Lecture 3: Basic of ML

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Plan for Today

- *Numerical Computation*

https://www.deeplearningbook.org/contents/numerical.html

- *Machine Learning Basic*

https://www.deeplearningbook.org/contents/ml.html

✔: Parts that we will cover

Machine Learning

- *"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E."*
- *A task T: classification, regression, etc.*
- *A performance measure P (typically on independent test dataset):*
  - *Example: for classifiers, accuracy/error rate, i.e., fraction of examples correctly/incorrectly classified*
- *An Experience E, provided as a training dataset on which an algorithm can try to improve its task solving skill*
  - *Supervised learning: learn to reproduce the ground-truth (e.g., flags in classification)*
  - *Unsupervised learning: learn the pdf of the dataset and use it to make probabilistic statements about new data (e.g., anomaly detection)*

learn some quantity x_i
from the other N-1 x_j

$$p(\mathbf{x}) = \prod_{i=1}^{n} p(\mathrm{x}_i \mid \mathrm{x}_1, \ldots, \mathrm{x}_{i-1}).$$

Machine Learning

- *Boundary between supervised and unsupervised are not so strict: the same approach can be used for supervised or unsupervised learning*

Learning the pdf of the data $p(\mathbf{x})$ is an unsupervised task

But it can be broken down in supervised tasks

from the other N-1 x_j

$$p(\mathbf{x}) = \prod_{i=1}^{n} p(\mathbf{x}_i \mid \mathbf{x}_1, \ldots, \mathbf{x}_{i-1}).$$

learn some quantity x_i

Learning some y from some $\mathbf{x}$, i.e., learning $p(y \mid \mathbf{x})$ is a supervised task

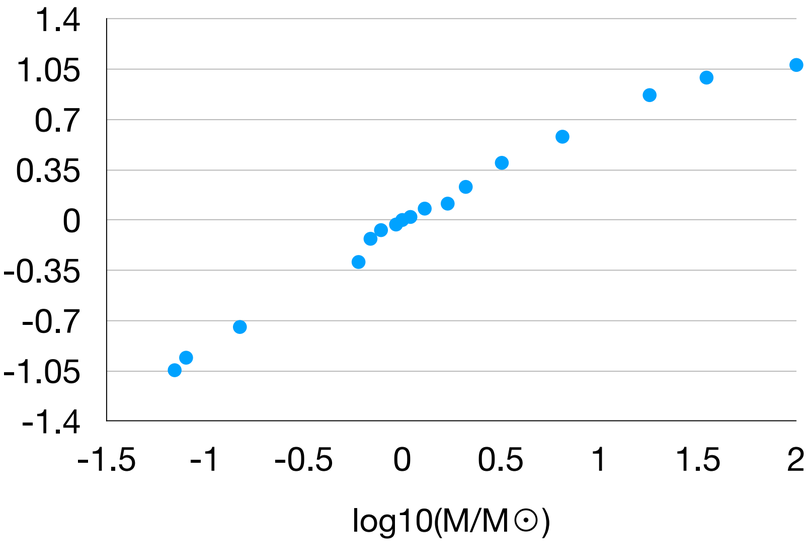
But this task can be approached with unsupervised technique, using the probability chain rule

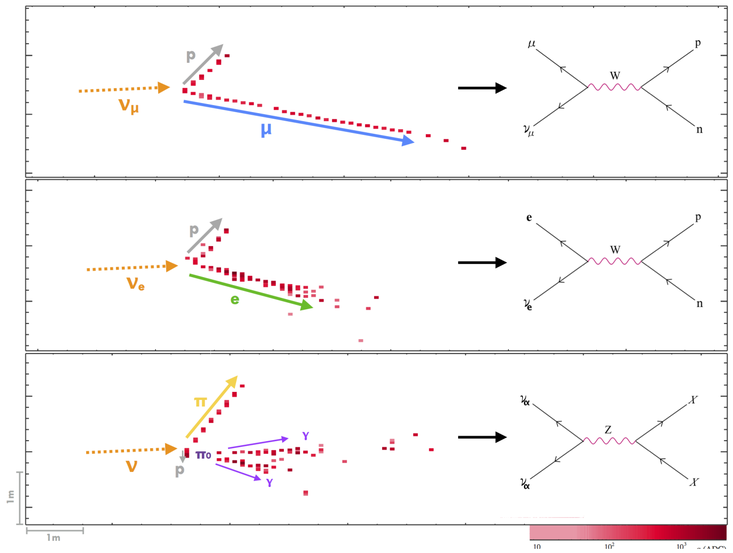
learning the full pdf

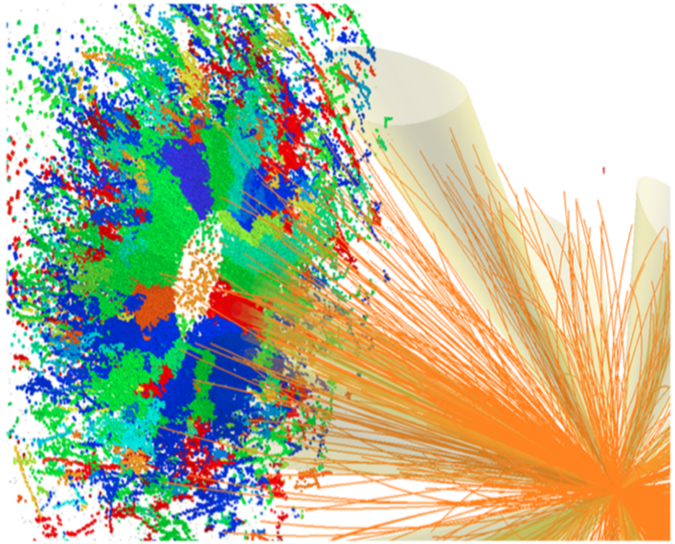
$$p(y \mid \mathbf{x}) = \frac{p(\mathbf{x}, y)}{\sum_y p(\mathbf{x}, y')}$$

learning the pdf $p(\mathbf{x})$

Machine Learning







Regression ***Supervised Learning***

- Prediction of continuous-valued vector $y \in \mathbb{R}^K$. E.g given some input, predict particle position, particle energy etc.
- Training set: Pairs of input signal and ground-truth value

Classification ***Supervised Learning***

- Predict value from a finite set $\{1,...,C\}$, e.g label (=cat) for an image X.
- Training set: Pairs of input signal and ground truth
- Usually predict one score per class, s.t correct class has maximum score

Density modelling ***Unsupervised Learning***

- Model probability density function of data μ_X
- Training set: values x_N without quantities to predict
- Trained model should allow for evaluation of pdf or sampling from it, or both

Machine Learning

- *We only have a finite training dataset*
- *We cannot measure the true test error*
- *Simple model classes underfit*
- *Complex model classes overfit*

Bias-variance trade-off

- *Goal: Select the model class with lowest test error*

Dataset Split

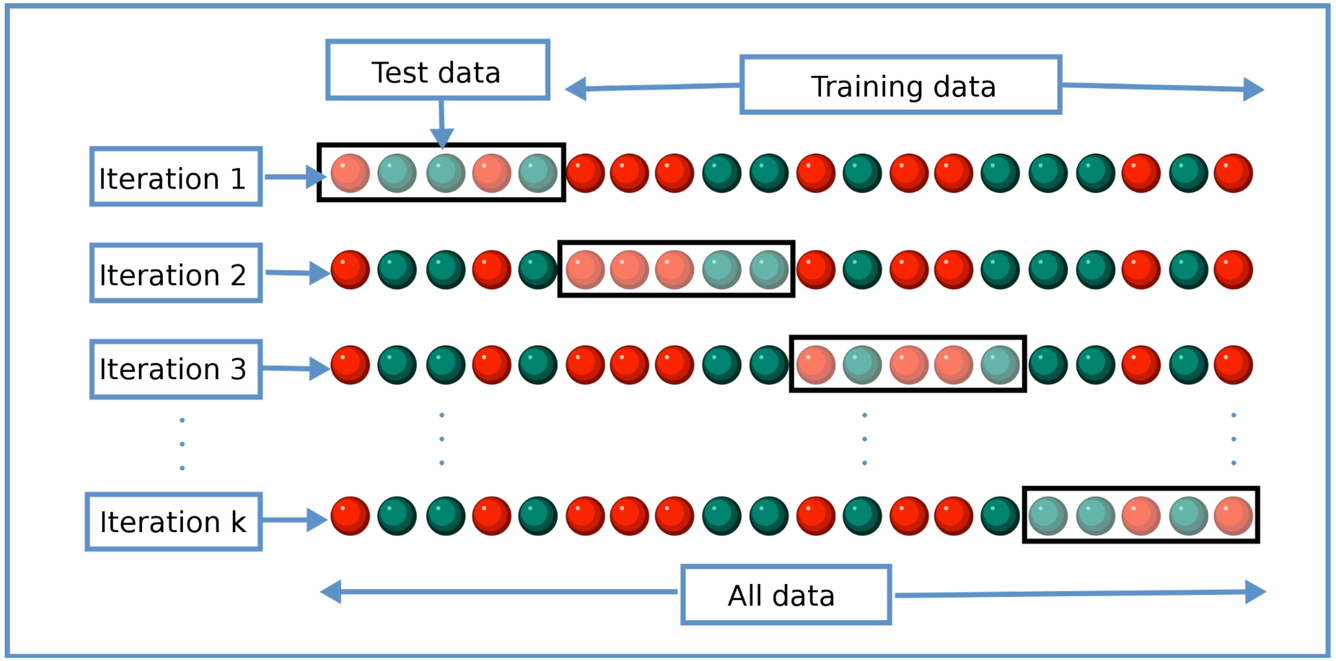
- *Split your sample in three:*
  - *Training: the biggest chunk, where you learn from*
  - *Validation: an auxiliary dataset to verify generalization and prevent overtraining*
  - *Test: the dataset for the final independent check*

- *What separates ML from optimisation is generalization!*

k-folding

Split the original dataset into k equal parts (e.g, k = 4)

- Train on the k – 1 parts and test on the remaining one
- Repeat for every choice of the k – 1 parts and average the validation errors



• Use all data as validation to improve the estimate of the test error (at the cost of more computation (k trainings))

k-folding

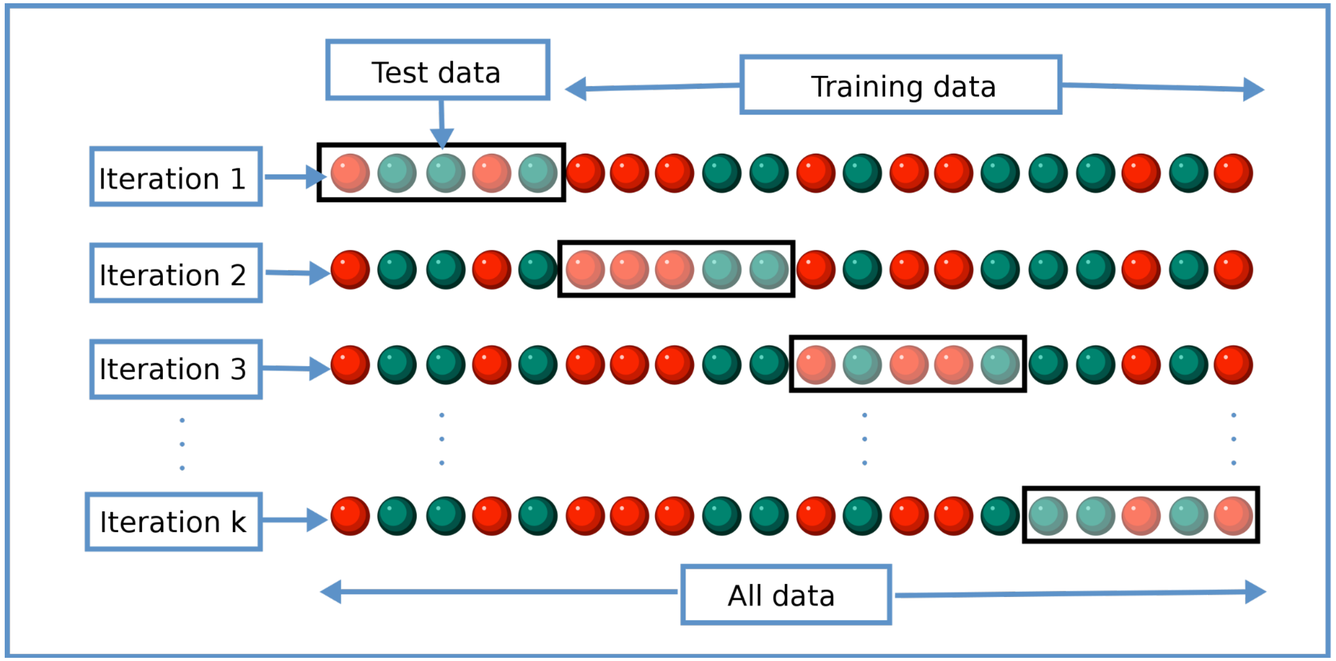
1. Training data
2. Model class
3. Loss function
4. Minimise Learning objective

$$\arg\min_{w} \sum_{i=1}^{N} L(y_i, f(x_i \mid w))$$

5. Cross-validation and model selection
6. Testing and deployment

Split the original dataset into k equal parts (e.g, k = 4)

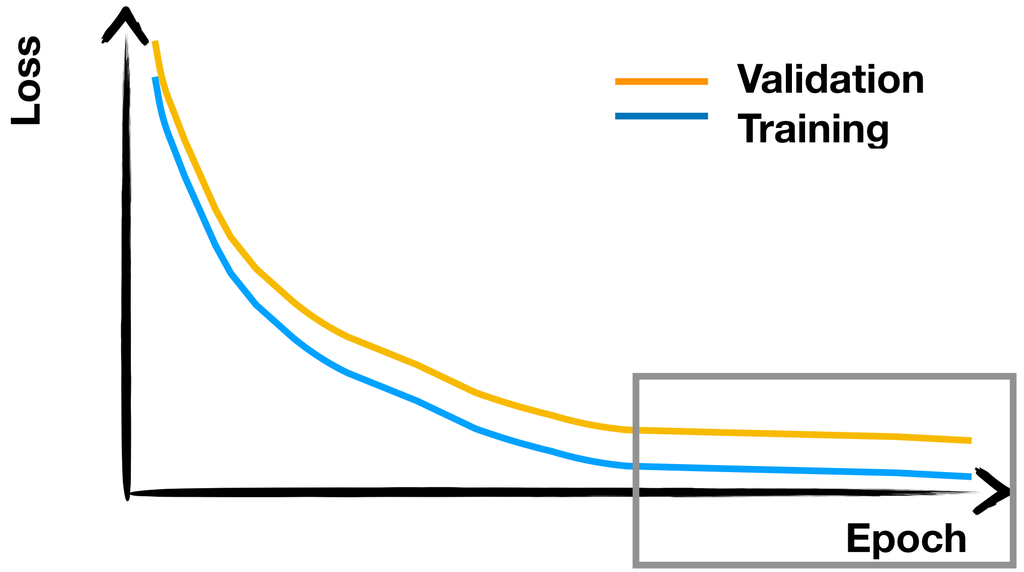
- Train on the k – 1 parts and test on the remaining one
- Repeat for every choice of the k – 1 parts and average the validation errors

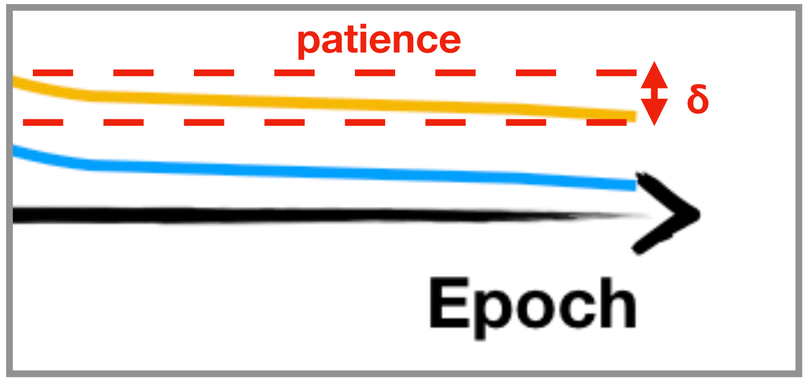


- Use all data as validation to improve the estimate of the test error (at the cost of more computation (k trainings))

