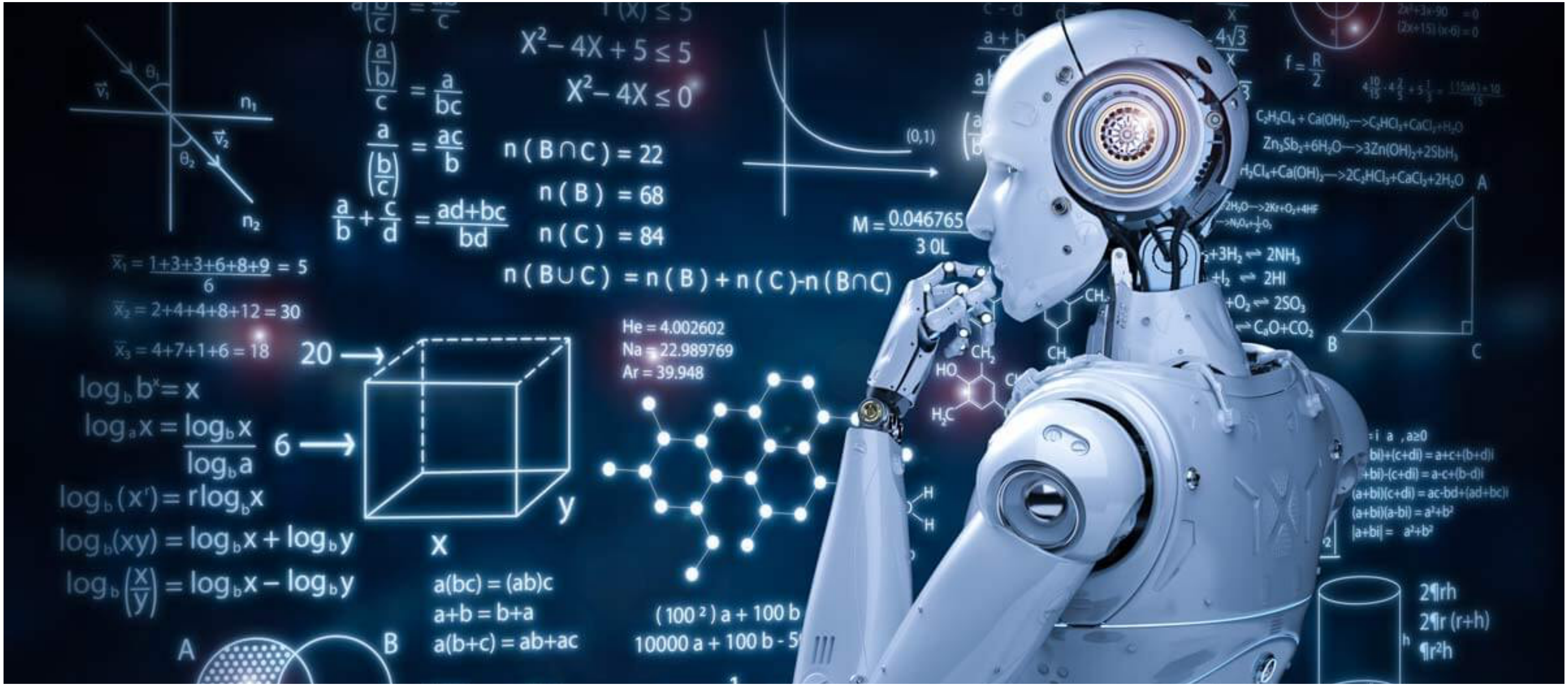
Deep Learning Applications for collider physics
Lecture 1

Maurizio Pierini

Plan for this week

	Day1	Day2	Day3	Day4	Day5
Lecture	Introduction	ConvNN	RNNs	Graphs	Unsupervised Learning
Tutorial	Fully Connected Classifier	ConvNN Classifier	RNNs Classifier	Graphs Classifier	Anomaly Detection



What is Machine Learning ?

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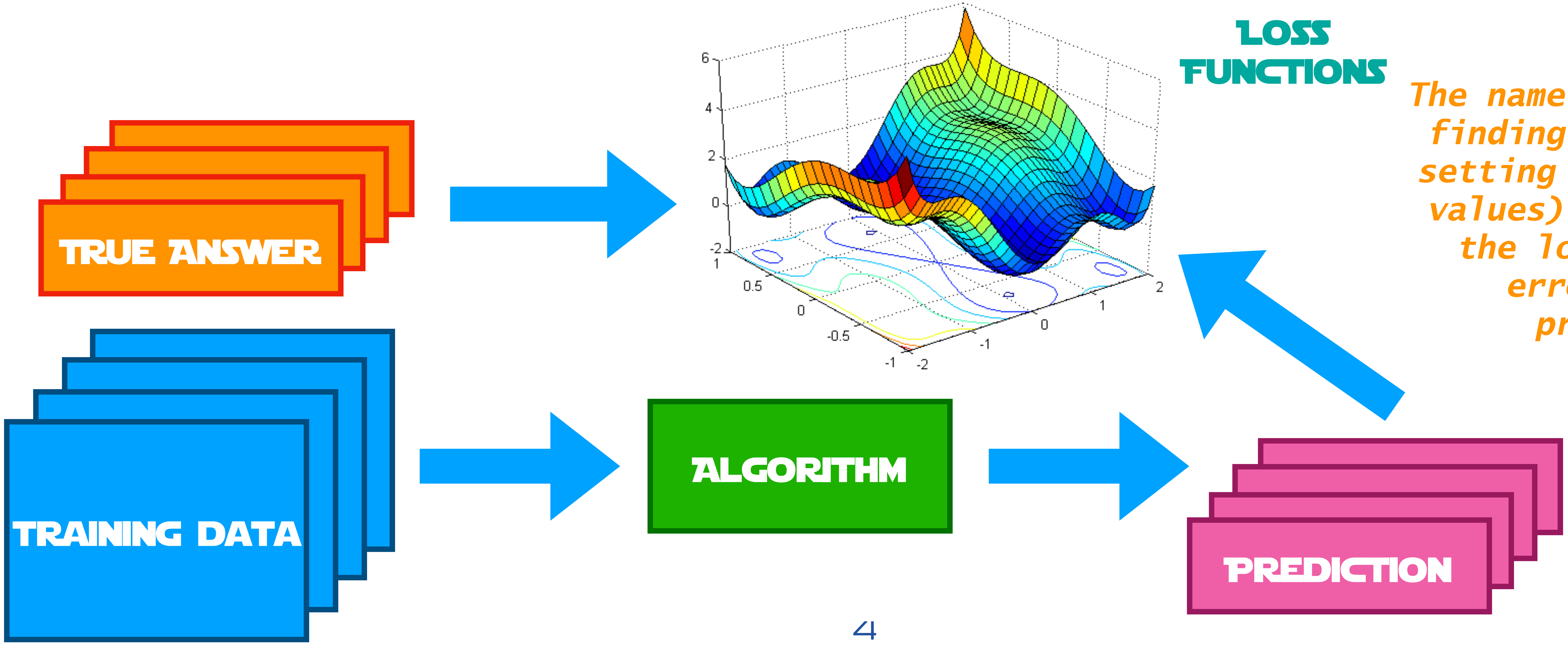
A definition (Wikipedia)

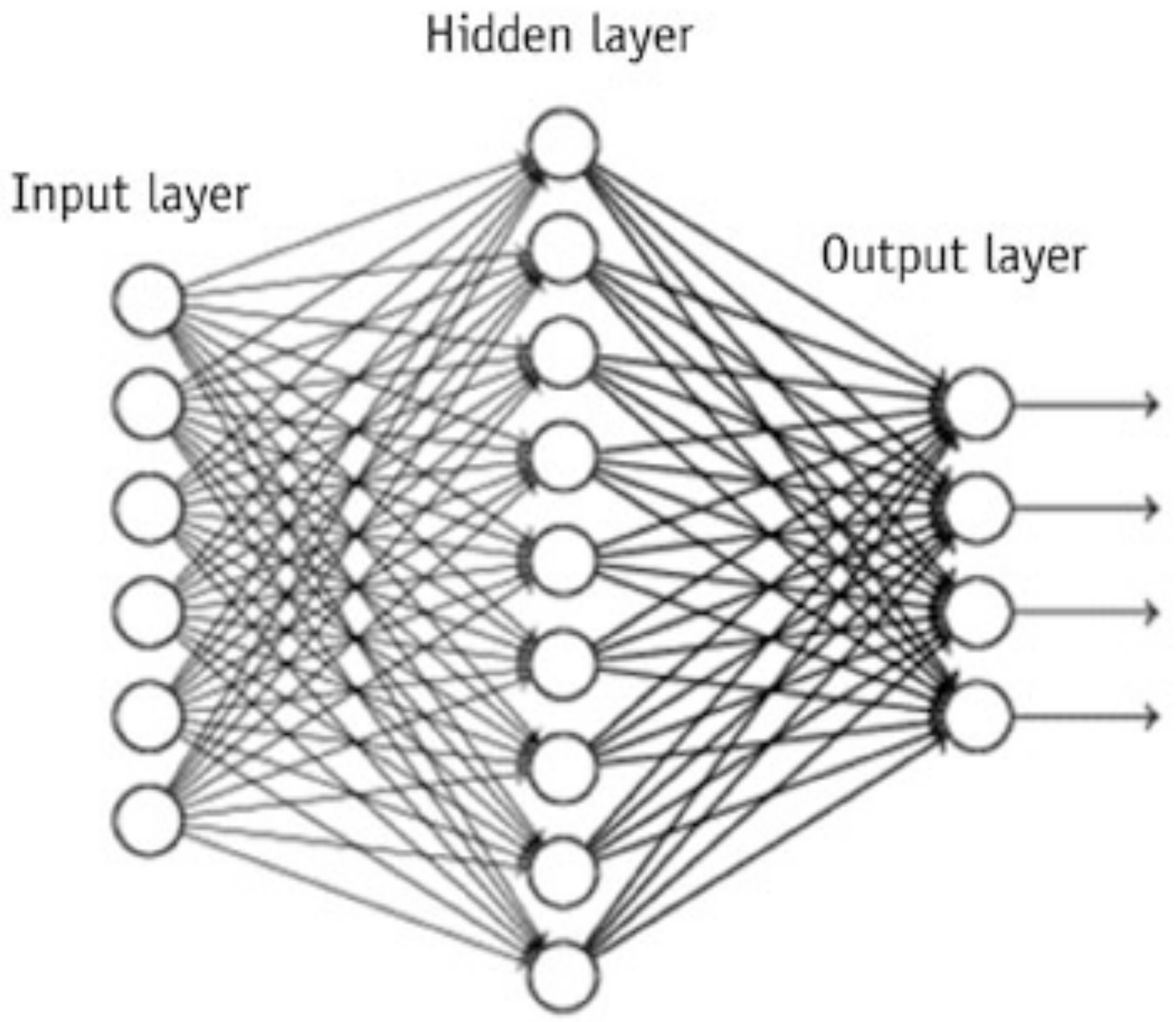
Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to progressively improve their performance on a specific task. Machine learning algorithms build a mathematical model of sample data, known as "training data", in order to make predictions or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

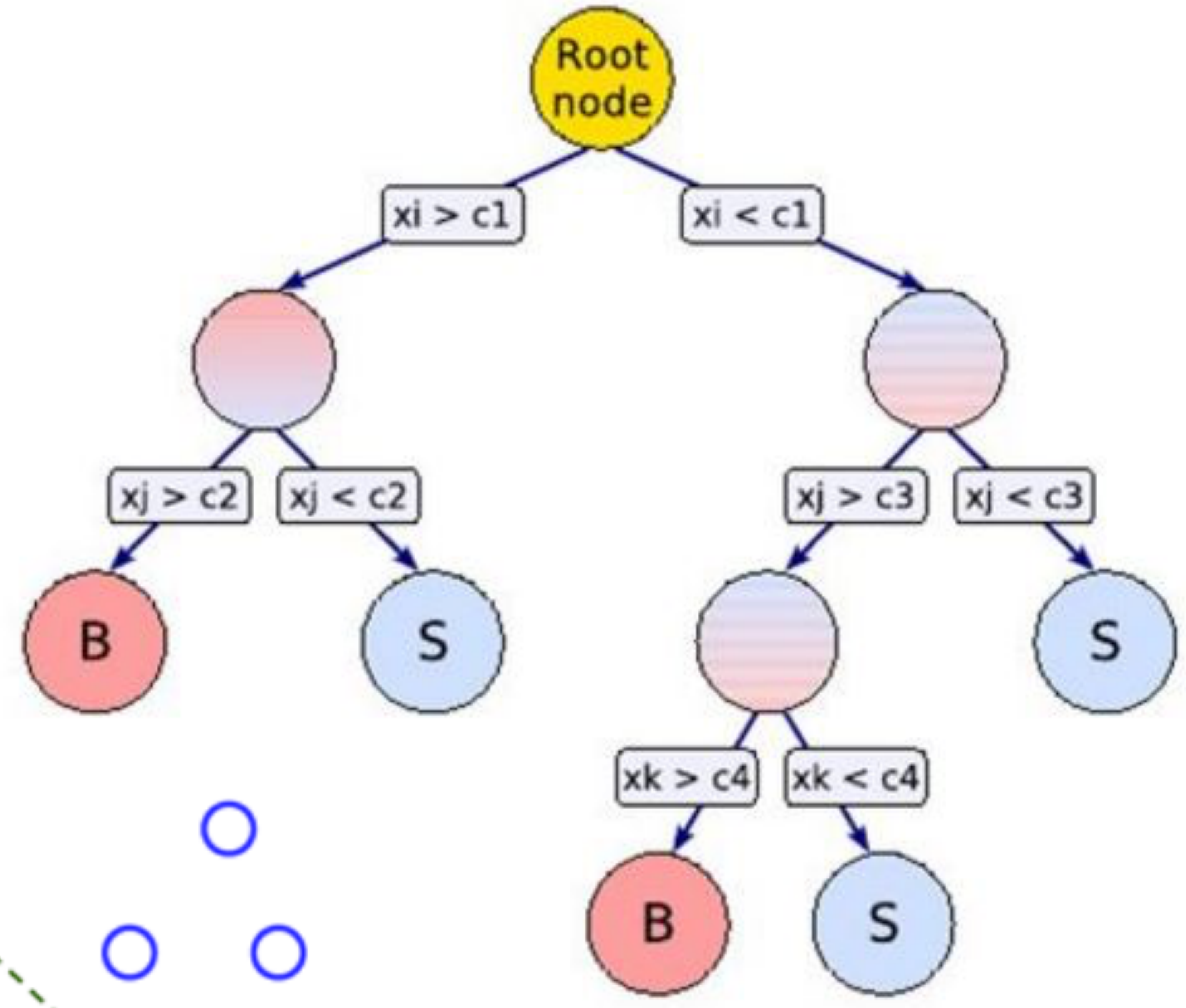


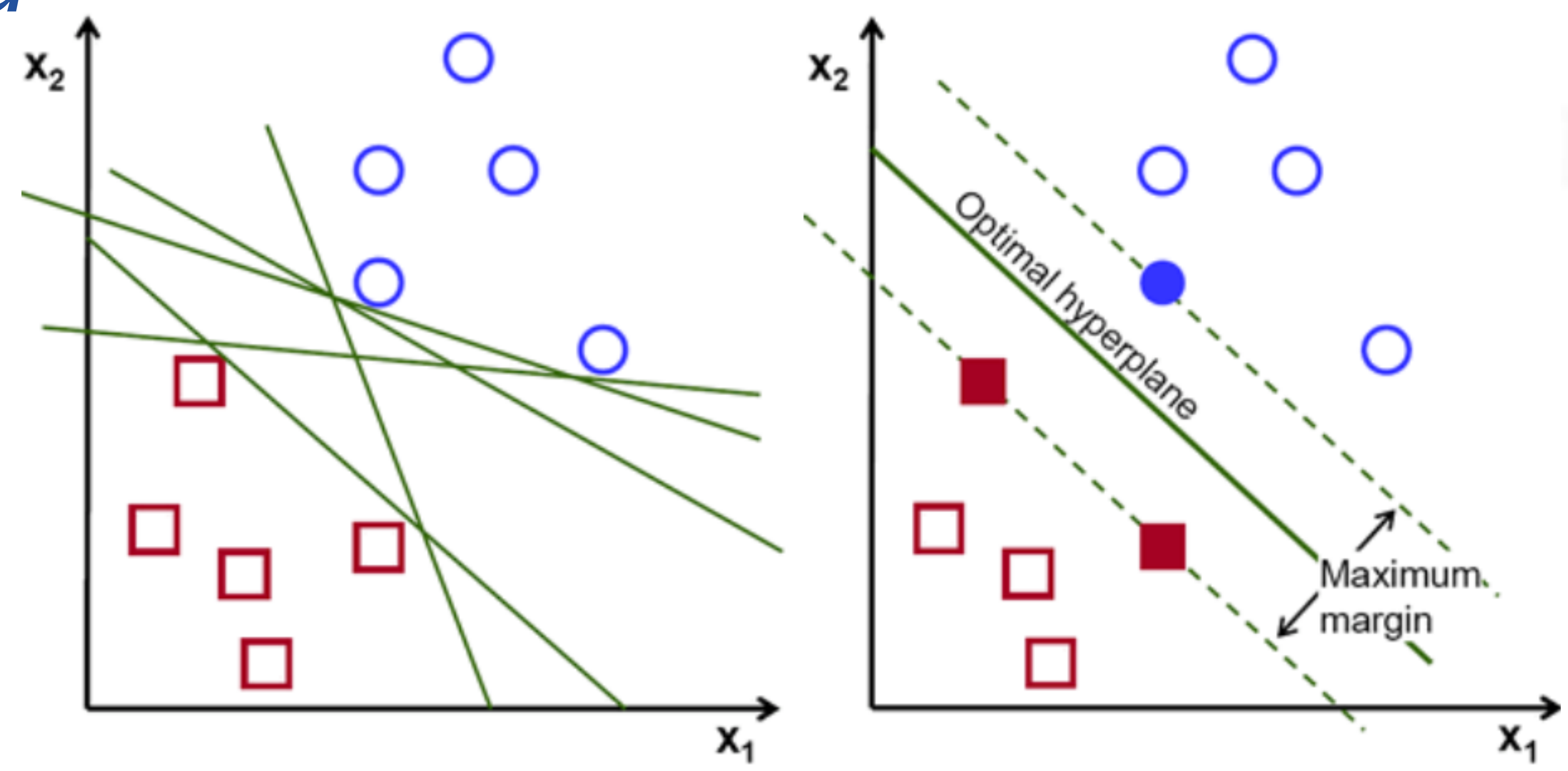
The name of the game is finding the algorithm setting (its parameter values) that minimise the loss, i.e. the error made in prediction

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

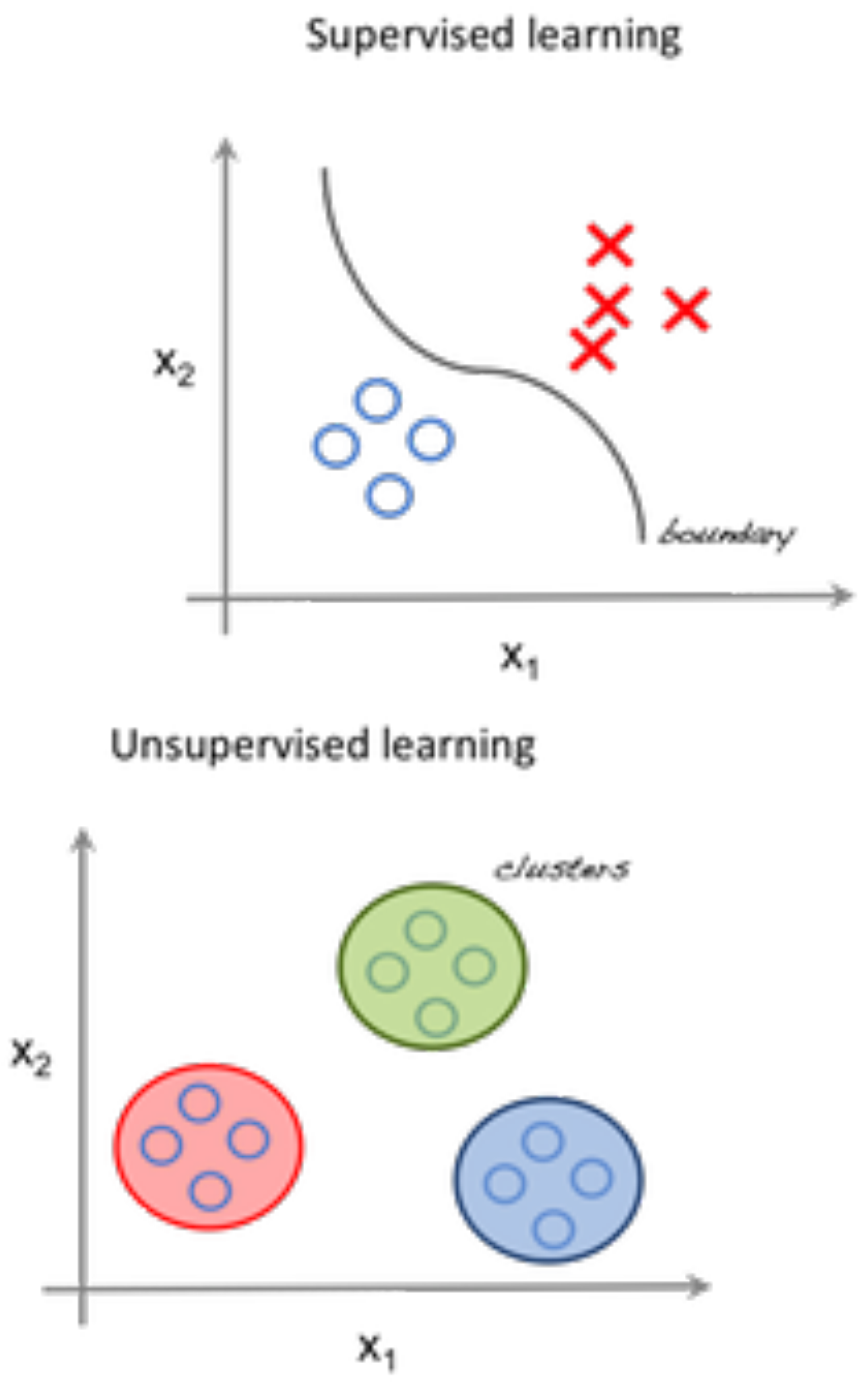






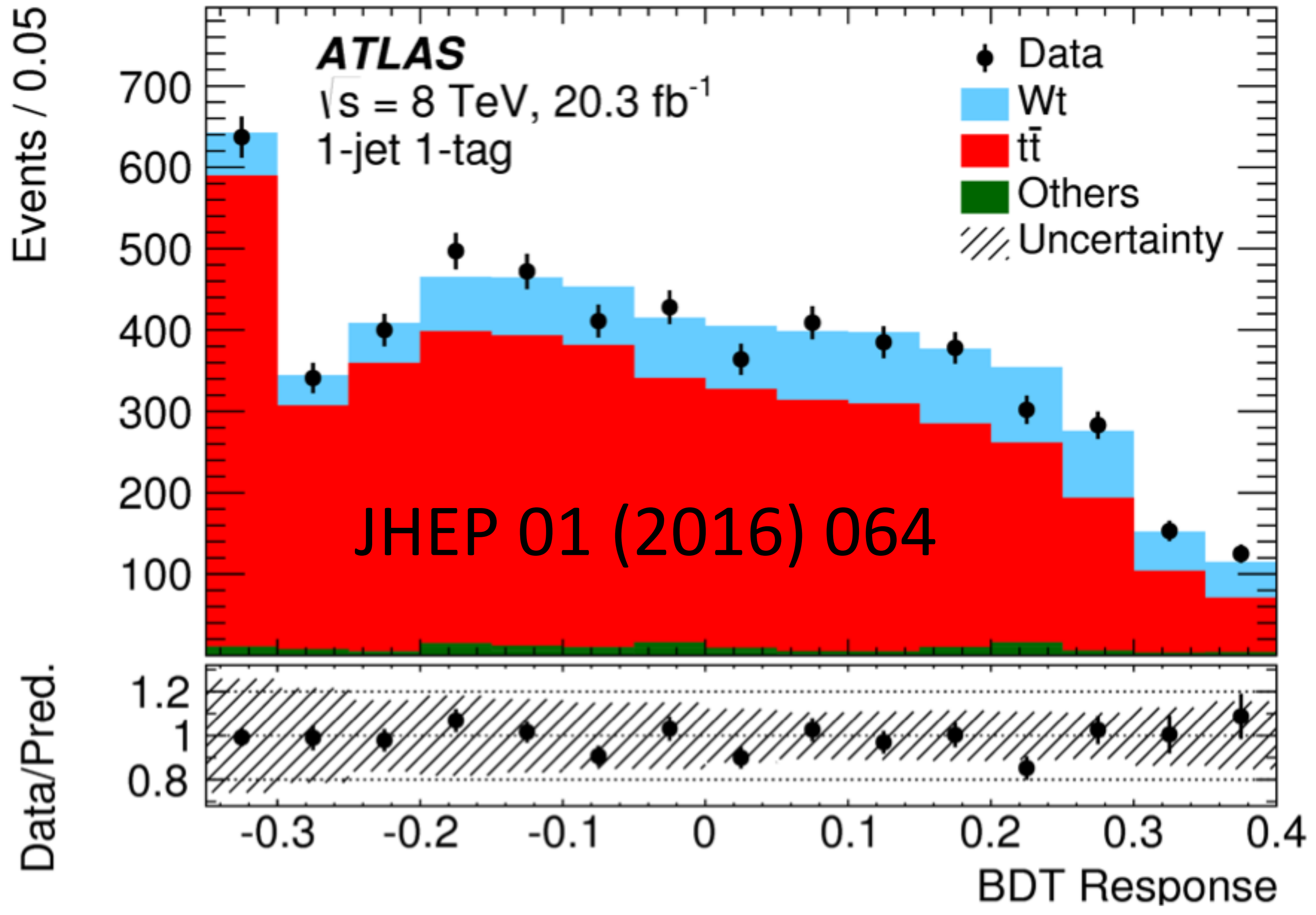
A two-steps process

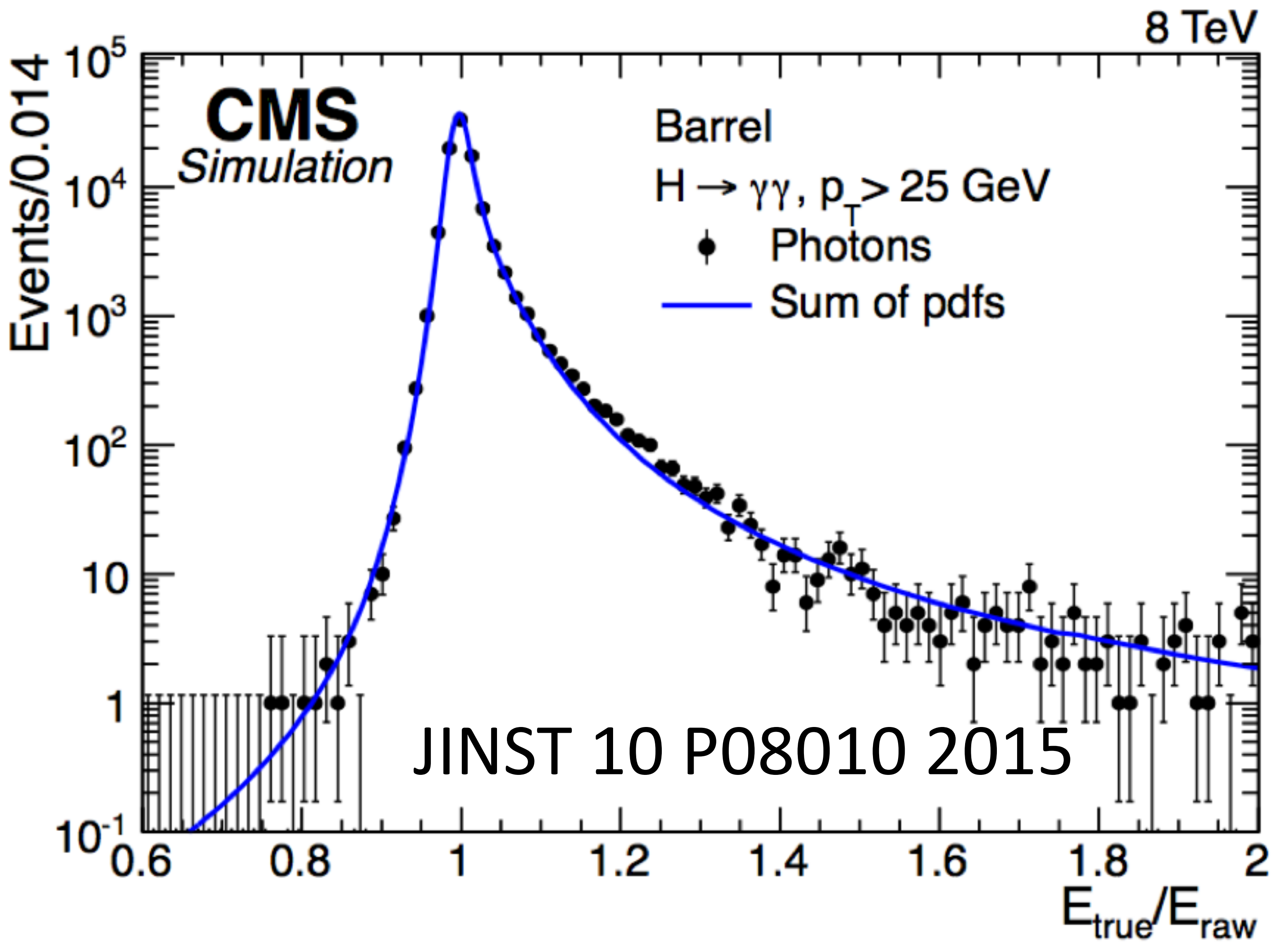
- ***Learning:*** *train the algorithm on a provided dataset*
    - ***Supervised:*** *the dataset X comes with the right answer y (right class in a classification problem). The algorithm learns the function*
    - ***Unsupervised****: the dataset X comes with no label. The algorithm learns structures 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*



Machine Learning in HEP

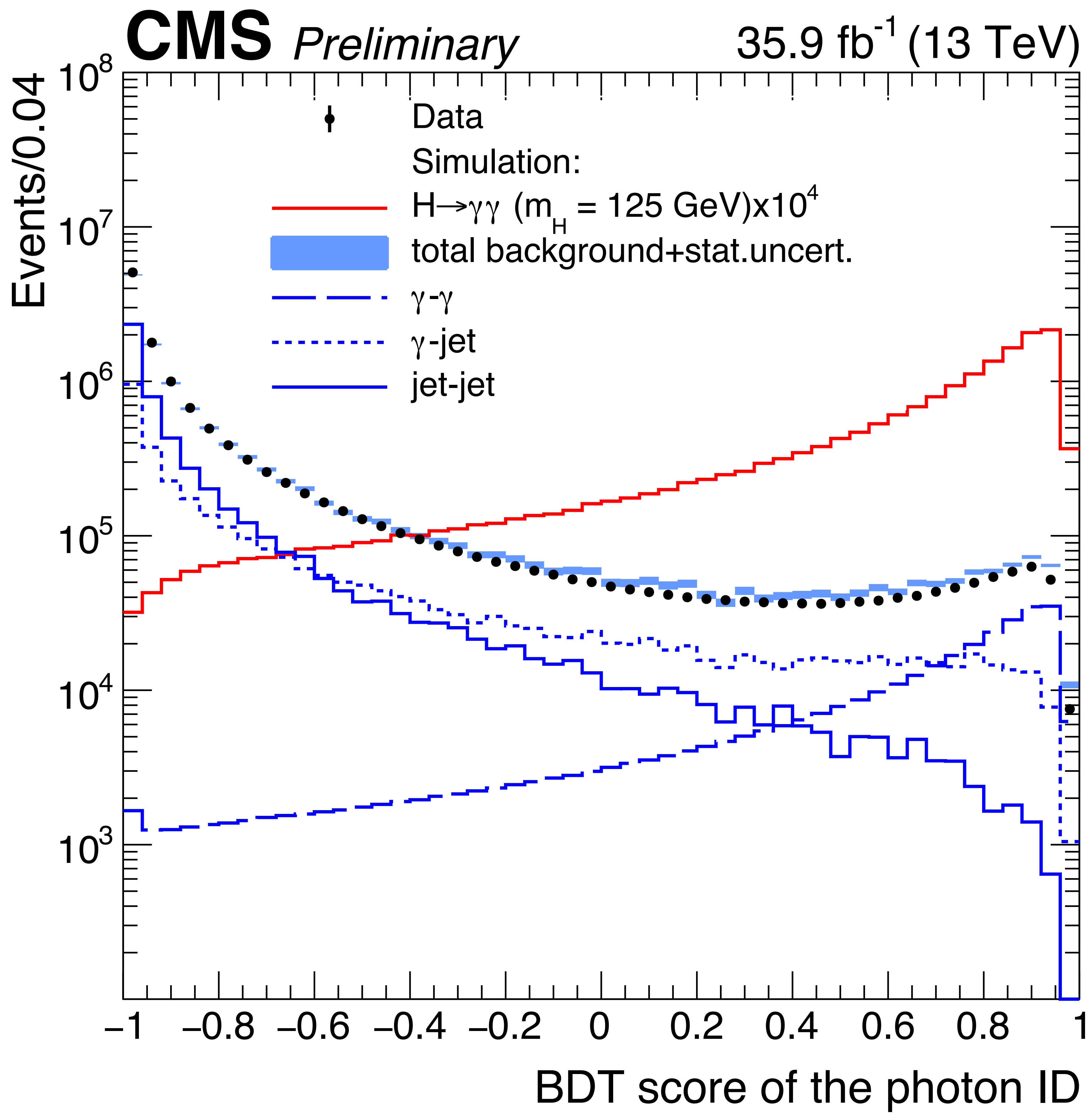
- Classification:
  - given an image, identify the object represented
  - in particle physics, given a particle shower, identify the particle kind
- Regression:
  - given a set of quantities x, learn some function f(x)
  - in particle physics, given a particle shower, learn its energy





