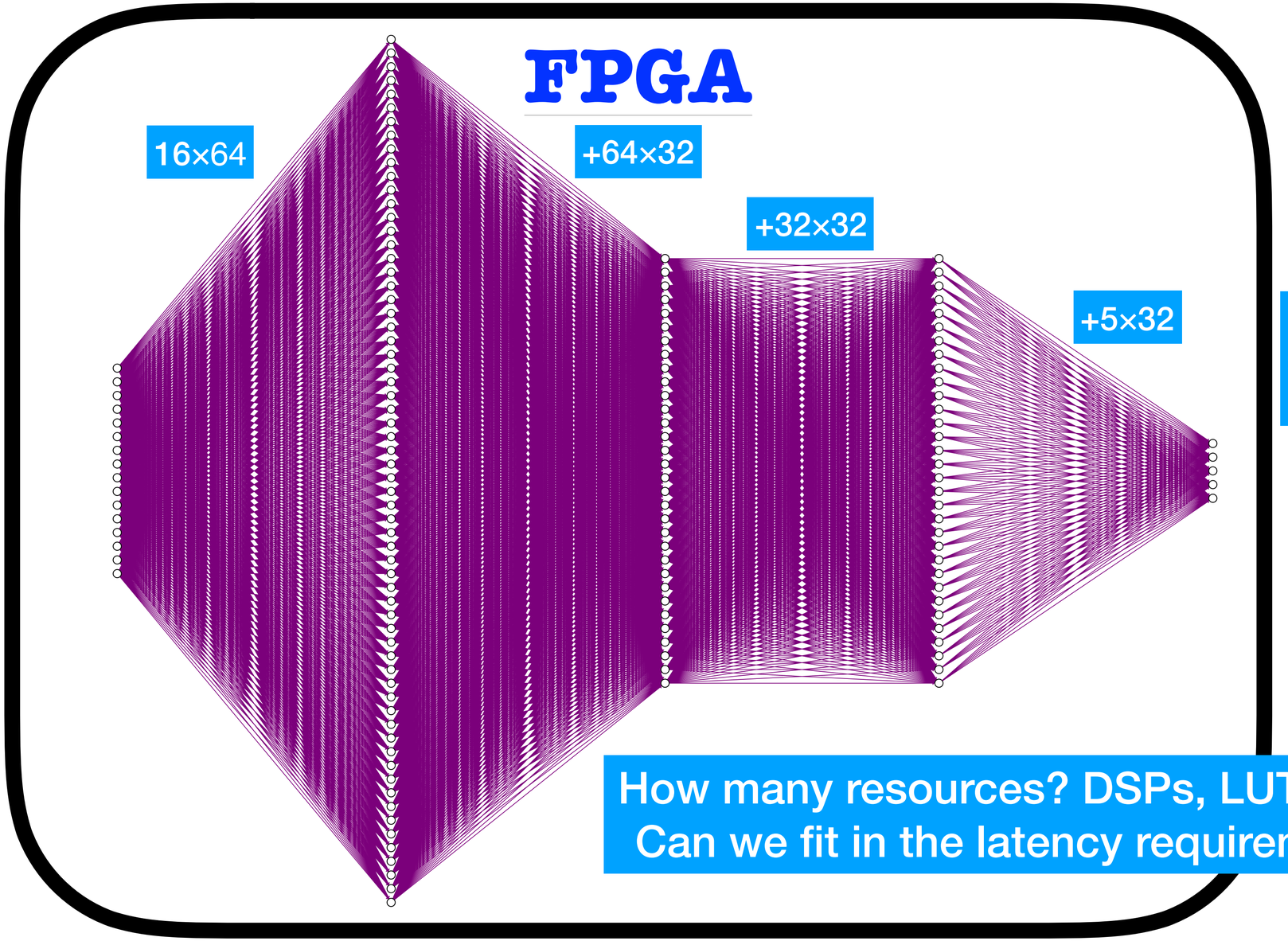
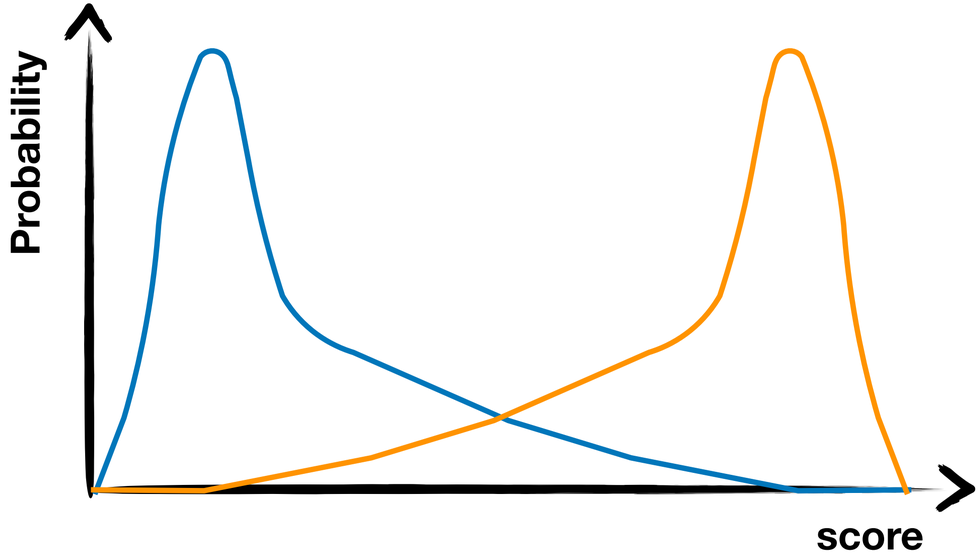