Learning history & Early Stopping

- *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)*

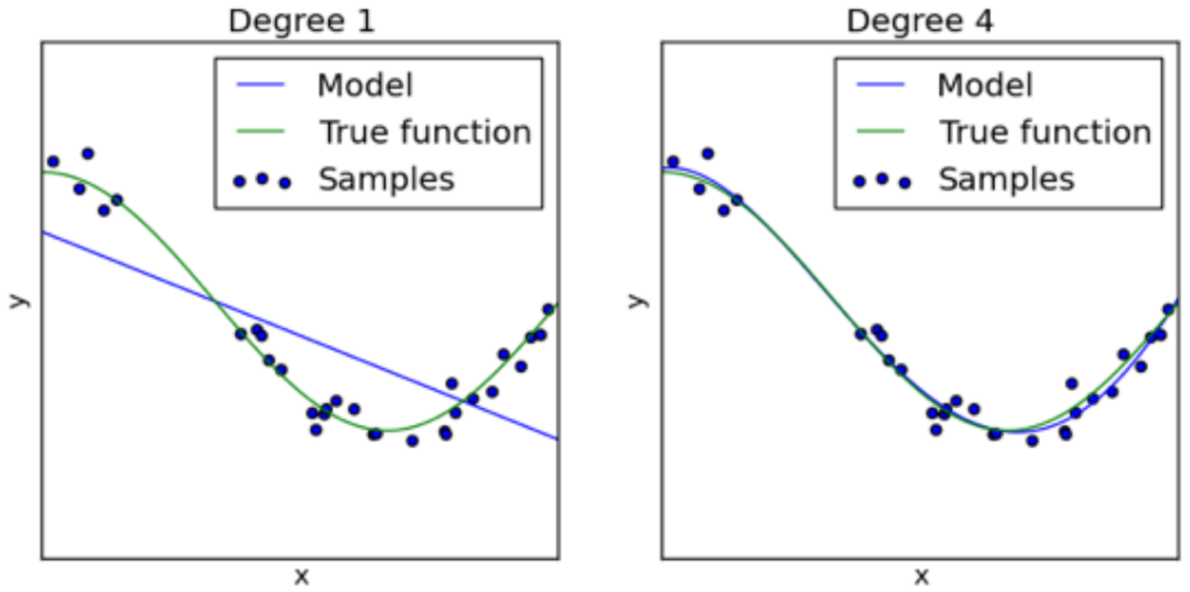


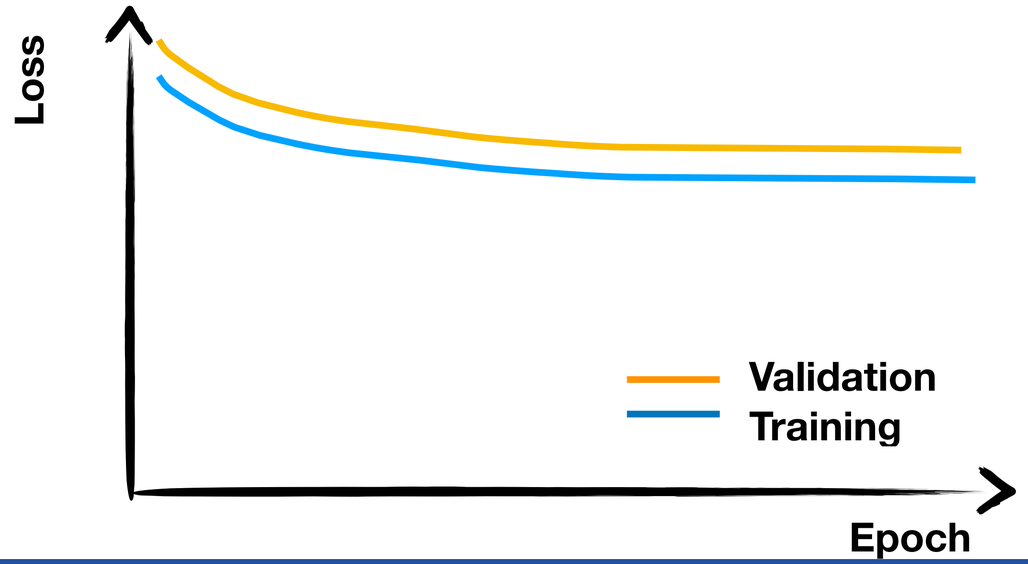


EARLY STOPPING: stop the train if the validation loss didn't change more than δ in the last n epochs (patience)

Undertraining

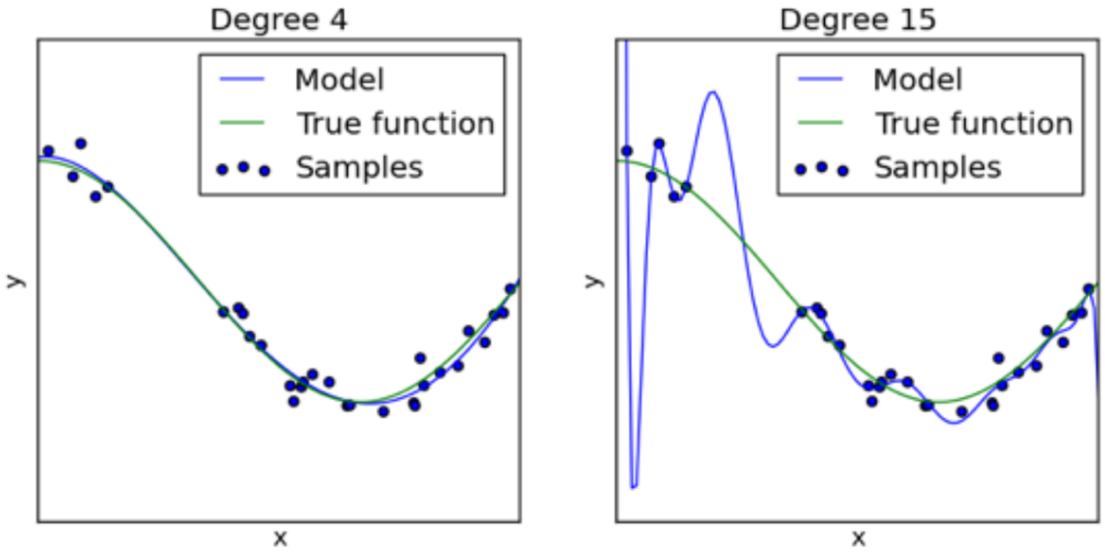
- *If your model has not enough flexibility, it will not be able to describe the data*
- *The training and validation loss will be close, but their value will not decrease*
- *The model is said to be underfitting, or being* ***biased***

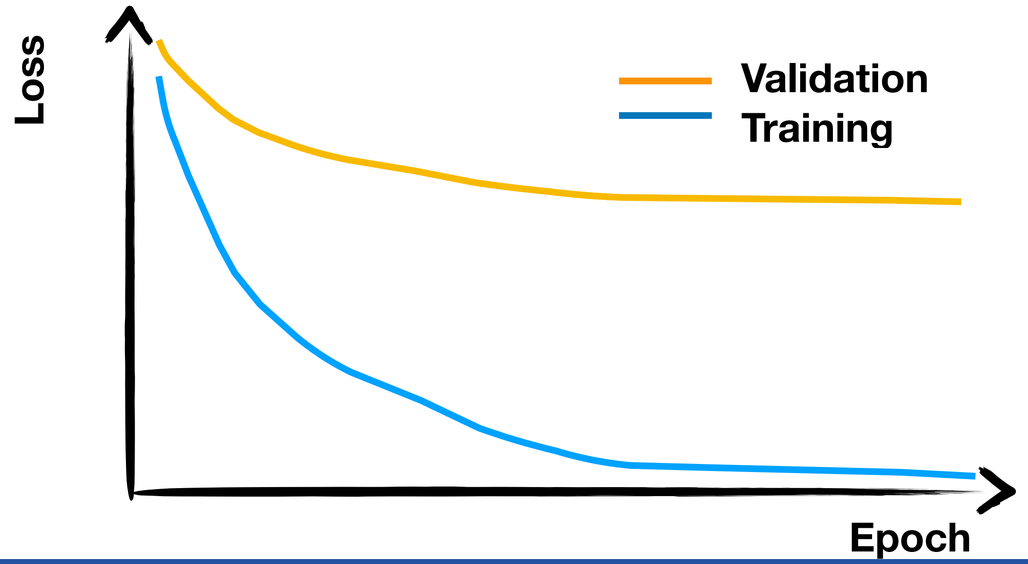




Overtraining

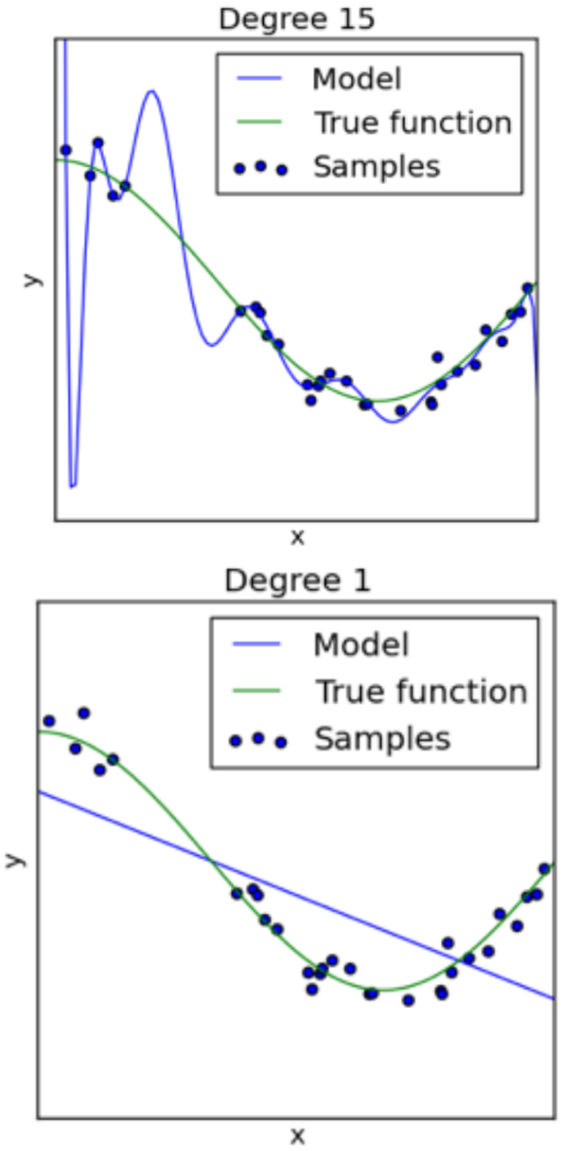
- *Your model can learn too much of your training dataset*
  - *e.g., its statistical fluctuations*
- *Such an overfitted model would not generalise*
- *So, its description of the validation dataset will be bad (i.e., **the model doesn't generalise**)*
- *This is typically highlighted by a divergence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





Bias vs Variance

- ***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)*



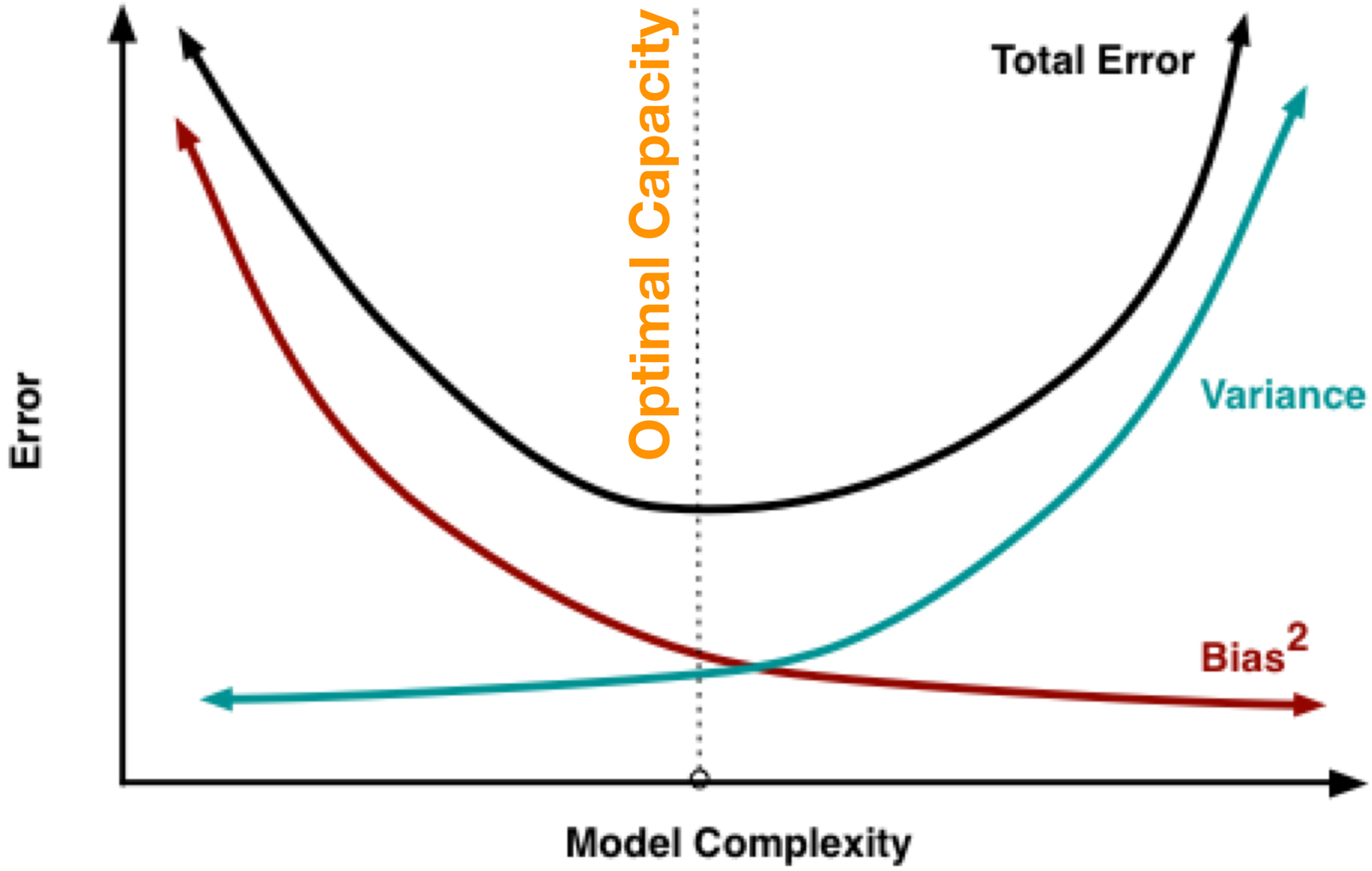
Bias vs Variance

- *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**

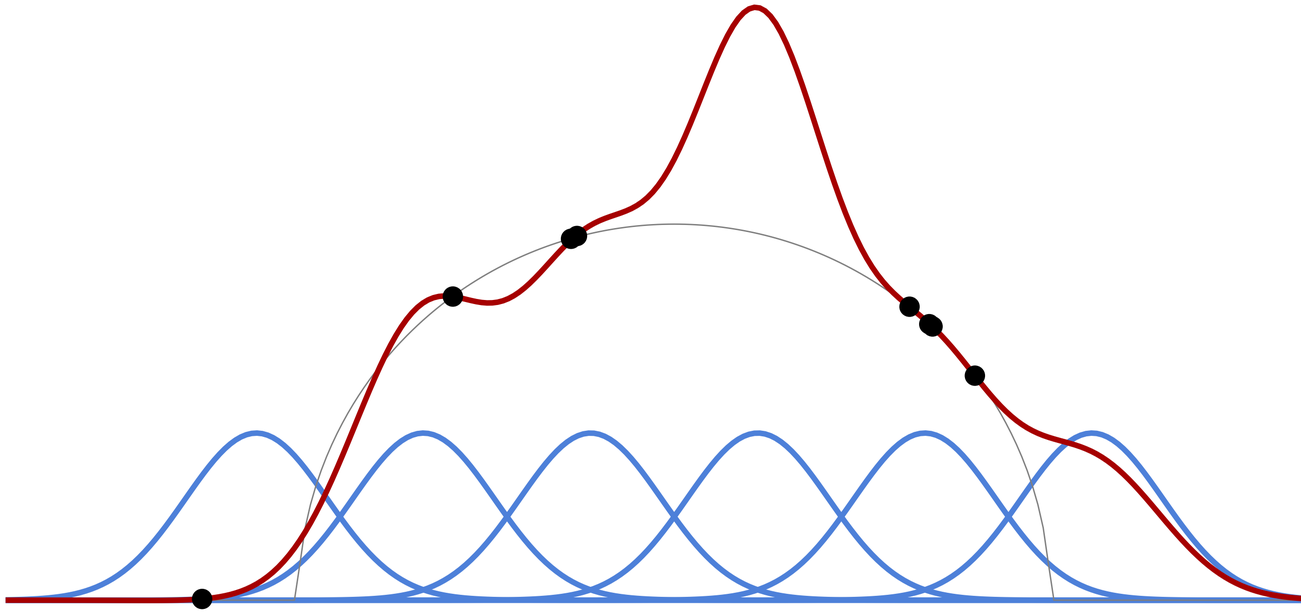
Bias vs Variance



Model capacity

<u>Model capacity</u>: flexibility and ability to fit diverse data

- Interplay between model capacity and amount/quality of your training data is highly important!
- Insufficient capacity → model cannot fit data, training error is high **<u>underfitting</u>**
- Insufficient data, training performance excellent but unrelated to underlying data structure (learn random noise in data) → **<u>overfitting</u>**



<u>Amount of training data small compared to model capacity!</u>

Model capacity

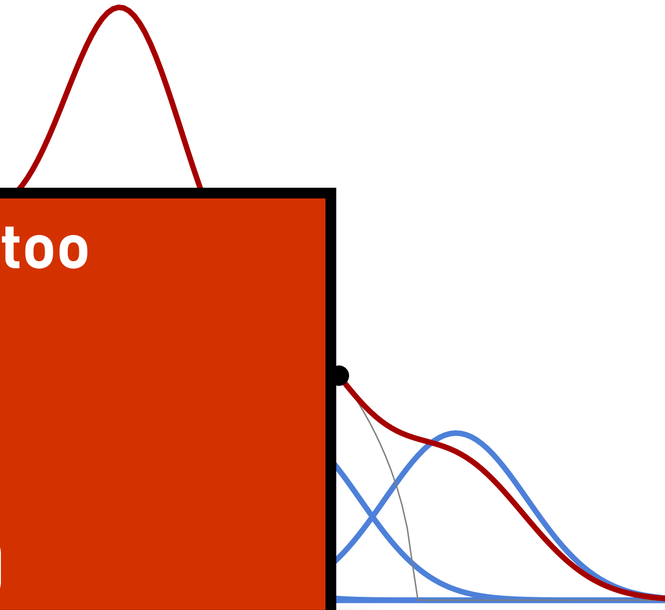
<u>Model capacity</u>: flexibility and ability to fit diverse data

- Interplay between model capacity and

What is applied ML all about? Design models that are not too flexible, but yet able to fit the data!

