Introduction to Artificial Neural Networks

Computing Methods for Experimental Physics and Data Analysis

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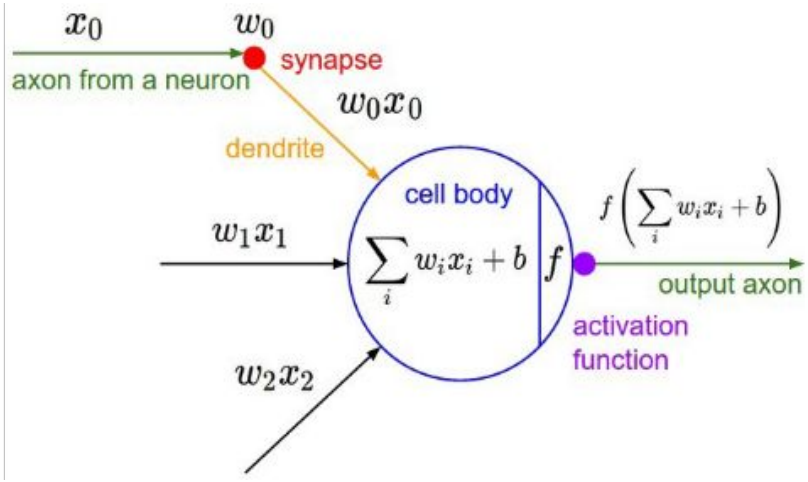
Recap of lecture 1

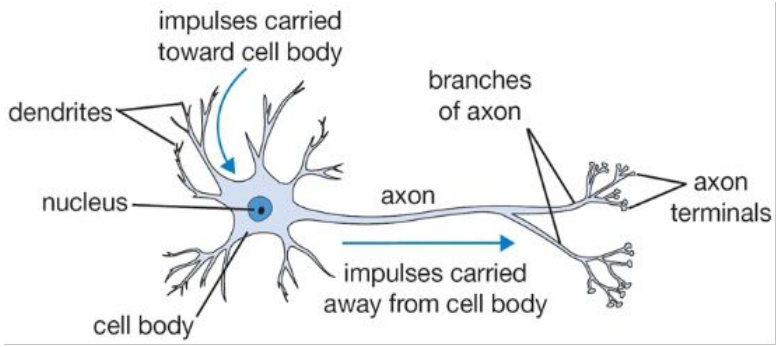
- ML techniques have common elements:
  - The function “f” to approximate
  - The model used to approximate “f” (e.g. polynomials functions)
  - The parameters of the model (e.g. the coefficients of the poly)
  - The hyper-parameters of the models (e.g. the grade of the polynomial, N=1 for linear)
  - The objective function (i.e. the loss such as MSE or binary cross entropy)
  - The variance-bias tradeoff (aka training vs generalization)
  - The regularization techniques
- Example of ML algorithms
  - Linear regression
  - PCA
  - Nearest Neighbours
  - Decision trees
    - Bagging vs boosting

Artificial Neural Networks

(Artificial) neural networks: the “Model”

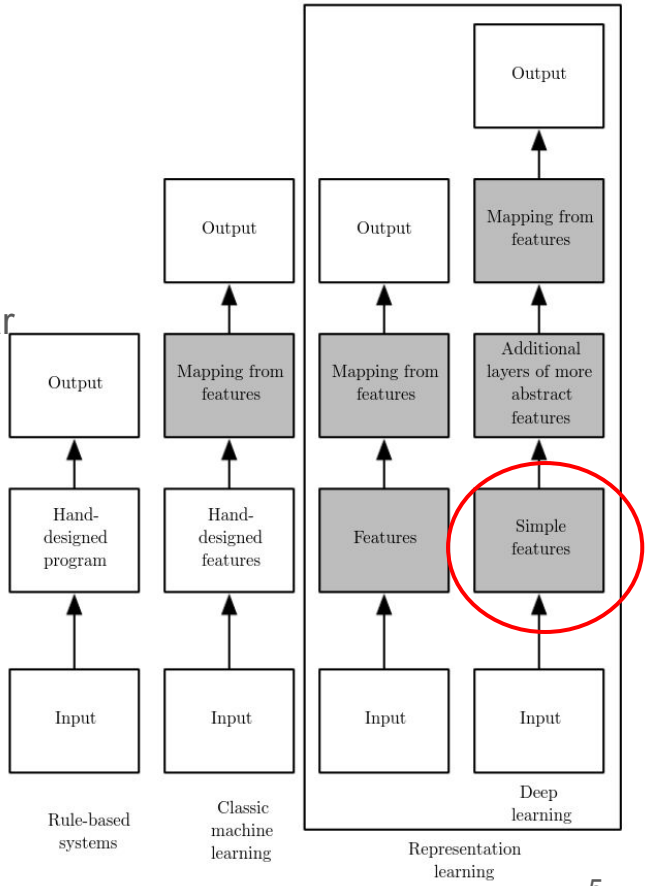
- Computation achieved with a network of elementary computing units (neurons)
- Each basic units, a neuron, has:
  - **Weighted** input connections to other neurons
  - A **non linear** activation function
  - An output value to pass to other neurons
- Biologically inspired to brain structure as a network of neuron
  - But artificial NN goal is not that of “simulating” a brain!
- Actual modern NN go much beyond the brain-inspired models