Machine Learning in HEP

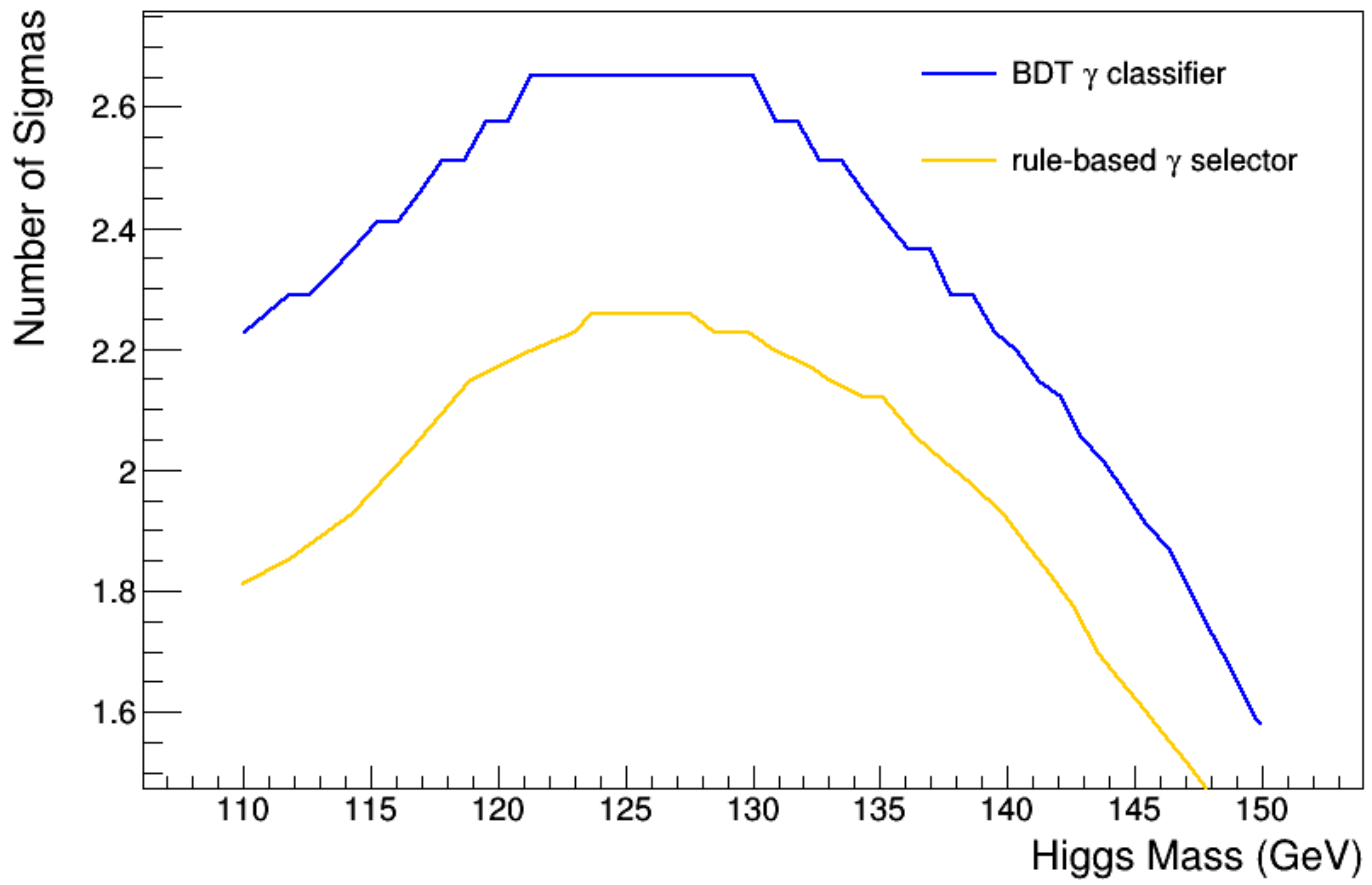
- *Classification:*
  - *identify a particle & reject fakes*
  - *identify signal events & reject background*
- *Regression:*
  - *Measure energy of a particle*
- *Up to now, these task mainly solved with BDTs*
  - *moved to Deep Learning for analysis-specific tasks*
  - *same will happen for centralised tasks (eventually)*

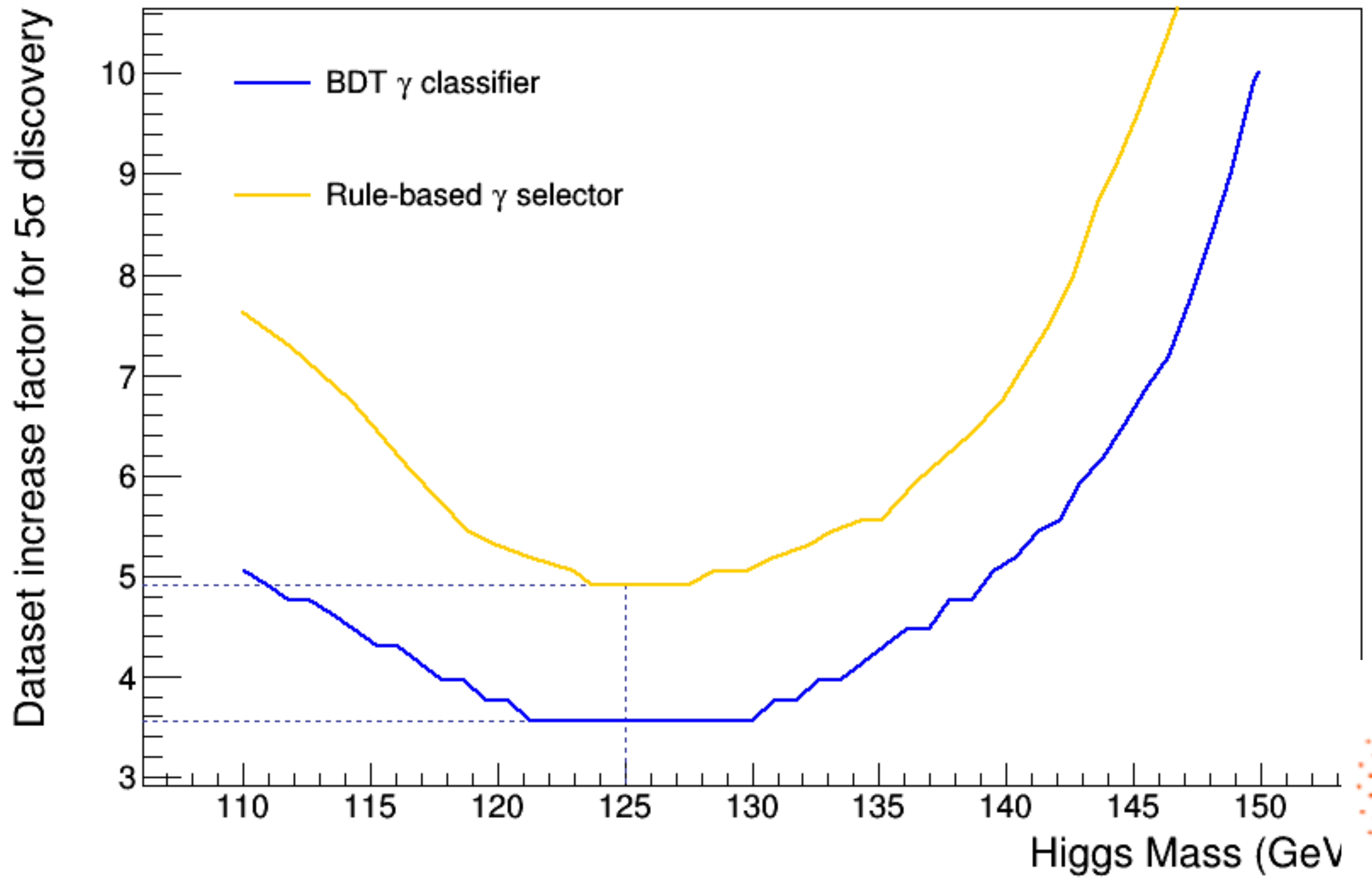


Centralised task (in online or offline reconstruction)
Analysis-specific task (by users on local computing infrastructures)

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*





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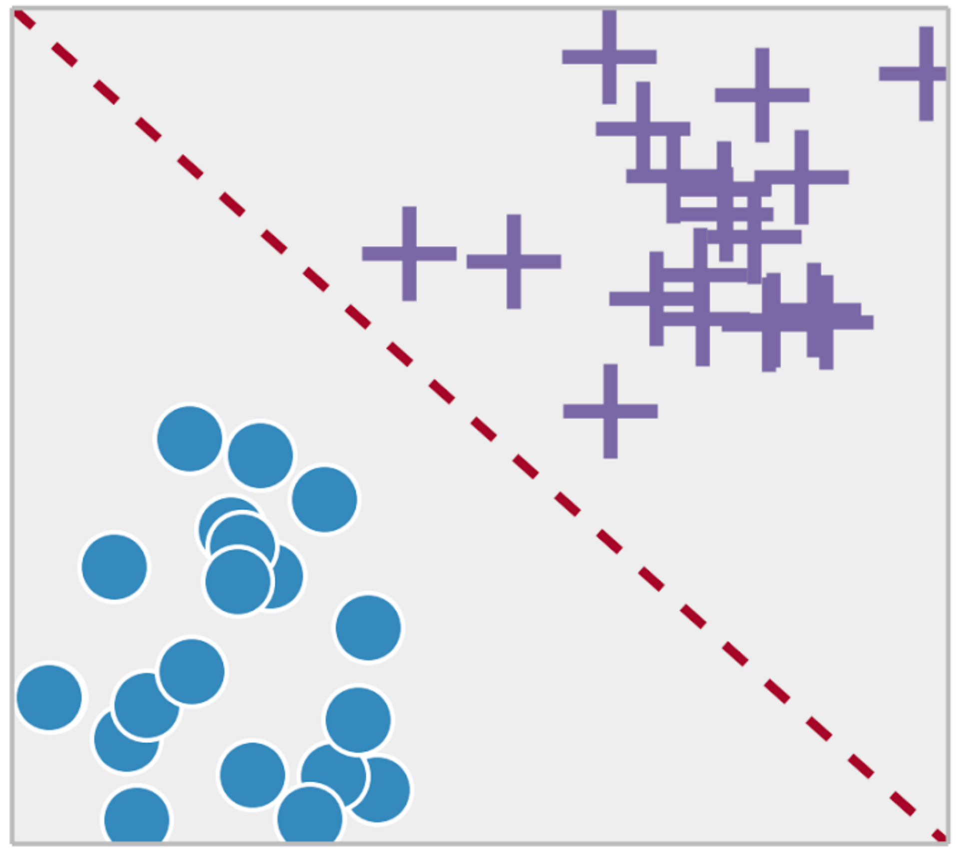
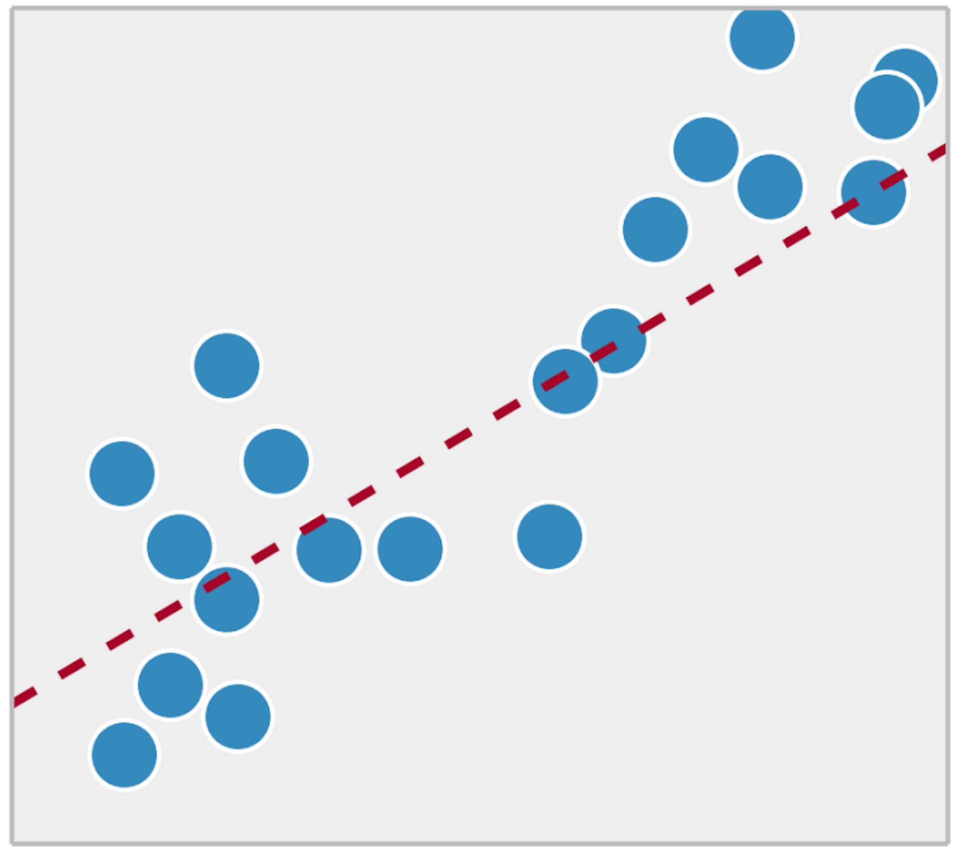
Typical problems

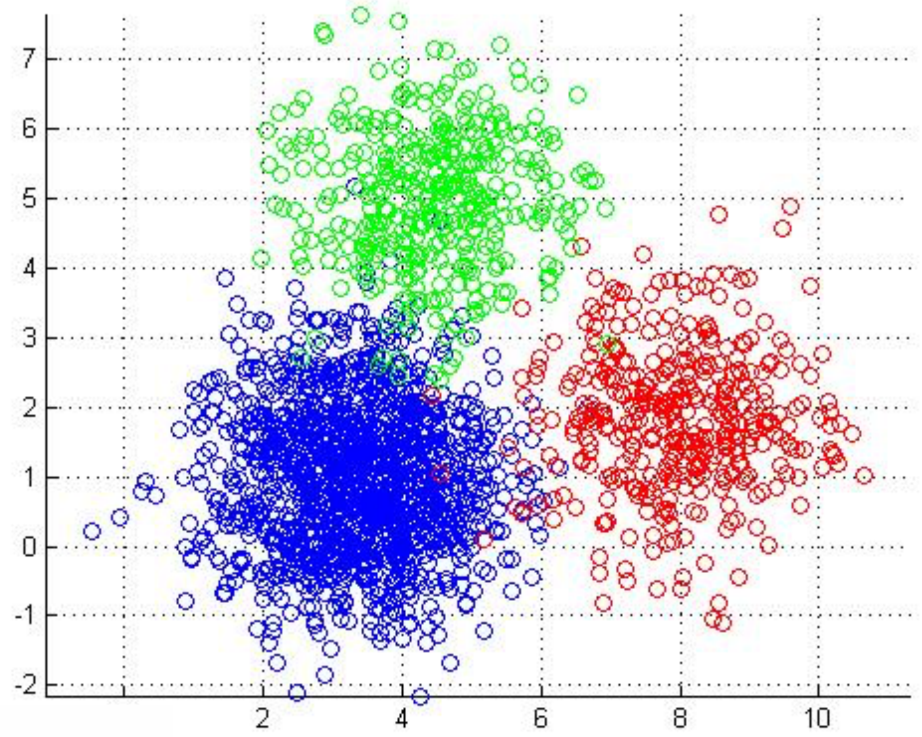
- ***Classification***: *associate a given element of a dataset to one of N exclusive classes*



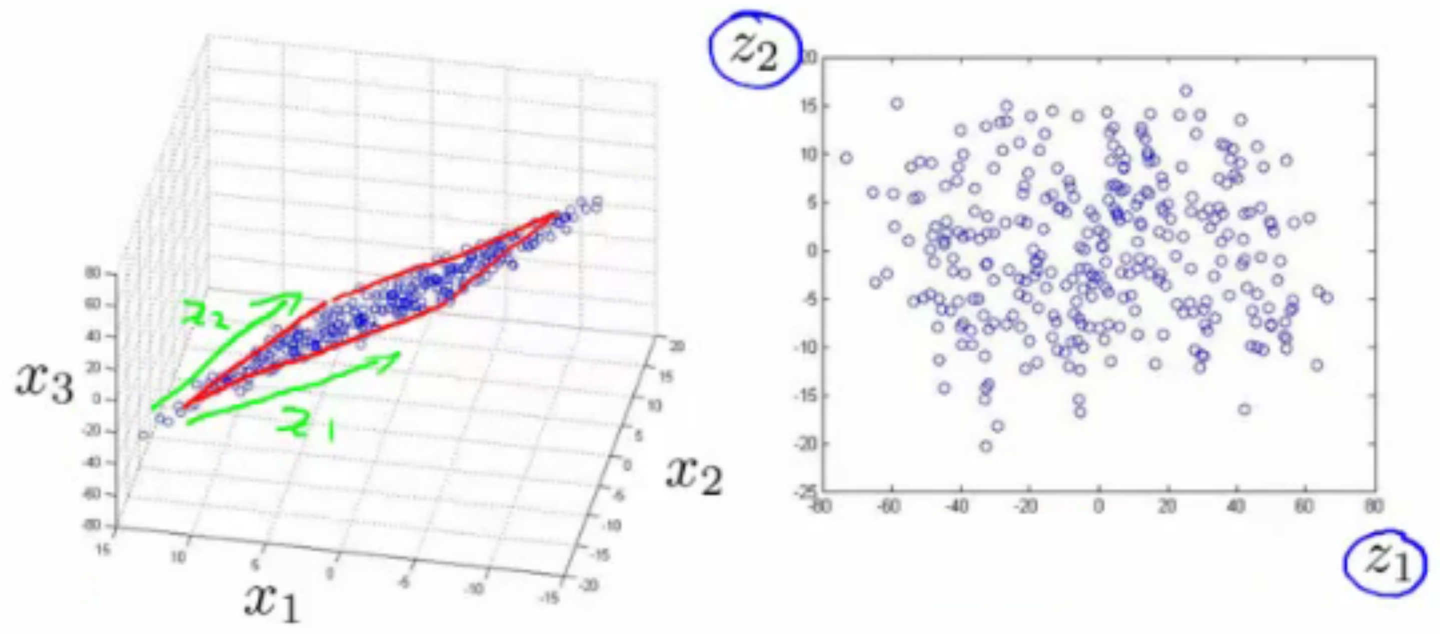
- ***Regression***: *determine a continuous value y from a set of inputs x*

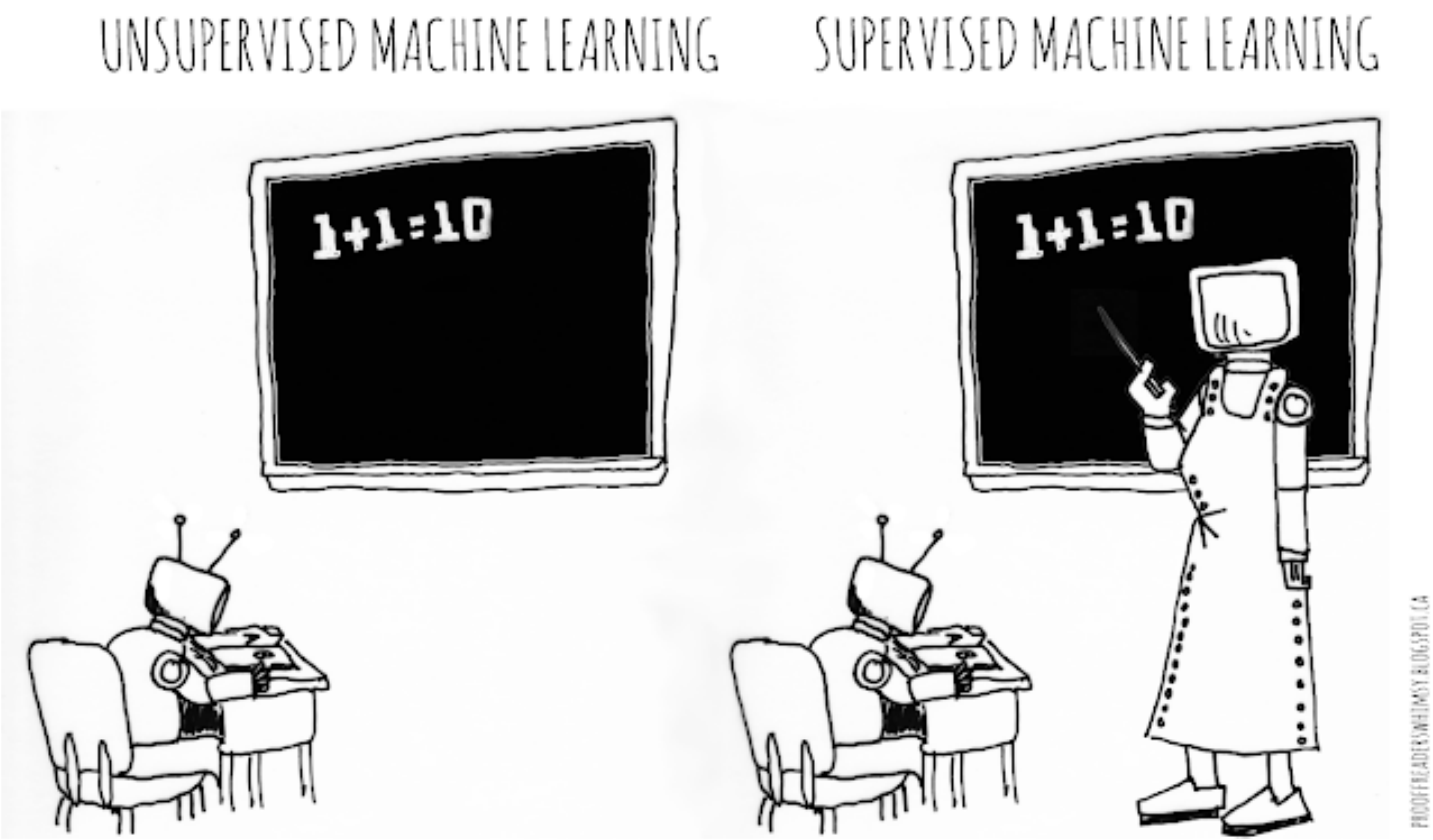


- ***Clustering***: *group elements of a dataset because of their similarity according to some learned metric*



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





Supervised Learning

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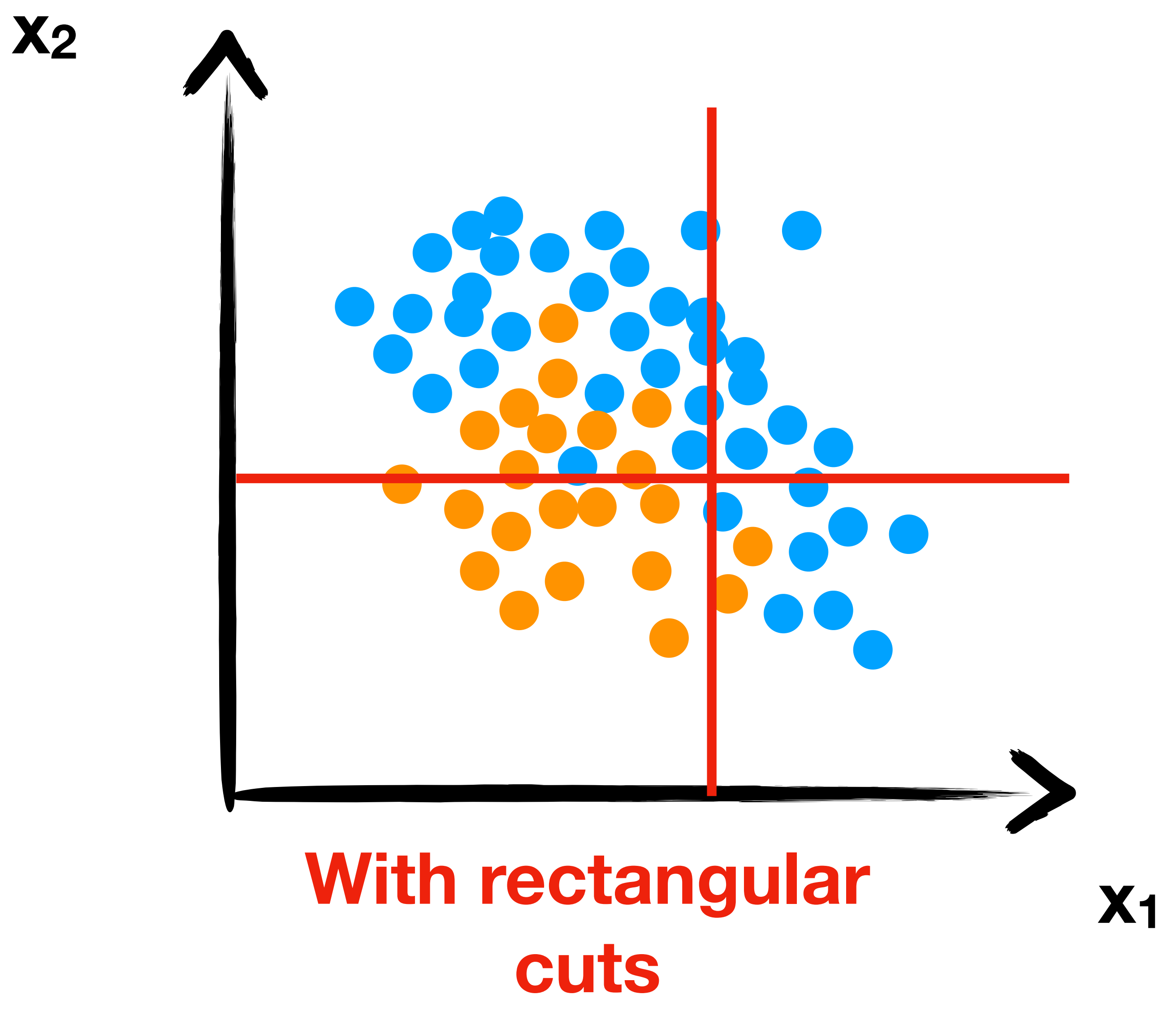
A simple example: S vs B selection

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



A simple example: S vs B selection

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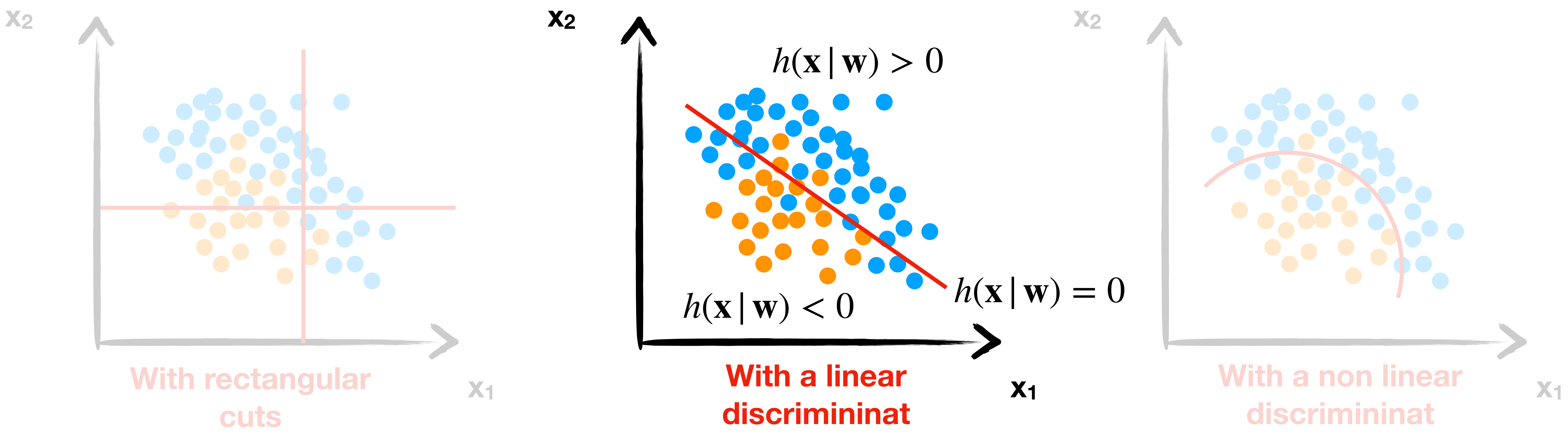


- Define a decision boundary which gives optimal separation

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

(Signed) distance between x and the boundary plane

Logistic Regression

- *Give as input pairs of inputs and outputs:*

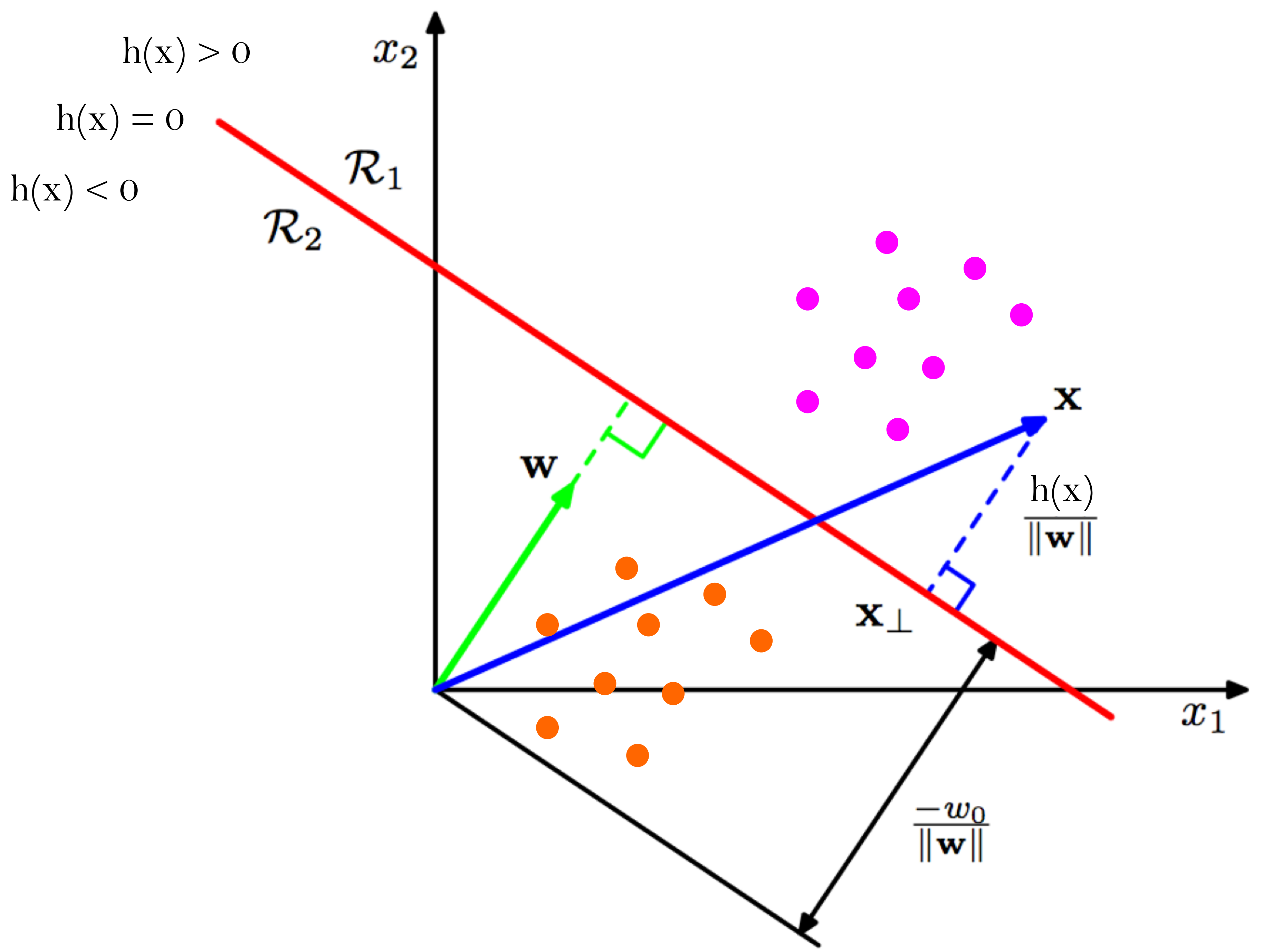
$$x_i \in \mathbb{R}^n \qquad\qquad y_i = \{0,1\}$$