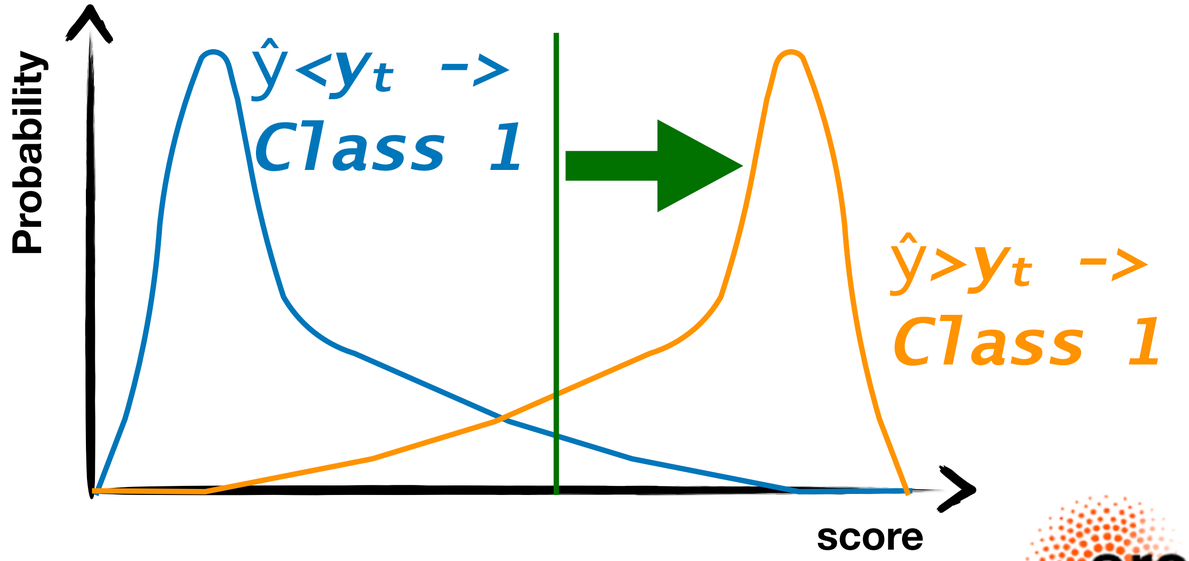