Brief history, highs and lows

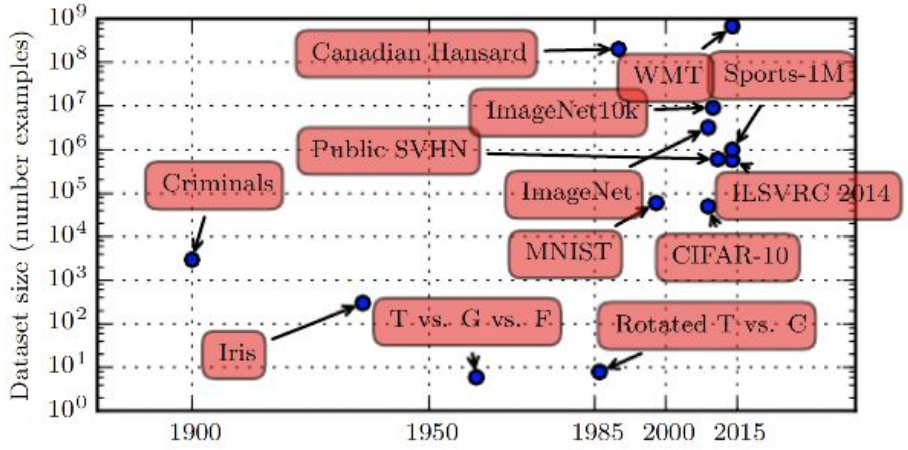
- First work originates back in ~1940-1960 “cybernetics”
  - Linear models
- Then called “connectionism” in ’80-’90
  - development of neural networks, backpropagation, non-linear activations (mostly sigmoid)
- High expectations, low achievements in the ‘90
  - A decade of stagnation
- New name, “Deep Learning”, from 2006
  - Deep architectures (see next slides)
  - Very active field in the past decade
  - Availability of GP-GPU game changing on typical “size”
  - Processing raw, low level, features
    - It doesn’t mean you **must** use “raw features” but that rather that you **can** use raw features!

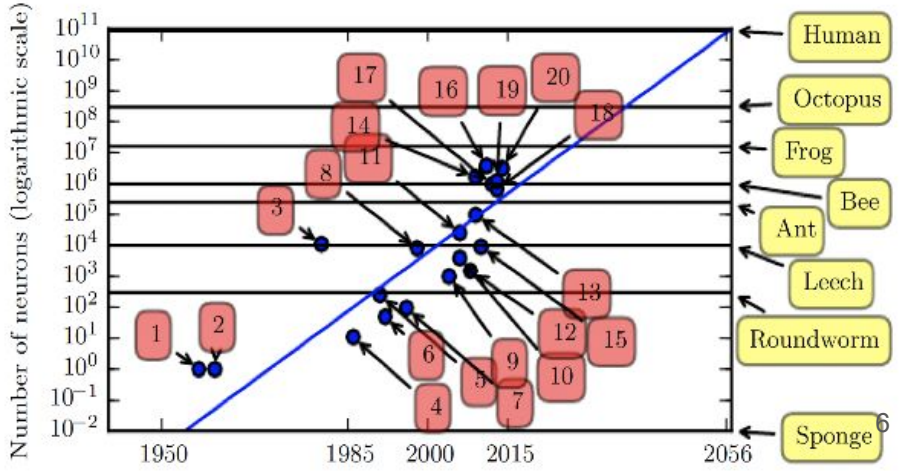


Complexity growth

- Dataset become larger and larger (“big data”)
  - Not just in “industry”, experimental scientific research is now producing multi PetaByte datasets
  - Digital era => everything can be “data”
- Increasing hardware performance

  => increasing complexity of the network (number of neurons and connections)
- 2020 largest ANN: OpenAI GPT3, 175 billion parameters (10^{11})
- 2021 “Switch transformer” and “Wu Dao 2.0” => trillion parameters models (10^{12})
- (for comparison) Human brain 10^{13} - 10^{15} synapses (~ parameters)





Performance on classic problems

- Image classification and speech recognition are the typical problems where ML (and Neural Networks) failed in the 90’
- Now it beats humans ...