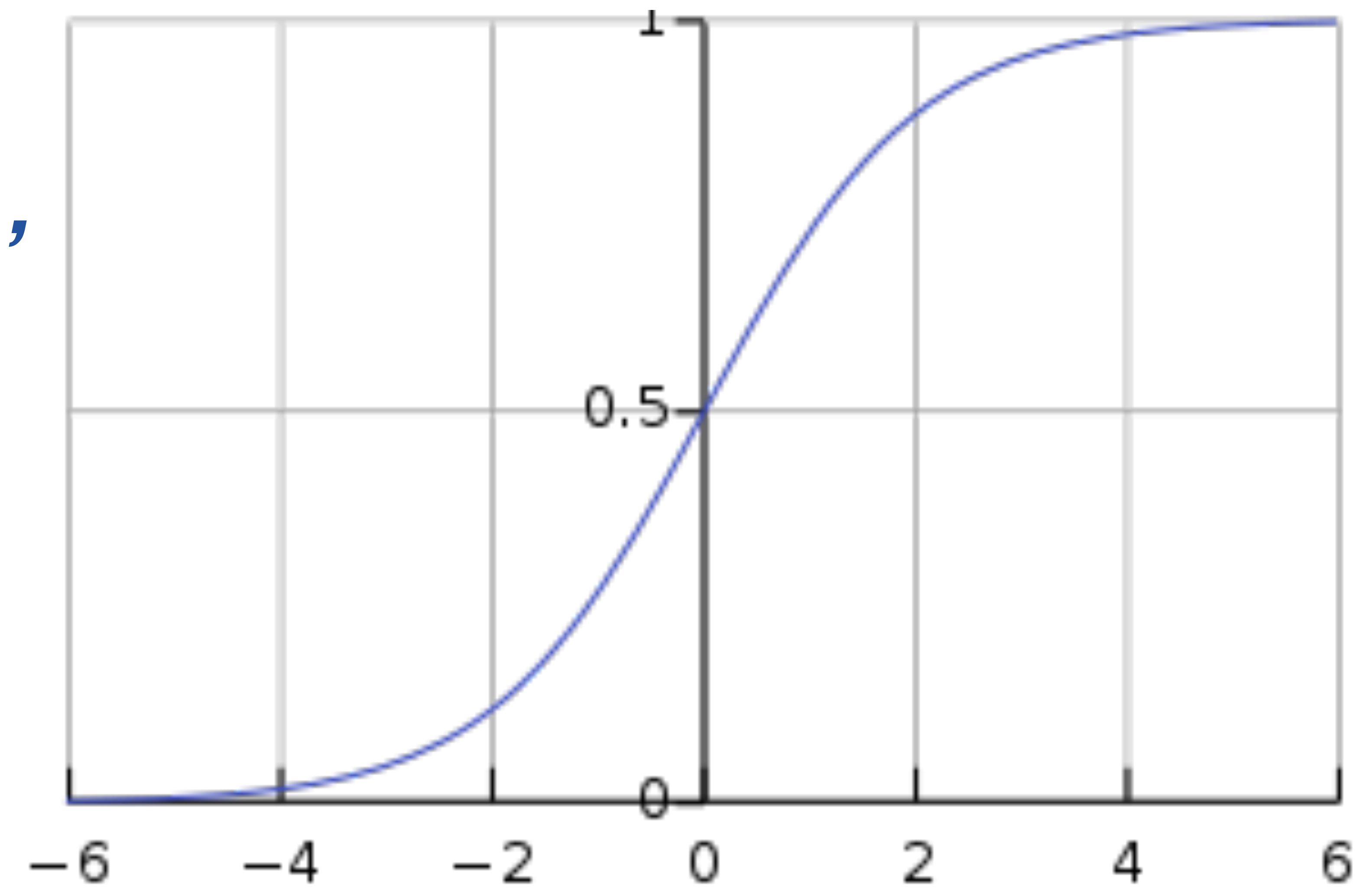
- *Model the probability of x to be signal (y=1) as*

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

  - *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 minimizing the binary cross entropy*
- *How do we minimise it?*

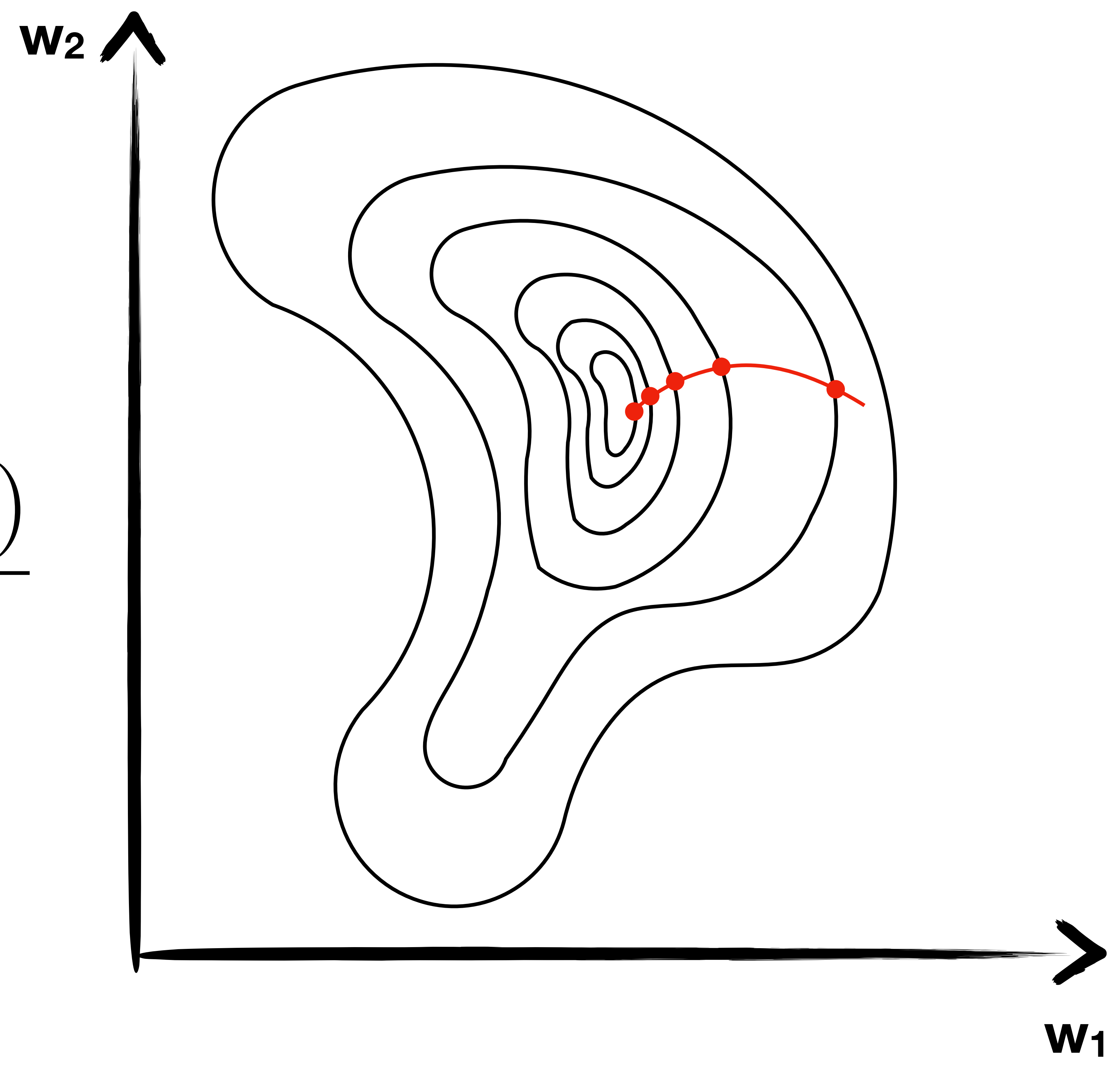
$$\mathcal{L} = \prod_i p_i^{x_i}(1-p_i)^{1-x_i}$$

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

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

Gradient Descent

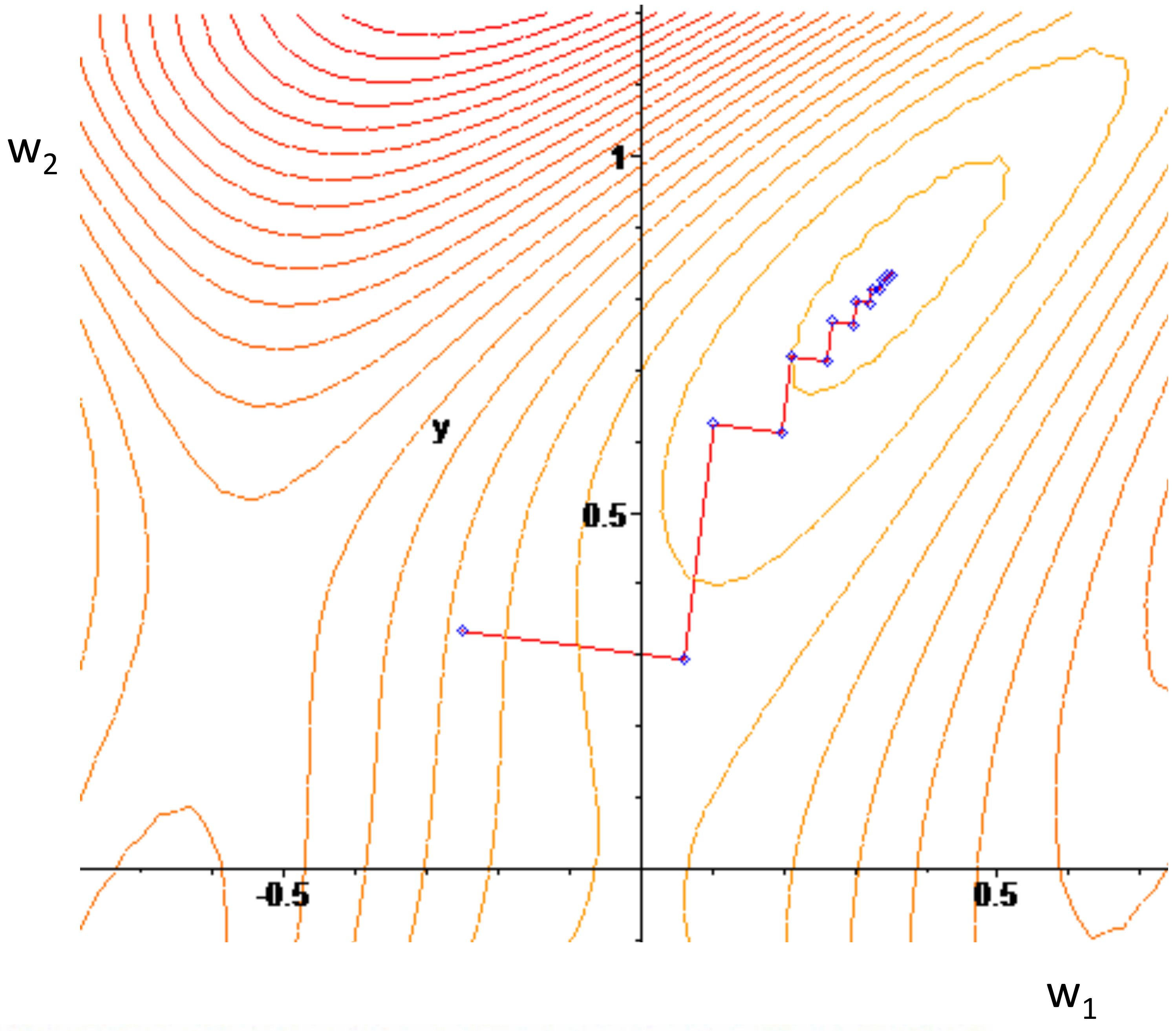
- *Gradient Descent is a popular minimisation algorithm*
  - *Start from a random point*
  - *Compute the gradient wrt the model parameters* $\dfrac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$
  - *Make a step of size η (the **learning rate**) towards the gradient direction*
  - *Update the parameters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

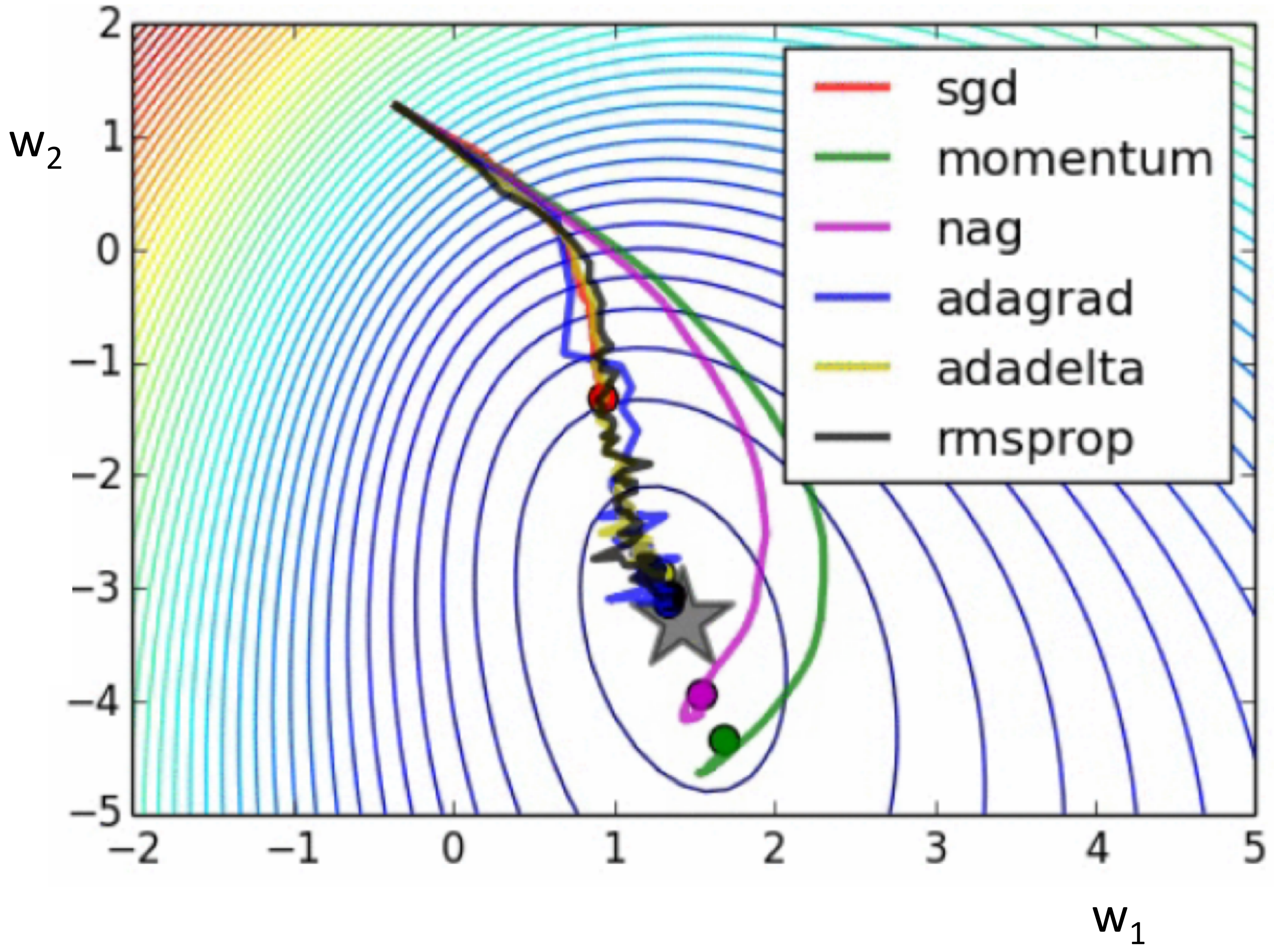


$$\mathbf{w}' \leftarrow \mathbf{w} - \eta \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$$

Stochastic Gradient Descent

- Make the minimisation more computationally efficient
  - Compute gradient on a small batch 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)

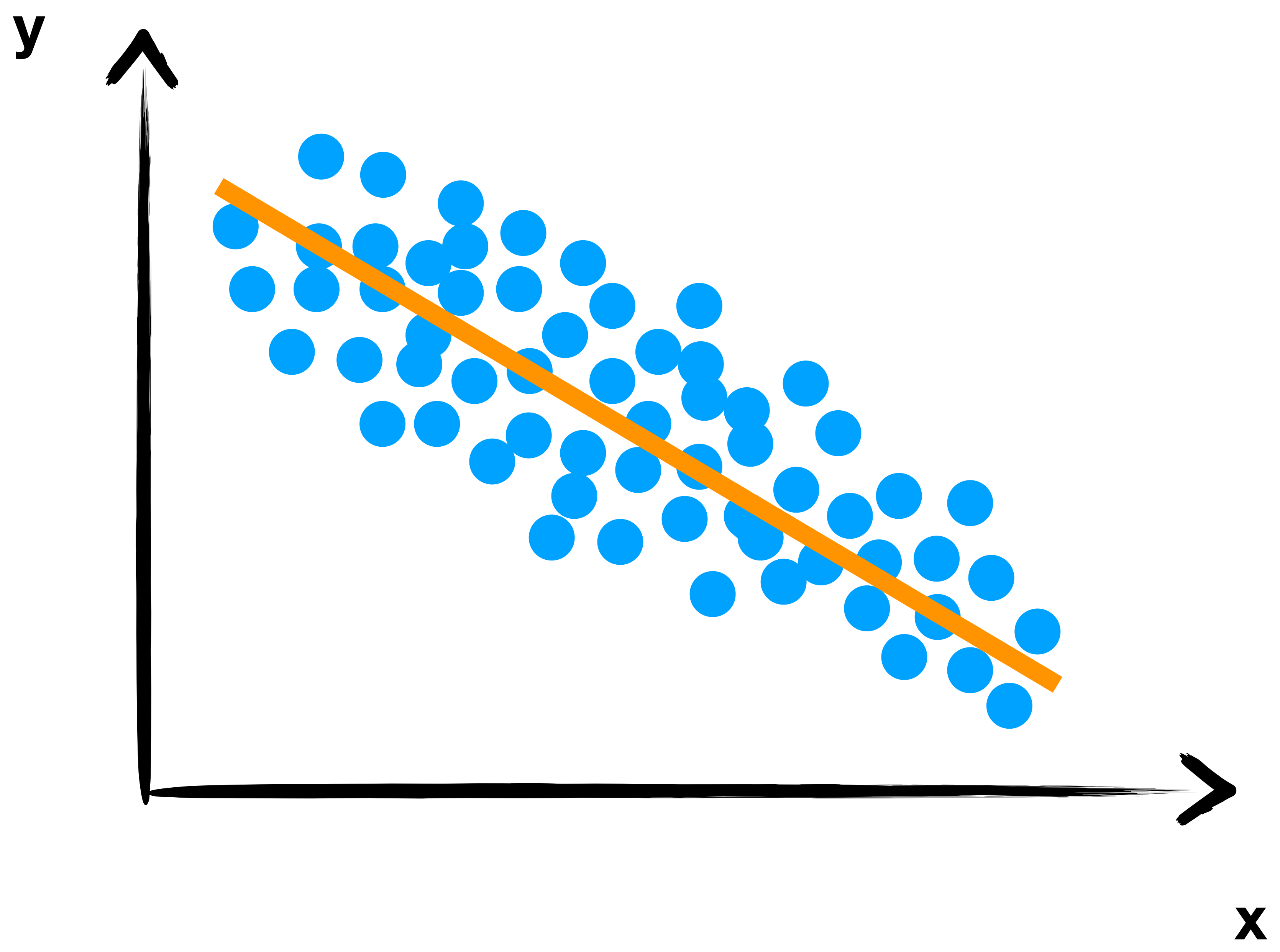




Example: regression & MSE

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

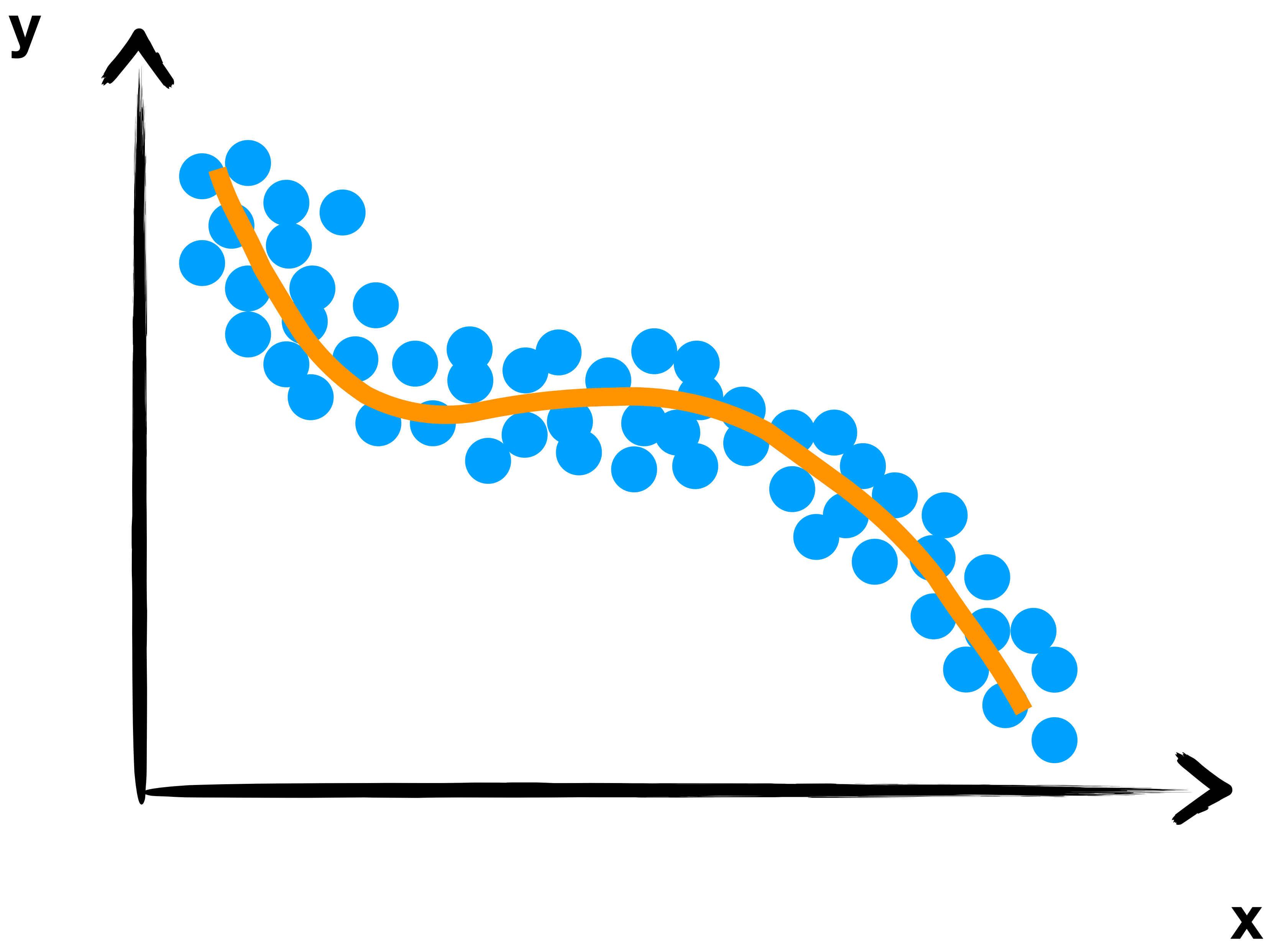
$$y_i = a x_i + b$$



  - *Can be a linear function of non-linear 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)*

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

- *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*

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

- *Write down the likelihood*

Example: regression & MSE

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

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

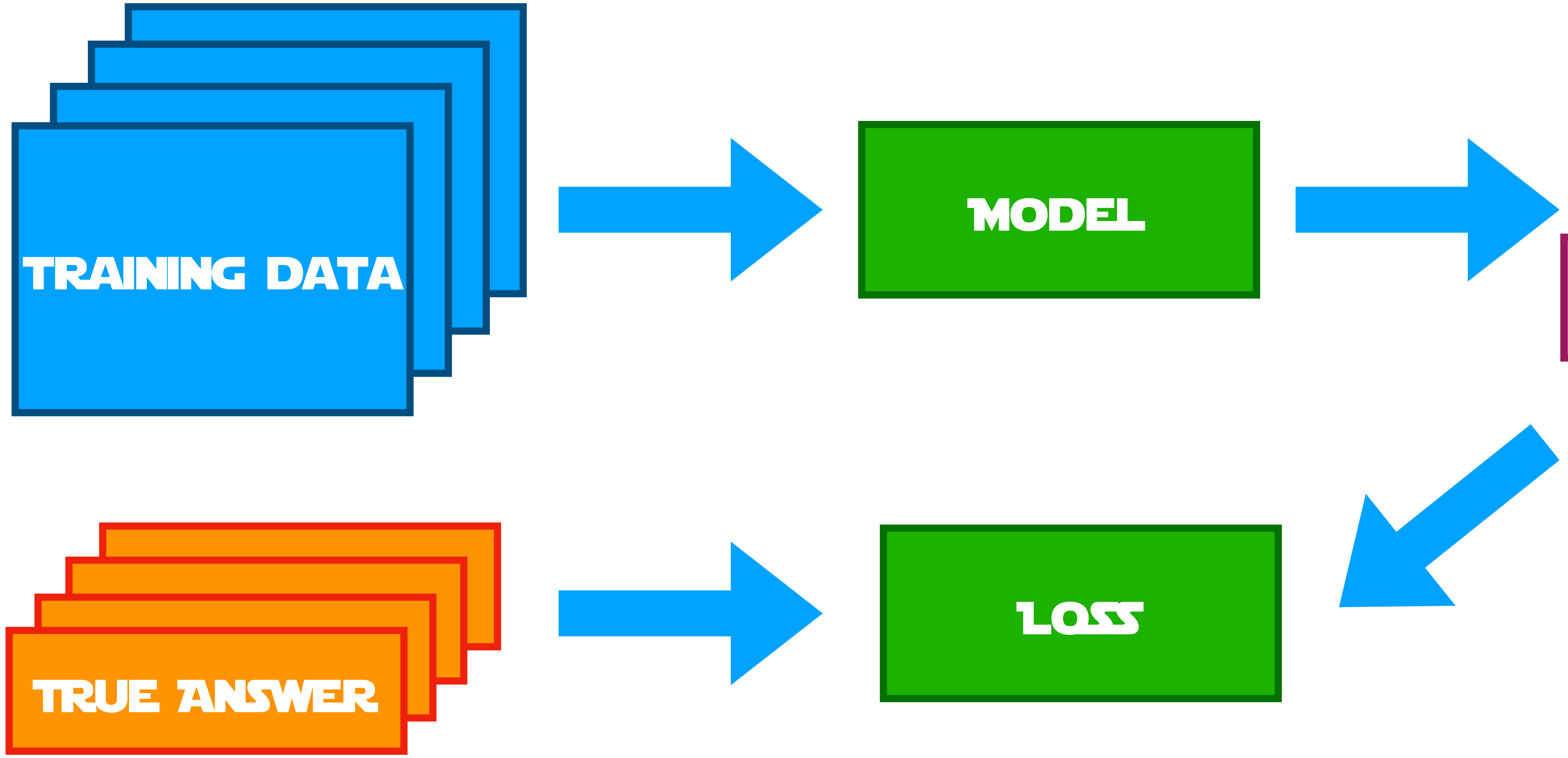
$$= argmin\Big[\sum_i \frac{(y_i-h(x_i))^2}{\sigma^2}\Big] = argmin\Big[\sum_i (y_i-h(x_i))^2\Big] = MSE$$

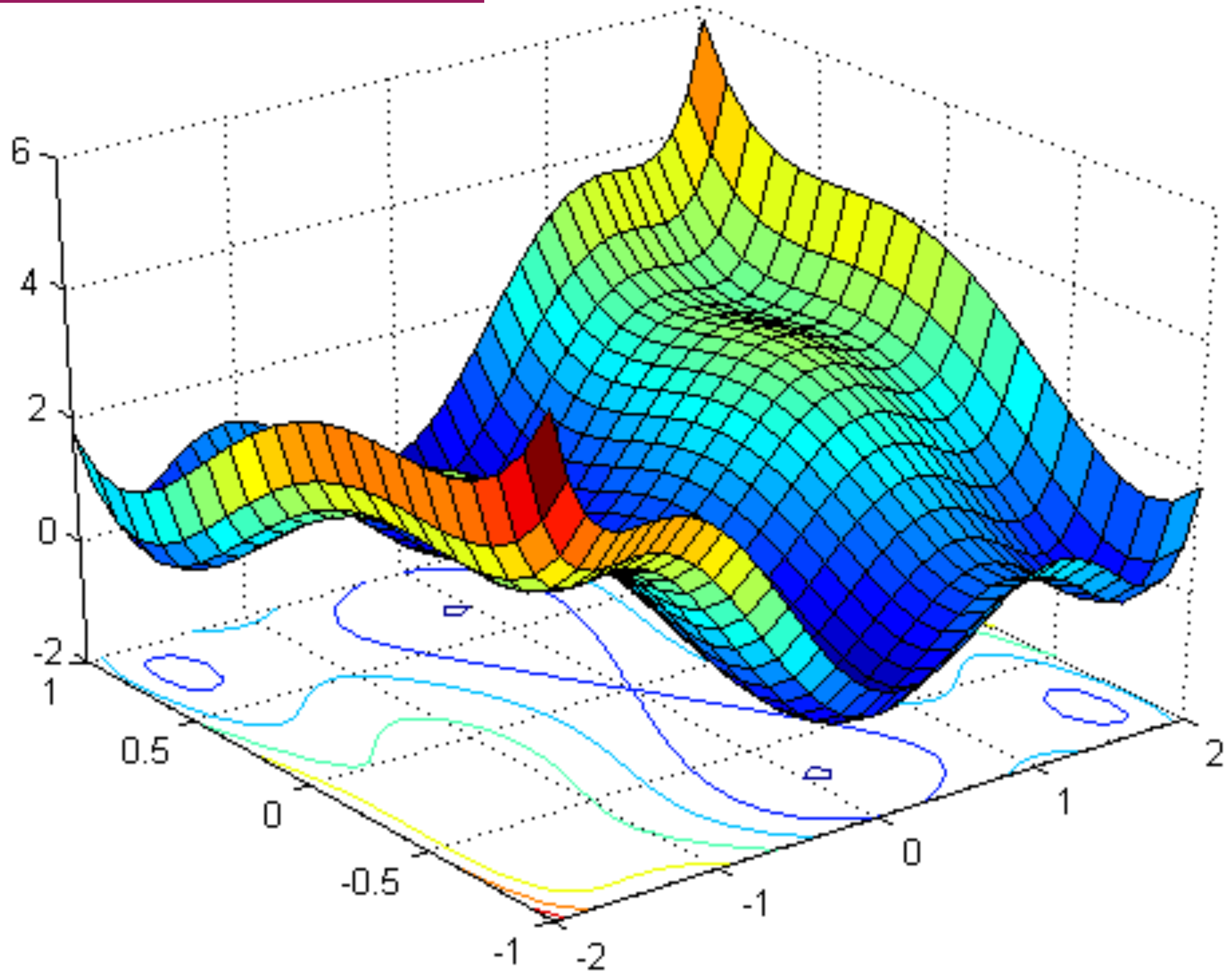
- *MSE is the most popular loss function when dealing with continuous outputs. We will use it a few times in the next days*