What is a ROC curve?

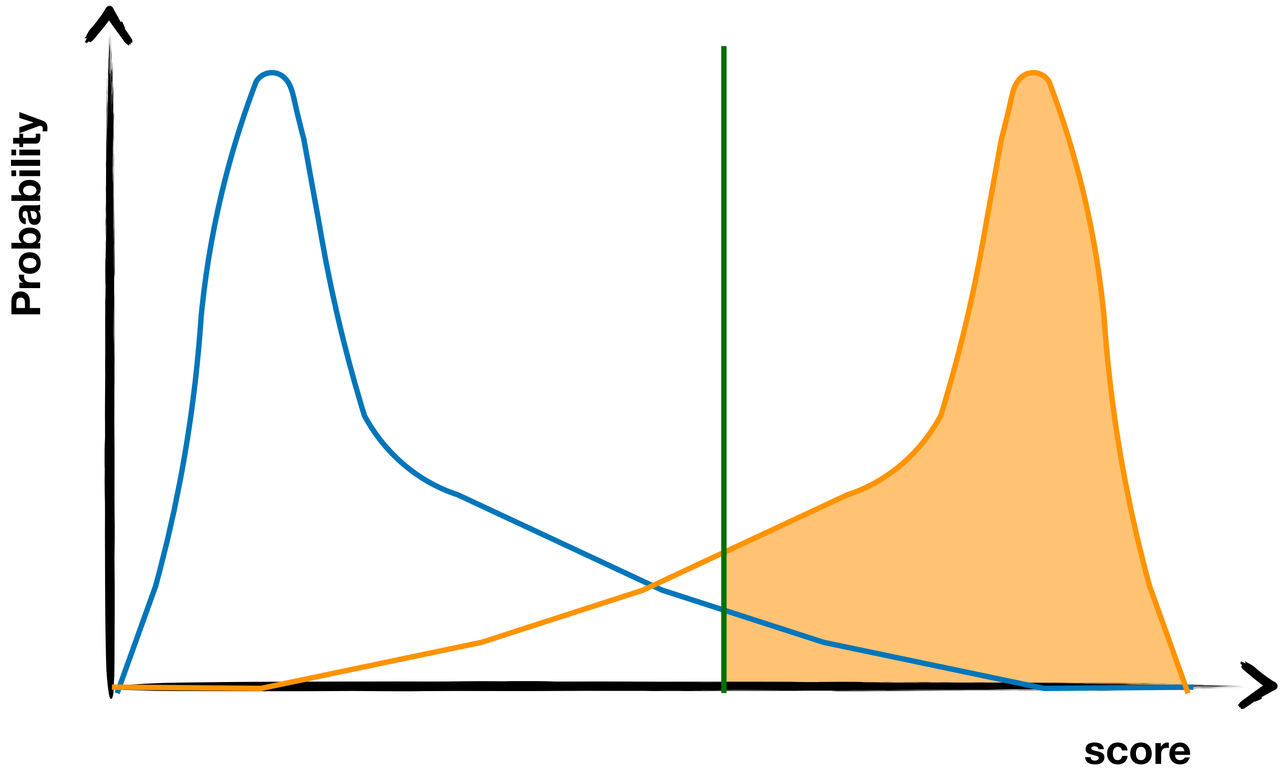
- Consider a binary classifier
- Its output $\hat{y}$ is a number in [0,1]
- If well trained, value should be close to 0 (1) for class-0 (class-1) examples
- One usually defines a threshold y_t such that:
  - $\hat{y} > y_t$ -> Class 1
  - $\hat{y} < y_t$ -> Class 0





What is a ROC curve?