Speech recognition

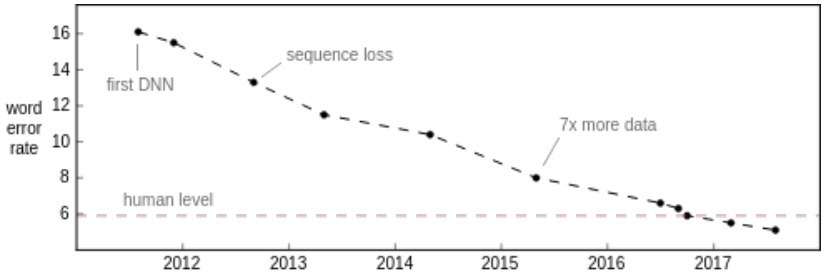
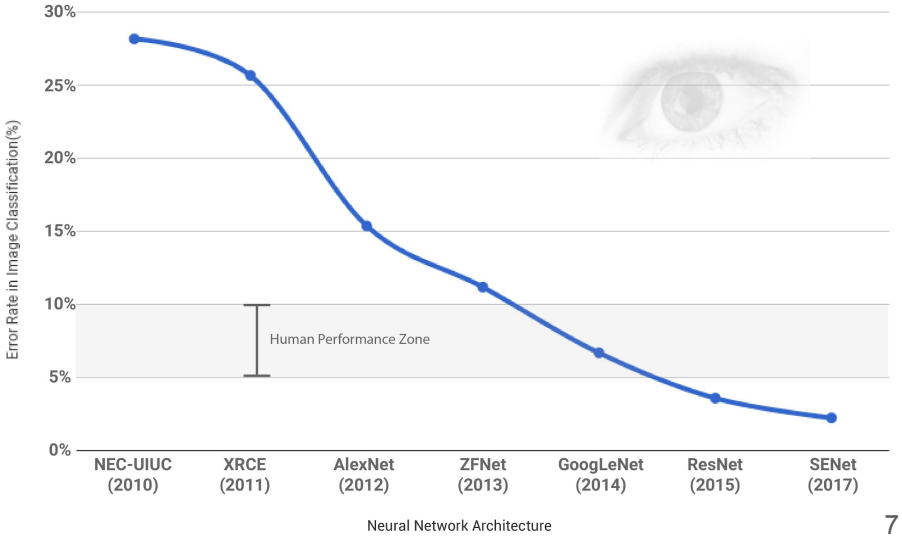
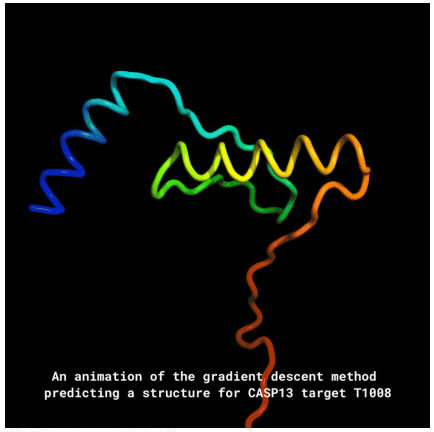


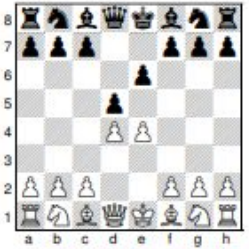
Image classification



My favorite performance examples

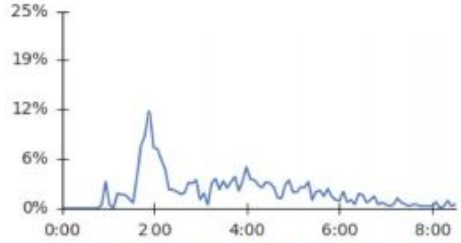
- Learning how to translate **without seeing a single translation example**, just having two independent monolingual corpora (https://arxiv.org/abs/1711.00043)
- Alpha-Fold: contest to predict protein folding, alphafold ranked first with 25 correct predictions out of 43 tests. The second ranked reached 3 out of 43.
  - 2021: Alpha-Fold2 !!
- AlphaGo => AlphaZero: AlphaGo beat humans at “Go”, learning from human matches and know-how. Then AlphaZero learned from scratch. AlphaZero beats AlphaGo 100-0
- AlphaZero learned chess too, and beat the best existing chess program
- AI recently proved math theorems, 1200 of them
- Microsoft and Alibaba AIs beated humans in text understanding test (SQuAD)
- DeepFake: never ever believe what you see on a screen, even in videos
- Image super-resolution arxiv:2104.07636



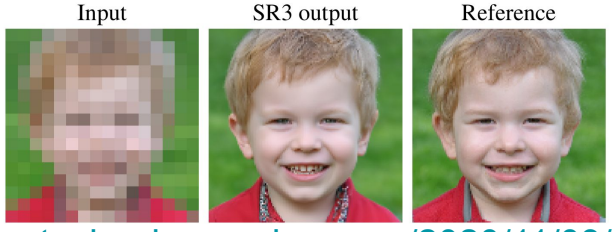


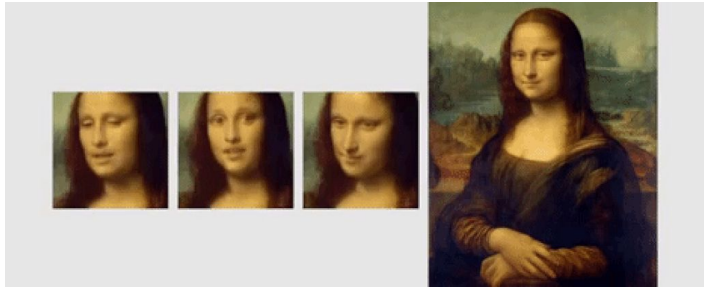
C00: French Defence

w 39/11/0, b 4/46/0



3.♘c3 ♘f6 e5 ♘d7 f4 c5 ♘f3 ♗e7





https://www.technologyreview.com/2020/11/03/1011616/ai-godfather-geoffrey-hinton-deep-learning-will-do-everything/