- ***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 if the RMS is not a constant?*

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

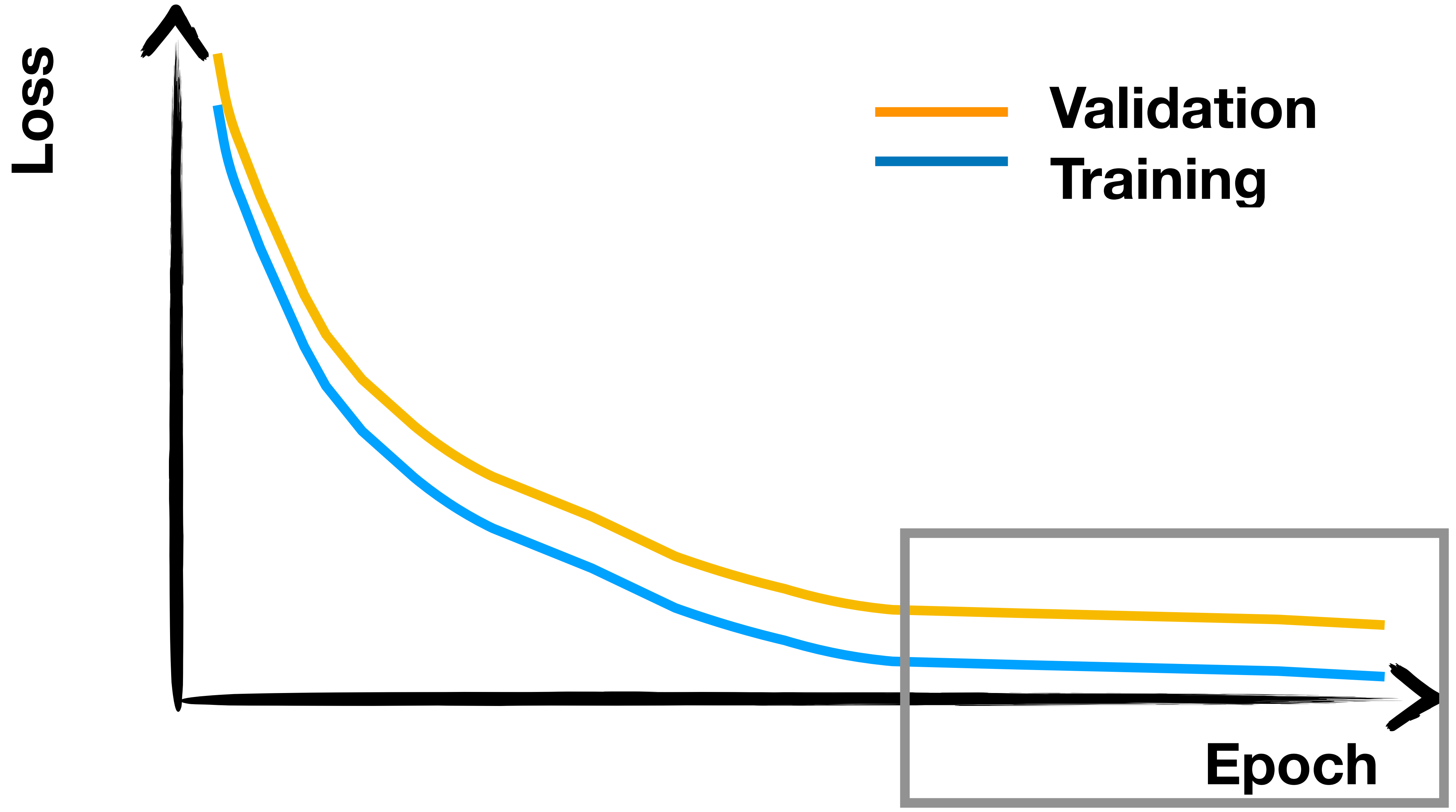
Training in practice

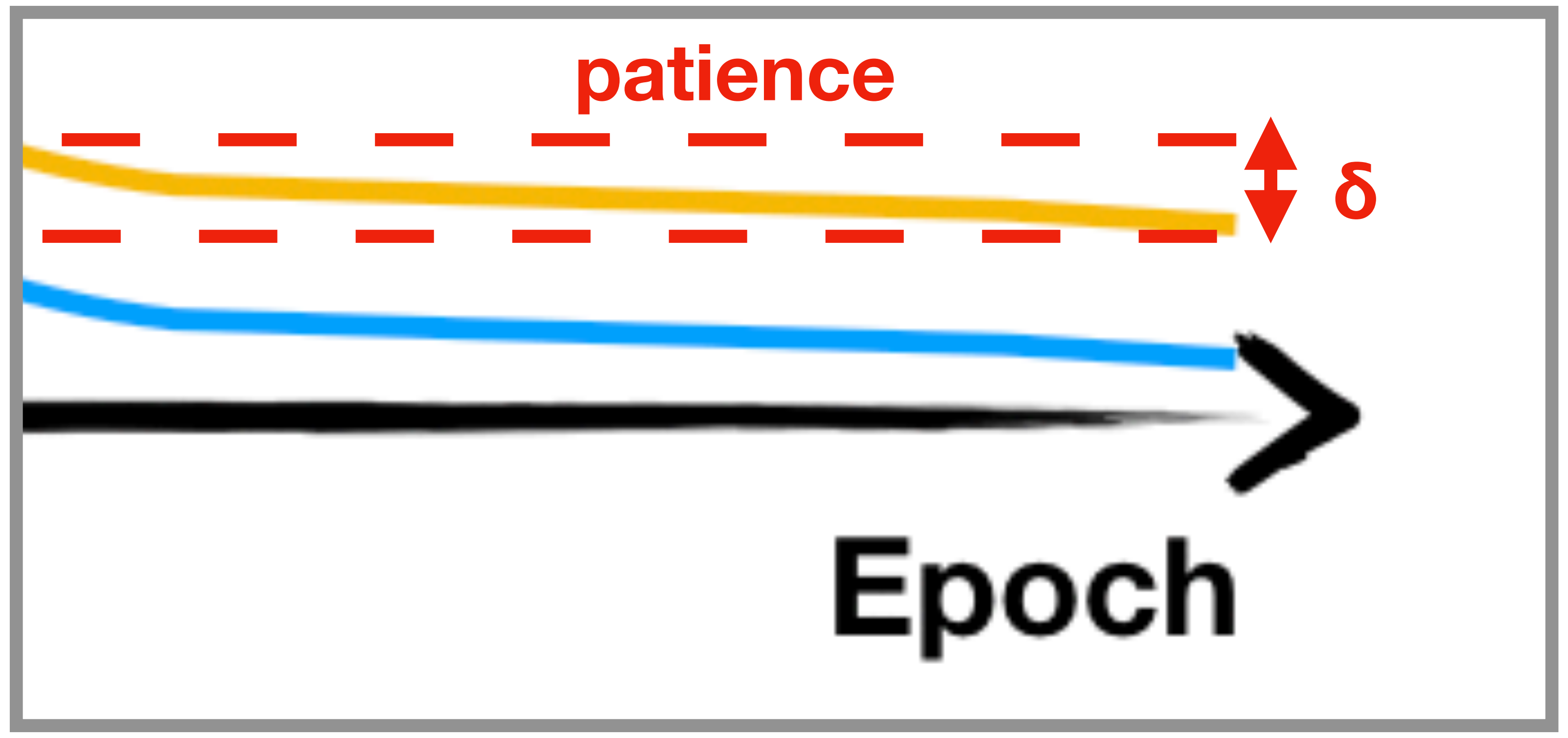
- *Split your sample in three:*
  - *Training: the biggest chunk, where you learn from*
  - *Validation: an auxiliary dataset to verify generalization and prevent overtraining*
  - *Test: the dataset for the final independent check*

Training | Validation | Test

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)

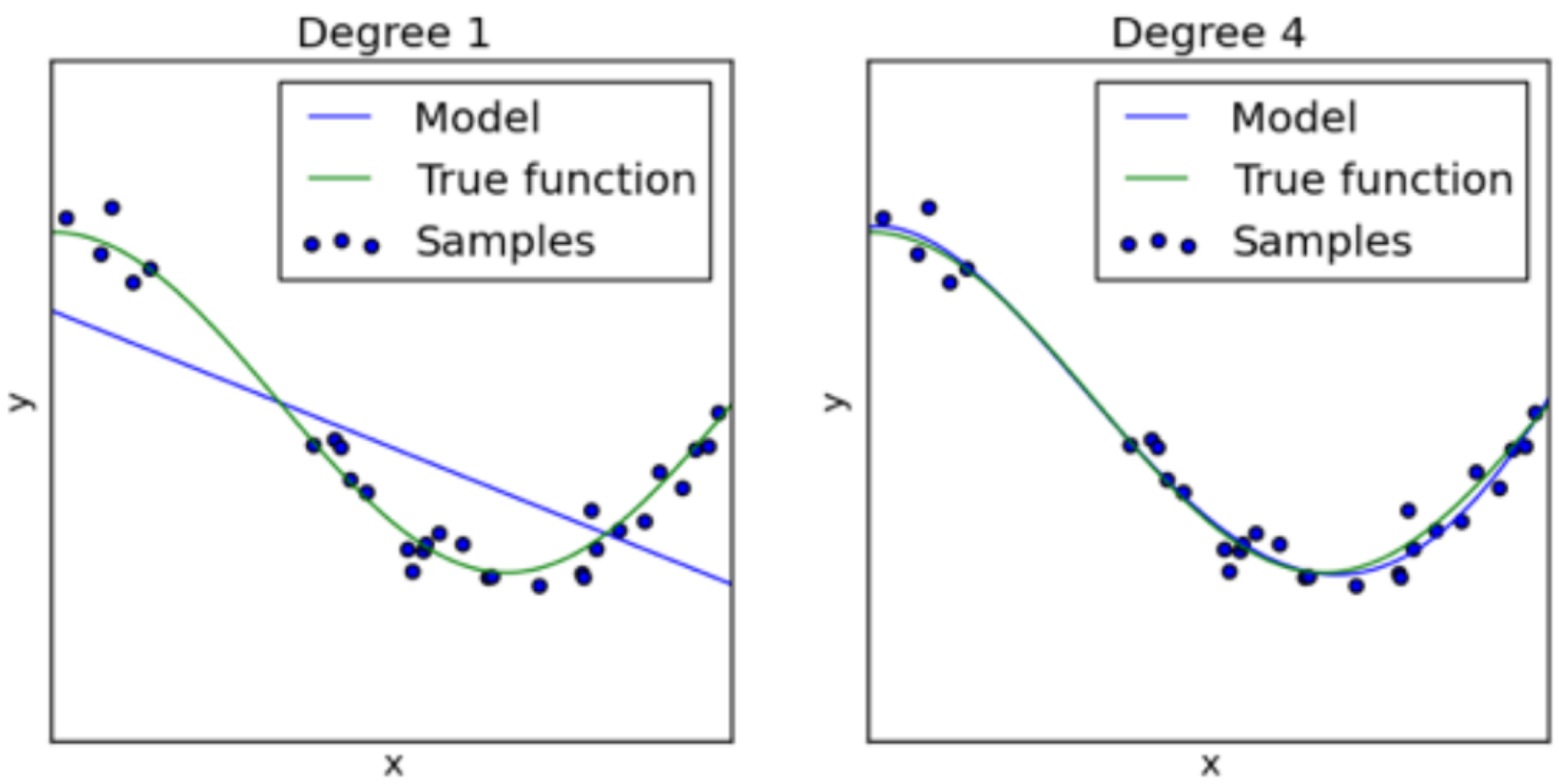


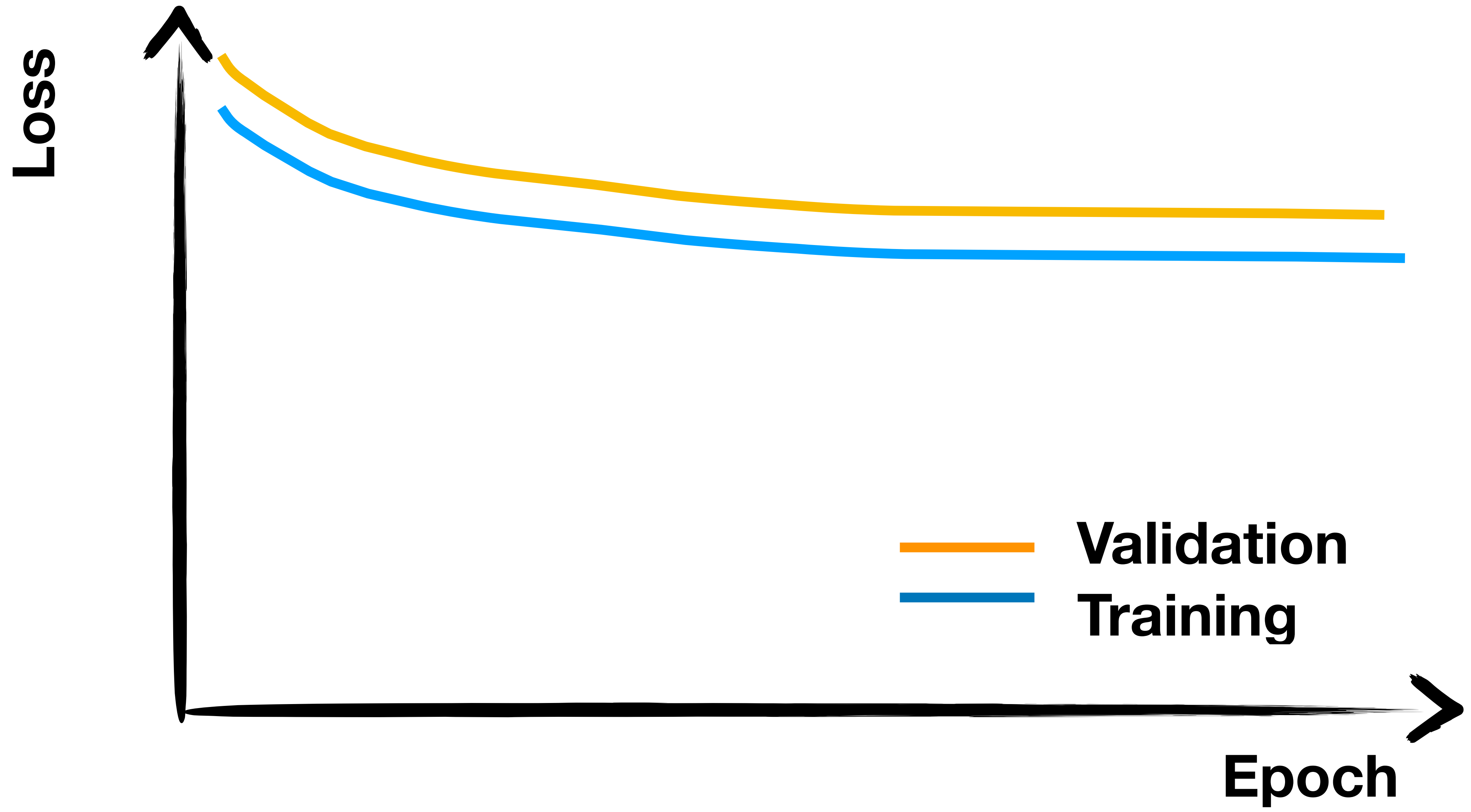


EARLY TOPPING: stop the train if the validation loss didn't change more than δ in the last n epochs (patience)

What can go wrong: underfitting

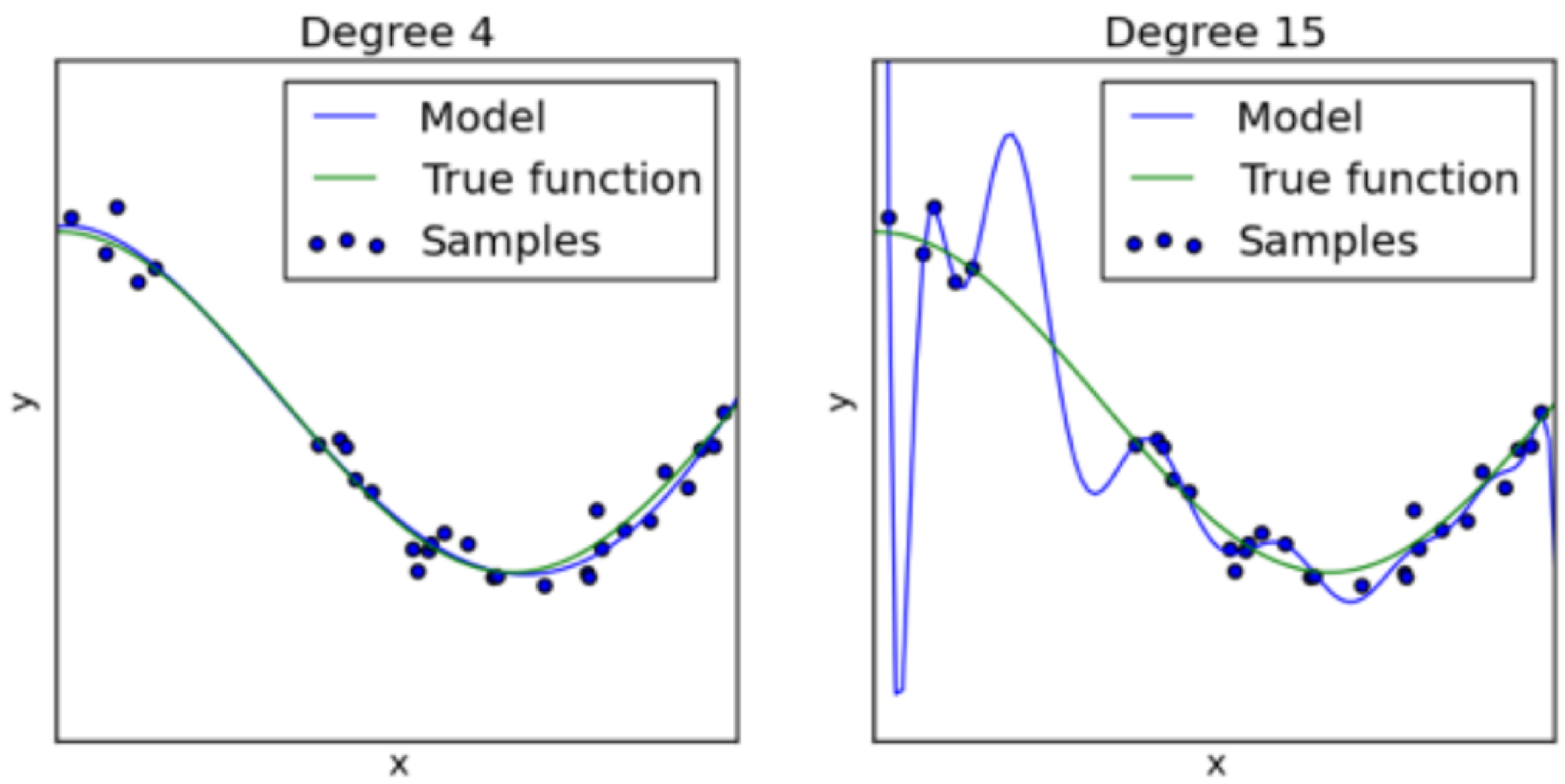
- *If your model has not enough flexibility, it will not be able to describe the data*
- *The training and validation loss will be close, but their value will not decrease*
- *The model is said to be underfitting, or being* ***biased***

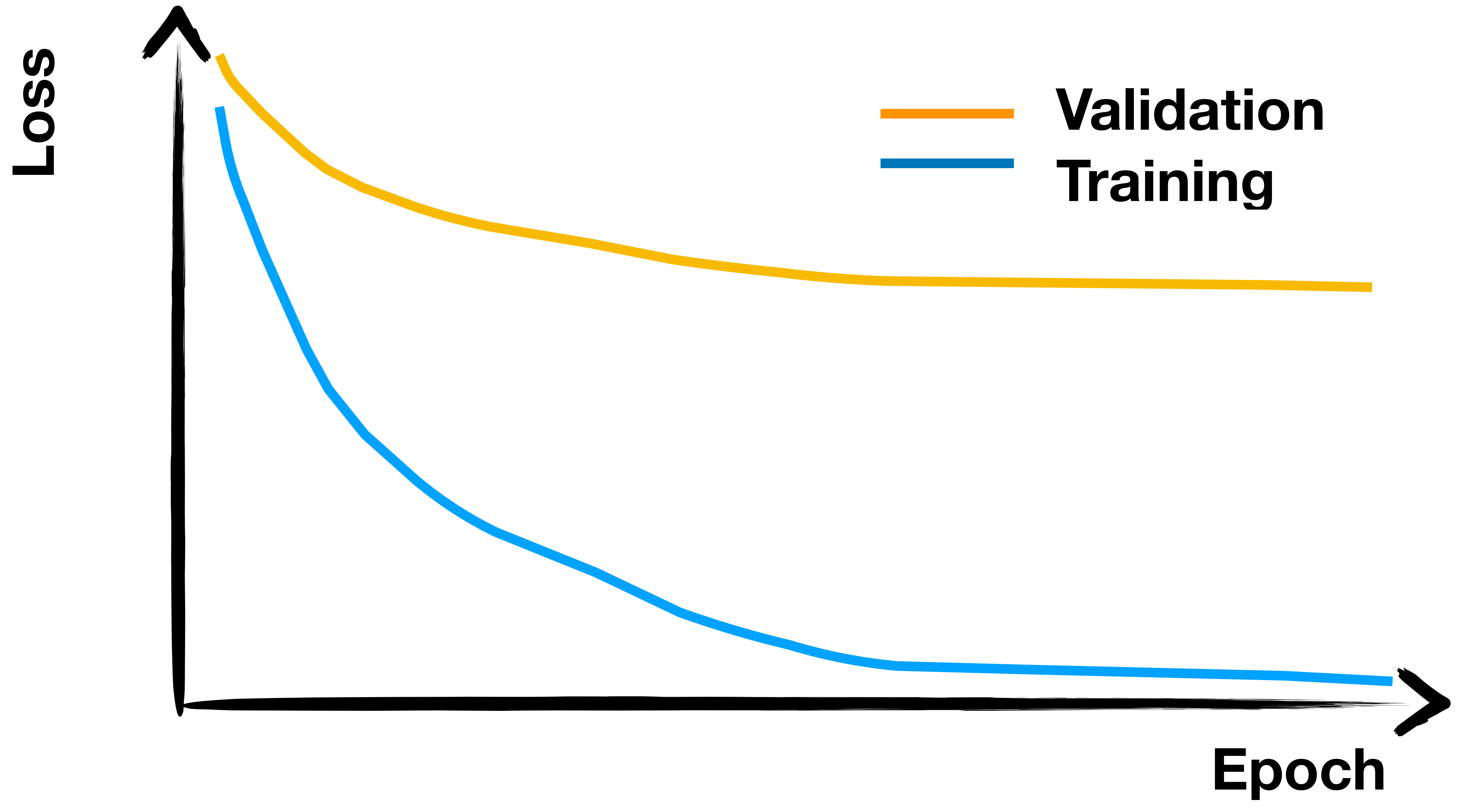




What can go wrong: overfitting

- *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*



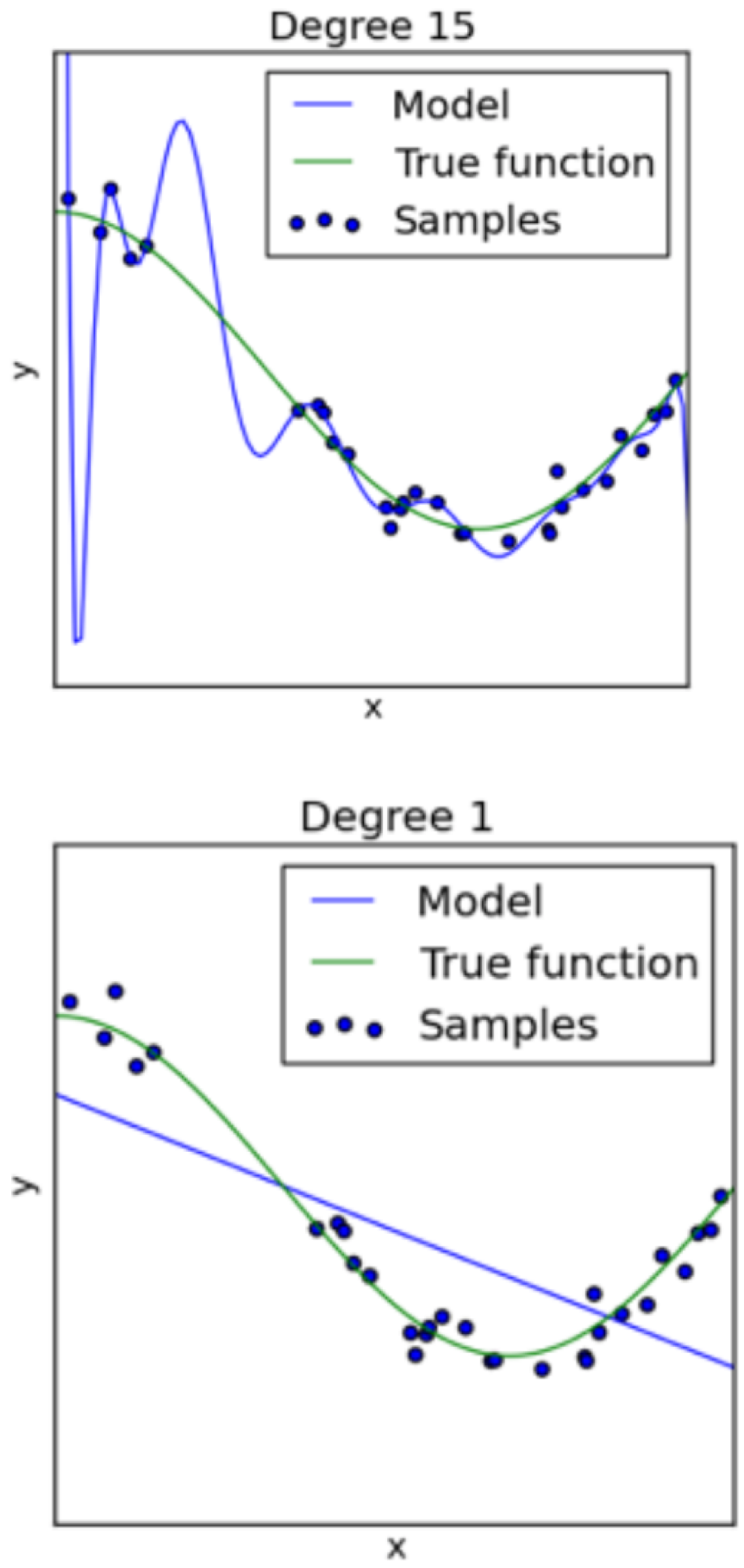


The Bias vs Variance tradeoff

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

- ***A model would overfit if 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)*



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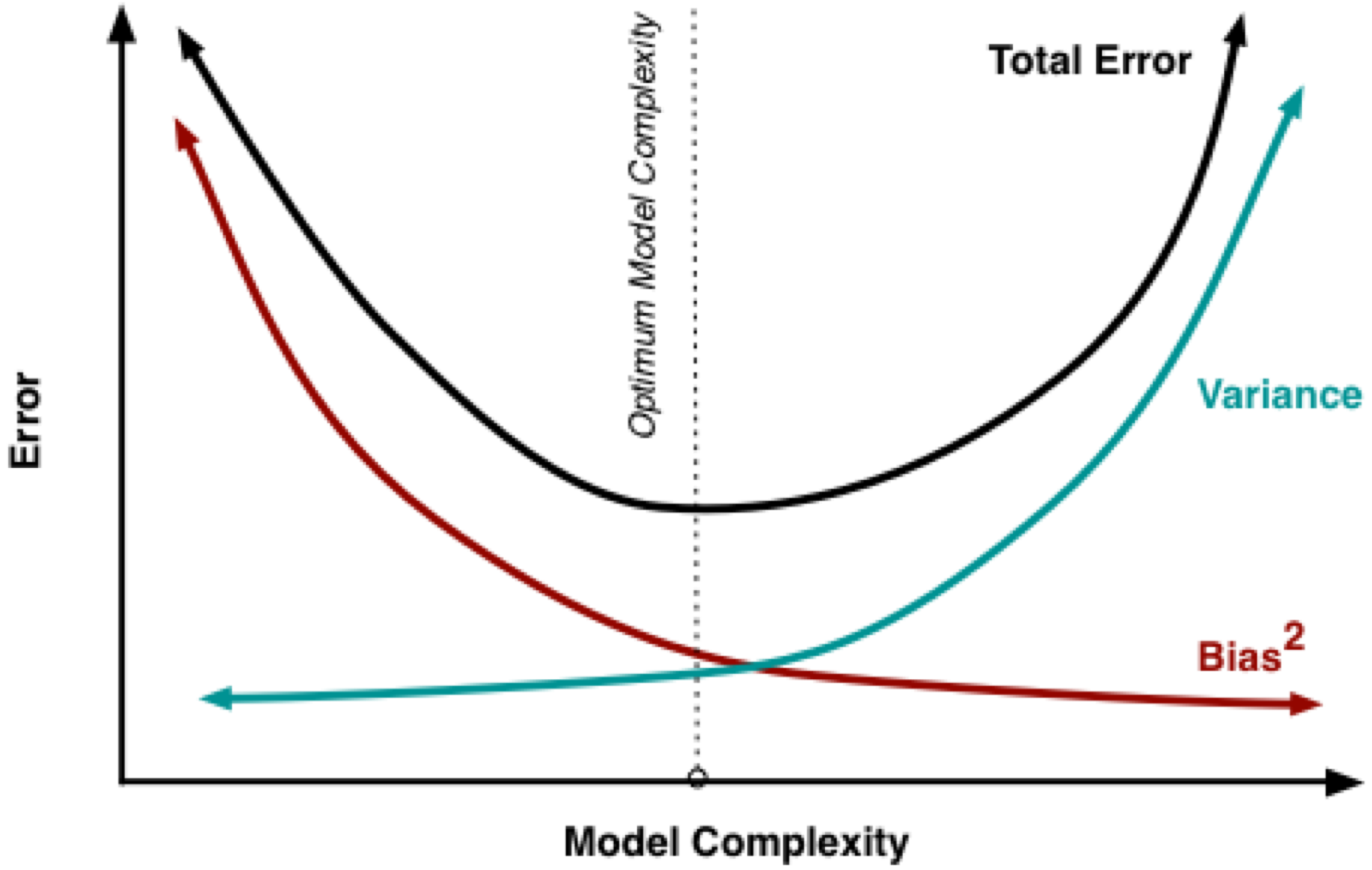
The Bias vs Variance tradeoff