- *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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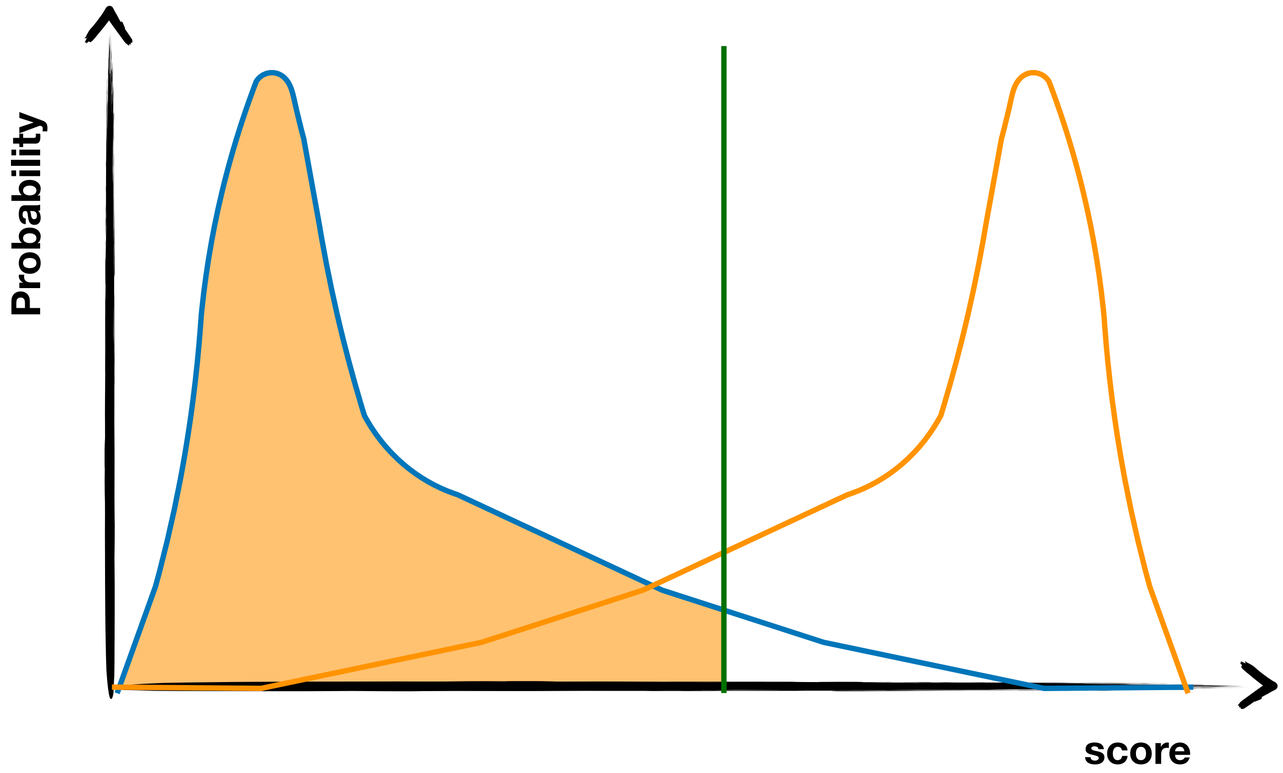

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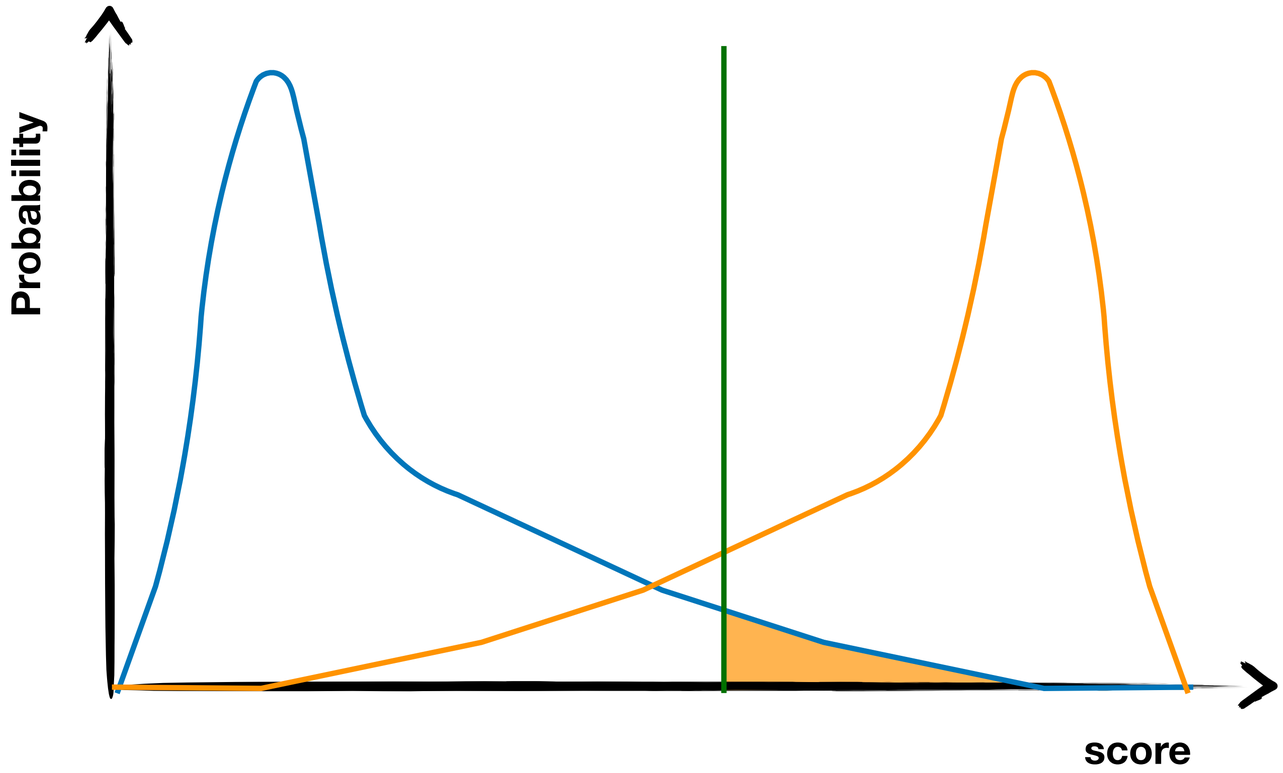