OpenAI GPT3

Generative Pre-trained Transformer

A 12M$ autocomplete (that is not really understanding what is talking about, but can still write better than most of us)

https://openai.com/blog/openai-api/

Solve for X:
X+40000=100000

X=50000

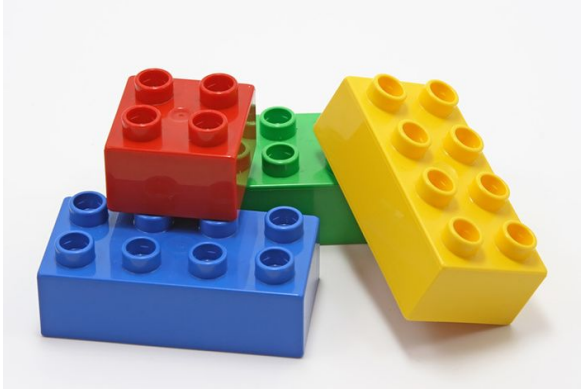
https://doi.org/10.1007/s11023-020-09548-1

Tanto gentile e tanto onesta pare
la donna mia, quand'ella altrui saluta,
ch'ogne lingua devèn, tremando, muta,
e li occhi no l'ardiscon di guardare.

Ella par che sia una cosa santa,
e in lei veder si può quanto bontà
di femmina è capace, e tanto valore
che già mai non fu da più bellezza.

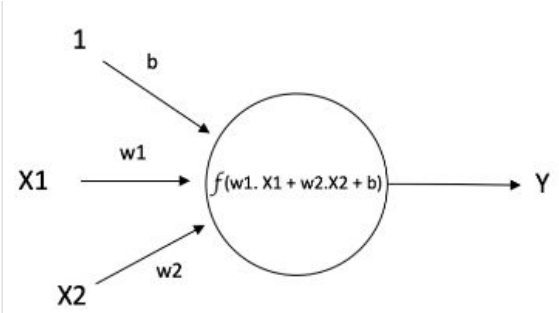
Ond'io per me la vo' sempre adorando,
et se mai la mente mia fosse offesa,
spero di far perdonando; et questo è quello
che fa ch'io son sì del tutto suo servitore.

Neural Nets Basic elements

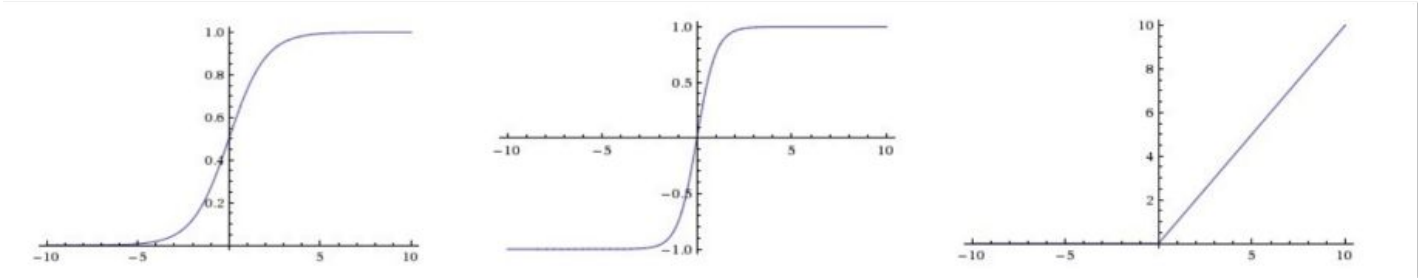


A neural network node: the artificial neuron

- The elementary processing unit, a neuron, can be seen as a node in a directed graph
- Inputs are **summed**, with **weights**, and an **activation function** is evaluated on such sum
- Nodes are typically also connected (with weight **b**) to an input “bias node” that has a fixed output value of 1
- Different activation functions can be used, common ones are: sigmoid, atan, relu (rectified linear unit)