- *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*

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

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

The Bias vs Variance tradeoff



Regularization

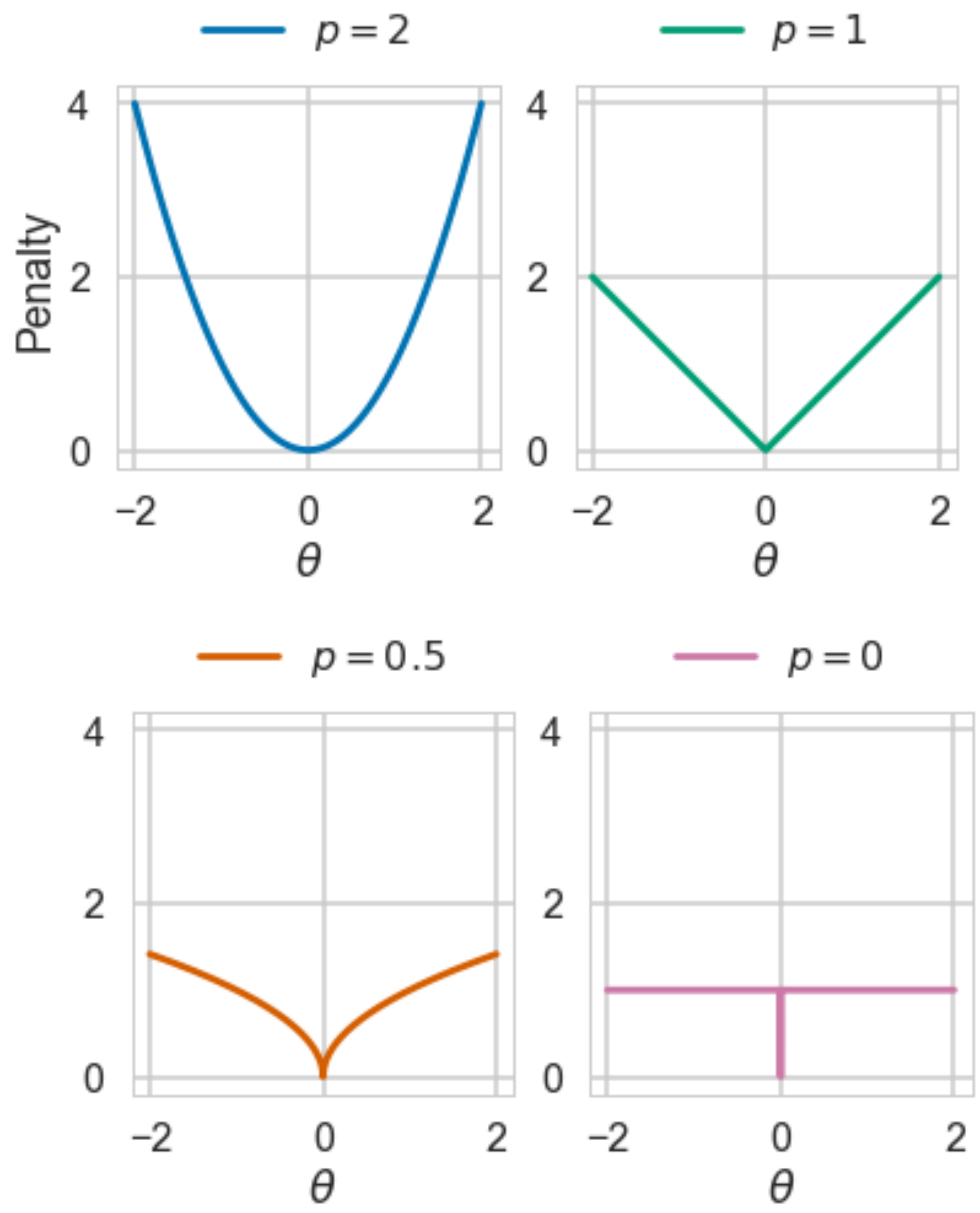
- Model complexity can be "optimized" when minimizing the loss
  - A modified loss is introduced, with a penalty term attache to each model parameter

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

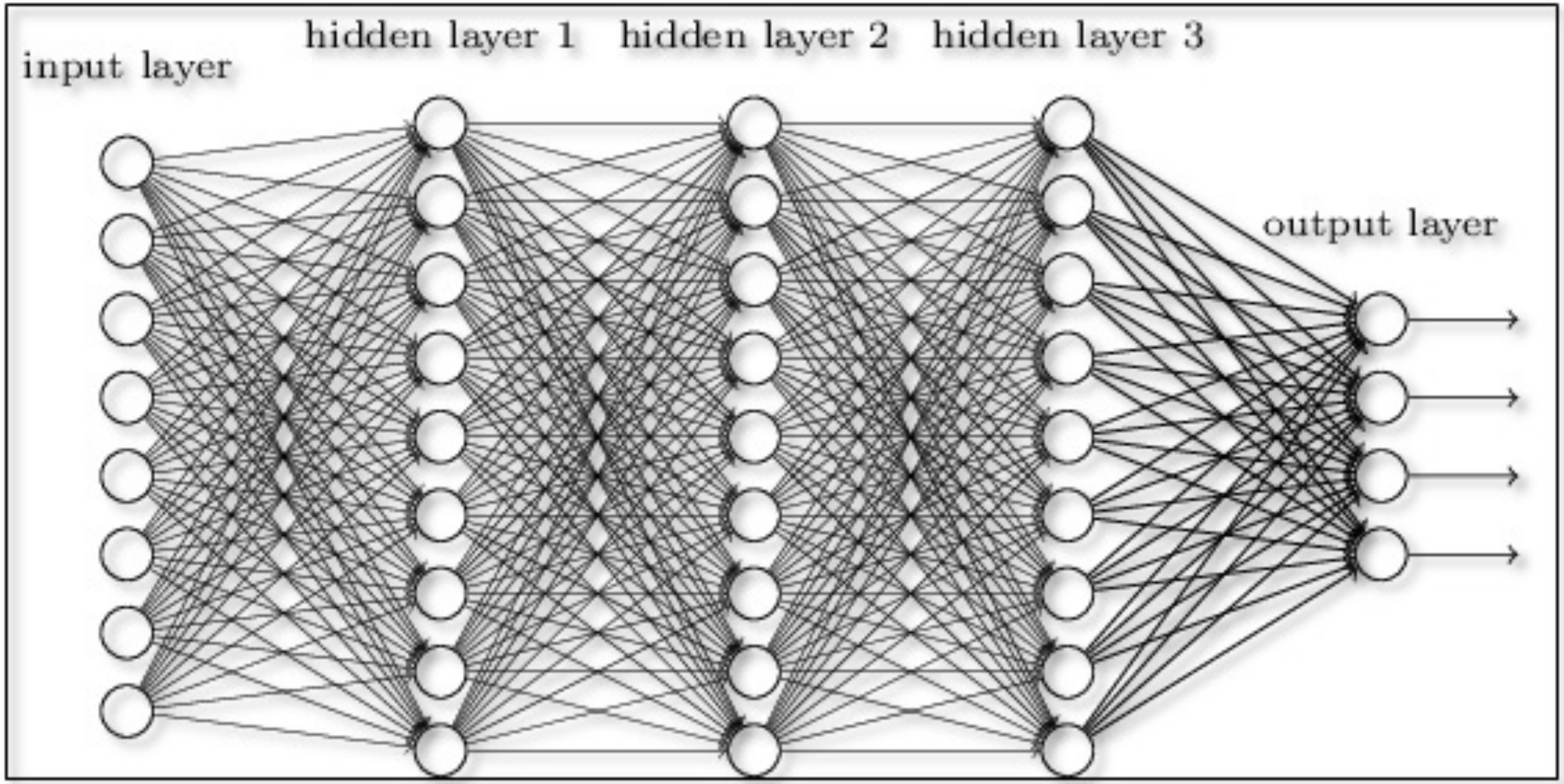
- For instance, Lp regularisation

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

- 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

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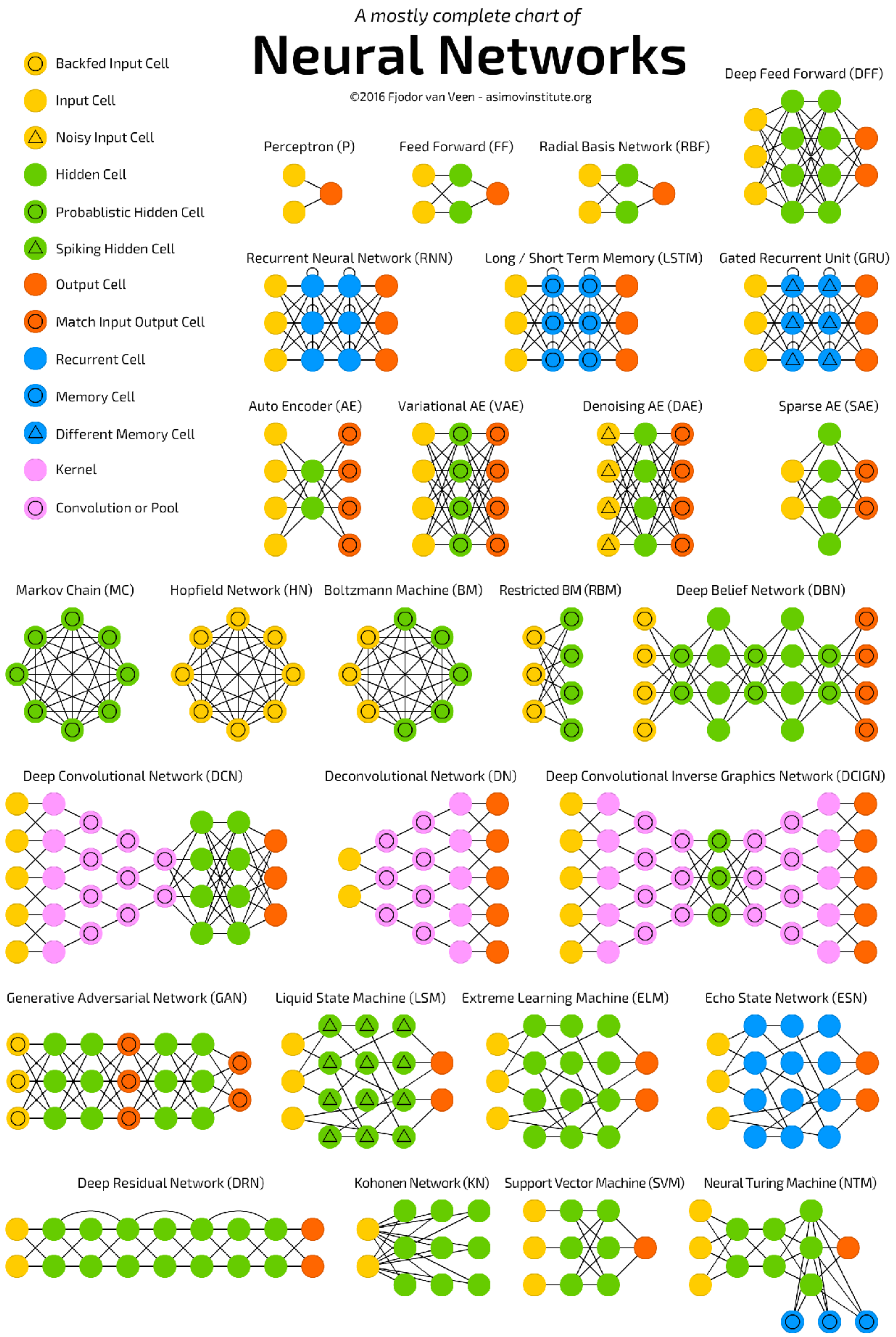
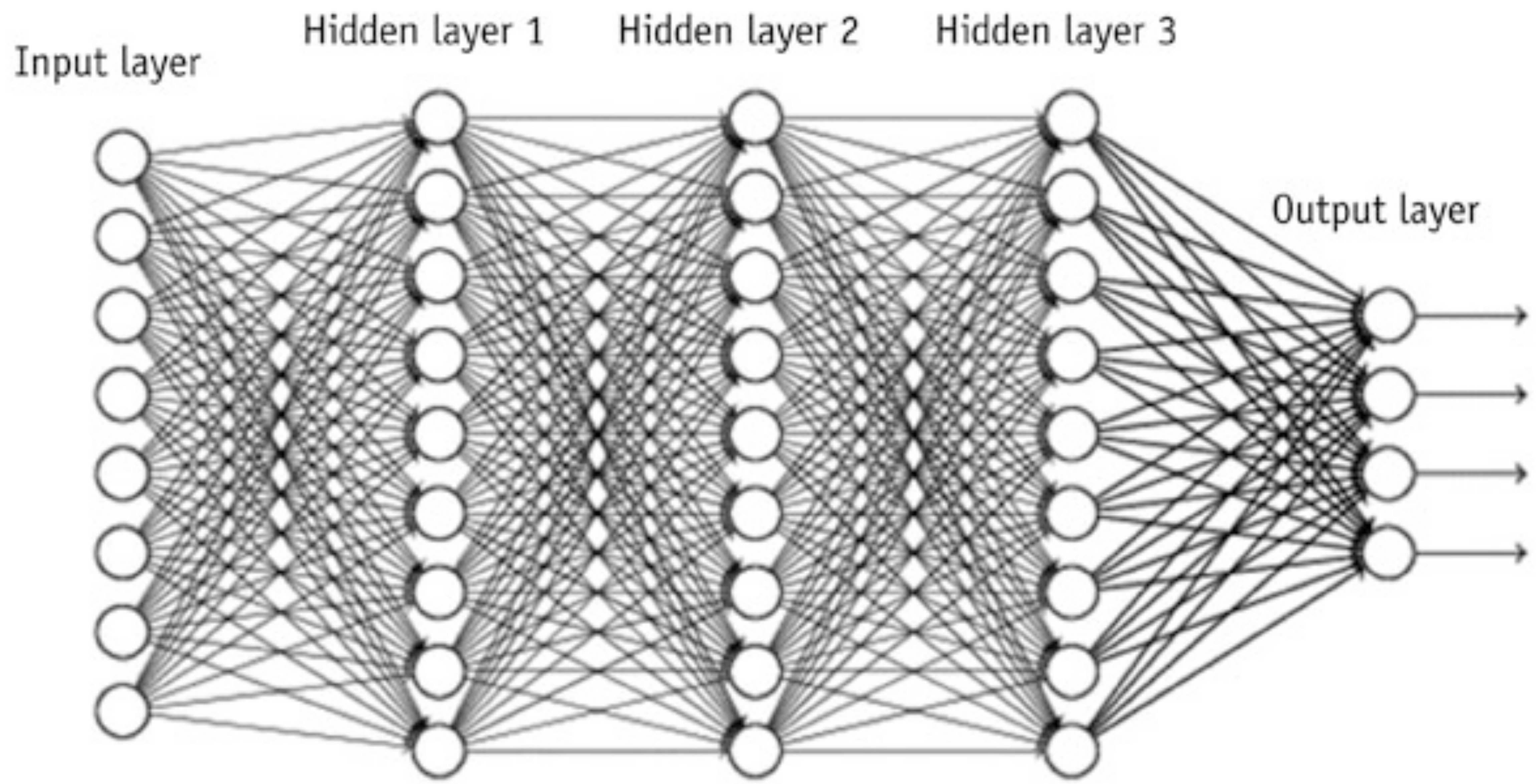
Neural Networks in a nutshell

- 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*
- *<u>Thanks to GPUs</u>, 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

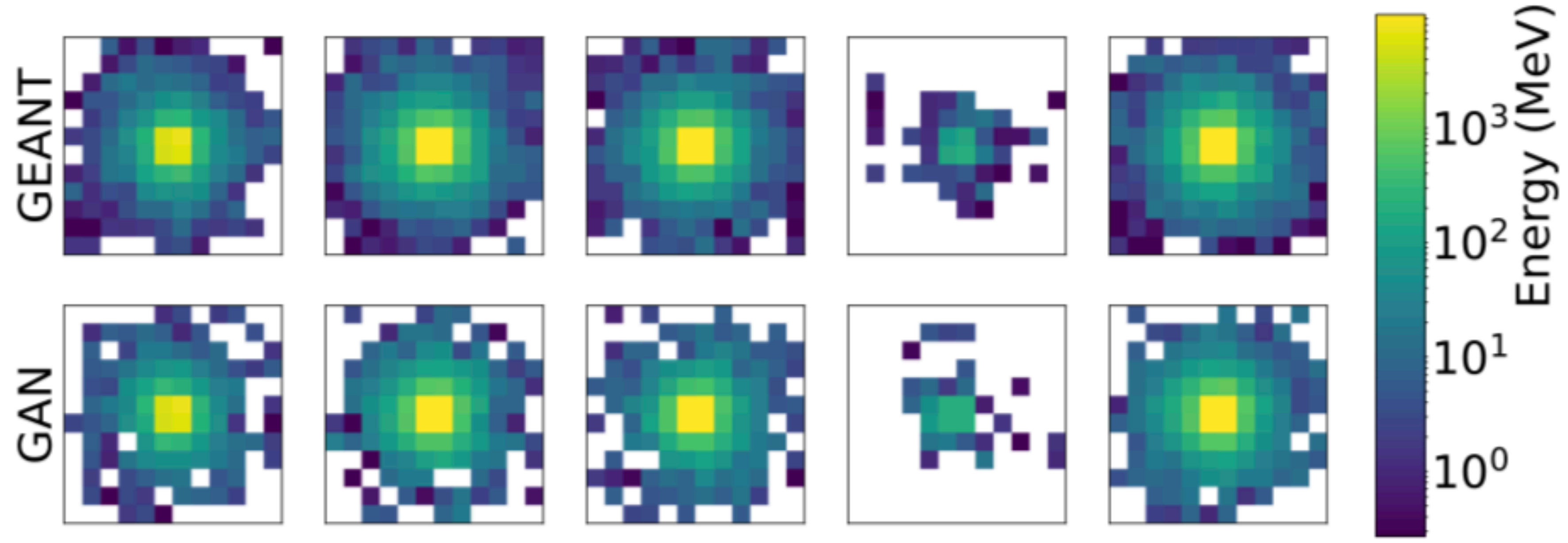
text/sound processing

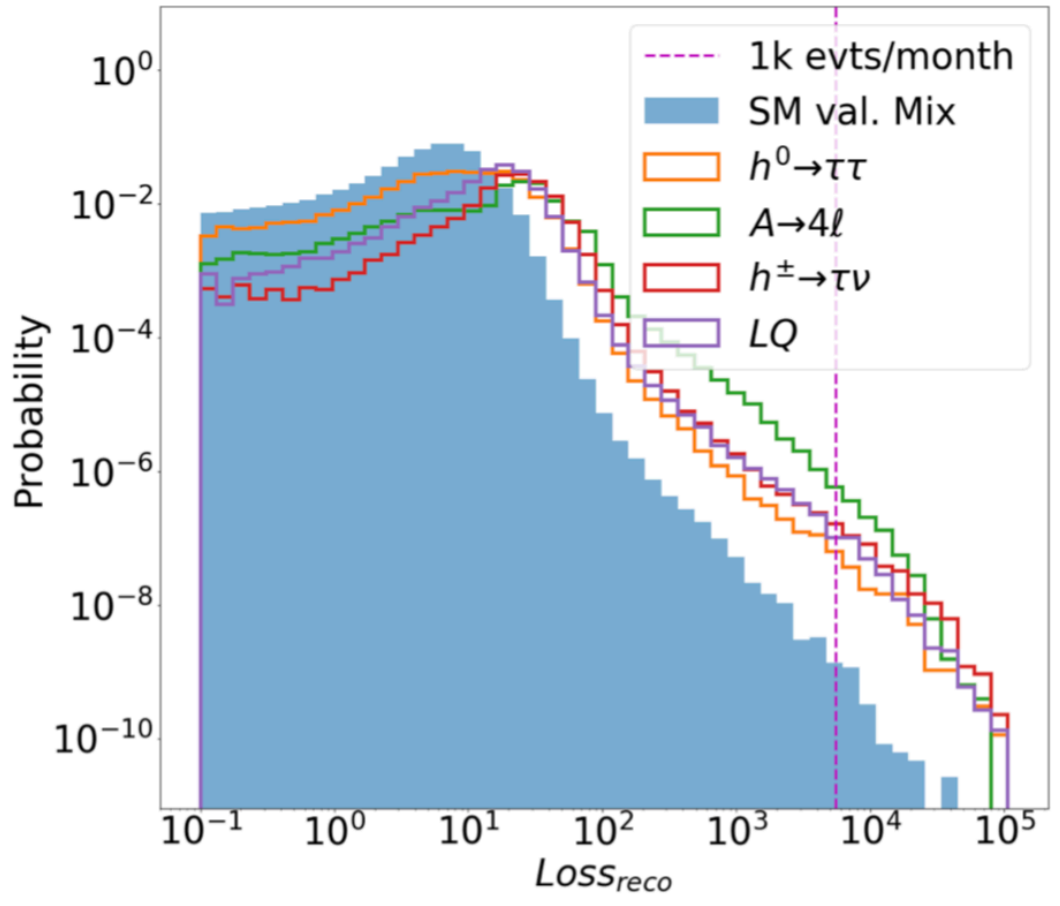
Reinforcement Learning

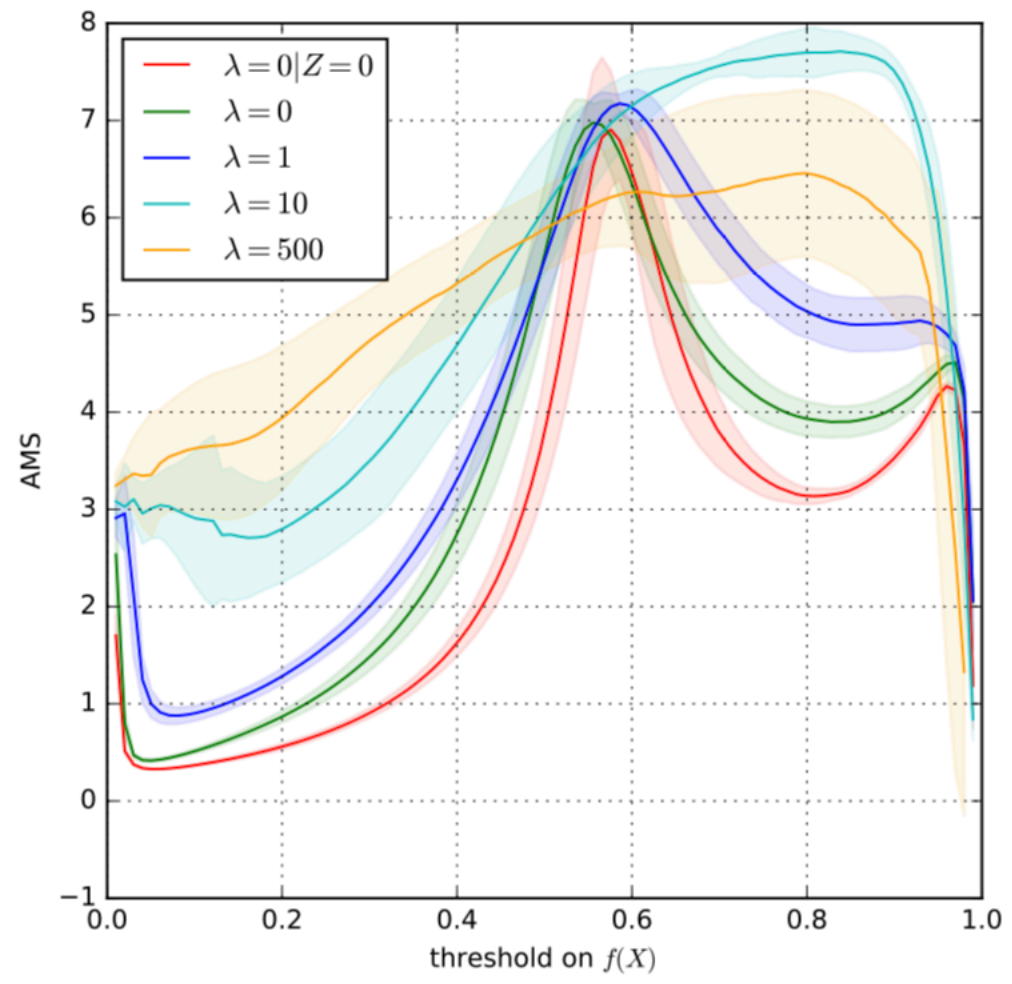
Clustering

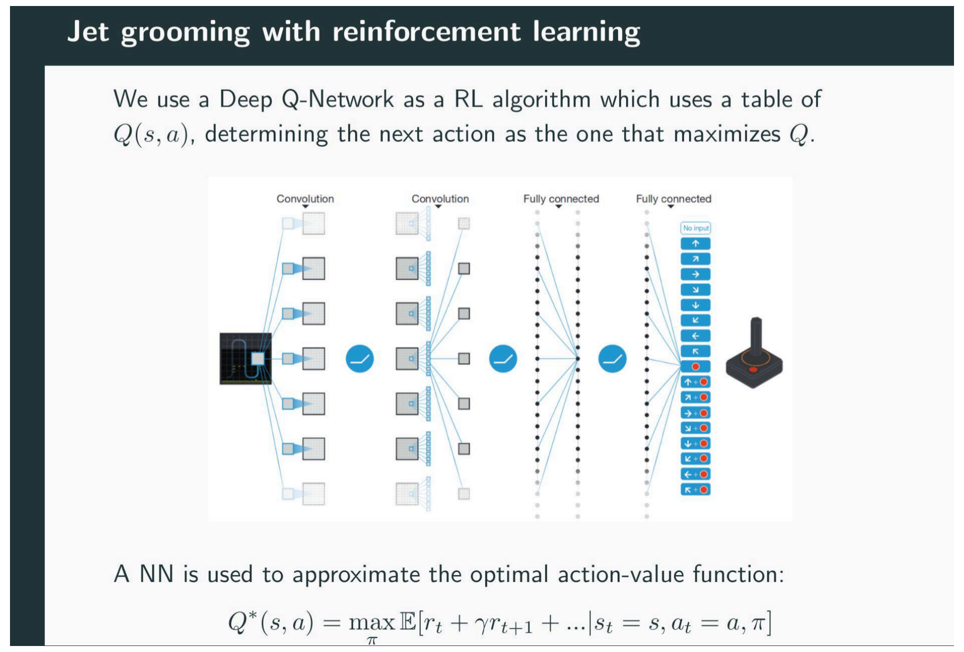
DL, HEP, and new opportunities

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



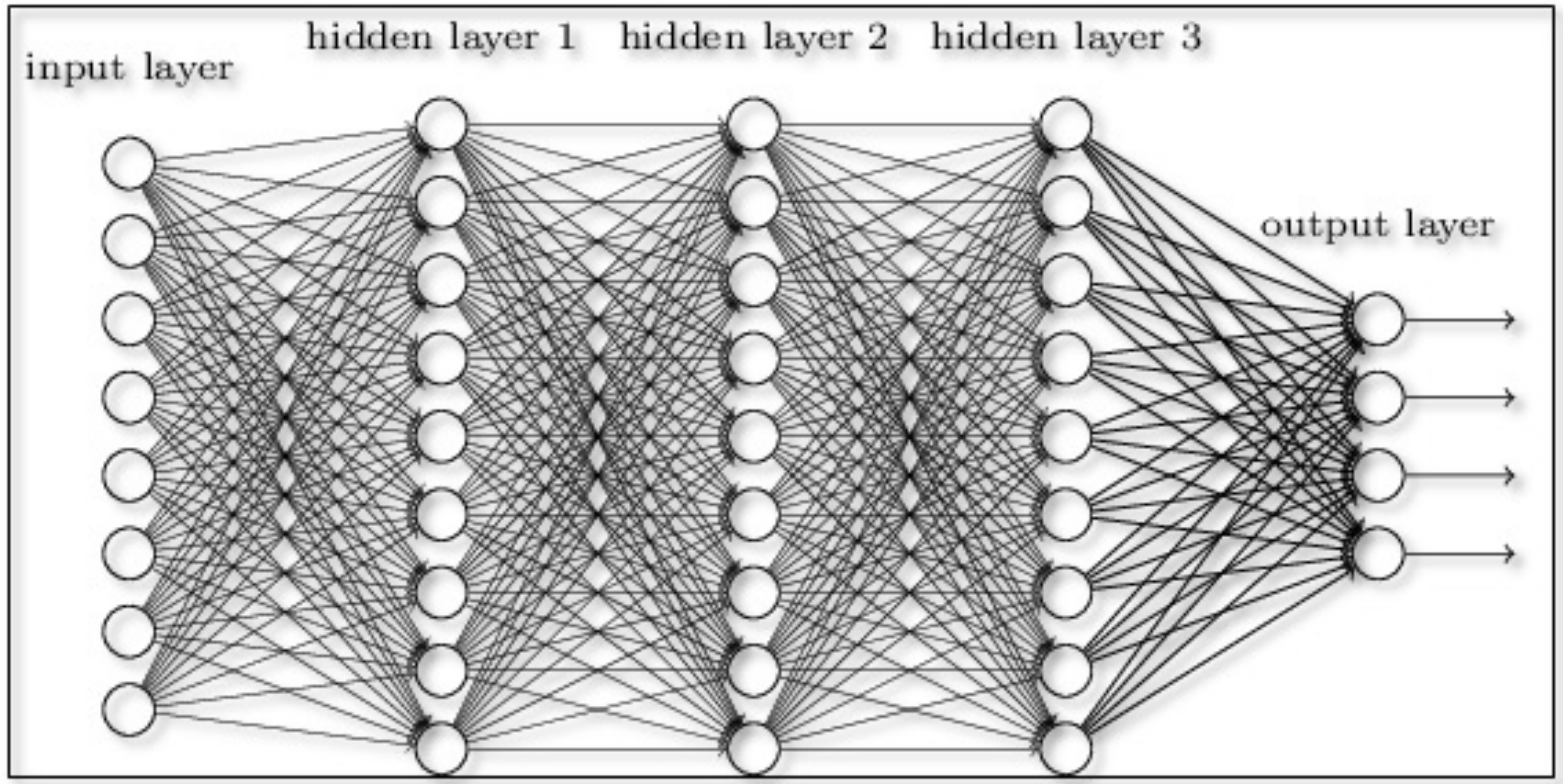






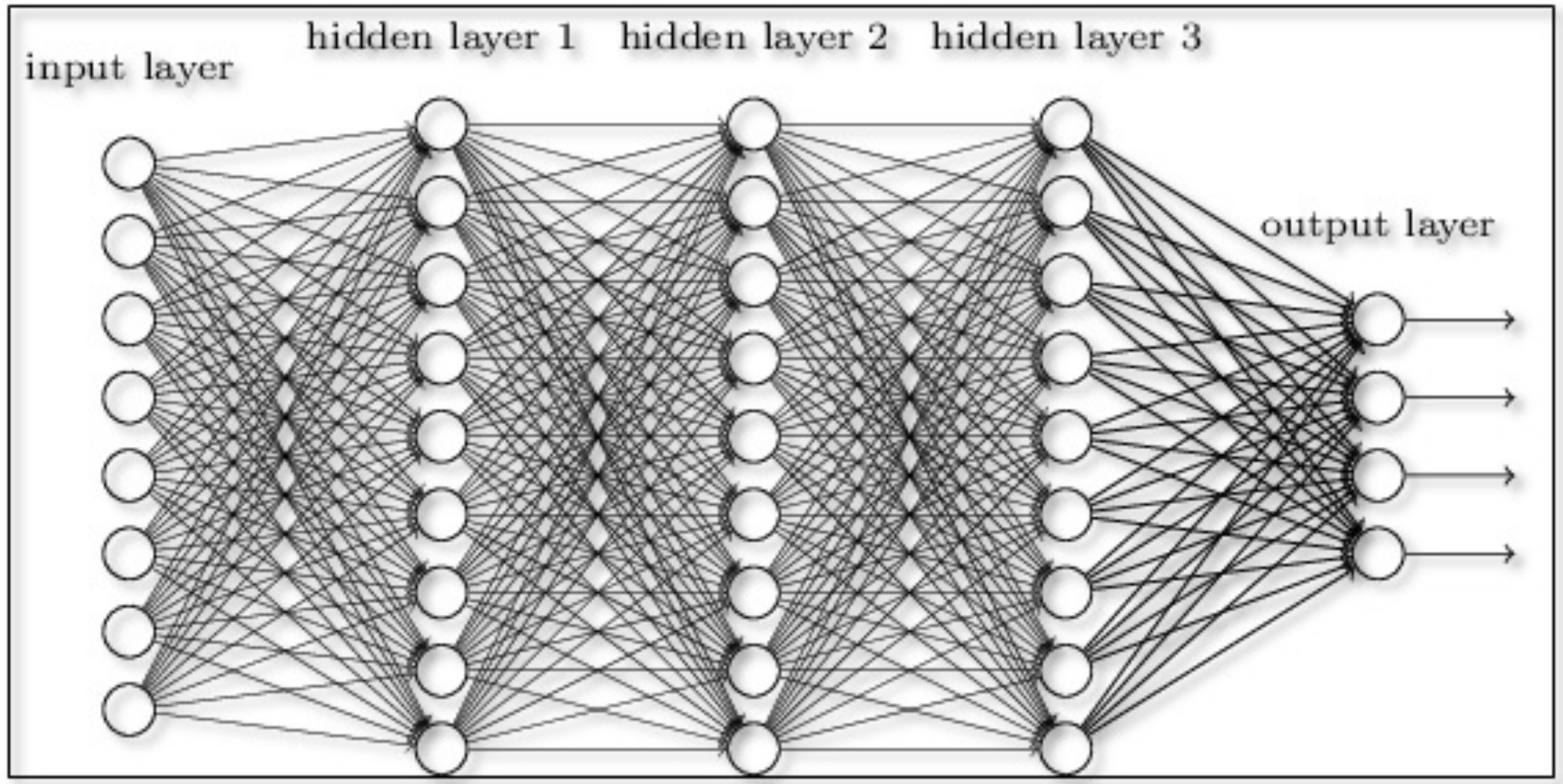
Feed-Forward NNs

- 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



$$w_{ij}x_j$$

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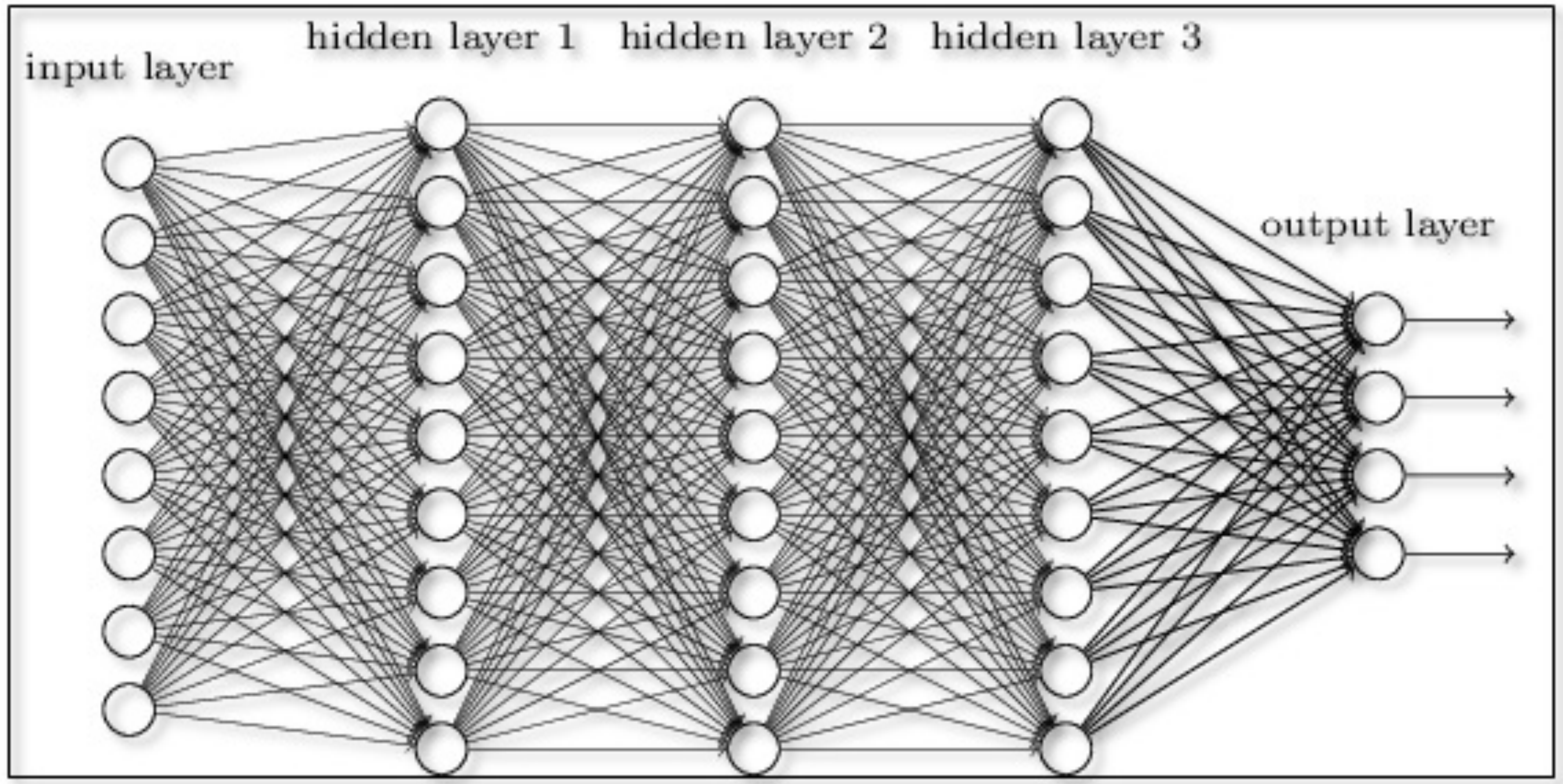