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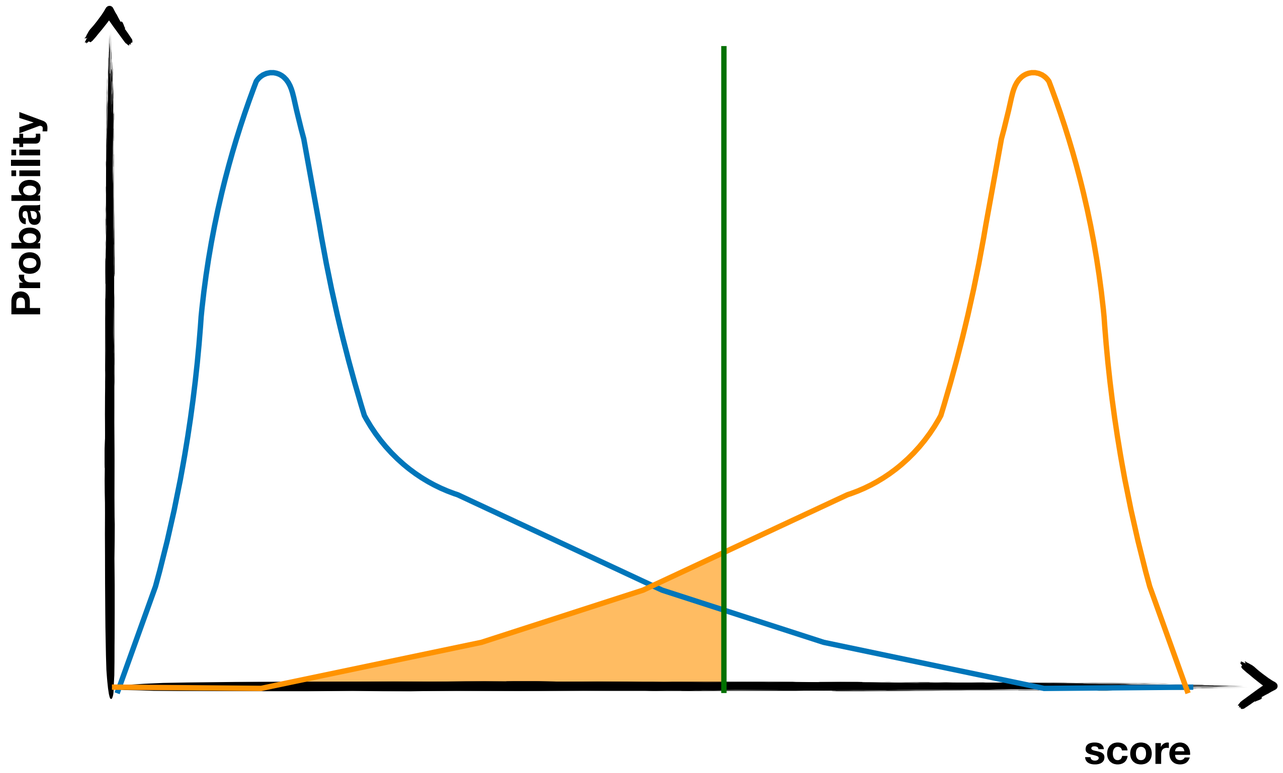
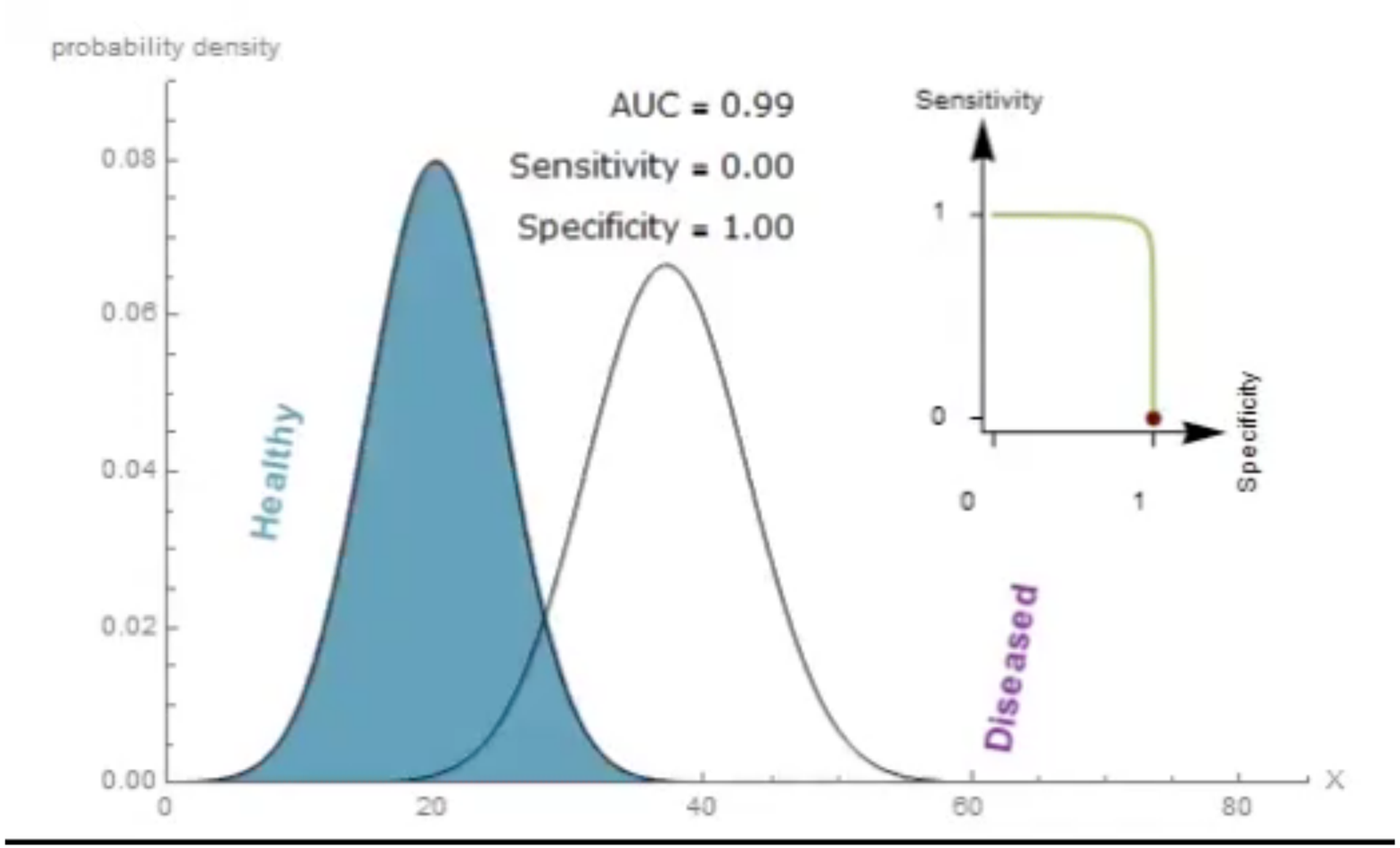