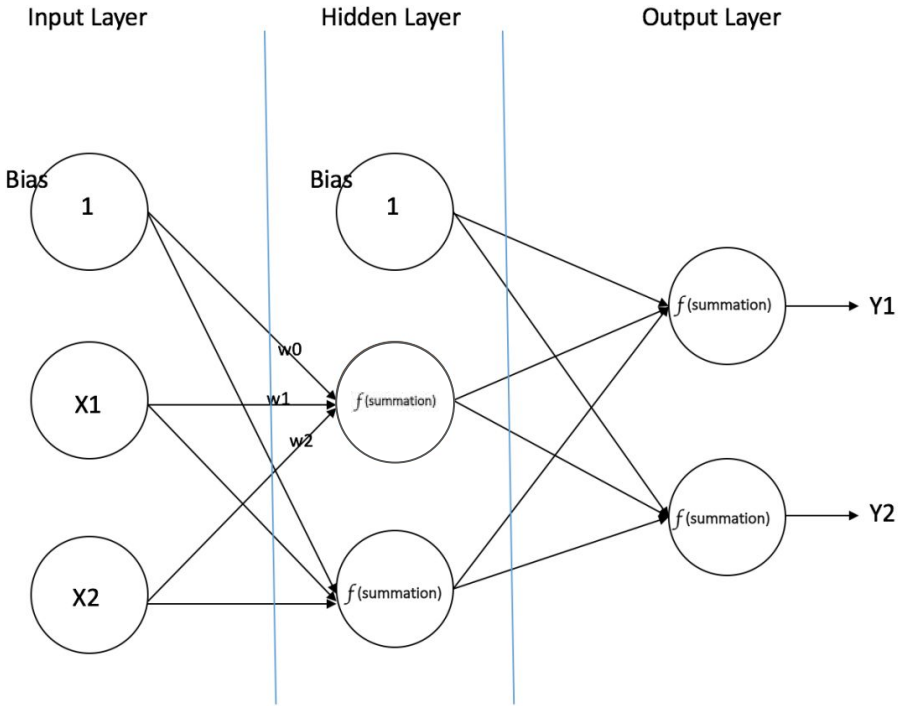


$$Y = f(w1.\,X1 + w2.X2 + b)$$



The MLP model

- The most common NN in the ‘90 was the Multi Layer Perceptron (MLP)
- Graph structure organized in “layers”
  - Input layer (nodes filled with input value)
  - Hidden layer
  - Output layer (node(s) where output is read out)
- Nodes are connected **only from one layer to the next** and **all possible connections** are present (known as “dense” or “fully connected” layer)
  - No intra-layer connections
  - No direct connections from input to output
- Size of input and output layers are fixed by the problem
- **Hyperparameters** are
  - The size of the hidden layers
  - The type of activation function
- The **parameters** to learn are the weights of the connections



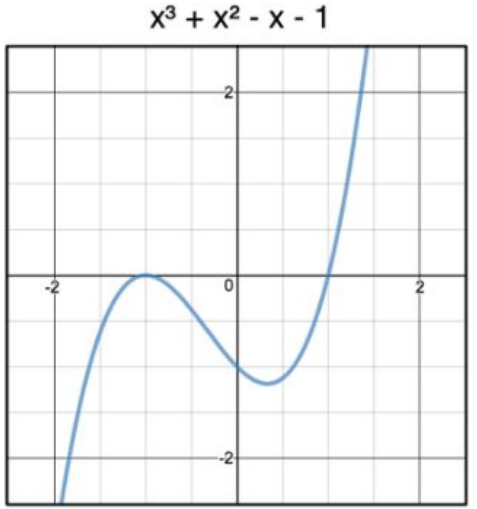
Universal approximation theorem

“One hidden layer is enough to *represent* (not *learn*) an approximation of any function to an arbitrary degree of accuracy” (I. Goodfellow et al. 2016)

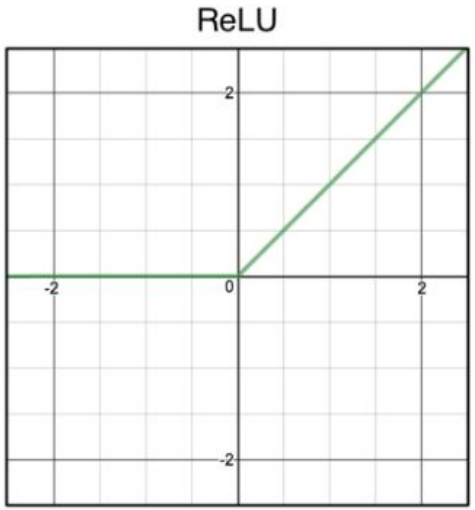
- You can approximate any function with arbitrary precision having **enough hidden nodes** and **the right weights**
- How do you get the right weights? You need a “training” for your network
  - The theorem does not say that one hidden layer (+ some training algorithm) is enough to find the optimal weights, just that they exists!
- Achieving some (even modest with some metric) level of accuracy may need an unmanageable hidden layer size
  - And may need an unreasonable number of “examples” to learn from

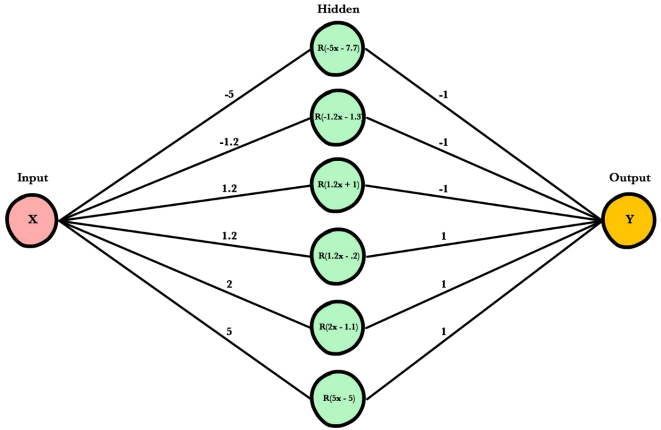
Example (1-D input)