- **Crafting right <u>inductive bias</u> in a model**
- **(structure corresponds to underlying structure of data)**

- Insufficient data, training performance excellent but unrelated to underlying data structure (learn random noise in data) → **<u>overfitting</u>**



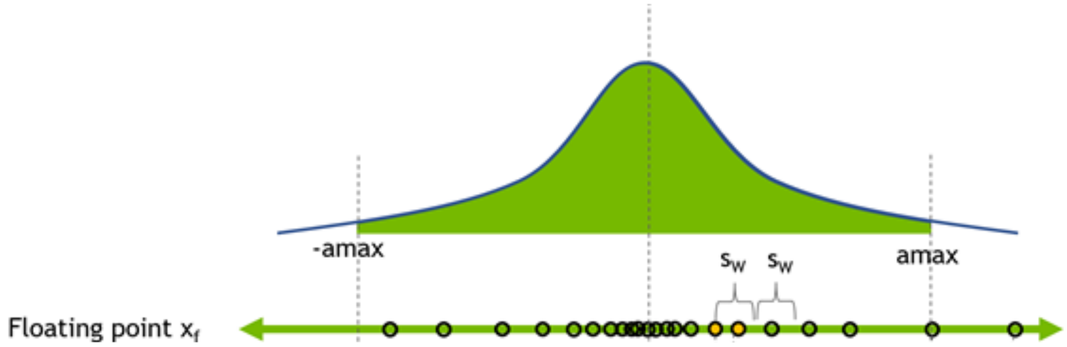
<u>Amount of training data small compared to model capacity!</u>

From theory to Practice

- *You can learn all Deep Learning theory, but an effective training requires skills and experience that are linked to your technical insight*
- *Many things can go wrong in training, and many of them have nothing to do with deep learning*
  - *Overflows, Underflows, out-of-memory, slow code due to ineffective I/O when handling the data*
- *Even if the training works, many things can be done better*
  - *Optimize I/O (data parallelism), distribute training on multiple GPUs, etc.*

Few things to keep in mind

- *PROBLEM: You are training on hardware that comes with limited numerical representation (e.g., 64 bits)*
  - *This implies rounding error, that could have large effects when training or using the algorithm in practice*
    - *Underflow: too small numbers are turned into 0, which kills your gradient and stop your training or give error (e.g., 1/0 -> NaN)*
    - *Overflow: number is too big -> NaN. And the following mathematic is compromised*



Floating point 32:
4B numbers in [-3.4e38, +3.4e38]

Few things to keep in mind

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    - *Overflow: number is too big -> NaN. And the following mathematic is compromised*
  - *Example: softmax activation function, used at the end of multi class classifier (takes a vector of scores and turns them into probabilities)*

$$\mathrm{softmax}(\boldsymbol{x})_i = \frac{\exp(x_i)}{\sum_{j=1}^{n} \exp(x_j)}$$

You can avoid NaN evaluating the function at z = x -max(x)

Few things to keep in mind

- *PROBLEM: You are looking for an optimal weight configuration computing gradients. You want to avoid 0 gradient*
  - *This is called conditioning, i.e., how rapidly a function changes wrt its input*
  - *Example: matrix inversion. You need to find* $f(x) = A^{-1}x$*, given* A*. Given* $\lambda=$ *eigenvalues of* A*, the condition number for A is* $\max_{i,j} \left| \frac{\lambda_i}{\lambda_j} \right|$*. Matrix inversion becomes numerically complicated when this number is large, i.e., when there is a big gap between the largest and smallest eigenvalue*

Regularisation in the loss

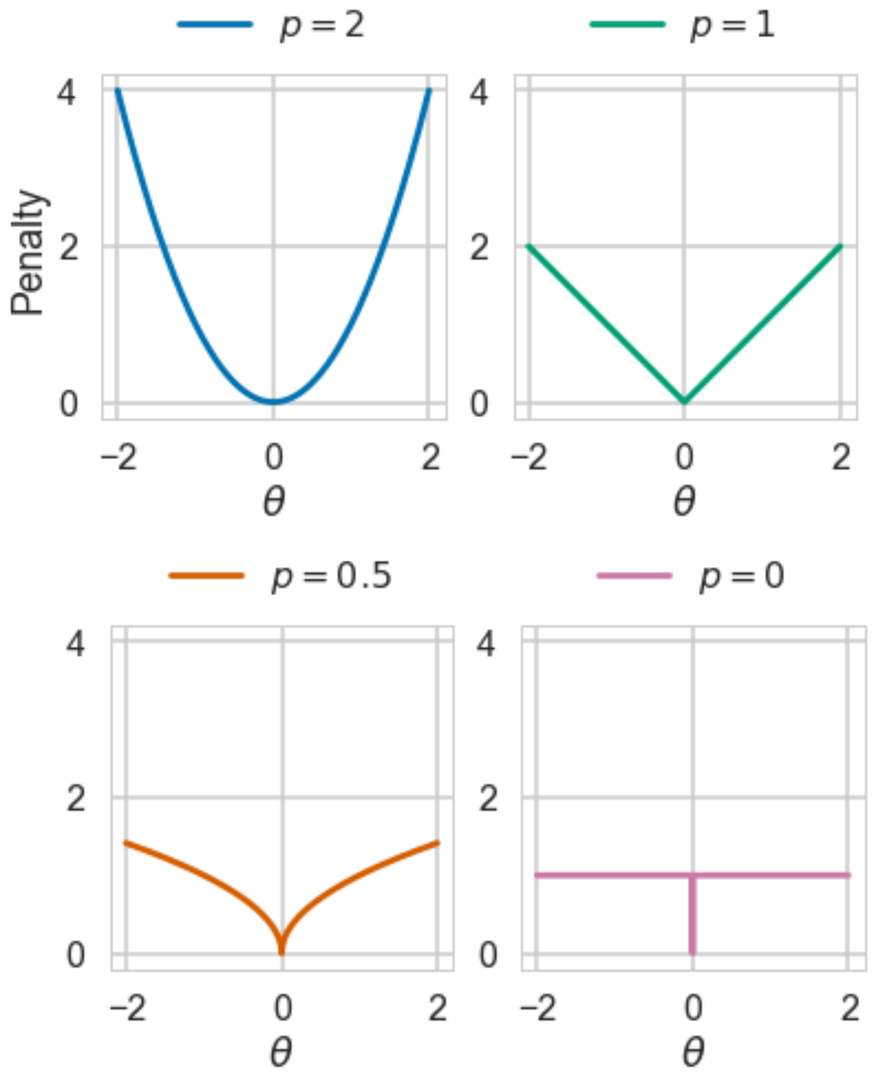
- *Model complexity can be “optimized” when minimizing the loss*
  - *A modified loss is introduced, with a penalty term attache to each model parameter*

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

- *For instance, Lp regularisation*

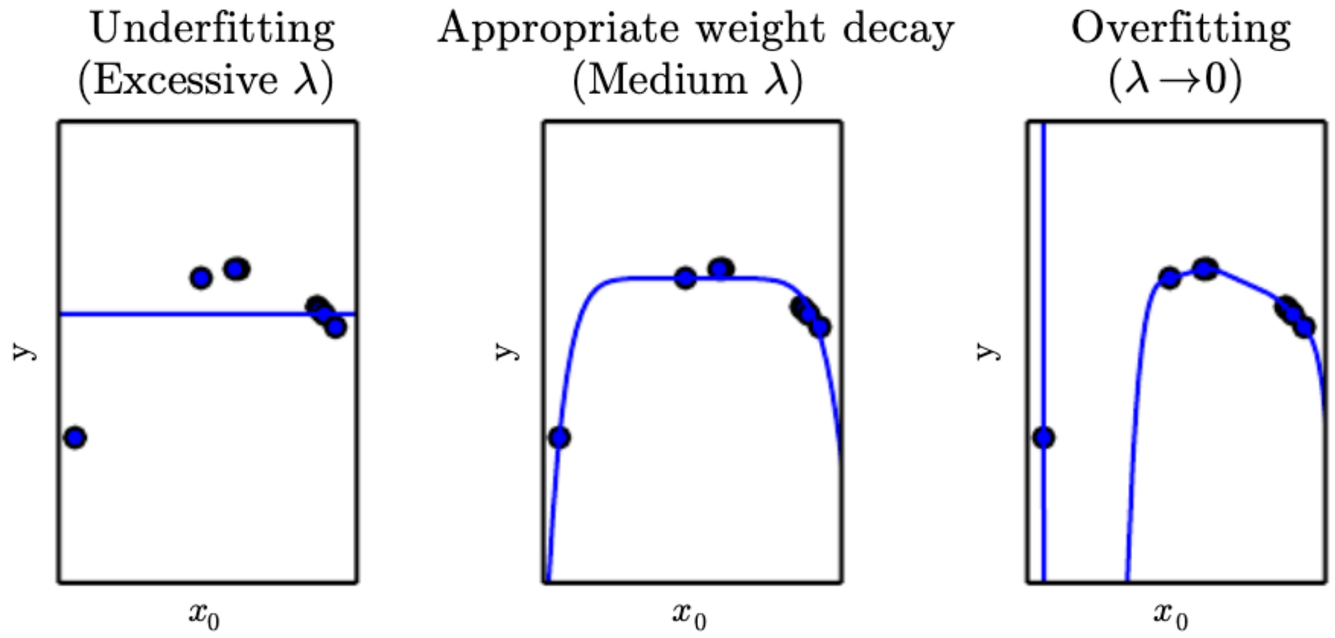
$$L_p = \|\mathbf{w}\|^p = \sum_i |w_i|^p$$

- *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

Regularisation in the loss



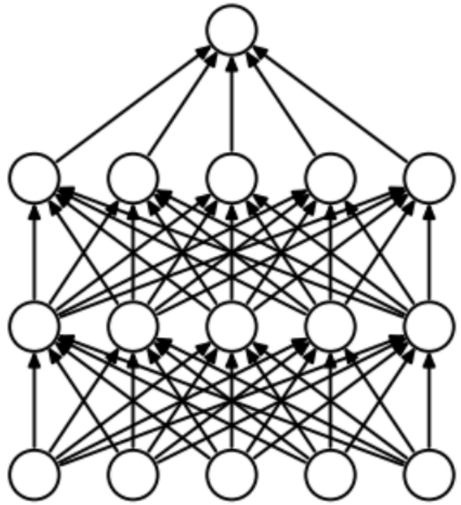
$$J(\boldsymbol{w}) = \mathrm{MSE}_{\mathrm{train}} + \lambda \boldsymbol{w}^\top \boldsymbol{w}$$

E.g adding L2 norm to a linear regression problem encourages weights to be small (put weight on fewer features, solutions with smaller slope)

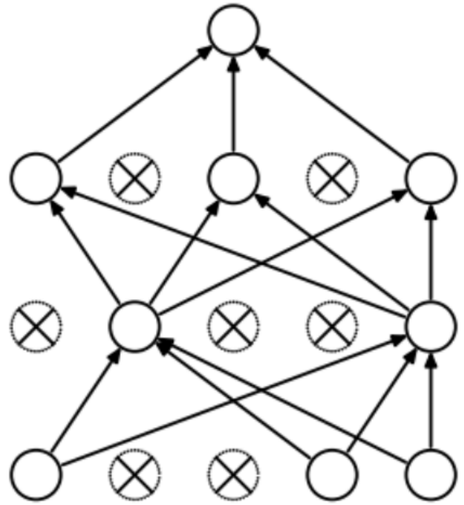
https://openreview.net/pdf?id=H1Y8hhg0b

Regularisation with Drop out

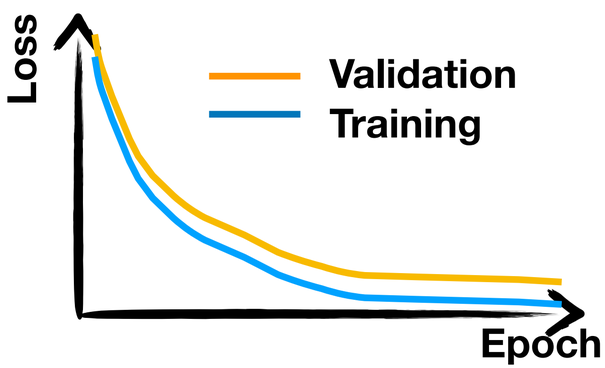
- *A special kind of layer, introduced for regularisation purpose*
- *Randomly drop links between neurons, with probability p*
- *The connections are re-established during the validation and inference steps*
- *Typical sign of it: invert hierarchy between training and validation loss*

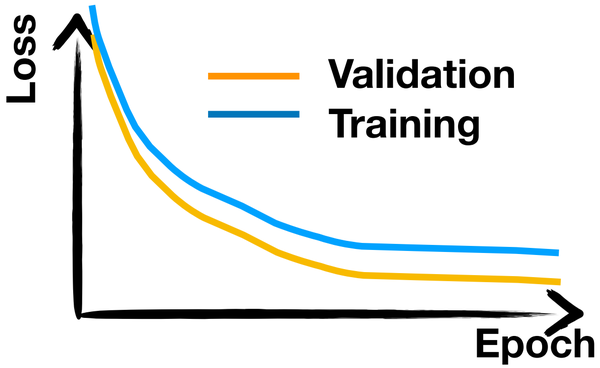


(a) Standard Neural Net



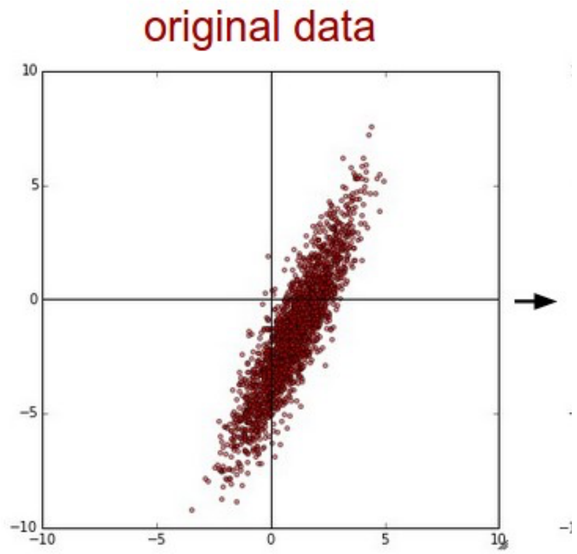
(b) After applying dropout.