$$\Sigma_j w_{ij} x_j$$

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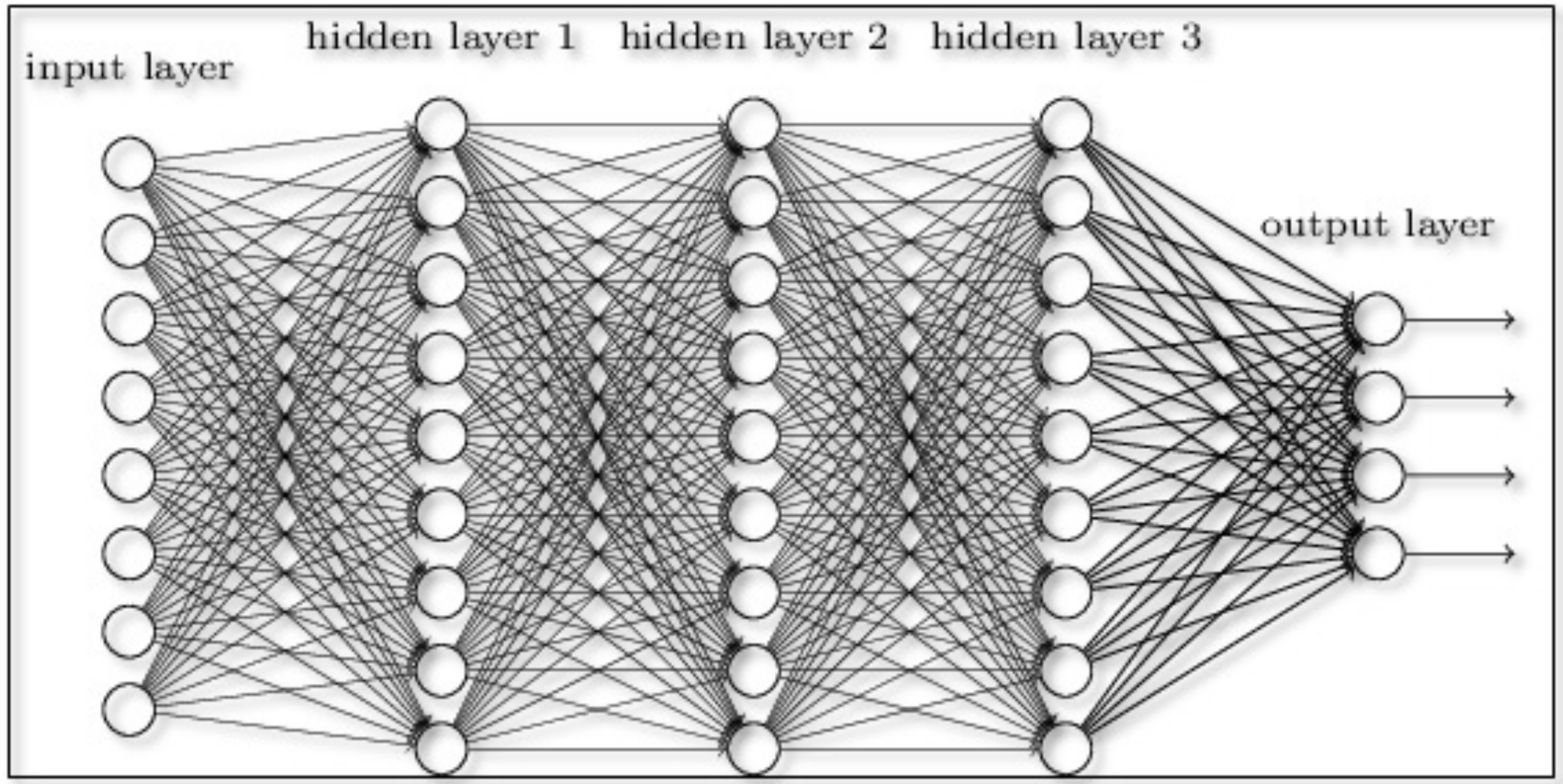
The role of a network node

- 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
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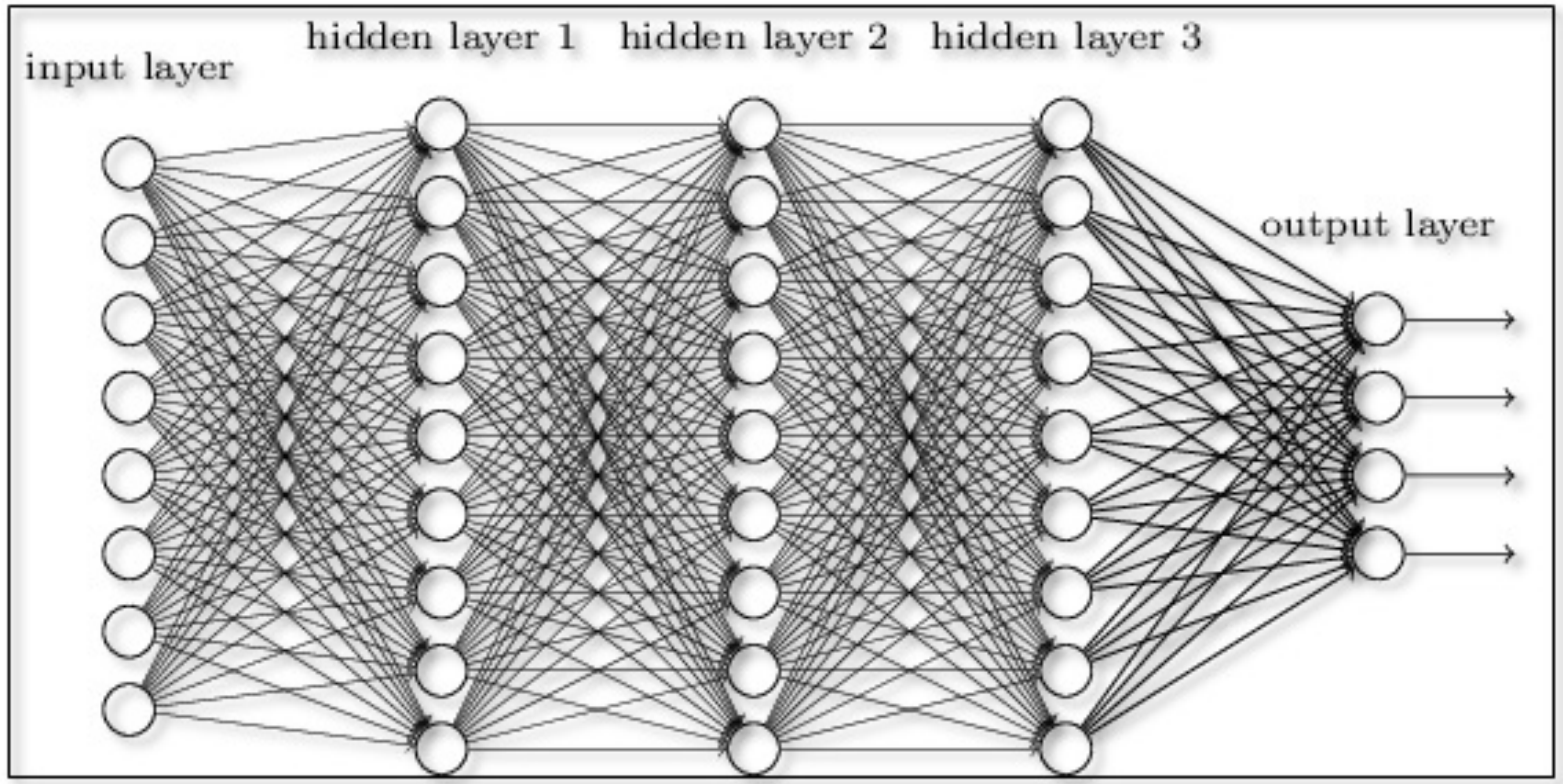
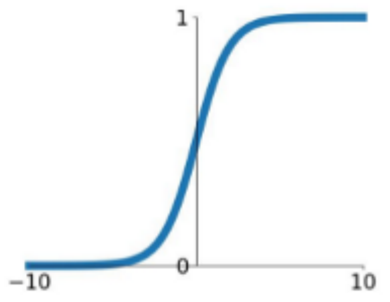
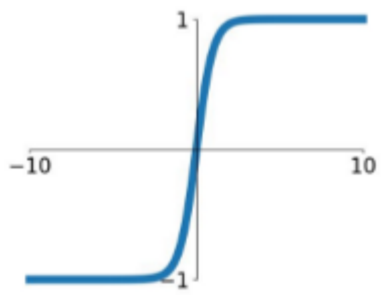


Activation Functions

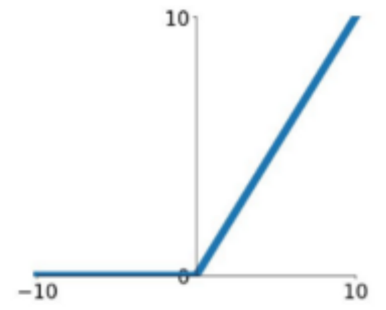
Sigmoid
$\sigma(x) = \frac{1}{1+e^{-x}}$



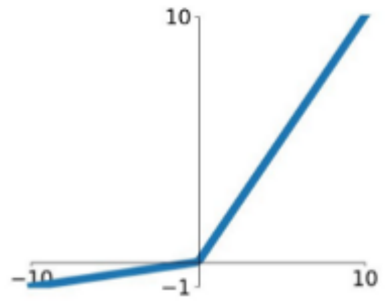
tanh
$\tanh(x)$



ReLU
$\max(0, x)$

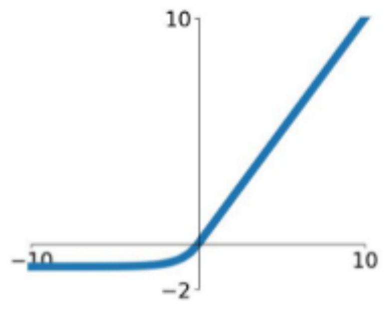


Leaky ReLU
$\max(0.1x, x)$



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

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

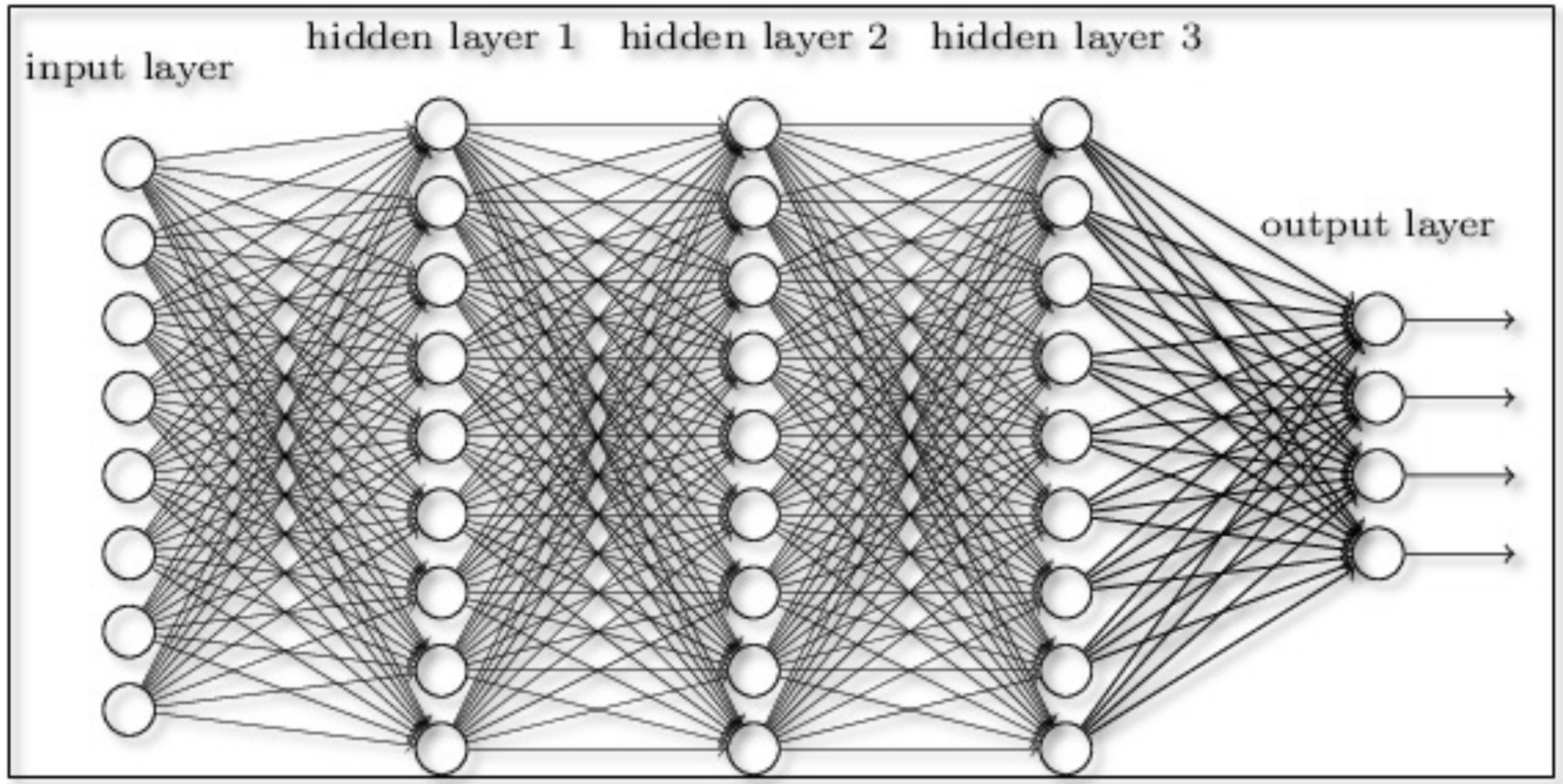


$$y_i = f(\Sigma_j w_{ij} x_j + b_i)$$

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*

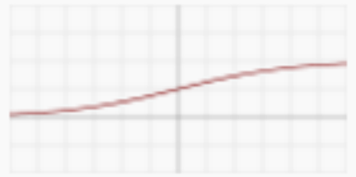
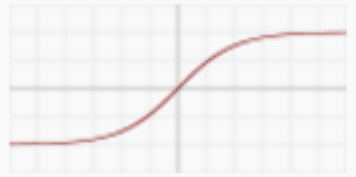
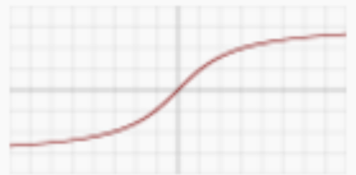
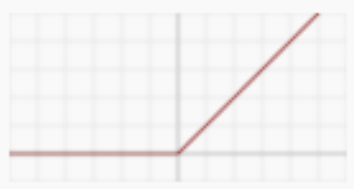
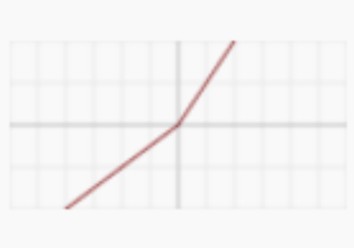
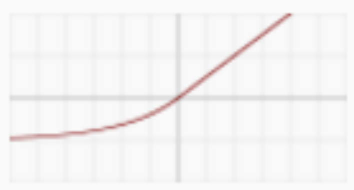
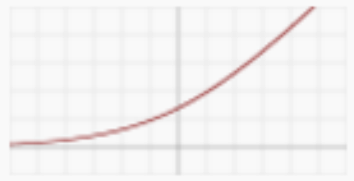


$$y_j = f^{(3)}(\Sigma_l w_{jl}^{(3)} f^{(2)}(\Sigma_k w_{lk}^{(2)} f^{(1)}(\Sigma_i w_{ki}^{(1)} x_i + b_k^{(1)}) + b_l^{(2)}) + b_j^{(3)})$$

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

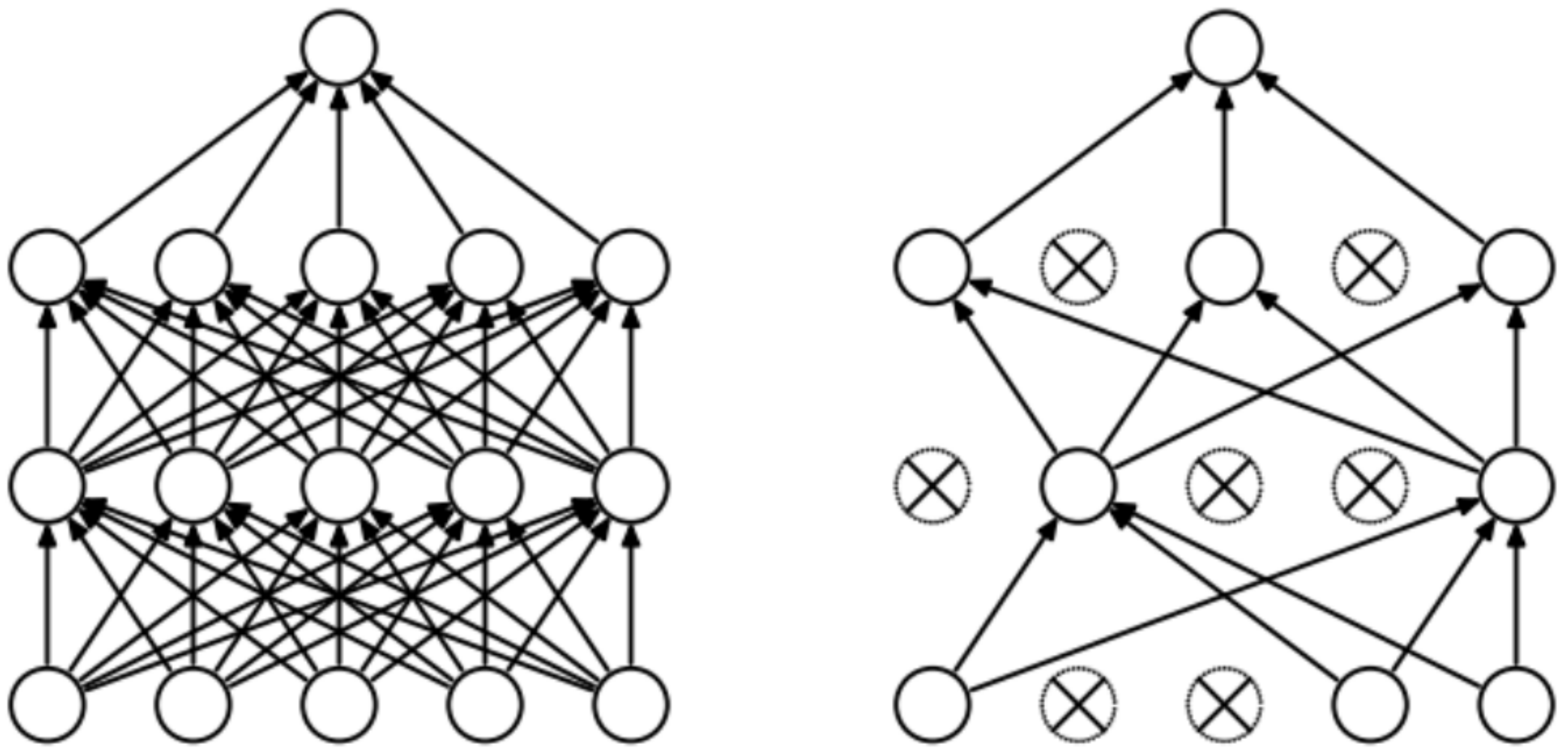
Activation Functions

- *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		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x \neq 0 \\ ? & \text{for} \quad x = 0 \end{cases}$
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)		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) [2]		$f(x) = \begin{cases} \alpha x & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Exponential Linear Unit (ELU) [3]		$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1+e^{-x}}$

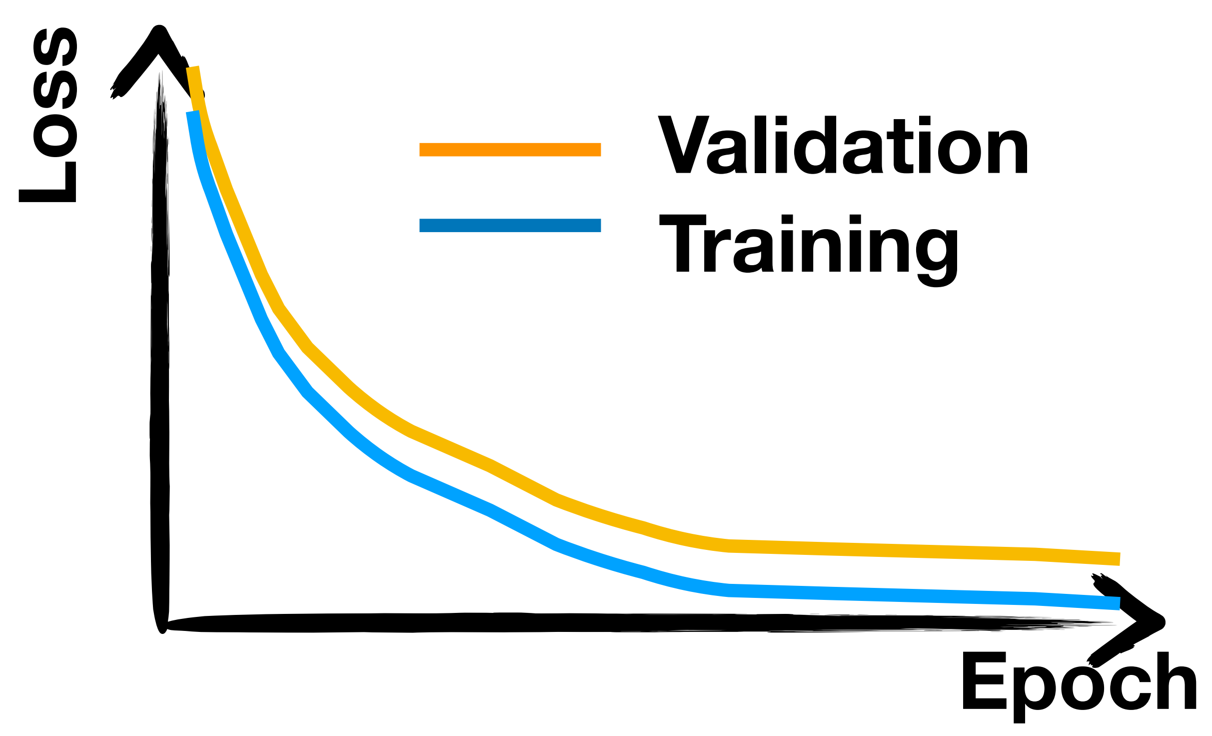
Dropout Layer

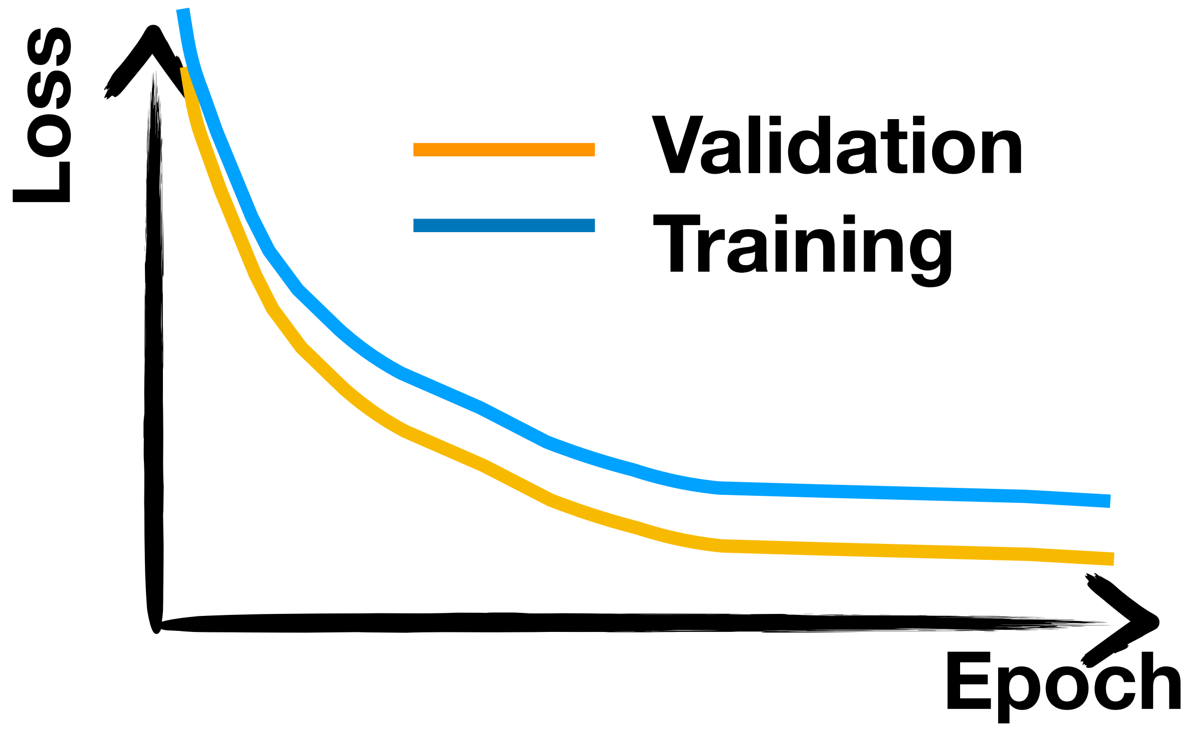
- *A special kind of layer, introduced for regularisation purpose*
- *Randomly drop links between neurons, with probability p*
- *The connections are re-established during the validation and inference steps*
- *Typical sign of it: invert hierarchy between training and validation loss*



(a) Standard Neural Net

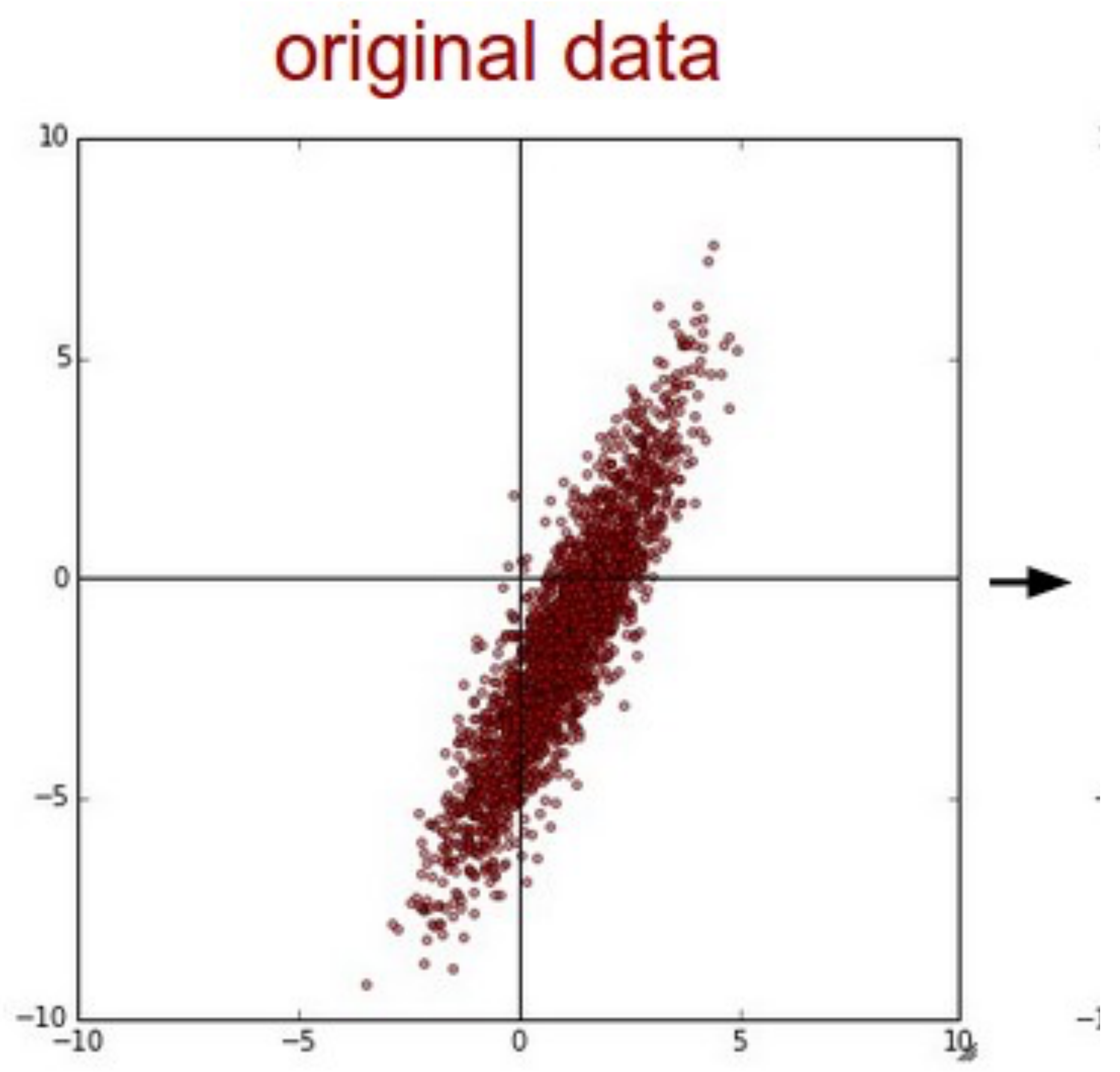
(b) After applying dropout.