Approximate this function



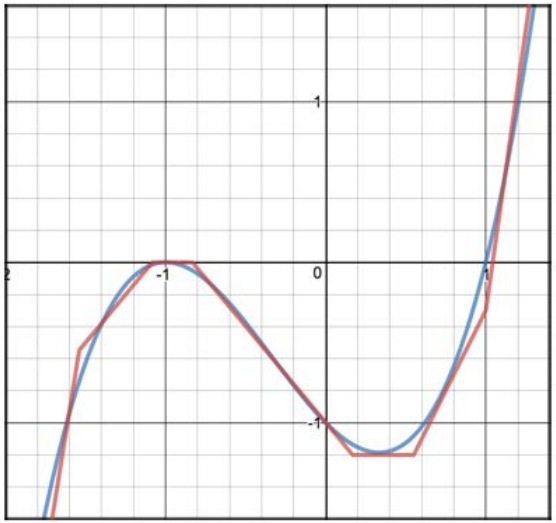
With a weighted sum of functions like this one





Example

- The Universal Approximation Theorem says that increasing #nodes I can increase the accuracy as much as I want
- More hidden nodes, higher “capacity” => more accuracy



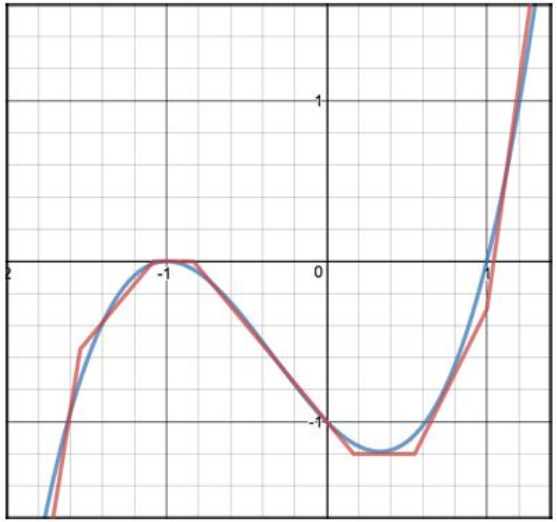
$$n_1(x) = Relu(-5x - 7.7)$$
$$n_2(x) = Relu(-1.2x - 1.3)$$
$$n_3(x) = Relu(1.2x + 1)$$
$$n_4(x) = Relu(1.2x - .2)$$
$$n_5(x) = Relu(2x - 1.1)$$
$$n_6(x) = Relu(5x - 5)$$

$$Z(x) = -n_1(x) - n_2(x) - n_3(x) + n_4(x) + n_5(x) + n_6(x)$$

https://towardsdatascience.com/can-neural-networks-really-learn-any-function-65e106617fc6

Training of an MLP

- How do I get the weights?
- Remember: we do not know the function we want to approximate, we only have some “samples”



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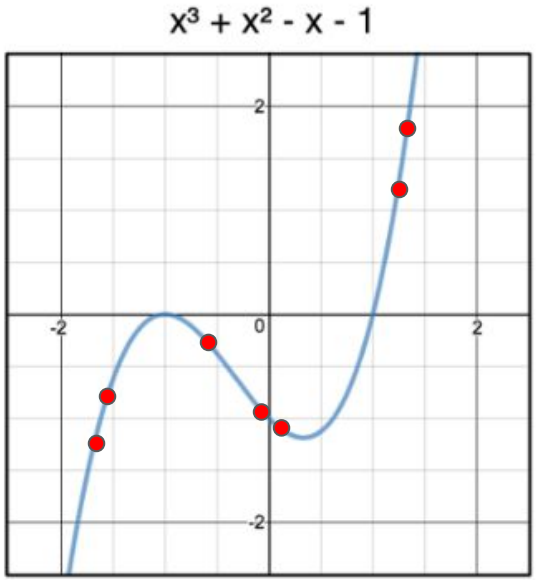
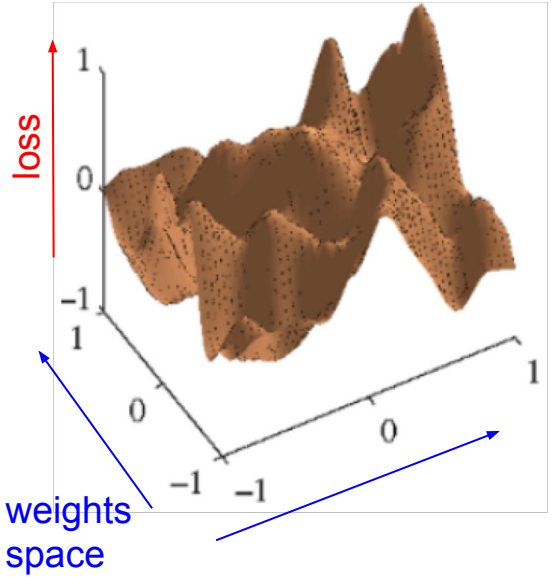