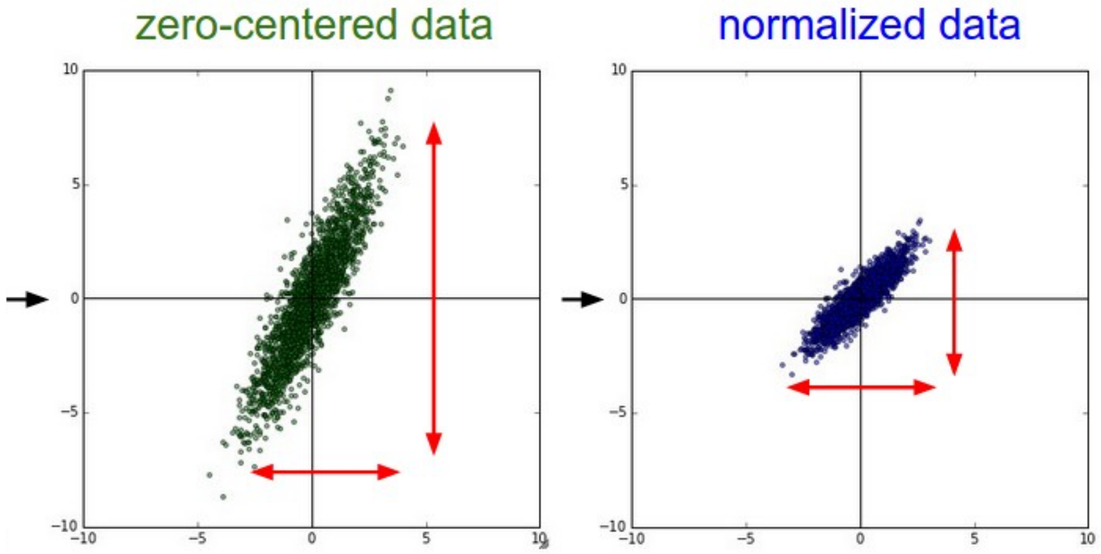




Data normalization

- *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*

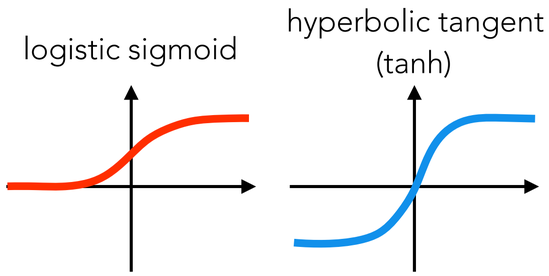




Non-linearities

Vanishing gradient:

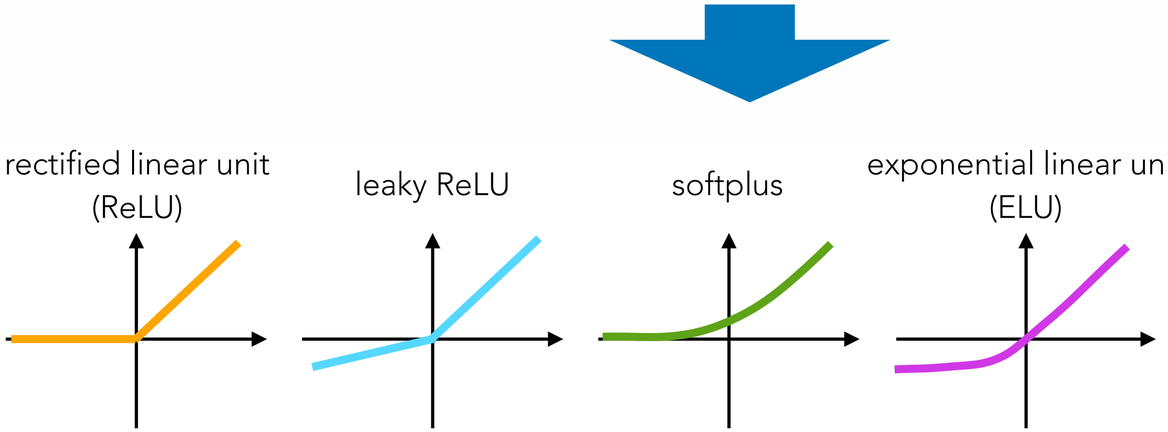
- Some activation functions have small derivatives almost everywhere
- In backpropagation, the product of many small terms goes to zero!→ Gradient "vanishes"



saturating

derivative goes to

zero at +∞ and -∞



non-saturating

non-zero derivative

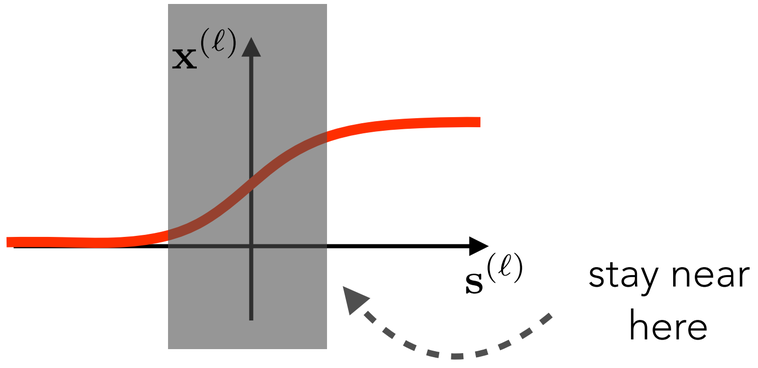
at +∞ and/or -∞

most often used

$$\mathrm{ReLU}(x) := \max(0, x)$$

Batch normalisation

Want to keep inputs within range of the non-linearity function!

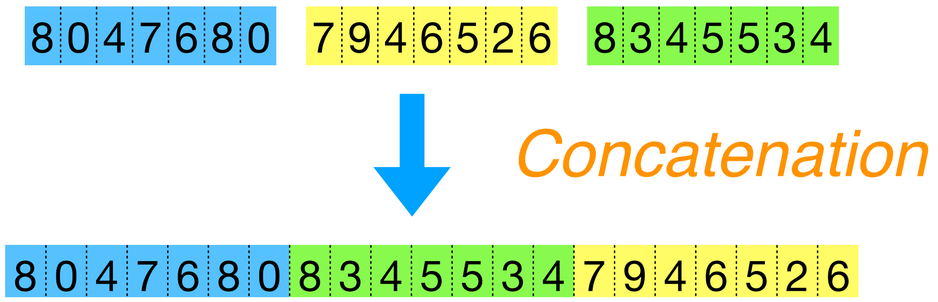


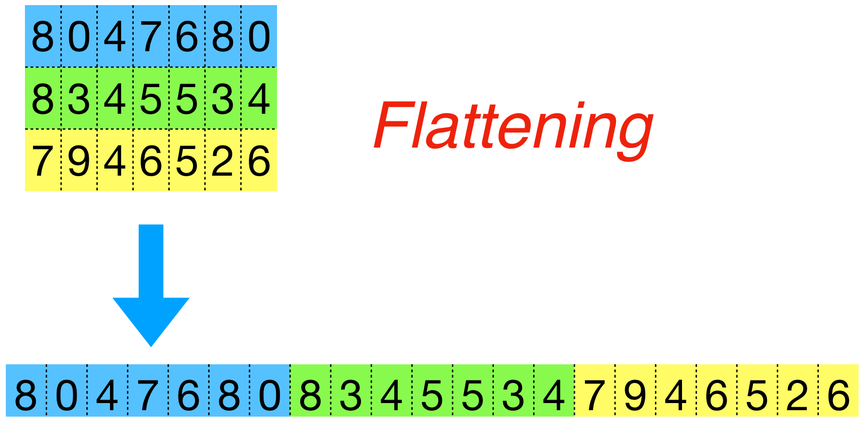
We can normalize the activations before applying the non-linearity

$$s \leftarrow \frac{s - shift}{scale}$$

Array Manipulation

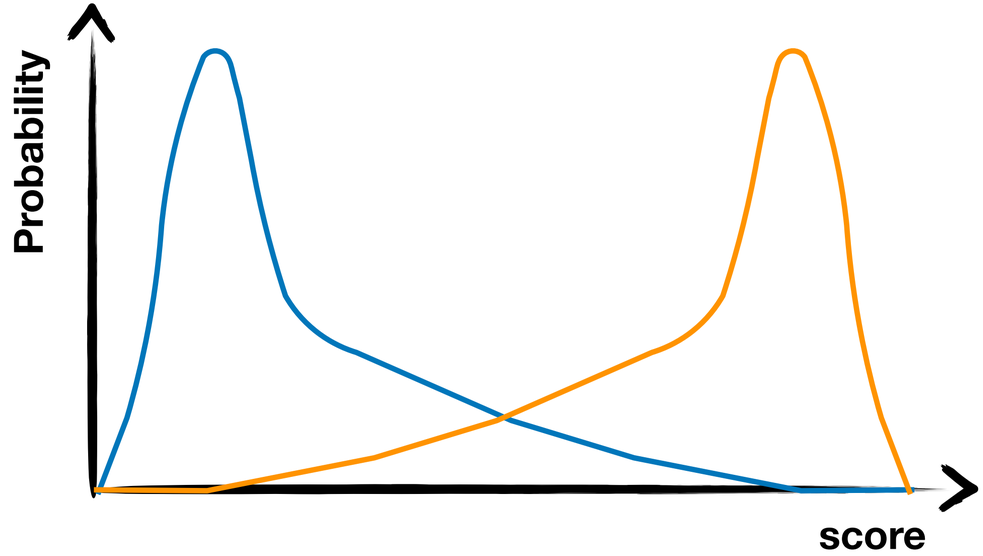
- *Dense NN architectures can be made more complex*
  - *Multiple inputs*
  - *Multiple outputs*
  - *Different networks branches*
- *This is possible thanks to layer-manipulation layers*
  - *Add, Subtract, etc.*
  - *Concatenation*
  - *Flattening*
- *All these operations are usually provided with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

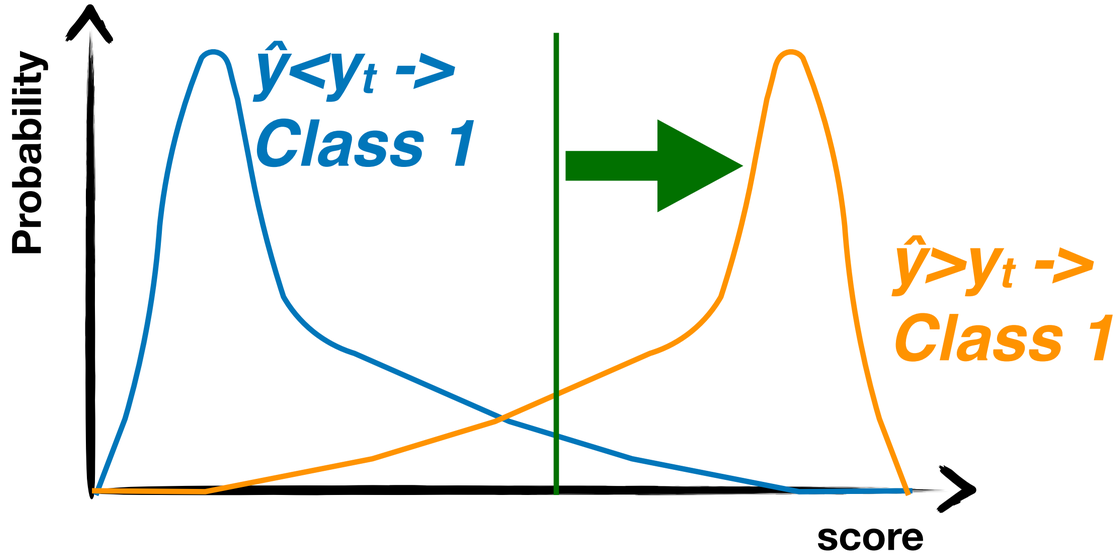




Classifier metrics

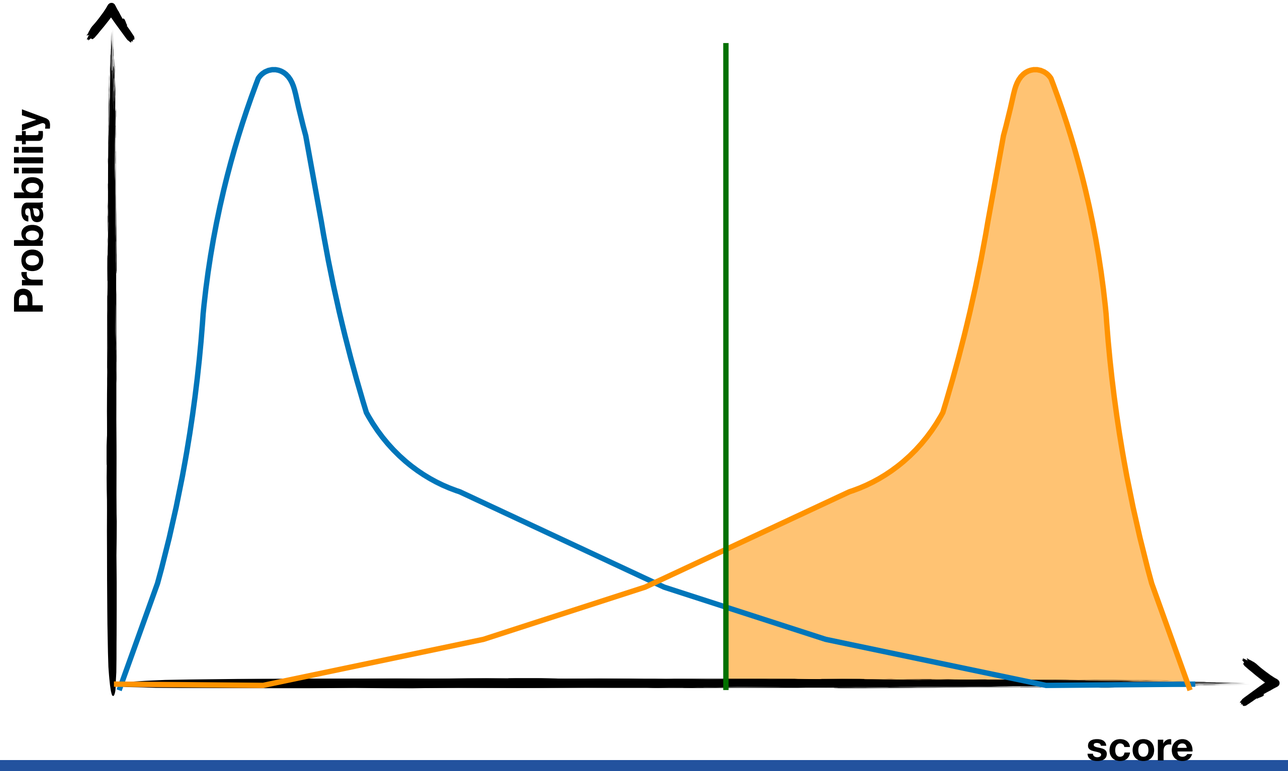
- *Consider a binary classifier*
- *Its output ŷ is a number in [0,1]*
- *If well trained, value should be close to 0 (1) for class-0 (class-1) examples*
- *One usually defines a threshold y_t such that:*
  - *$\hat{y}>y_t$ -> Class 1*
  - *$\hat{y}<y_t$ -> Class 0*