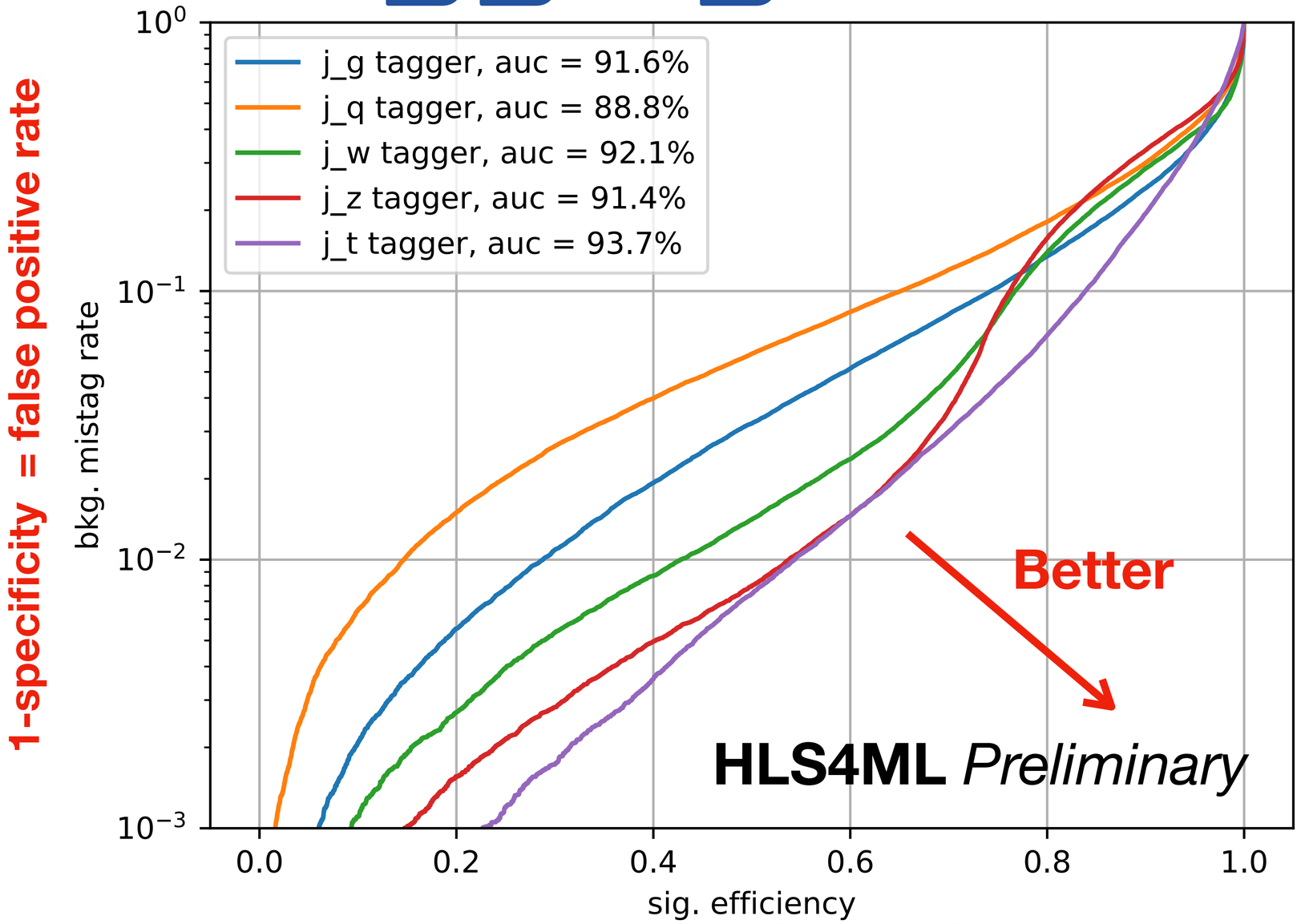
Classifier metrics

- *Accuracy: (TP+TN)/Total*
  - *The fraction of events correctly classified*
- *Sensitivity: TP/(Total positive)*
  - *We call it signal efficiency*
- *Specificity: TN/(Total negative)*
  - *We call it 1-mistag*
- *These metrics depend o the chosen threshold*
- *To build a threshold-independent metric, we need a ROC curve*

What is a ROC curve?



Jet tagging ROC curve



1-specificity = false positive rate

Sensitivity = True Positive Rate

Summary of Lecture 1

- *ML models are adaptable algorithms that are trained (and not programmed) to accomplish a task*
- *The training happens minimizing a loss function on a 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*
- *It could be relevant to the future of HEP, e.g., to face the big-data challenge of the High-Luminosity LHC*

References

- *Michael Kagan, CERN OpenLab classes on Machine Learning*
  - *Source of inspiration for this first lesson*
- *Pattern Recognition and Machine learning (Bishop)*
- *I. Goodfellow and Y. Bengio and A. Courville, "Deep Learning" MIT press*