Training a NN

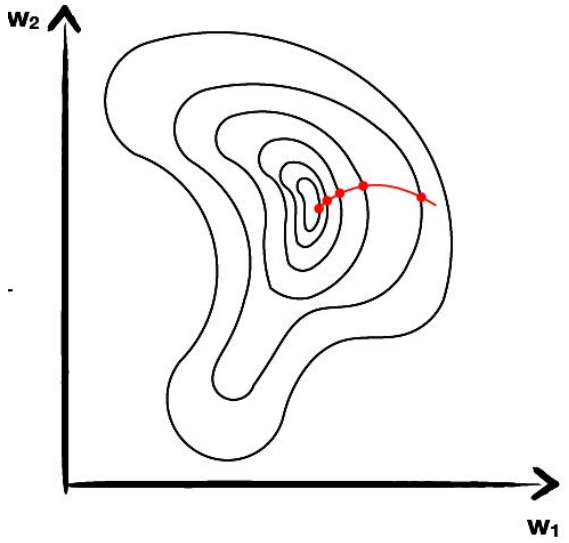


- The goal of training is to minimize the objective function (possibly both on the training and validation sample)
  - I.e. we want to minimize the loss as a function of the model parameters (i.e. the weights)
- For a MLP the basic idea is the following
  a. Start with random weights
  b. Compute the prediction y_pred for a given input ***x*** and compare target *y_true* computing the loss (repeat for a few example, aka “one batch”)
  c. Estimate an update for the weights that **reduces the loss**
  d. Iterate from point (b), repeating for all samples
  e. When the sample has been used completely (end of an epoch), iterate from (b) again on all samples
  f. Repeat for multiple epochs
- The important point is how to implement point (c) => (stochastic) gradient descent

How to find a minimum?

Gradient Descent

- We know the loss function value in a point in the weights phase space (e.g. the initial set of random weights, or the iteration N-1), computed numerically as the mean or the sum of the losses for each of our training examples
- We can compute the gradient of the loss function in that point, we expect the minimum on “the way down” hence we adjust our set of weights doing a “step” in the direction pointed by the gradient with a step size that is proportional to the length of the gradient

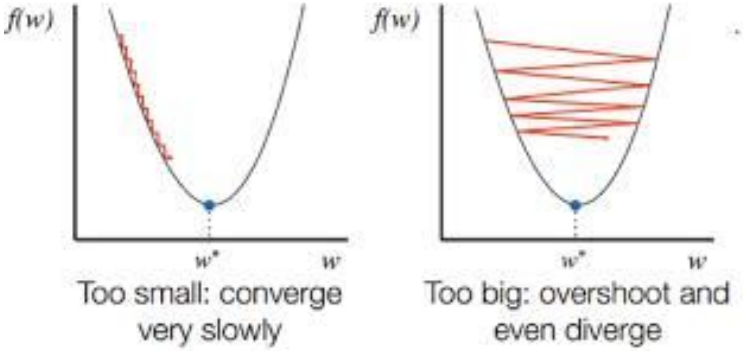


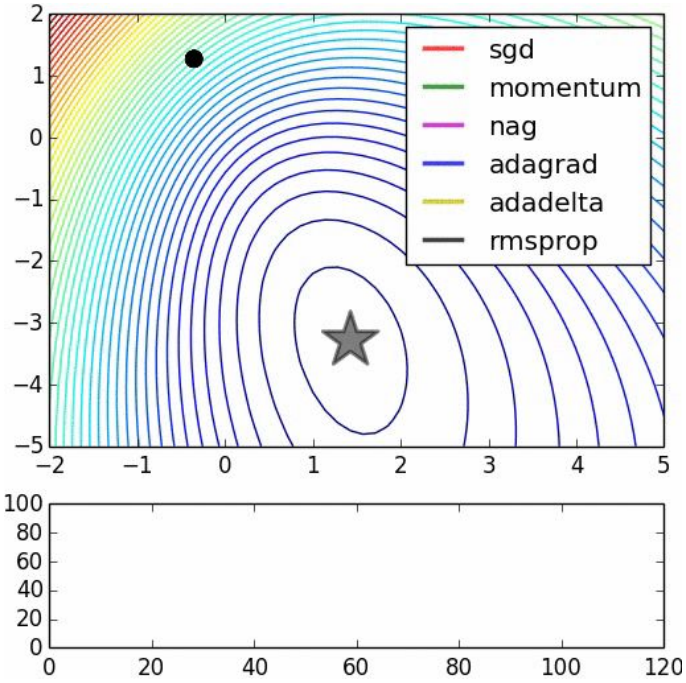
Stochastic Gradient Descent (SGD):

- Compute the gradient on “**batches**” of events rather than full sample
- The “noise” may help avoiding local minima