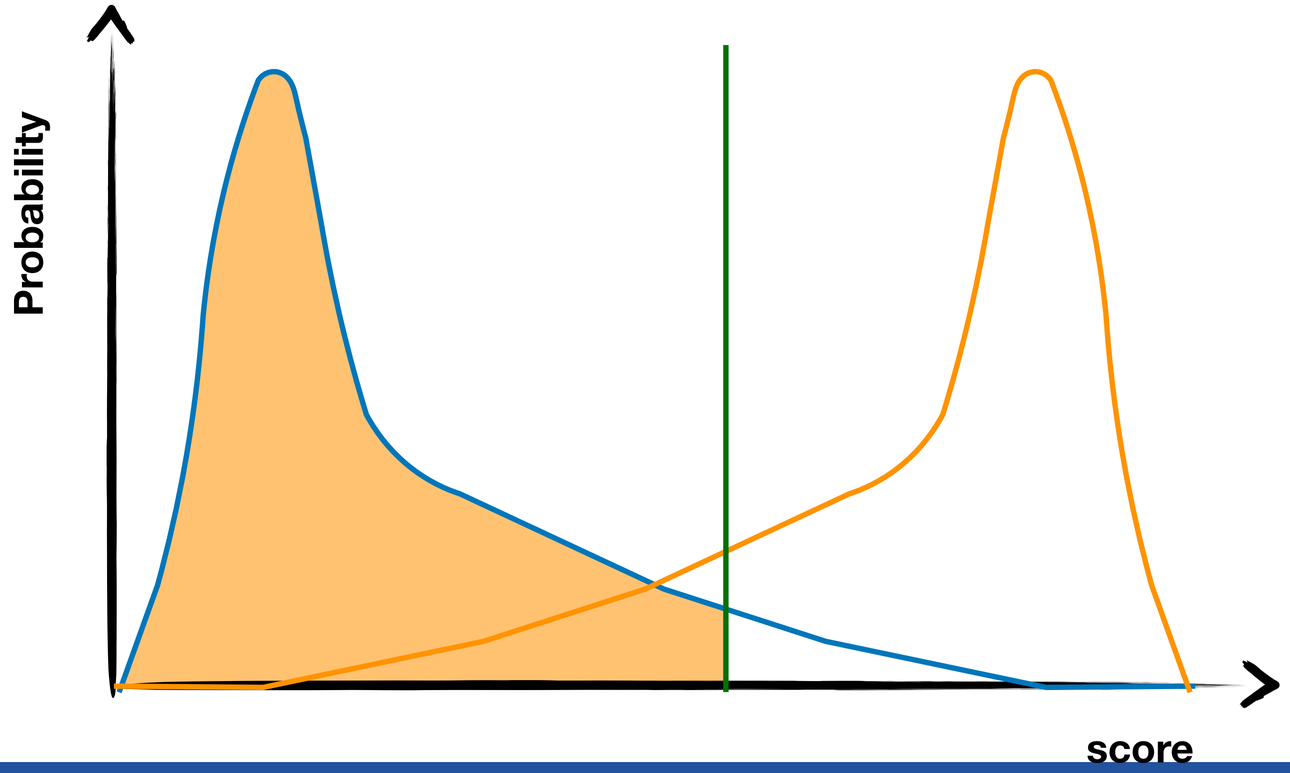
Classifier metrics

- *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*



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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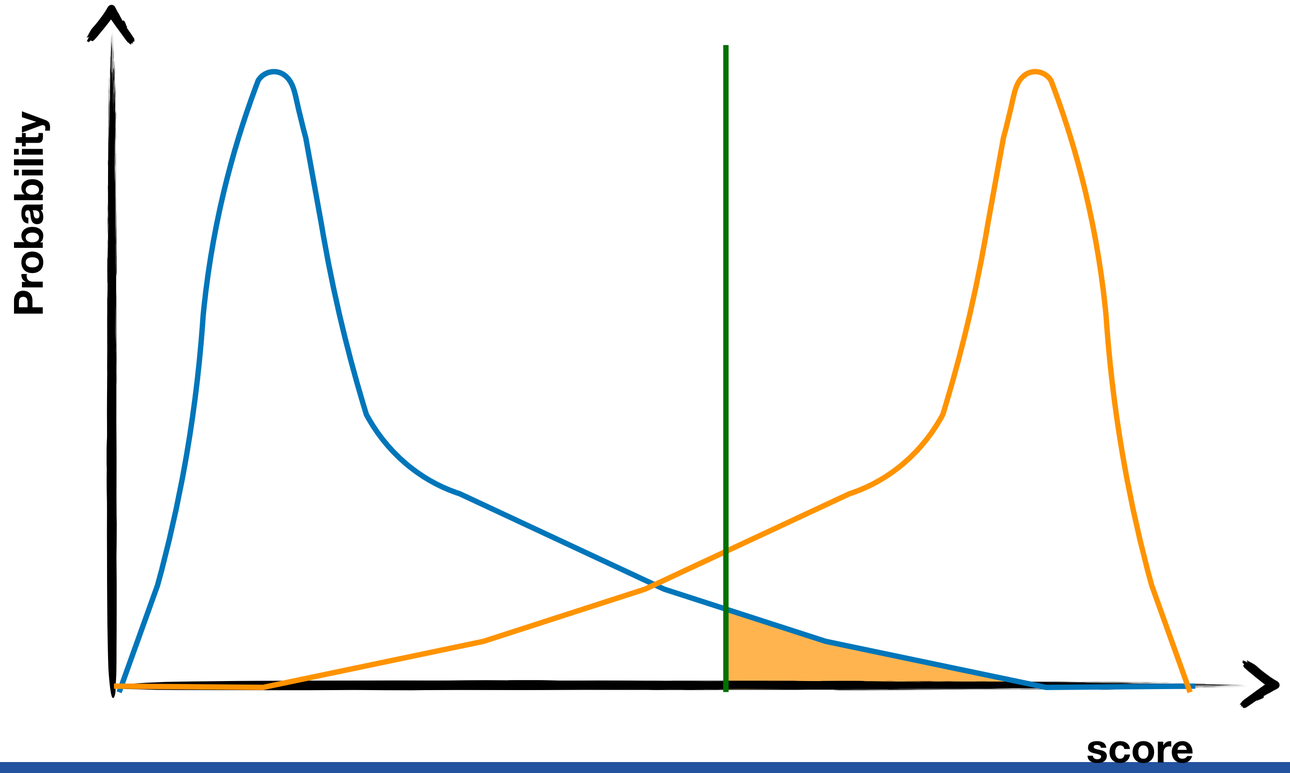

Classifier metrics

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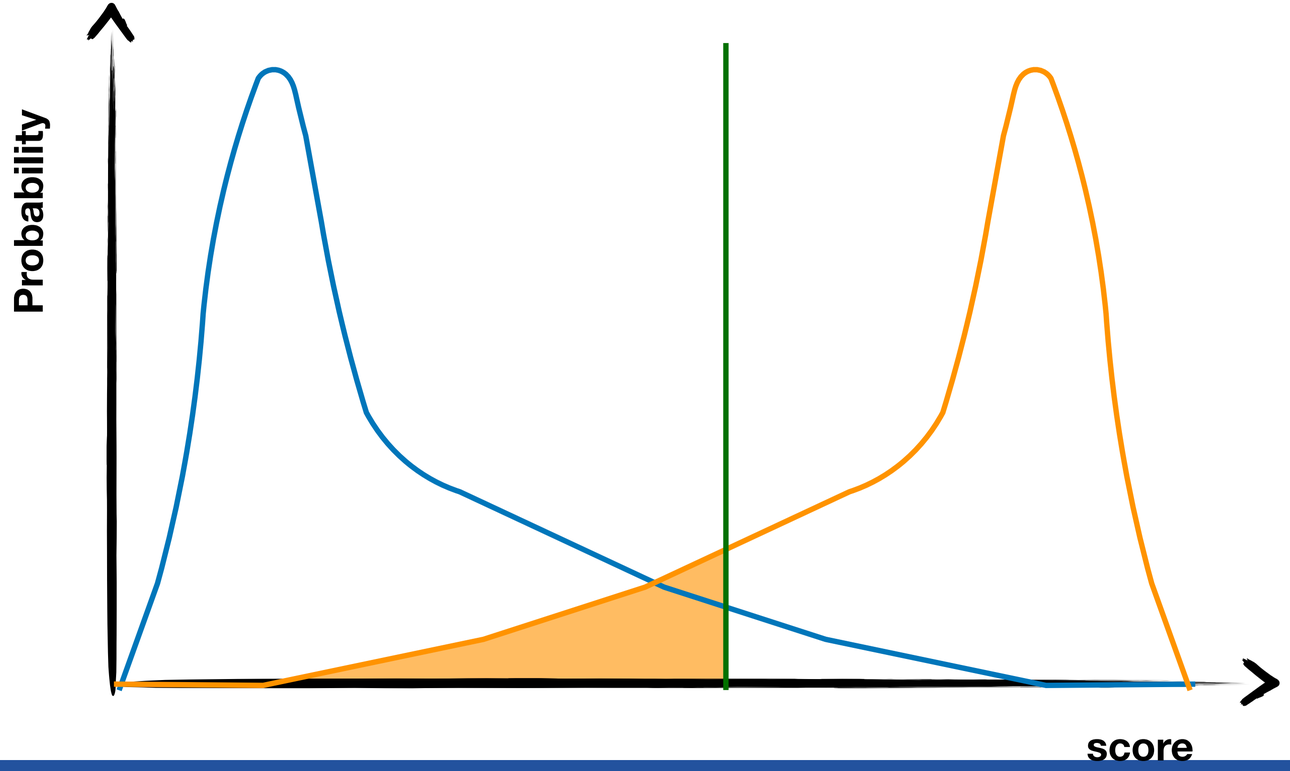
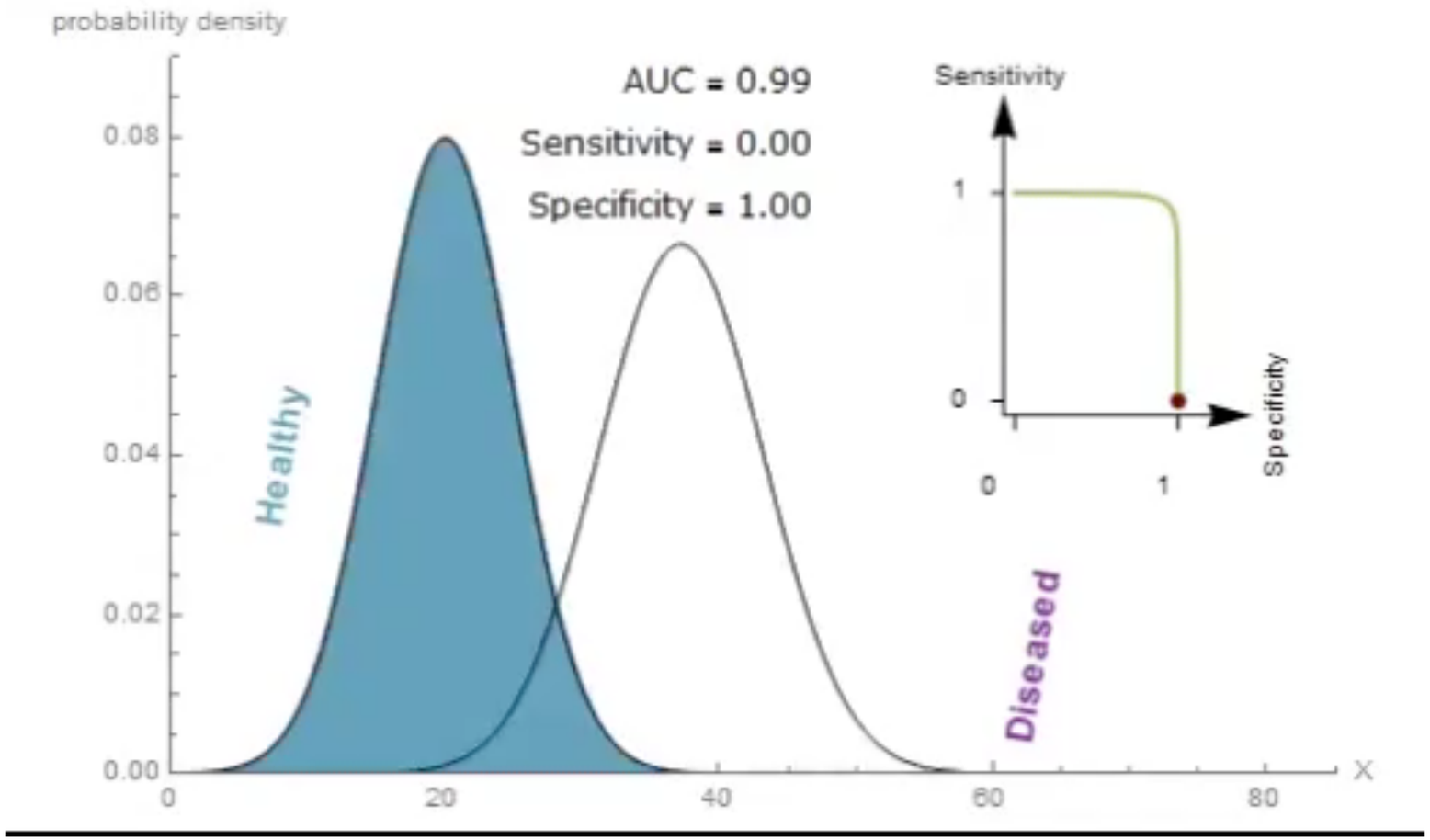