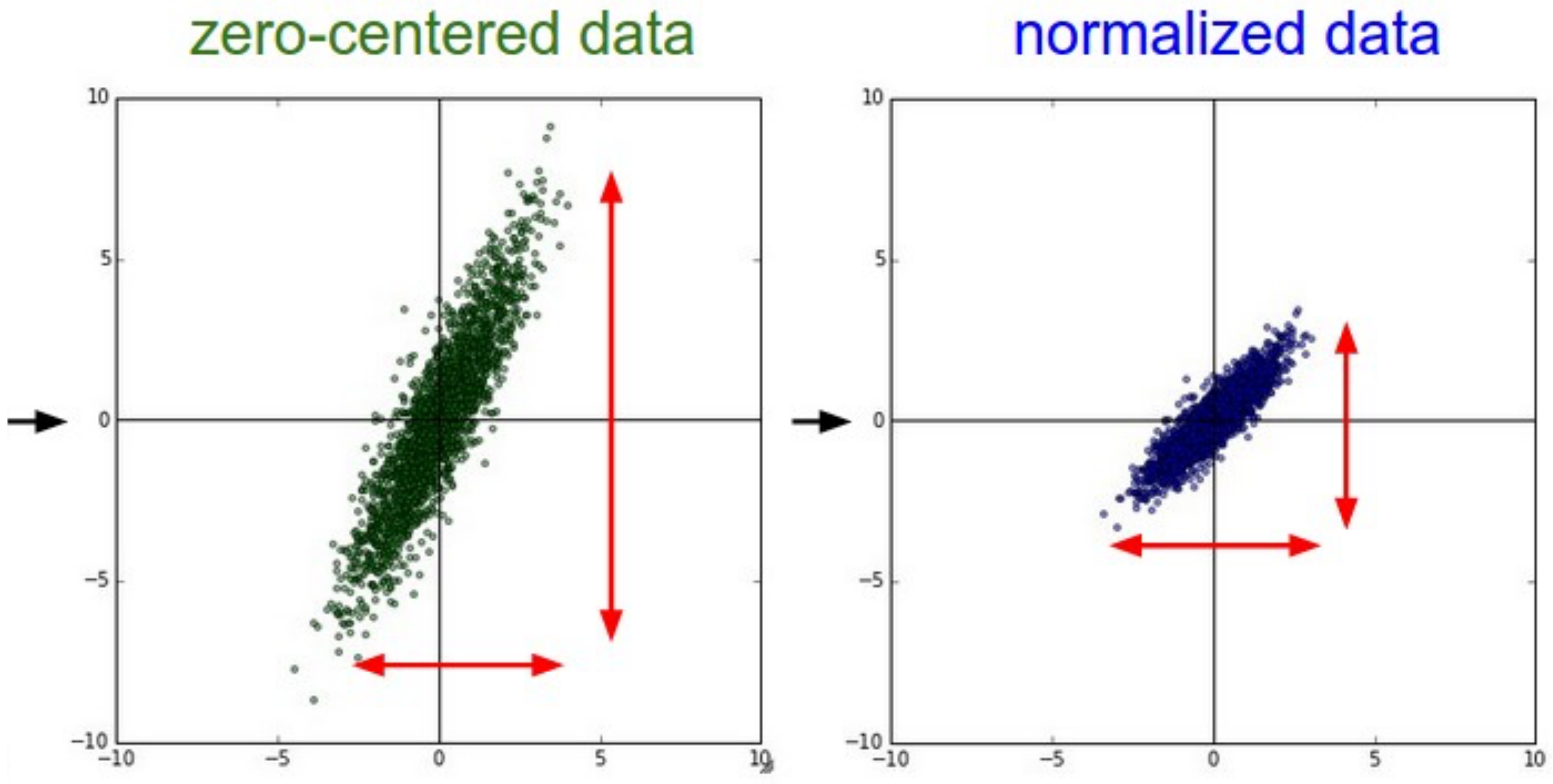


BatchNormalization Layer

- *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*

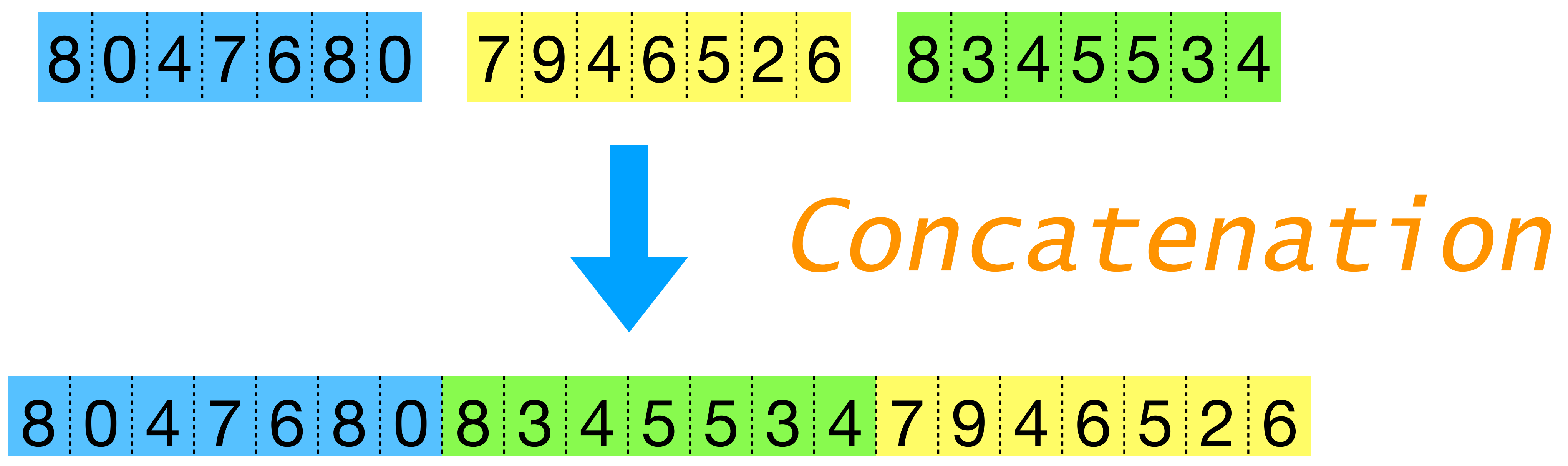


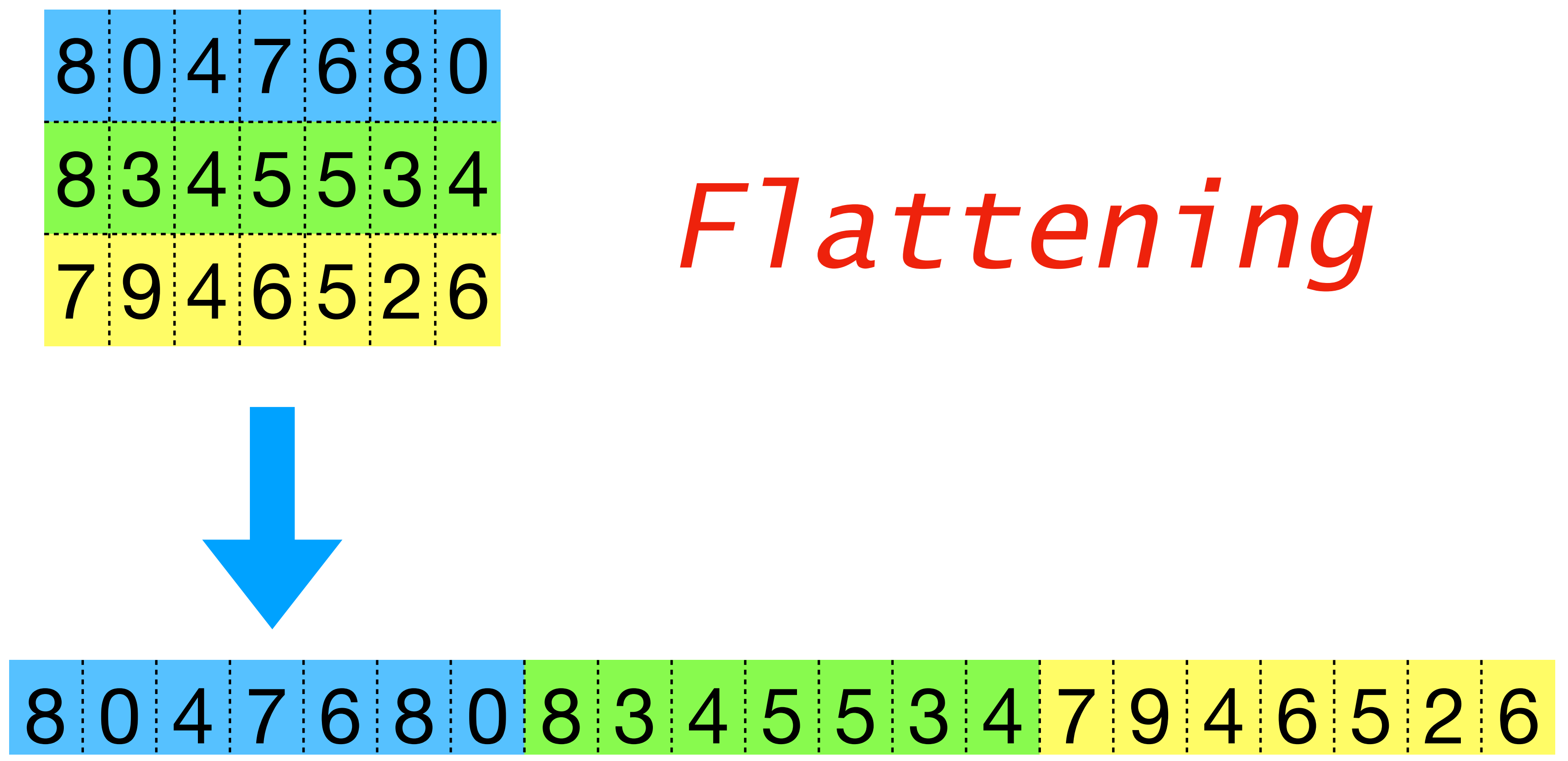
- *This can be done automatically with BatchNormalization*
  - *non-learnable shift and scale parameters, adjusted batch by batch*



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*



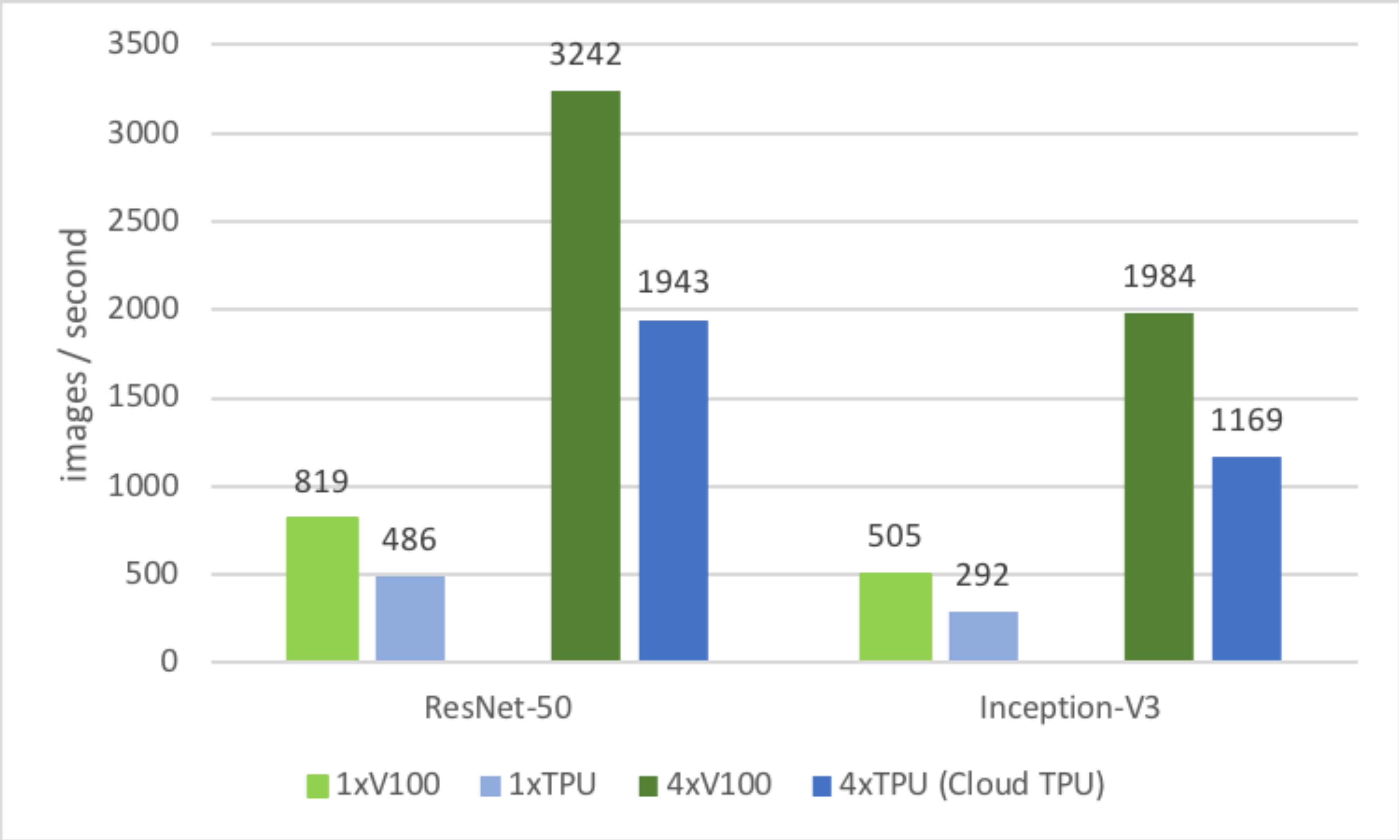


Training Libraries

- 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)

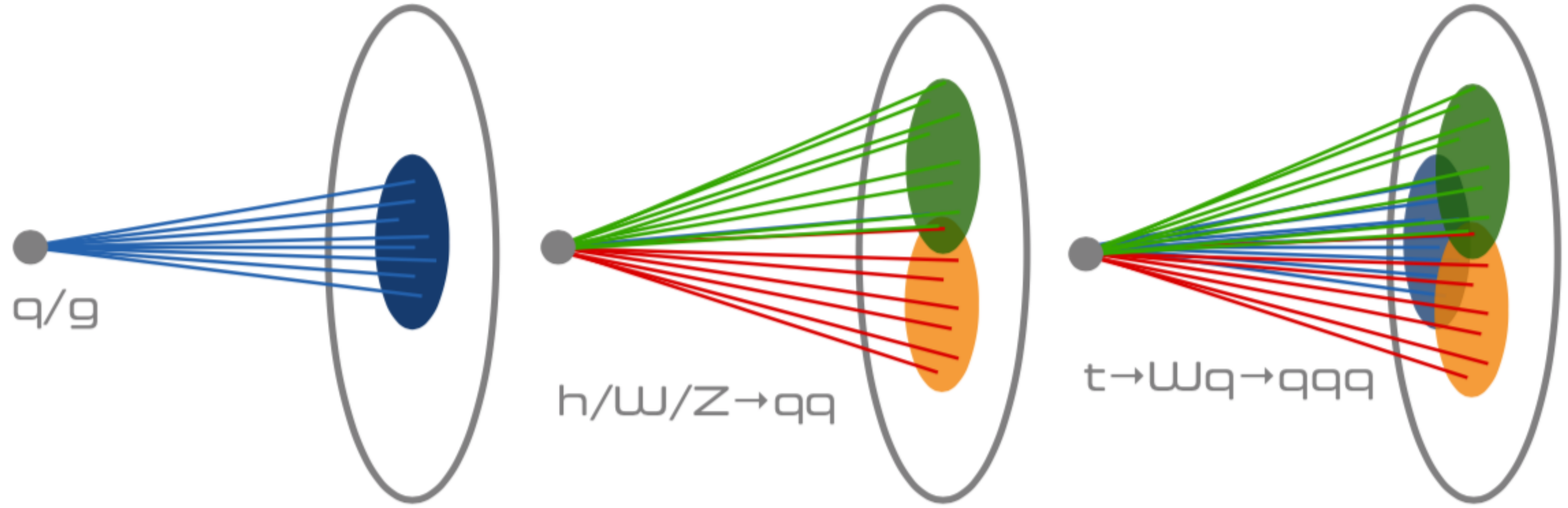
GPUs & TPUs

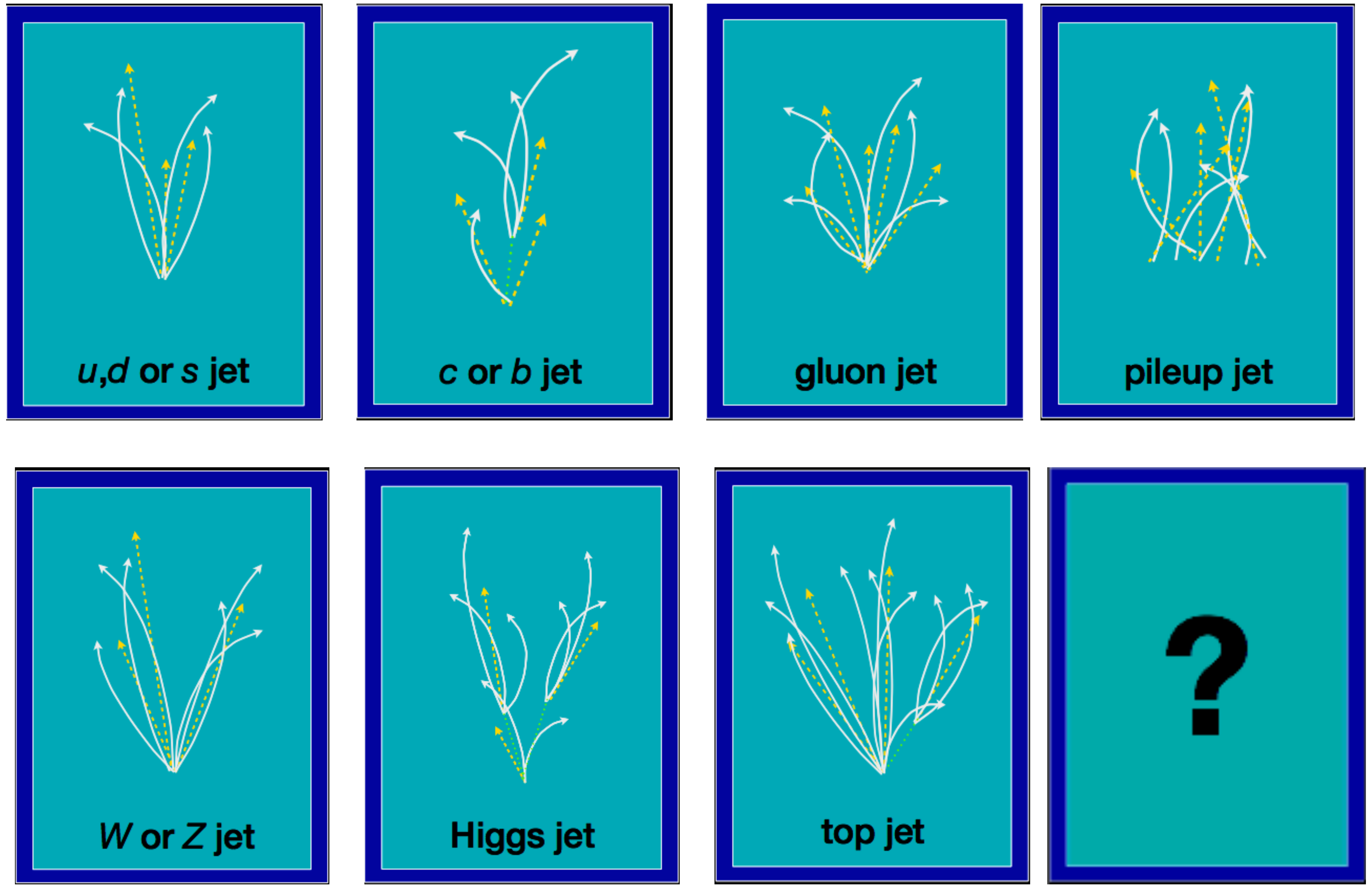
- All codes come with GPU support, through CUDA
    - They work on nVidia GPUs
- GPUs are very suitable to train neural networks
    - dedicated VRAM provides large memory to load datasets
    - architecture ideal to run vectorised operations on tensors
    - can also paralyse training tasks (e.g., processing 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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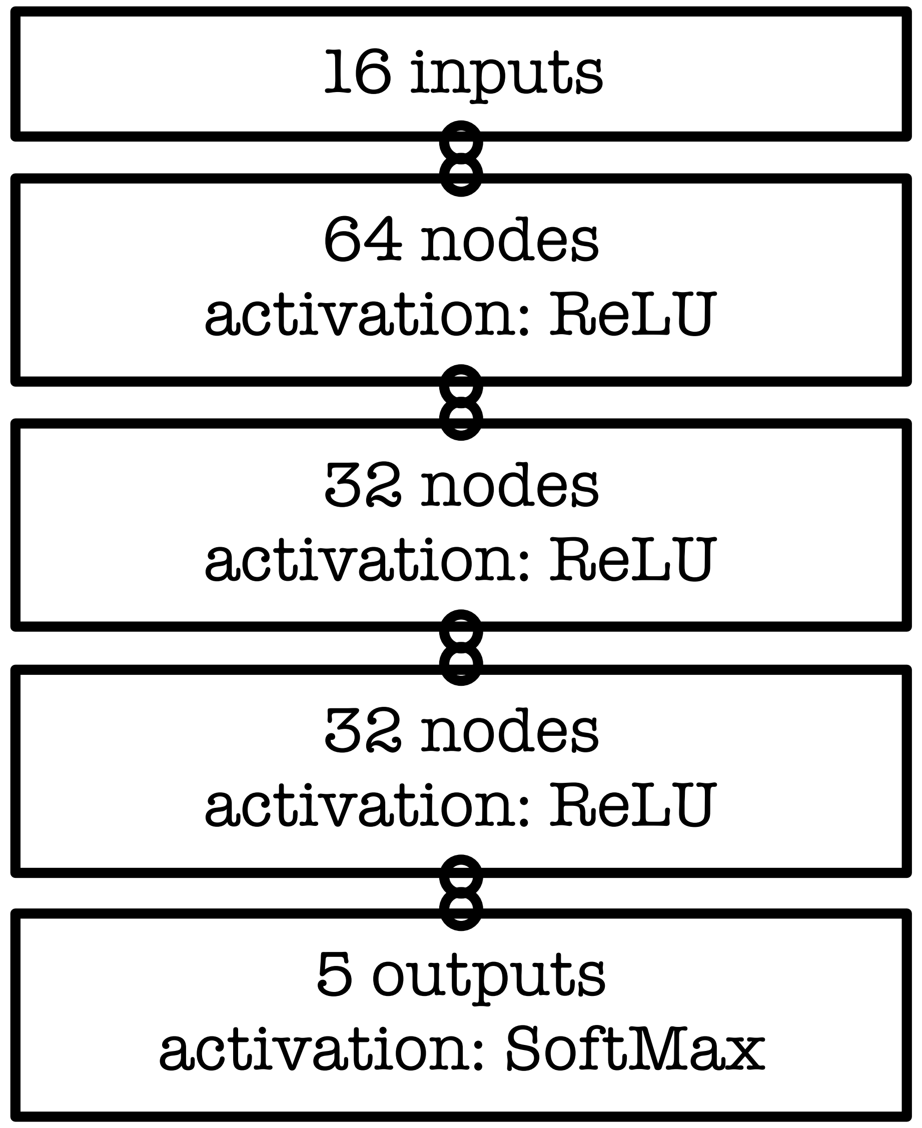

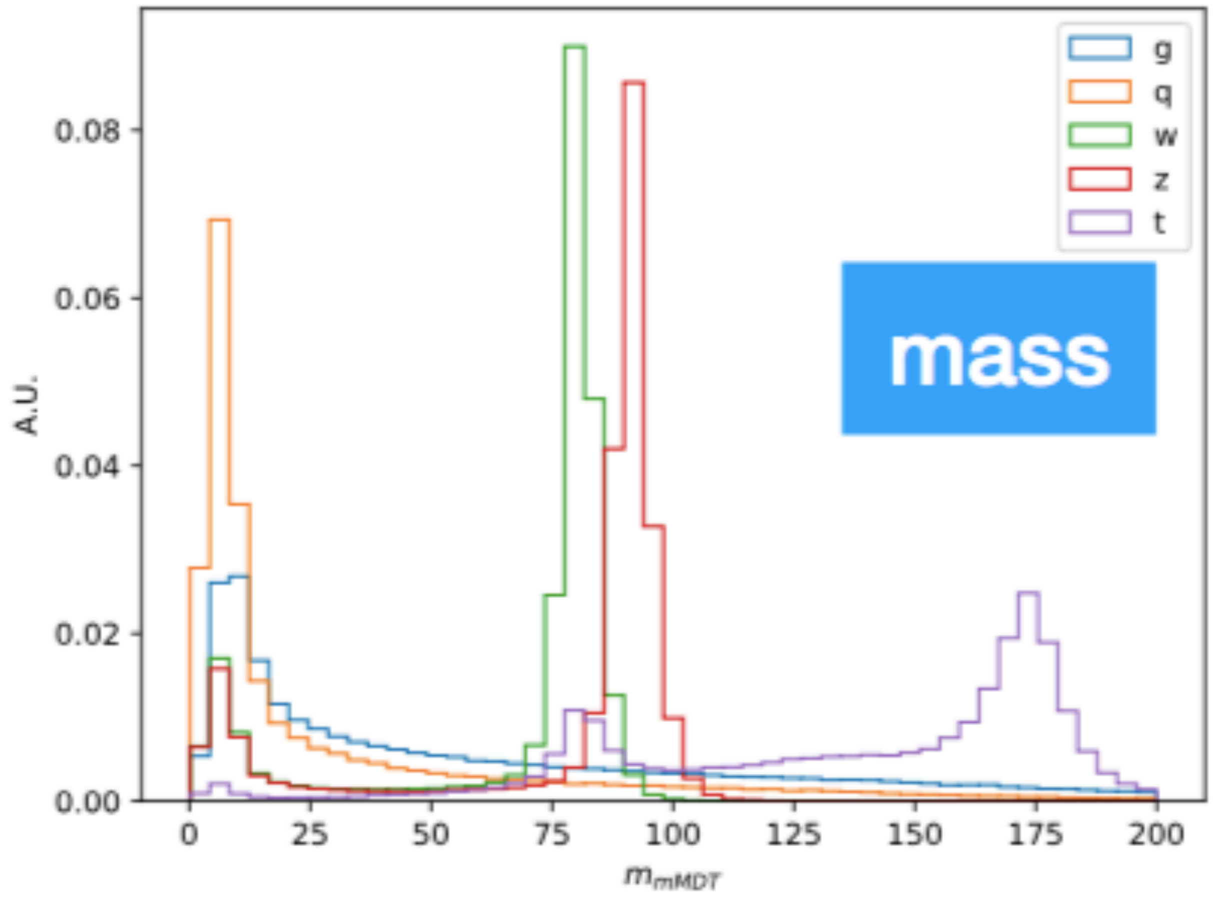

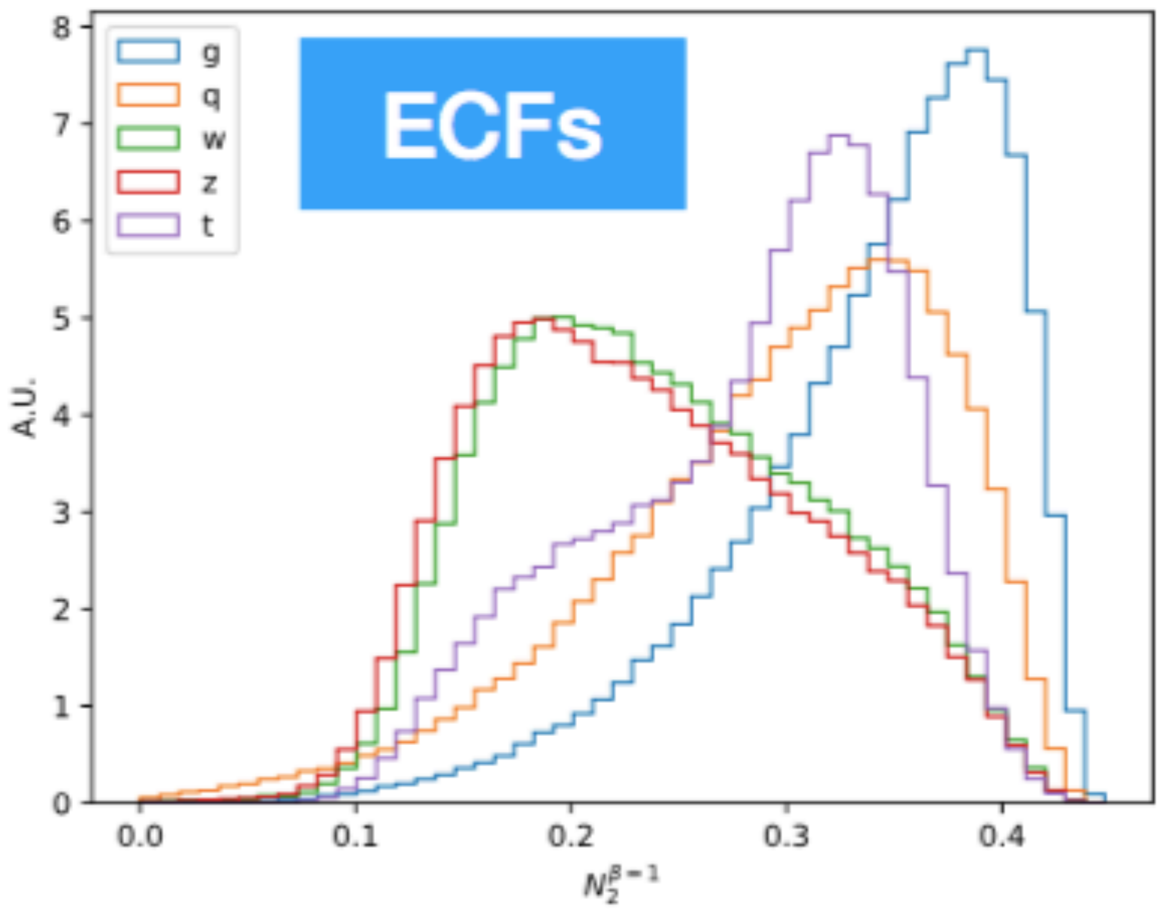

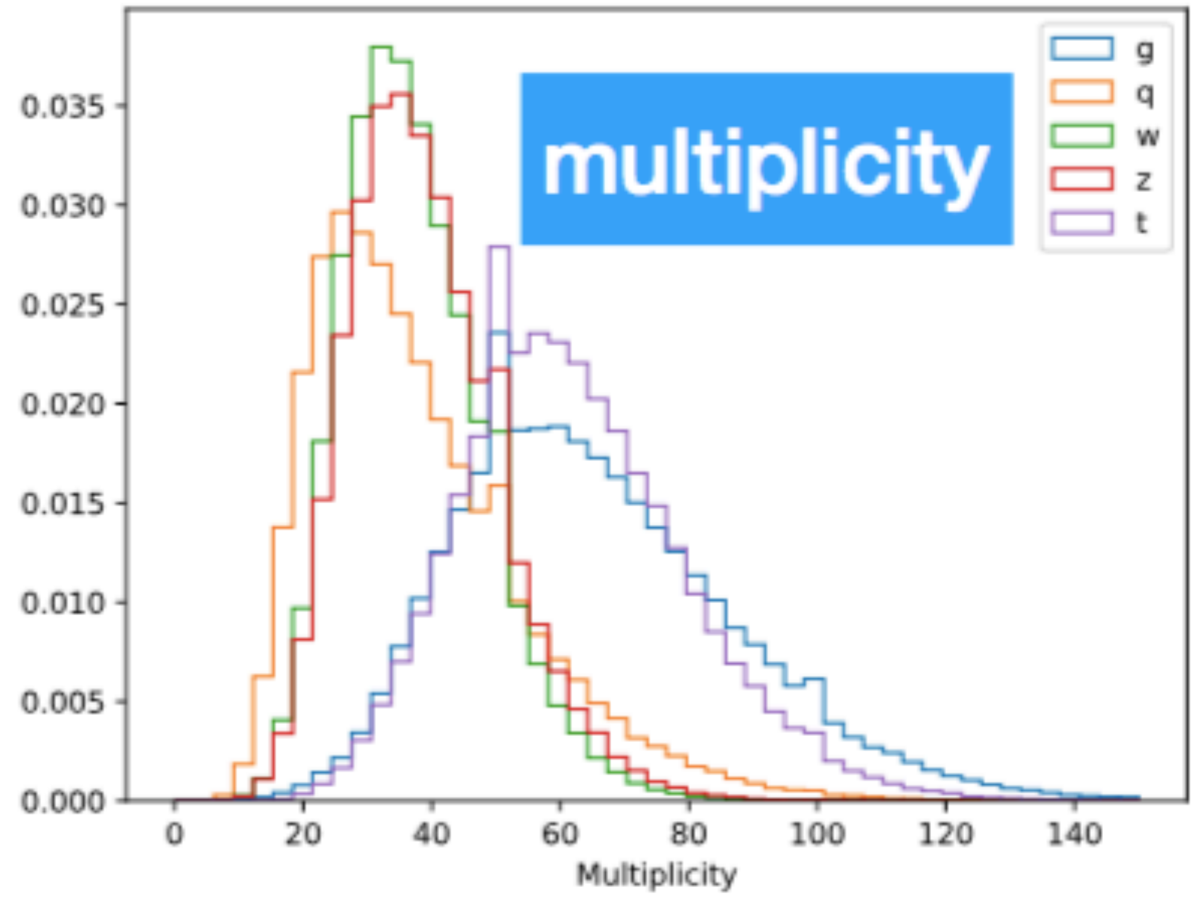

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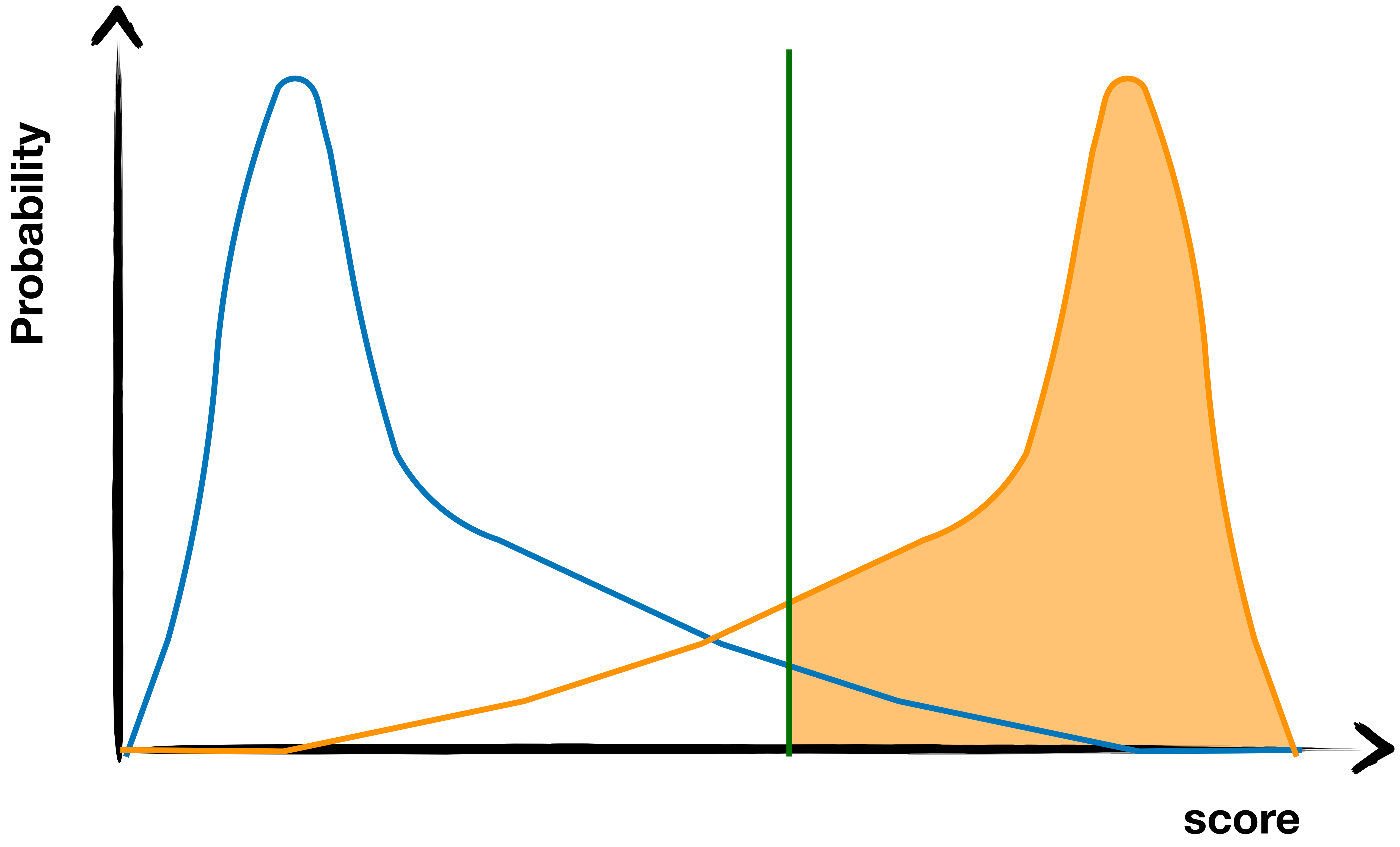
Classifier metrics

- 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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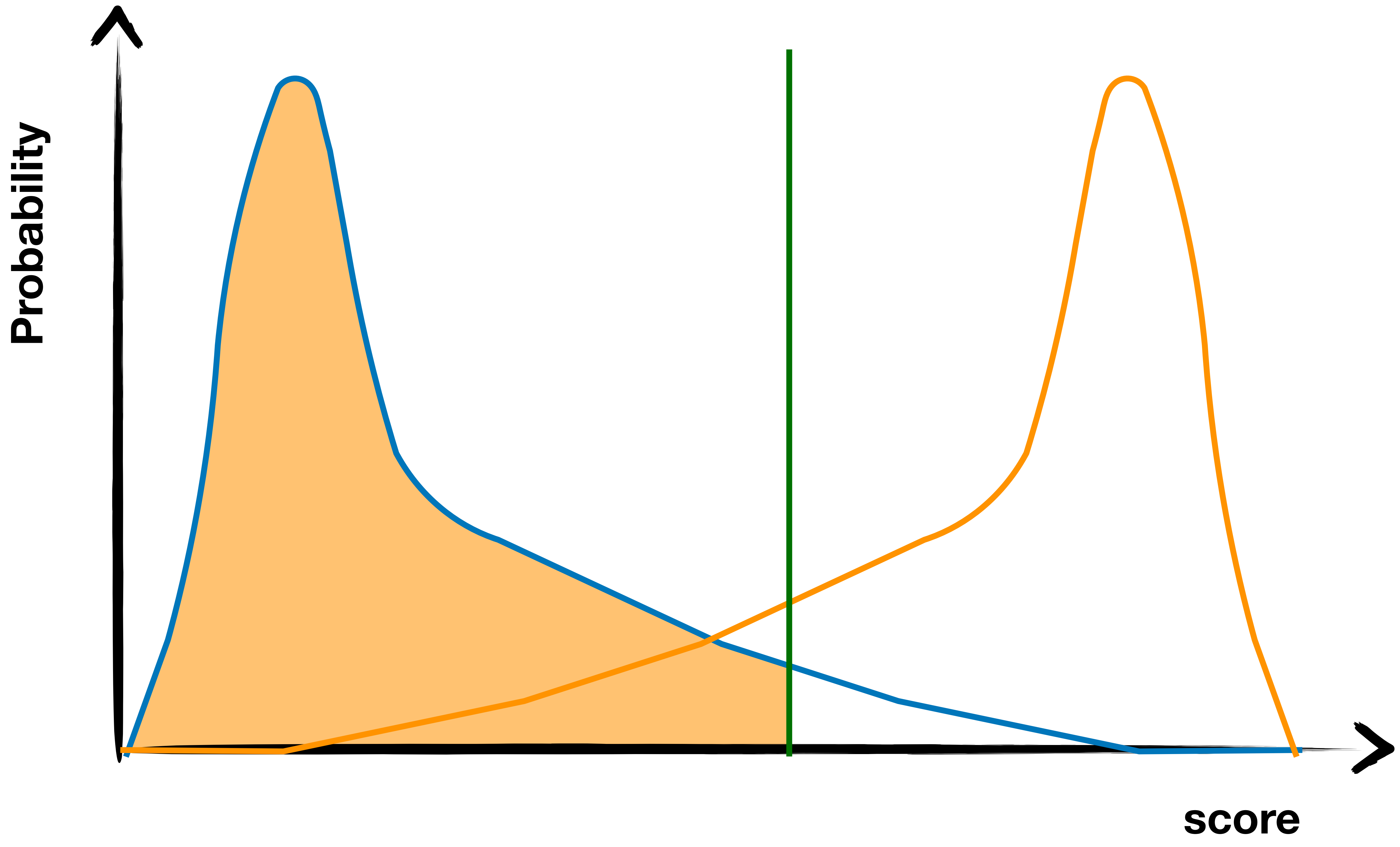

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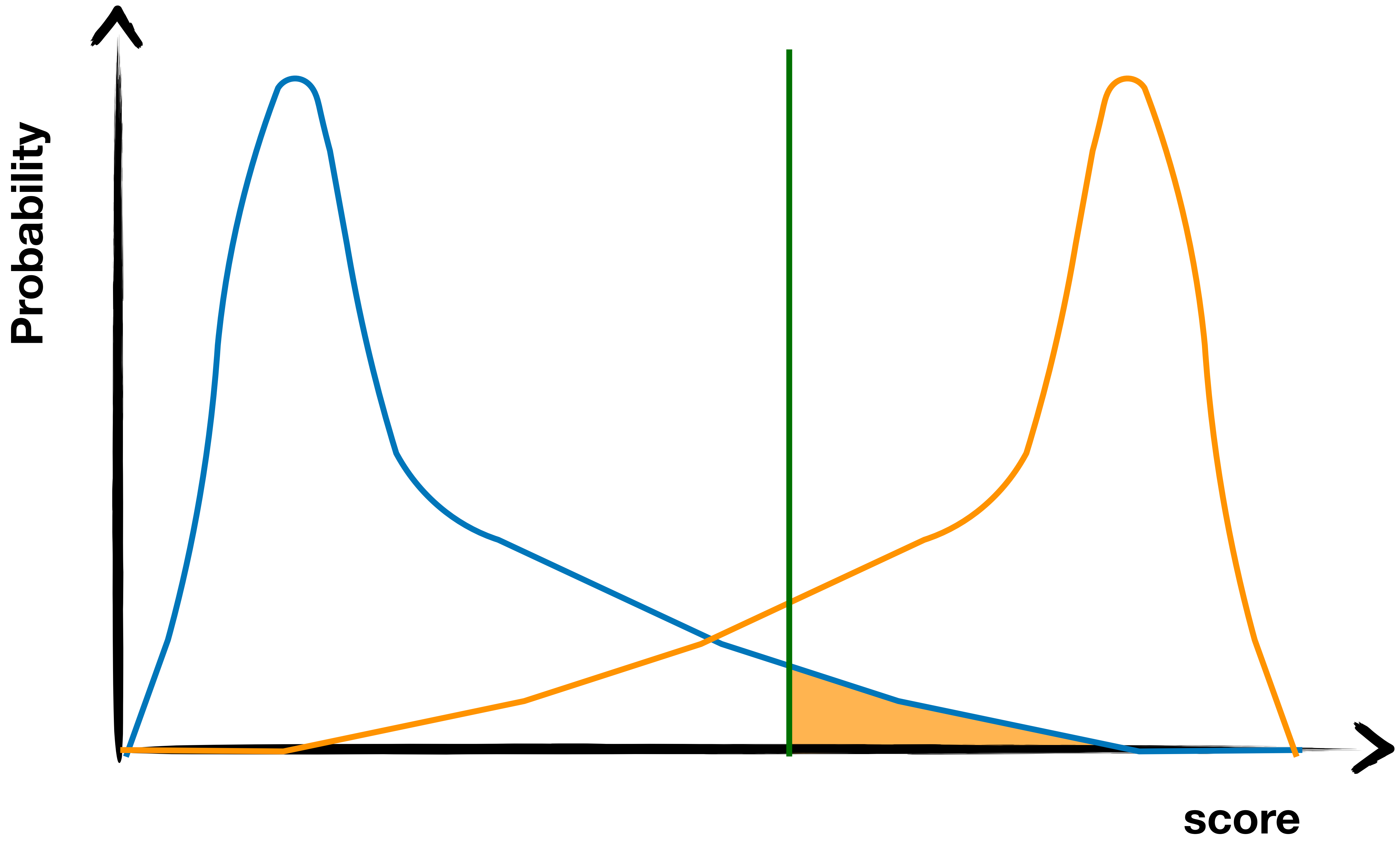

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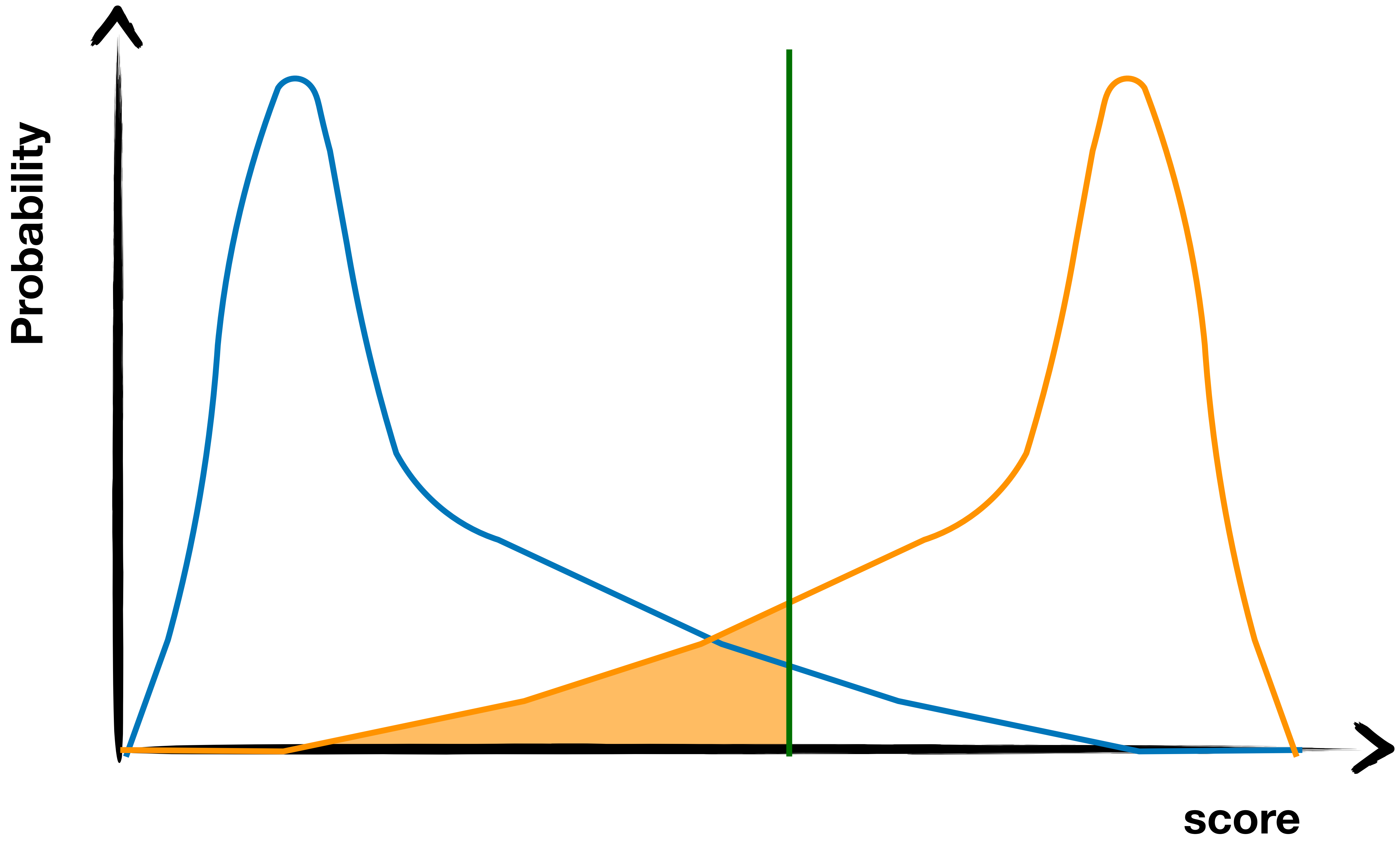
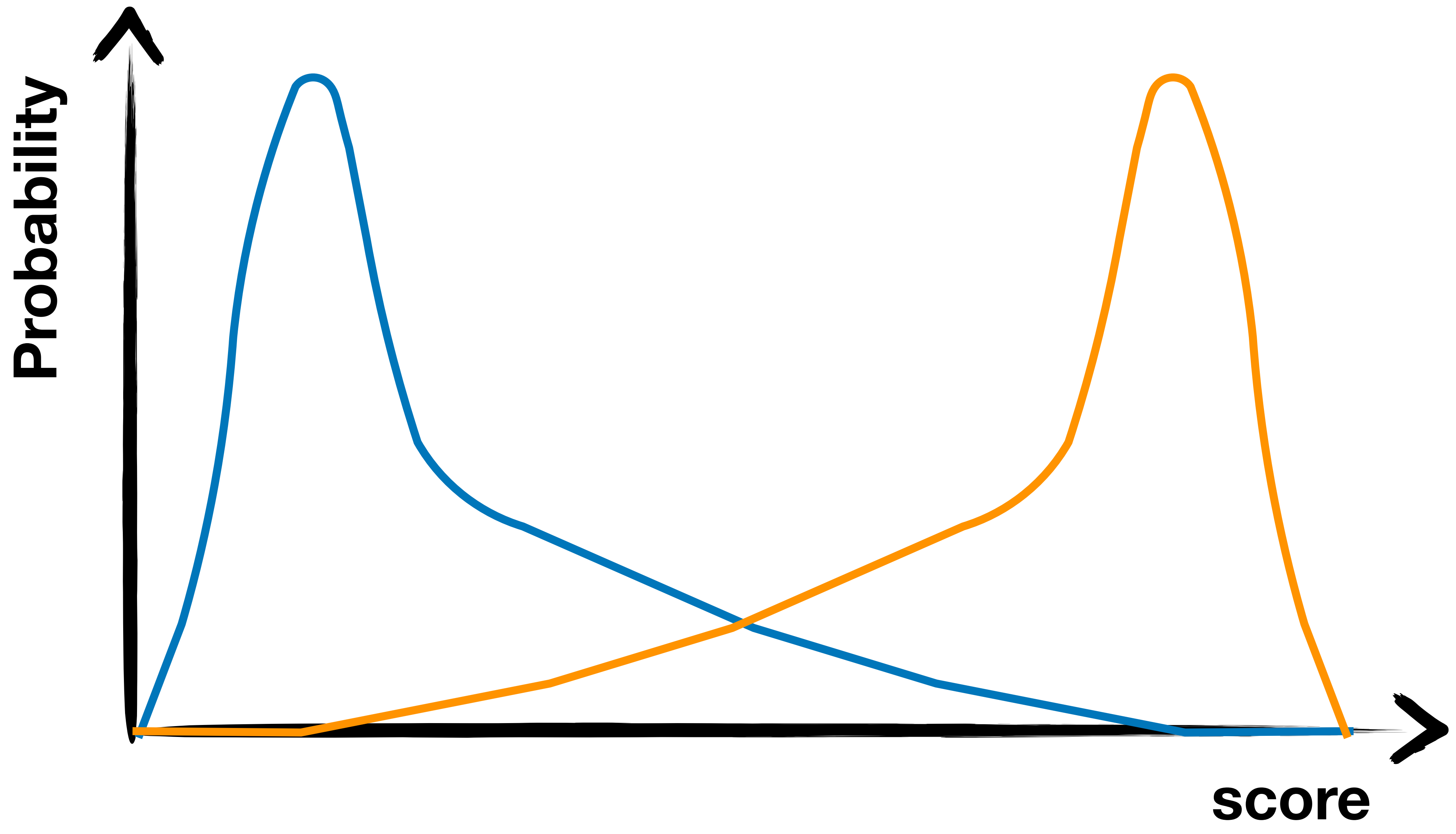
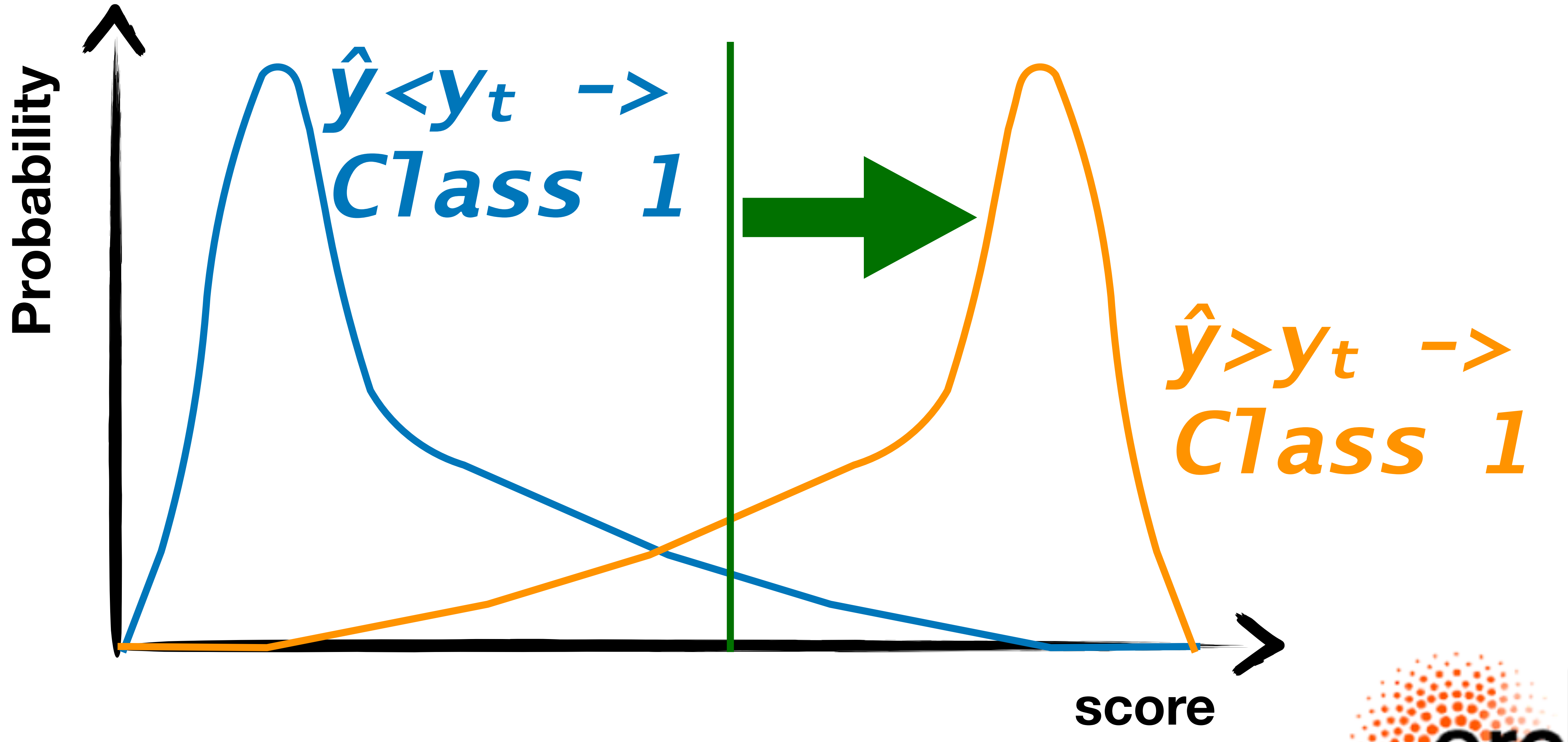


Classifier metrics

- *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*

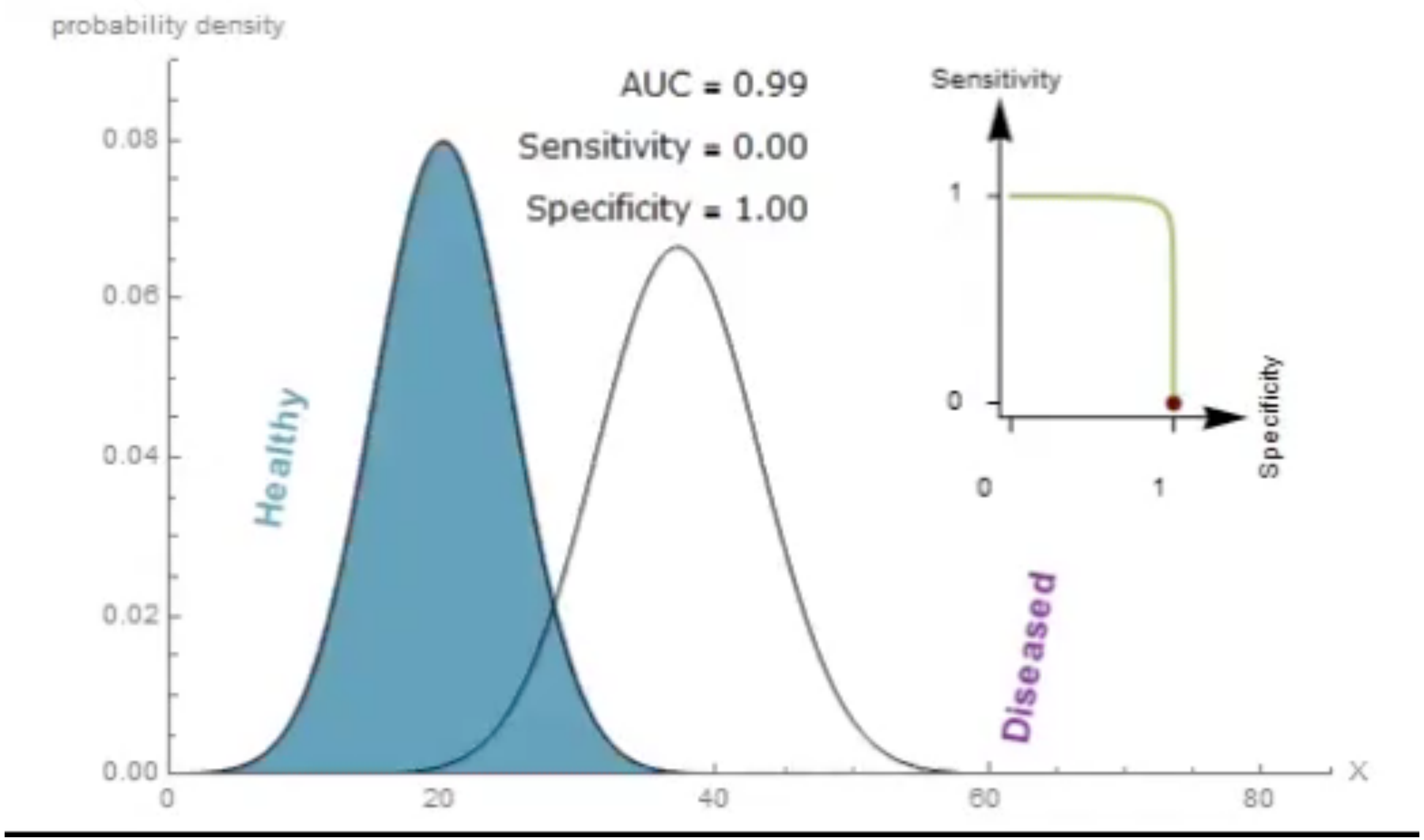




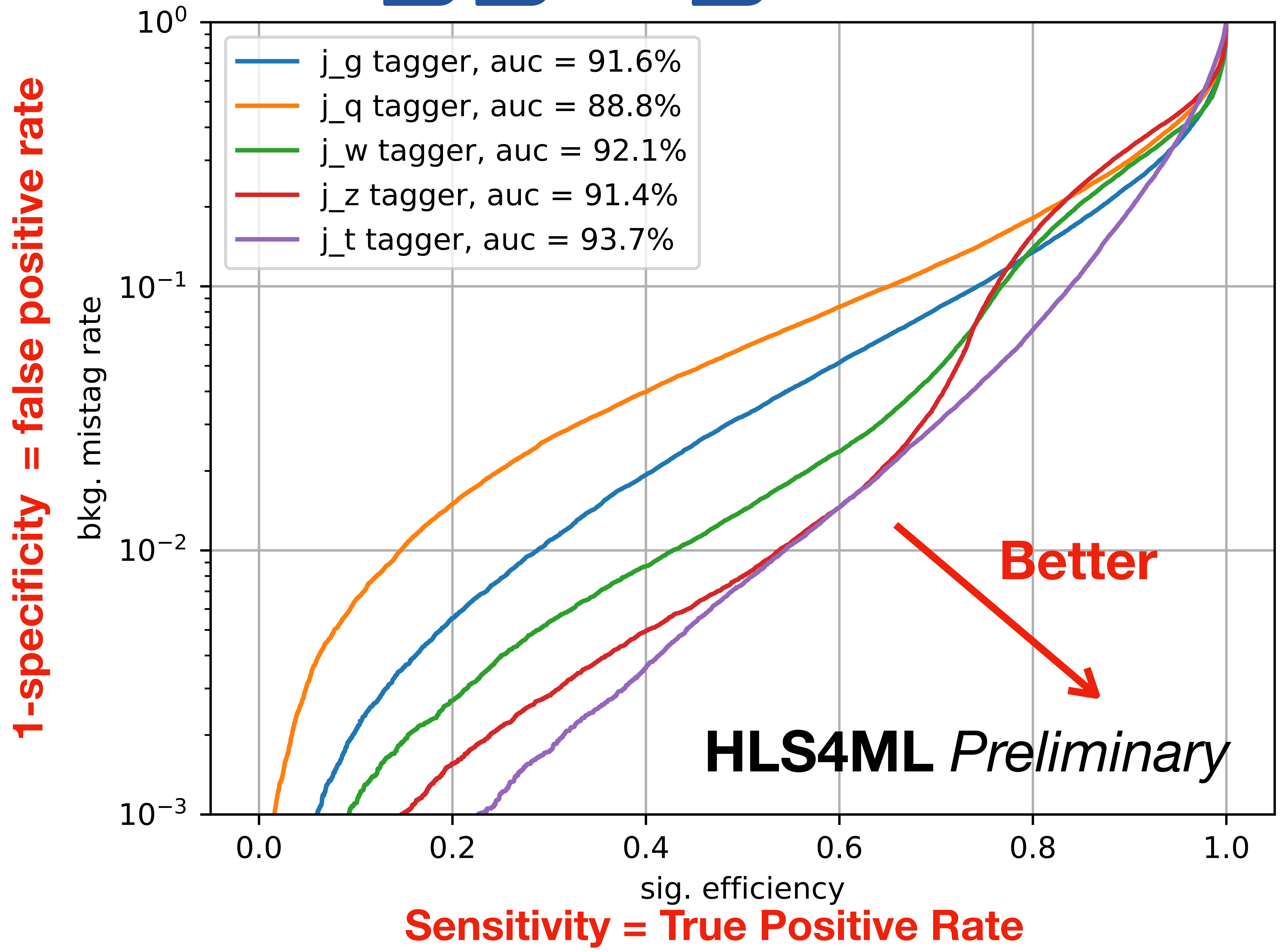
Classifier metrics

- *Starting ingredients are true positive (TP) and true 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*

Receiver operating characteristic



Jet tagging ROC curve



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*

- *Main reference for tutorial exercise: https://arxiv.org/abs/1908.05318*
- *All notebooks and classes are/will be on GitHub: https://github.com/pierinim/tutorials/tree/master/GGI_Jan2021*
- *Full dataset available at: https://zenodo.org/record/3602260*

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