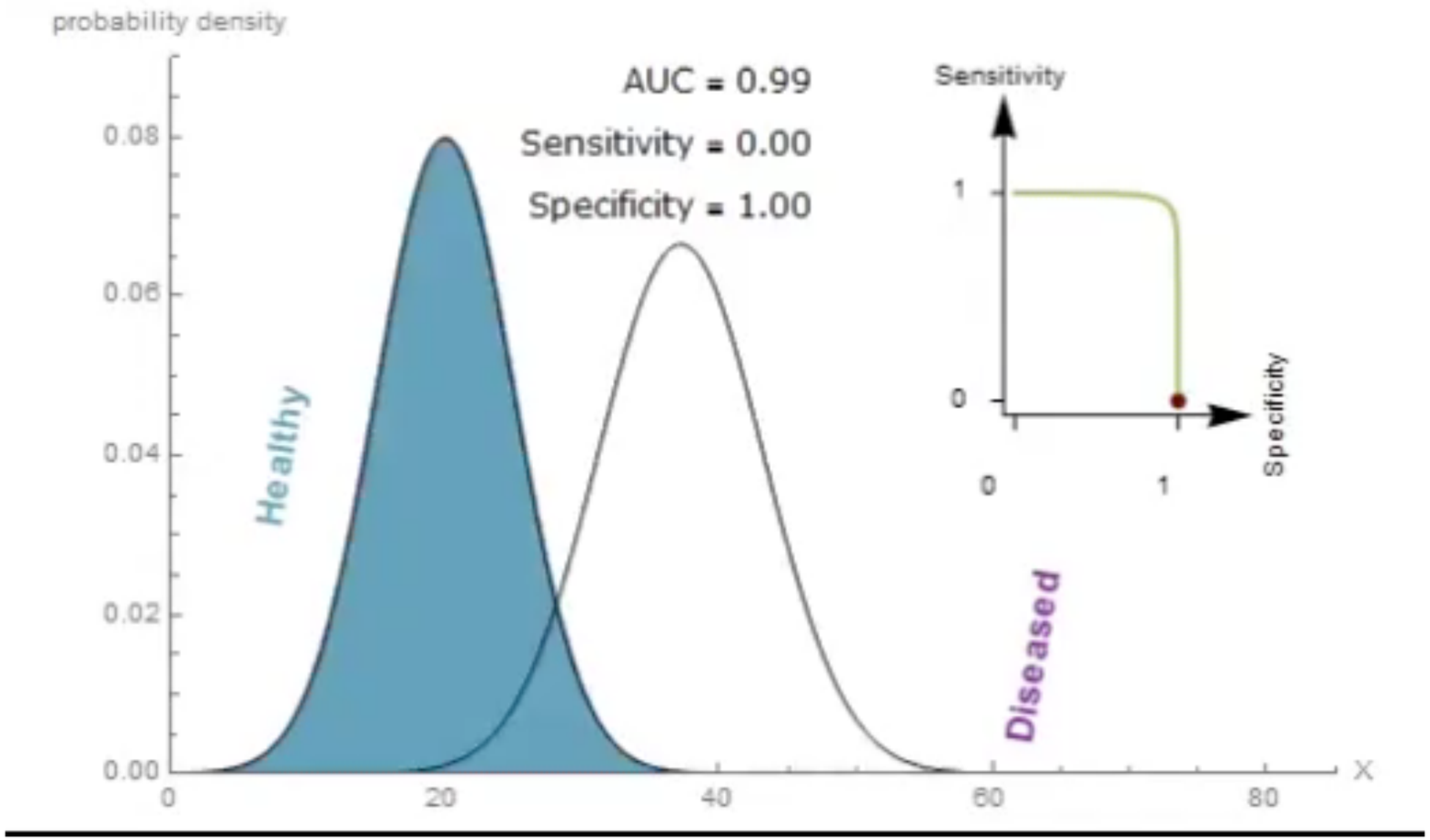
Classifier metrics

- *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*

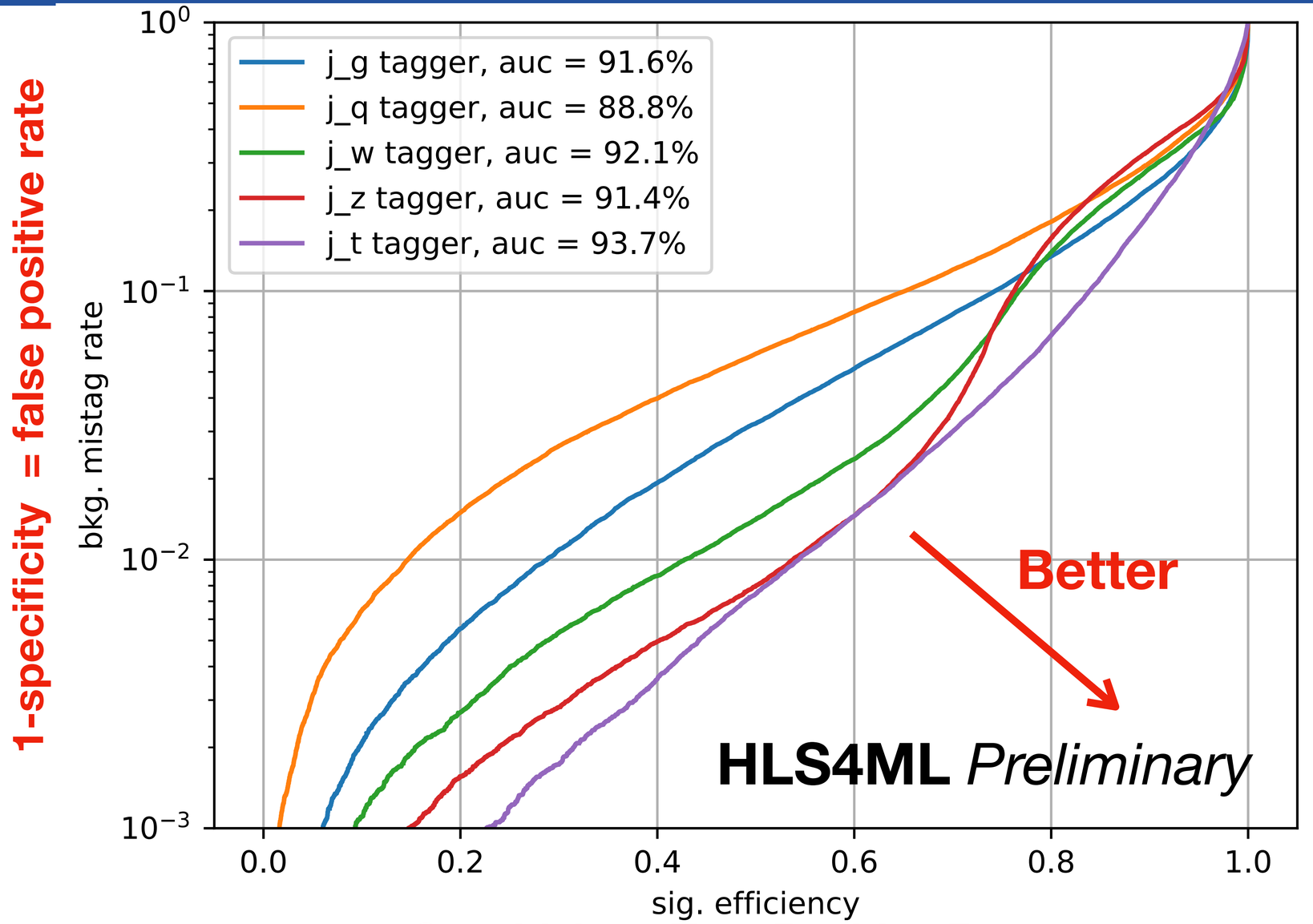
Receiver operating characteristic



Receiver operating characteristic



ROC curve

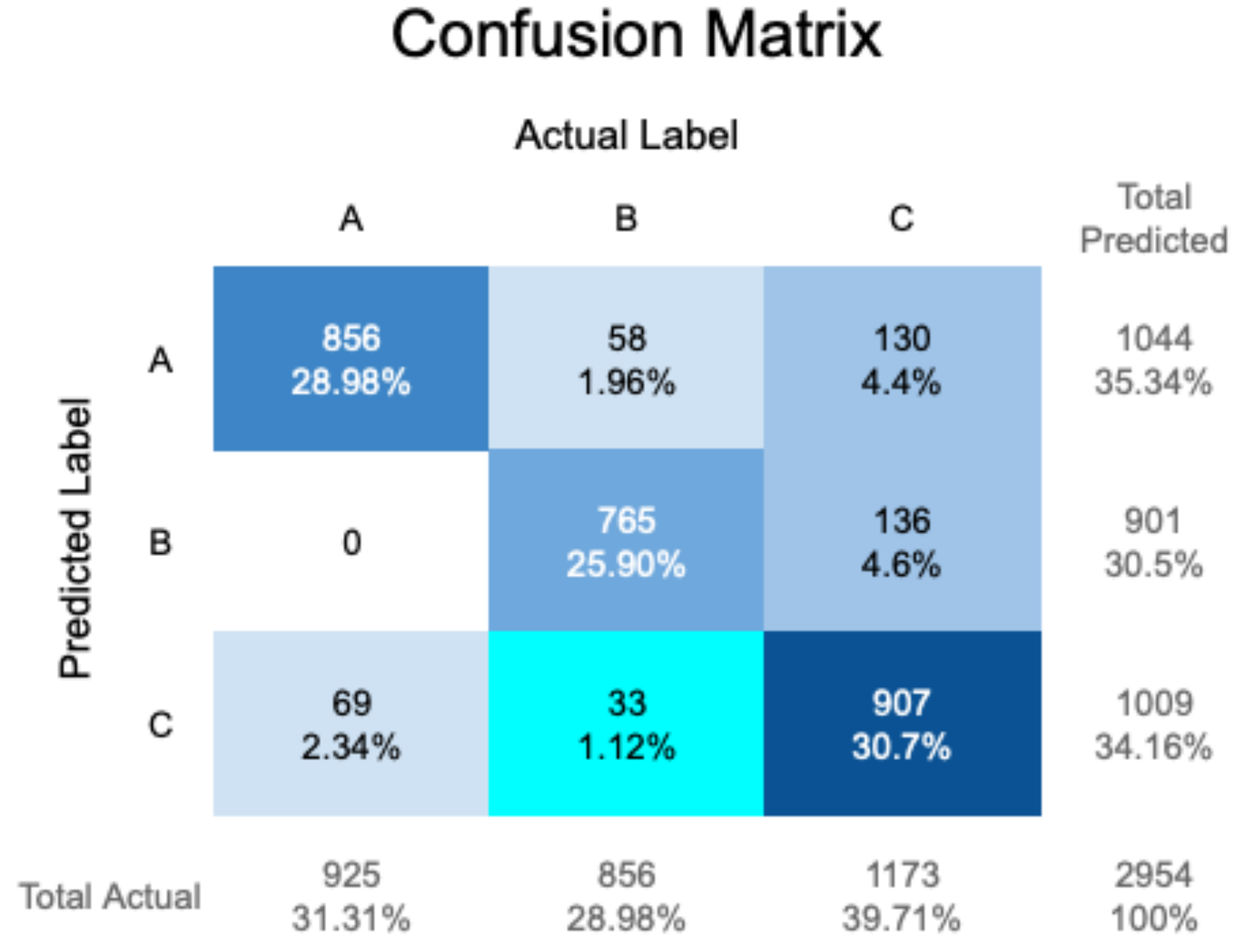


1-specificity = false positive rate

Sensitivity = True Positive Rate

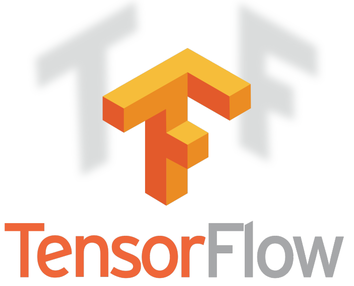
Confusion matrix

- *A very effective visual tool to understand where your classifier works and where it doesn't*
  - *Fill a matrix A_{ij} the fraction of examples of class C_i classified as class C_j*
  - *Ideally, one would like to see the identity matrix*
  - *In practise, one can look for large off-diagonal elements to see which classification is problematic*



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)*



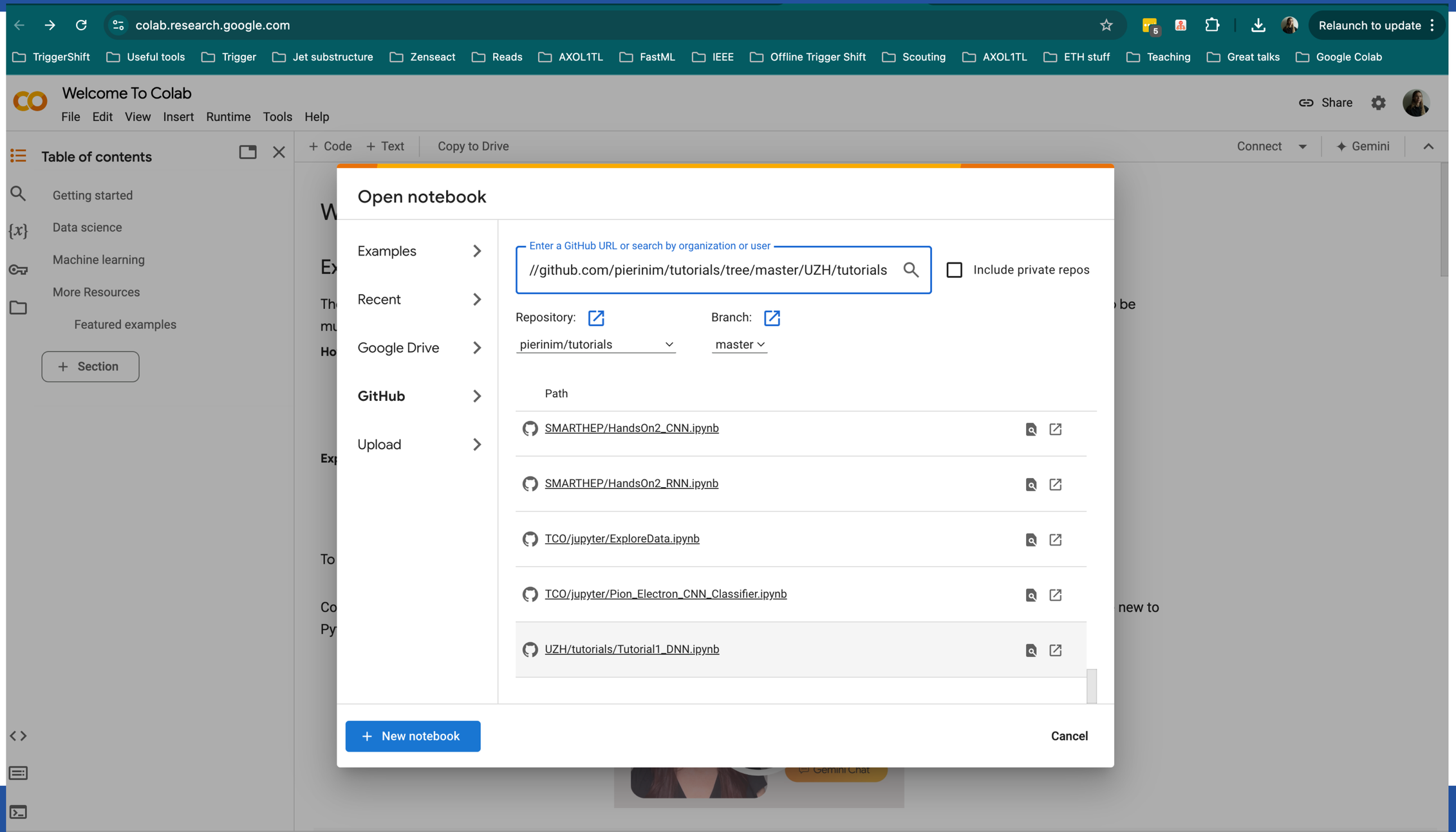
Summary

- *Training a network requires work*
  - *To prepare the data (dataset split, normalization, etc)*
  - *To optimize the training efficiency (early stopping, regularization, etc.)*
  - *To perform post-training diagnostic: training convergence, bias vs variance, accuracy, confusion*
- *Things might not work out of the box, but insight on pre-training, training and post-training techniques make your work easier*

Setting up COLAB

https://github.com/pierinim/tutorials/blob/master/GGI_Jan2021/Lecture1/Tutorial_Colab.pdf

Tutorial


colab.research.google.com
Relaunch to update
TriggerShift
Useful tools
Trigger
Jet substructure
Zenseact
Reads
AXOL1TL
FastML
IEEE
Offline Trigger Shift
Scouting
AXOL1TL
ETH stuff
Teaching
Great talks
Google Colab
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//github.com/pierinim/tutorials/tree/master/UZH/tutorials
Include private repos
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Branch:
pierinim/tutorials
master
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SMARTHEP/HandsOn2_CNN.ipynb
SMARTHEP/HandsOn2_RNN.ipynb
TCO/jupyter/ExploreData.ipynb
TCO/jupyter/Pion_Electron_CNN_Classifier.ipynb
UZH/tutorials/Tutorial1_DNN.ipynb
New notebook
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Tutorial

Tutorial1_DNN.ipynb

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Gemini

Muliclass classifier on IRIS dataset

16s

```
# Import necessary libraries
import numpy as np
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.datasets import load_iris
from sklearn.preprocessing import OneHotEncoder
from sklearn.metrics import roc_curve, auc, confusion_matrix, ConfusionMatrixDisplay
import matplotlib.pyplot as plt
import seaborn as sns
from tensorflow.keras.models import Sequential
from tensorflow.keras.layers import Dense
from tensorflow.keras.utils import to_categorical
from sklearn.preprocessing import label_binarize
```

0s

```
[2] # Load the Iris dataset
    iris = load_iris()
    X = iris.data  # Features
    y = iris.target  # Labels
```

0s

```
[3] # One-hot encode the labels: use (1,0,0), (0,1,0), (0,0,1)
    y = to_categorical(y)
```

0s

```
[6] print(y.shape)
    print(X.shape)
```

```
(150, 3)
(150, 4)
```



```
[12] # Add layers
     from tensorflow.keras.layers import Input
     model.add(Input(shape=(X_train.shape[1],)))
```

Tutorial

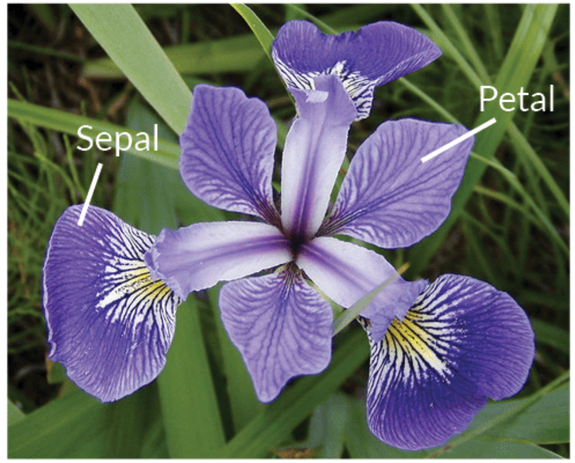
The Iris Dataset

This data sets consists of 3 different types of irises' (Setosa, Versicolour, and Virginica) petal and sepal length, stored in a 150x4 numpy.ndarray

The rows being the samples and the columns being: Sepal Length, Sepal Width, Petal Length and Petal Width.

The below plot uses the first two features. See here for more information on this dataset.

```
# Code source: Gaël Varoquaux
# Modified for documentation by Jaques Grobler
# License: BSD 3 clause
```



Iris Versicolor

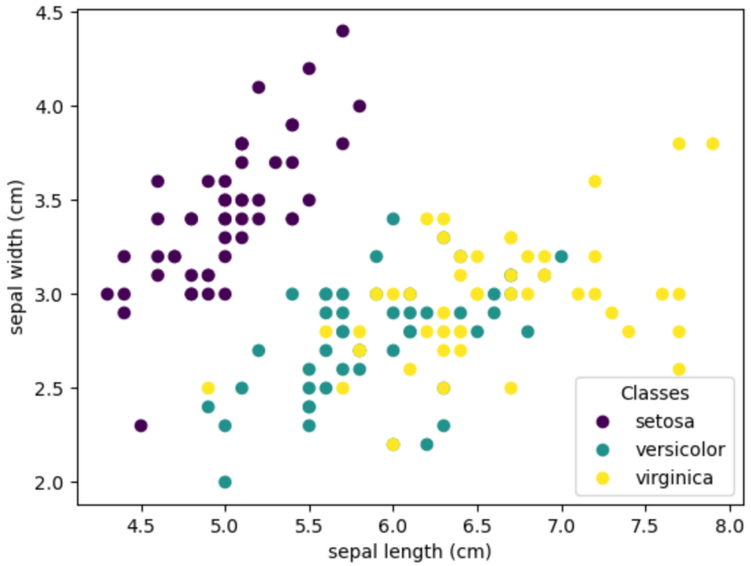
Iris Setosa

Iris Virginica

Loading the iris dataset

```
from sklearn import datasets

iris = datasets.load_iris()
```



https://scikit-learn.org/stable/auto_examples/datasets/plot_iris_dataset.html

Tutorial

```
[12] # Add layers
     from tensorflow.keras.layers import Input
     model.add(Input(shape=(X_train.shape[1],)))
     model.add(Dense(16, activation='relu', input_shape=(X_train.shape[1],)))
     model.add(Dense(16, activation='relu'))
     model.add(Dense(16, activation='relu'))
     model.add(Dense(y_train.shape[1], activation='softmax'))  # Output layer
```

```
/usr/local/lib/python3.10/dist-packages/keras/src/layers/core/dense.py:87: UserWarning: Do n
  super().__init__(activity_regularizer=activity_regularizer, **kwargs)
```

```
# Compile the model
model.compile(optimizer='adam', loss='categorical_crossentropy', metrics=['accuracy'])
```

Tutorial

Data Dictionary

Variable	Definition	Key
survival	Survival	0 = No, 1 = Yes
pclass	Ticket class	1 = 1st, 2 = 2nd, 3 = 3rd
sex	Sex	
Age	Age in years	
sibsp	# of siblings / spouses aboard the Titanic	
parch	# of parents / children aboard the Titanic	
ticket	Ticket number	
fare	Passenger fare	
cabin	Cabin number	
embarked	Port of Embarkation	C = Cherbourg, Q = Queenstown, S = Southampton

In this challenge, we ask you to build a predictive model that answers the question: “what sorts of people were more likely to survive?” using passenger data (ie name, age, gender, socio-economic class, etc).

https://www.kaggle.com/c/titanic/overview

Tutorial

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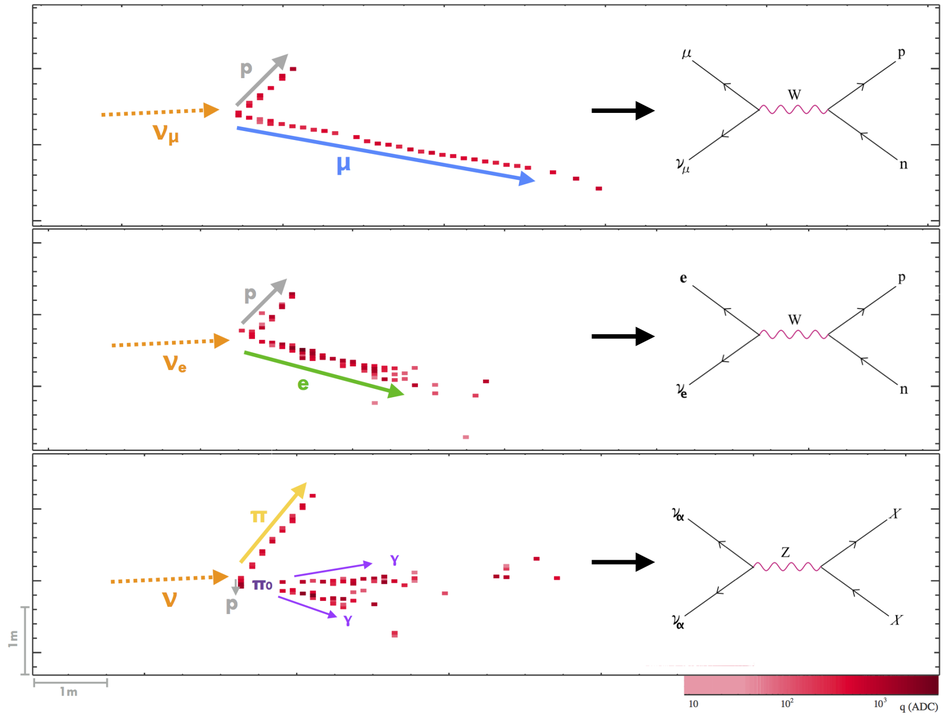
Losses

MSE is a standard loss when predicting a continuous value (e.g regression)

What about classification?
Labels (y_i) 1 for correct class, 0 for the rest

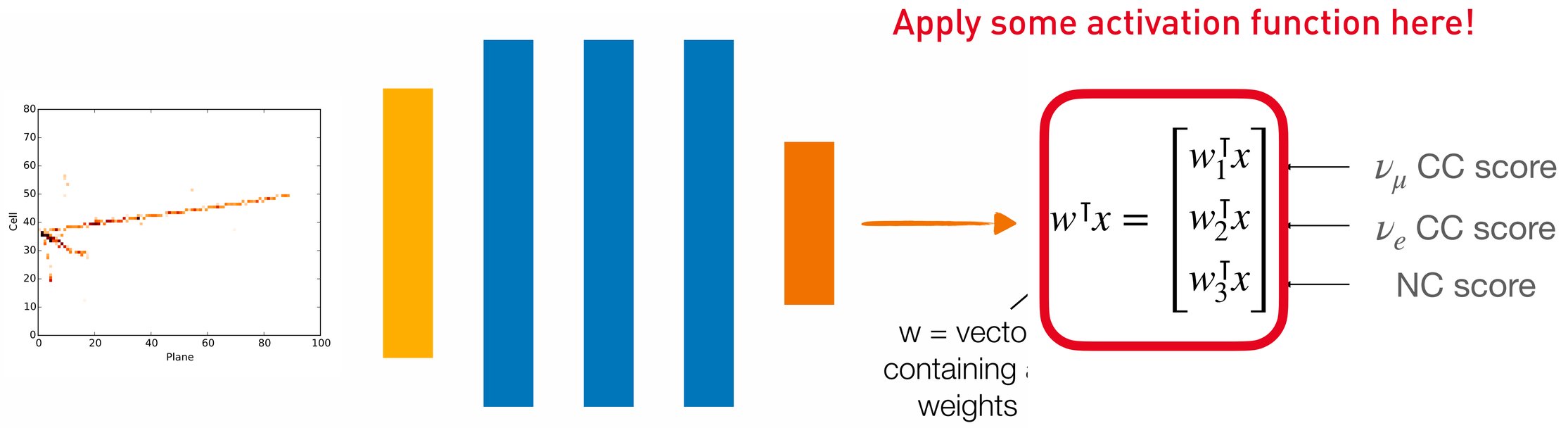


$$w^\intercal x = \begin{bmatrix} w_1^\intercal x \\ w_2^\intercal x \\ w_3^\intercal x \end{bmatrix} \begin{matrix} \leftarrow \nu_\mu \text{ CC score} \\ \leftarrow \nu_e \text{ CC score} \\ \leftarrow \text{NC score} \end{matrix}$$

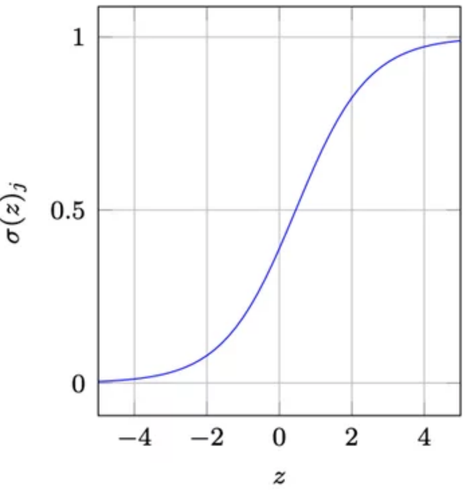
Softmax

Apply an activation function to final output layer (in our case (3,1) for each interaction type):

- should push each value to be between 0 and 1, and
- should make sure the sum (in our case, across all 3) is equal to 1



Softmax



$$\text{softmax}\left(\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_K \end{bmatrix}\right) = \frac{1}{\sum_{k=1}^{K} \exp(a_k)} \begin{bmatrix} \exp(a_1) \\ \exp(a_2) \\ \vdots \\ \exp(a_K) \end{bmatrix}$$

Probability of each class $\in \{0,1\}$

These are often called the logits ***Normalisation factor to make sum of probabilities==1***

$$\begin{bmatrix} 1.2 \\ 0.9 \\ 0.4 \end{bmatrix} \rightarrow \boxed{\text{Softmax}} \rightarrow \begin{bmatrix} 0.46 \\ 0.34 \\ 0.20 \end{bmatrix}$$

Softmax

$$\text{softmax}\left(\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_K \end{bmatrix}\right) = \frac{1}{\sum_{k=1}^{K} \exp(a_k)} \begin{bmatrix} \exp(a_1) \\ \exp(a_2) \\ \vdots \\ \exp(a_K) \end{bmatrix}$$

Probability of each class $\in \{0,1\}$

These are often called the logits

Normalisation factor to make sum of probabilities==1

In contrast to other activation functions (like ReLu), softmax takes a vector as input and has a vector as output (since it needs to normalise across classes

- argmax of output is the model class!
- Why exp? Because it hugely increase the probability of the **biggest** score and decrease the probability of the lower scores

Crossentropy loss

Given y, try to make probability for corresponding entry in output vector as high as possible:

$$\hat{y} = \begin{bmatrix} 0.9 \\ 0.02 \\ 0.08 \end{bmatrix} \quad y = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

How? Cross-entropy. The cross-entropy loss for a softmax output layer is given by

$$L(y, \hat{y}) = -\sum_{i=1}^{n} y_i \log(\hat{y}_i),$$

y: True probability distribution (one-hot encoded)

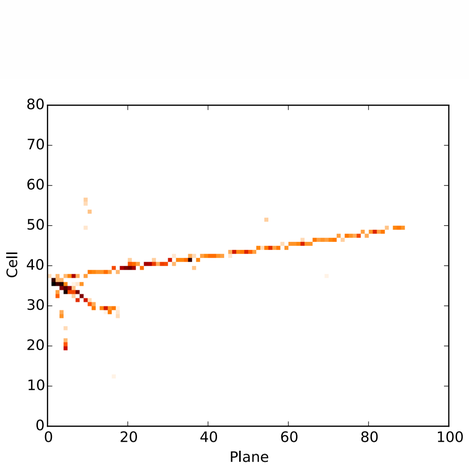
$\hat{y}$: Predicted probability distribution (softmax output)

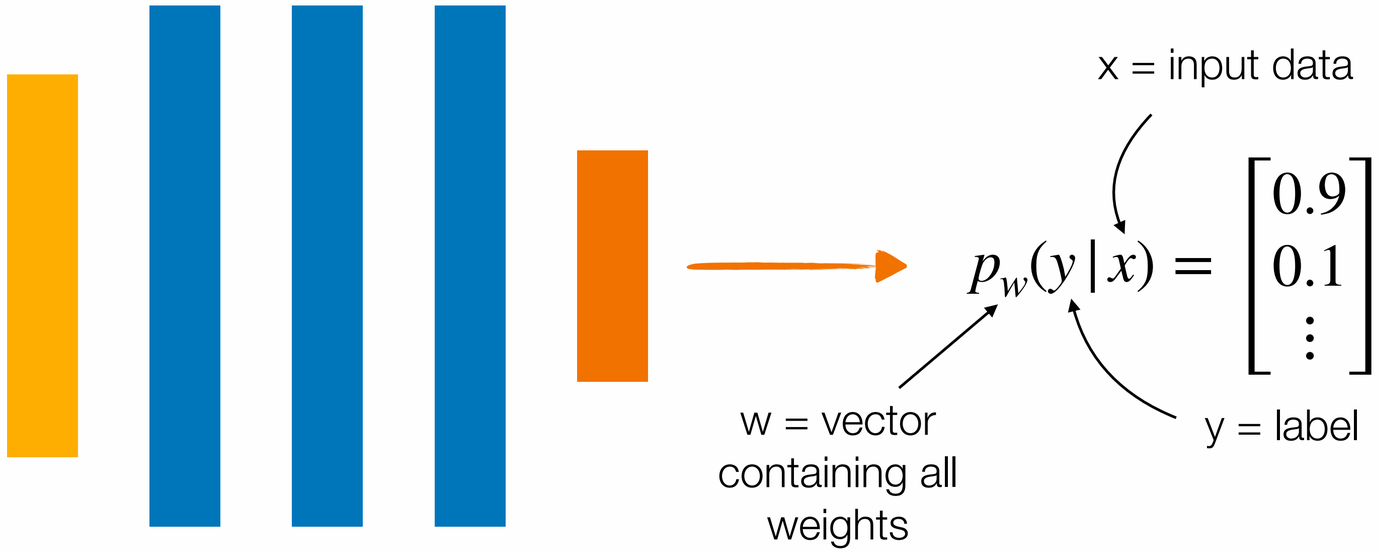
n: Number of classes

All terms with 0 in y, will be zero! Only term left is "correct class" term, in our case $-\hat{y}_1 log y_1$

Gradient descent wants to make this term small, must make y_1 as large as possible (can be at most 1)!

Training





Train such that w^* maximise the log likelihood of the data under our model:

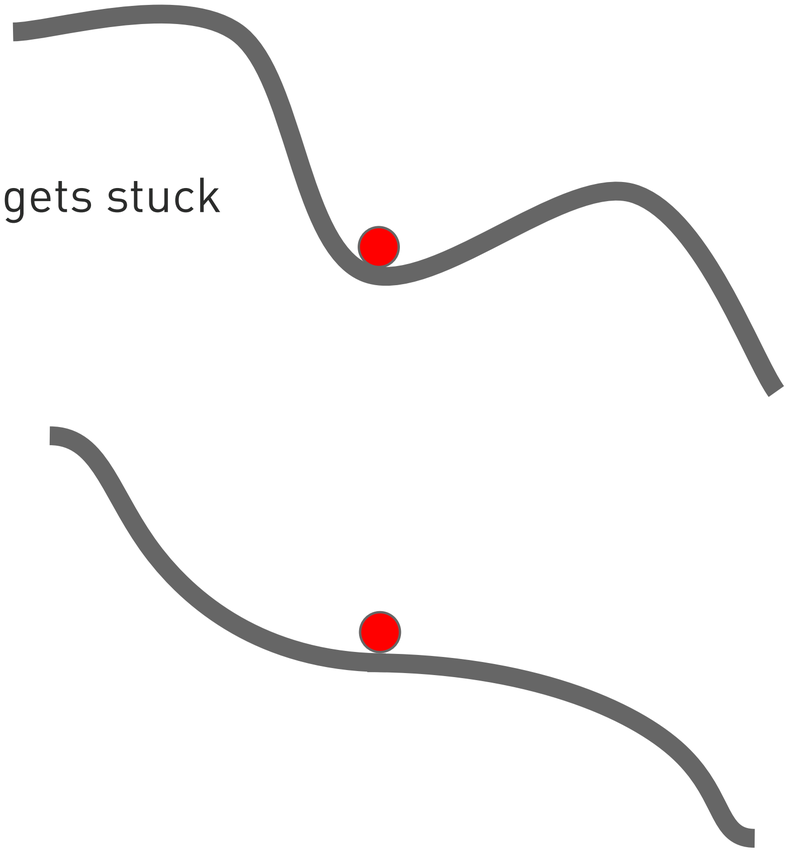
$$\mathscr{L}_{cross-entropy}(w) = -\frac{1}{N}\sum_{n=1}^{N} \log \hat{P}(Y = y_N | X = x_N) = -\frac{1}{N}\sum_{n=1}^{N} \log \frac{e^{f(x_N;w)_{y_N}}}{\sum_z e^{f(x_N;w)_z}}$$

(Negative log-likelihood loss, or cross-entropy loss)

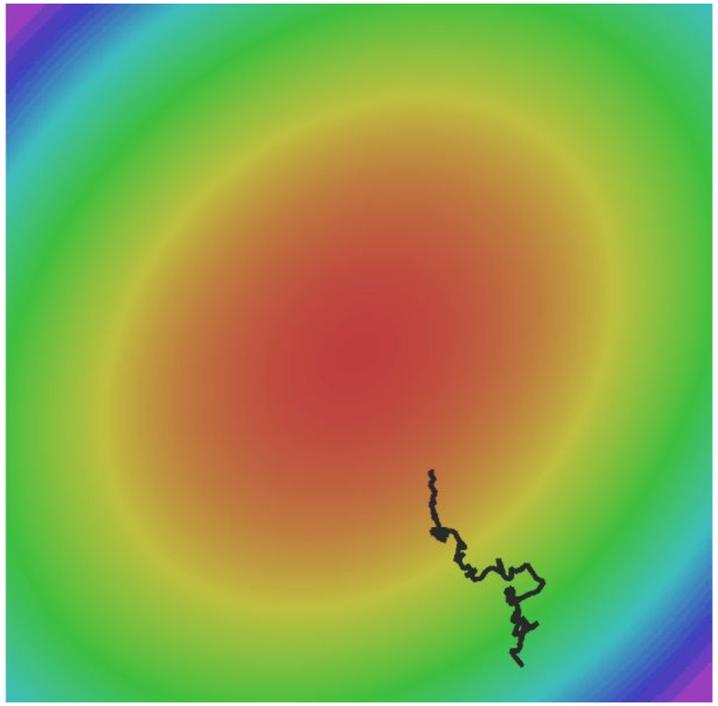
Optimisers

What if the loss function has local minima or saddle point?

- Zero gradient, function has a gradient descent local minima or gets stuck
- Saddle points much more common in high dimension



Our gradients come from mini batches so they can be noisy!

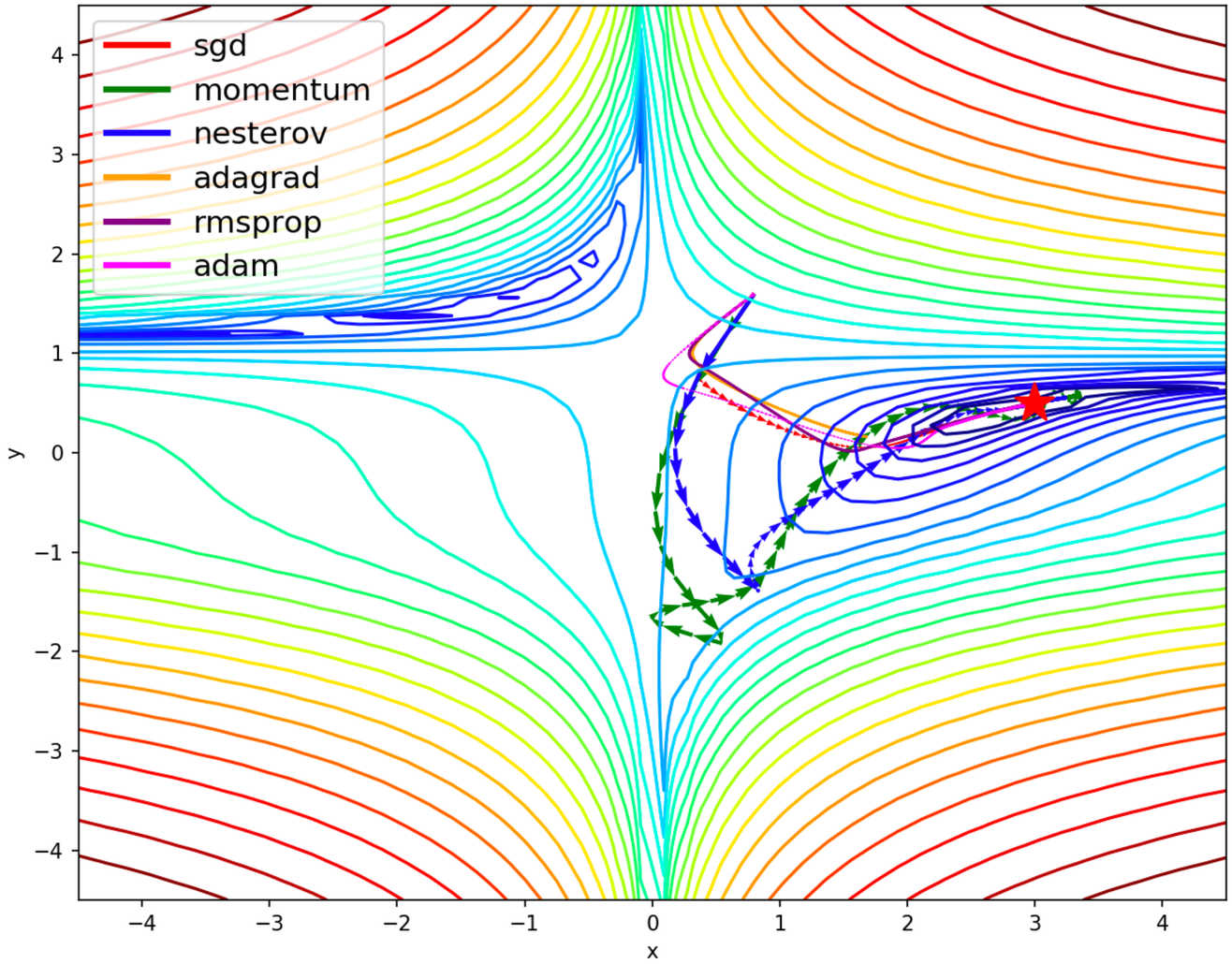


Optimisers

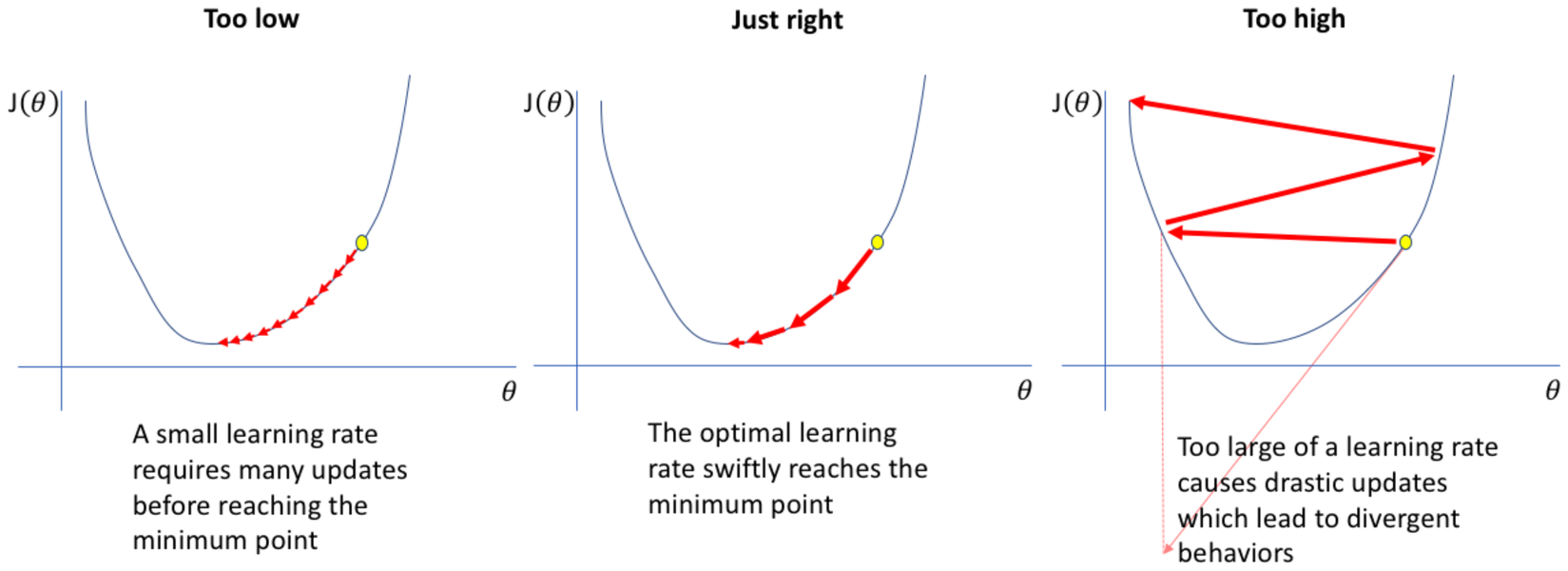
Several alternative optimisation algorithms to stochastic gradient descent exists

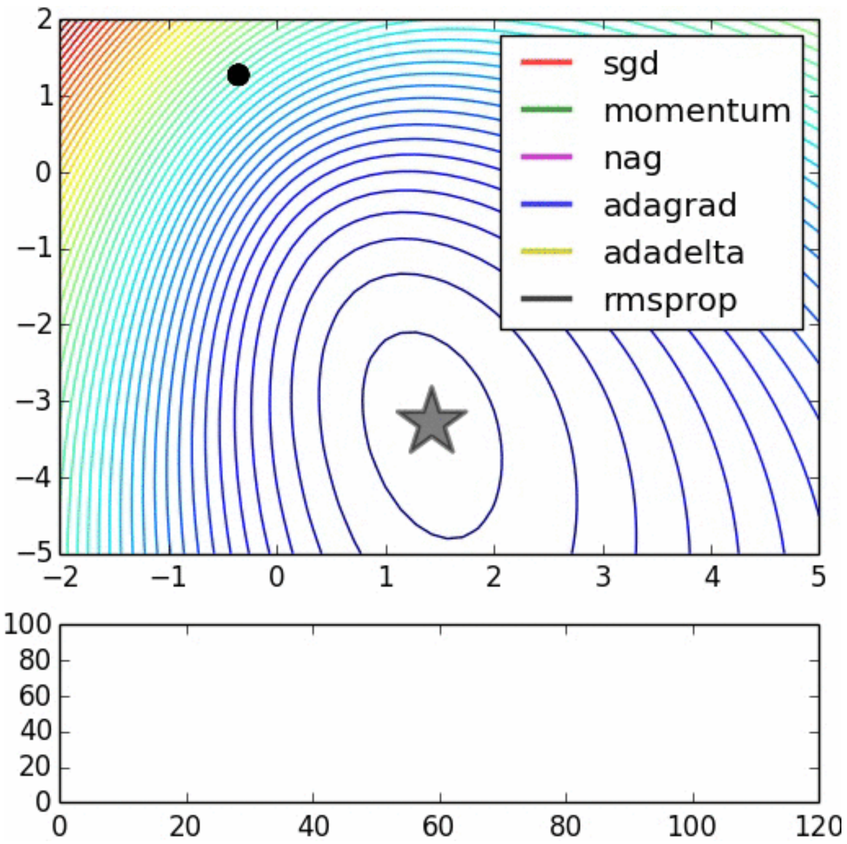
- AdaGrad
- RMSProp
- Adam (per parameter lr)

All based on estimating moments of the gradients and/or iteratively changing learning rate



Other (popular) options





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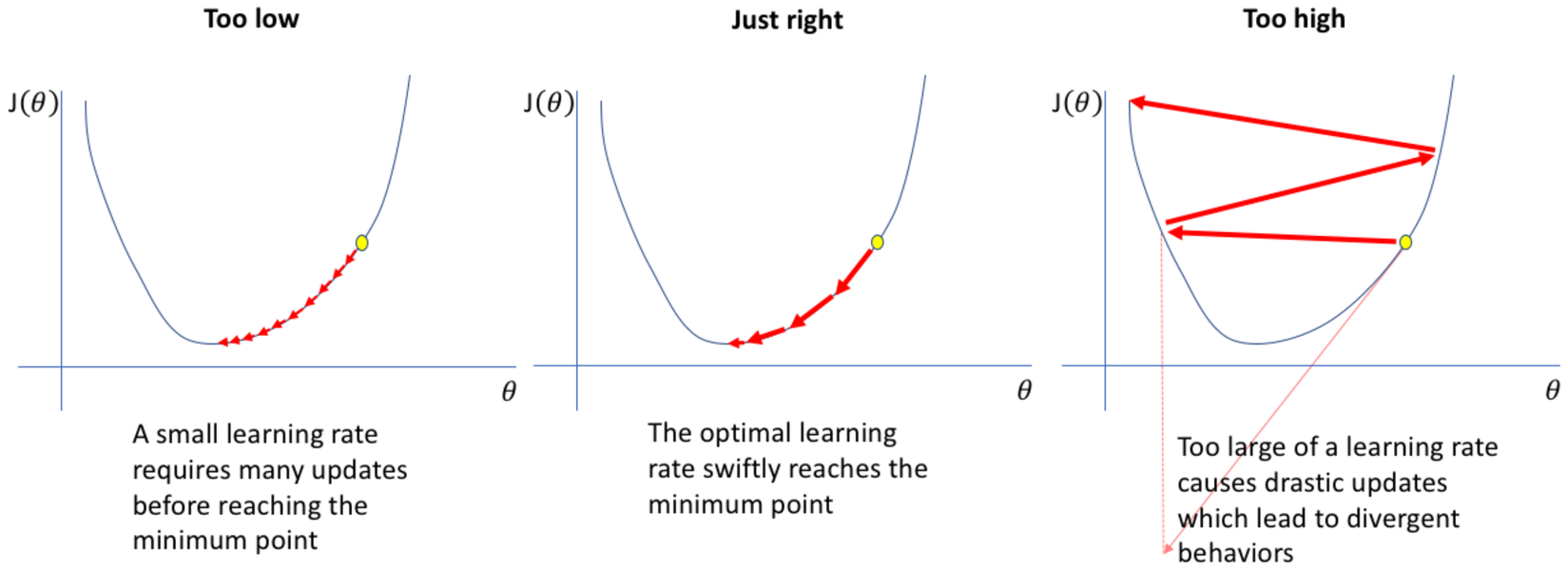
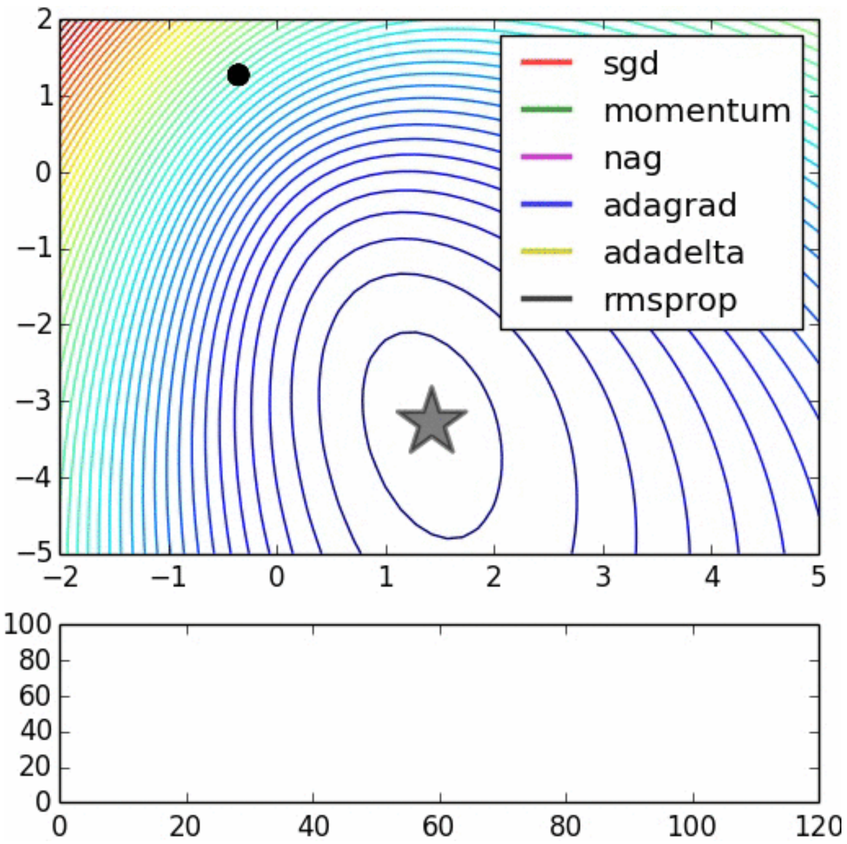
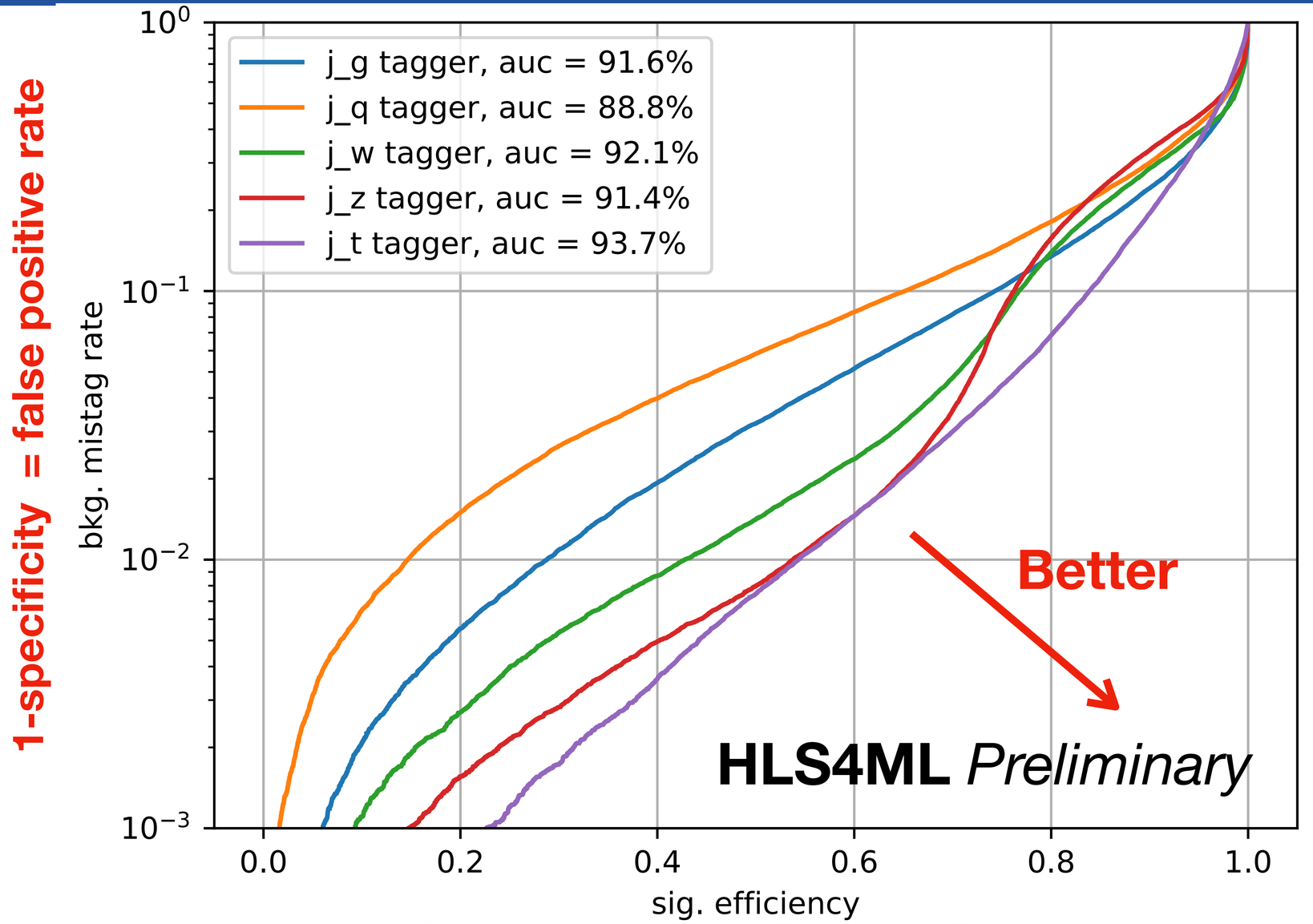




Homework

```python
from tensorflow.keras.utils import to_categorical
from sklearn.datasets import fetch_openml
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import LabelEncoder, StandardScaler
import numpy as np

seed = 0
np.random.seed(seed)
import tensorflow as tf

tf.random.set_seed(seed)
import os

data = fetch_openml('hls4ml_lhc_jets_hlf')
X, y = data['data'], data['target']

print(data['feature_names'])
print(X.shape, y.shape)
print(X[:5])
print(y[:5])
```

Homework



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Sensitivity = True Positive Rate