Not as simple as you would imagine

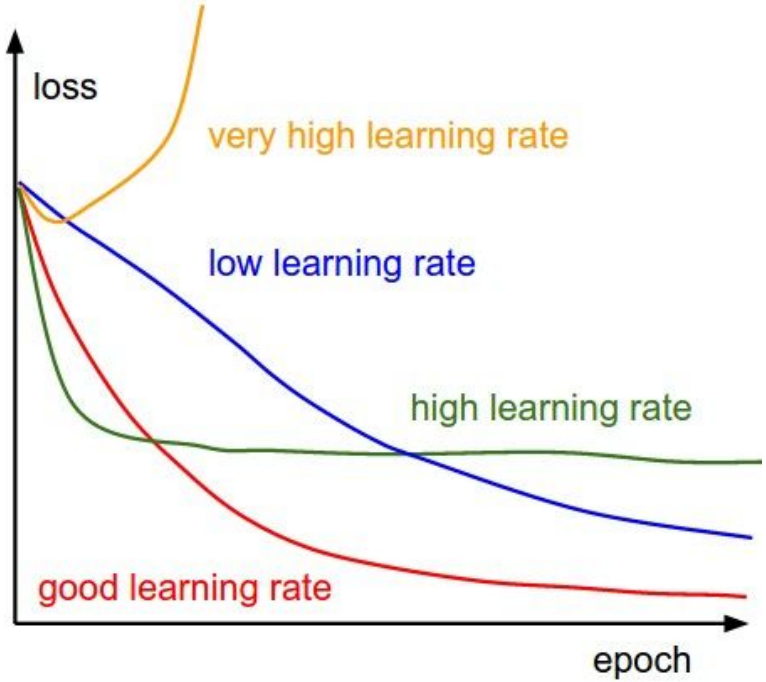
- A parameter named **learning rate** controls how big the step in the direction of the gradient is
  - A too large step may let you bounce back and forth on the walls of your “valley”
  - A too small step would make your descent lasting forever
- Several variants of SGD
  - Include “momentum” from previous gradient calculations (may help overcome local obstacles)
  - Reduce step size over time
  - Adadelta, Adagrad, Adam, and many more



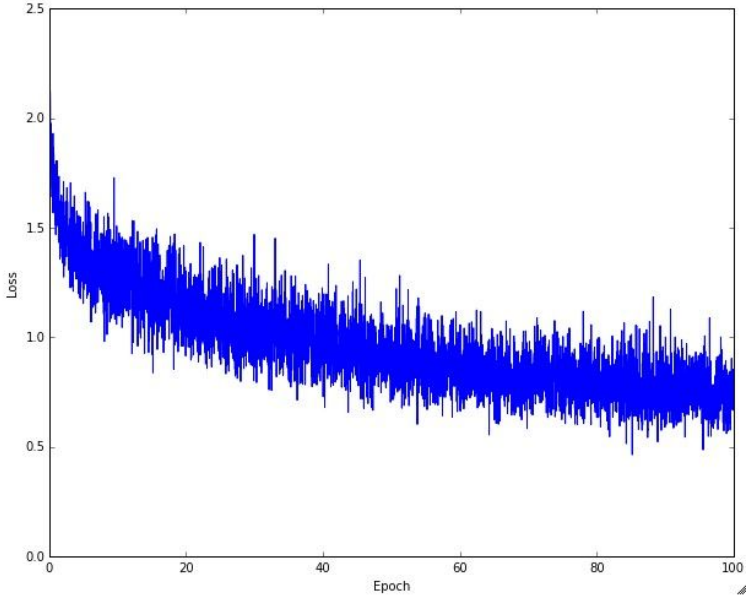


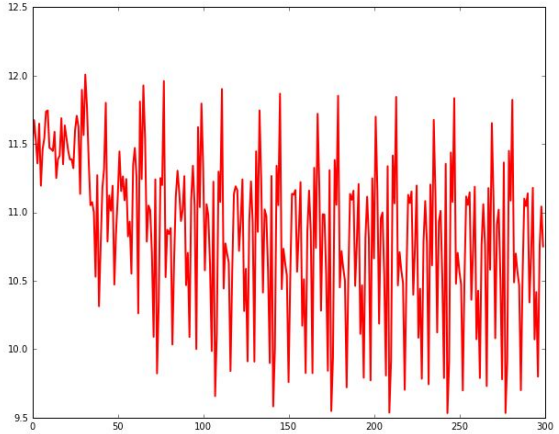
Learning rate, epochs and batches

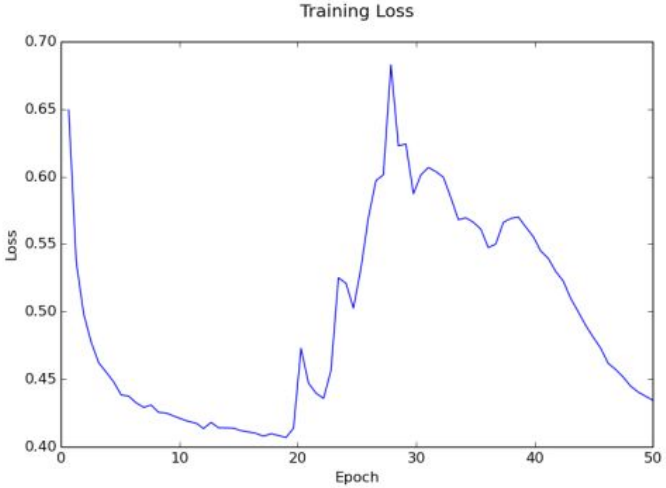
- The gradient update (in SGD) is repeated for each “batch” of events
- A full pass of the whole dataset (i.e. all batches) is called an **epoch**
- A typical training foresee iteration on multiple epochs
- The size of the update step can be controlled with a multiplicative factor called “**learning rate**”
    - Learning rate can be adapted over time



In reality

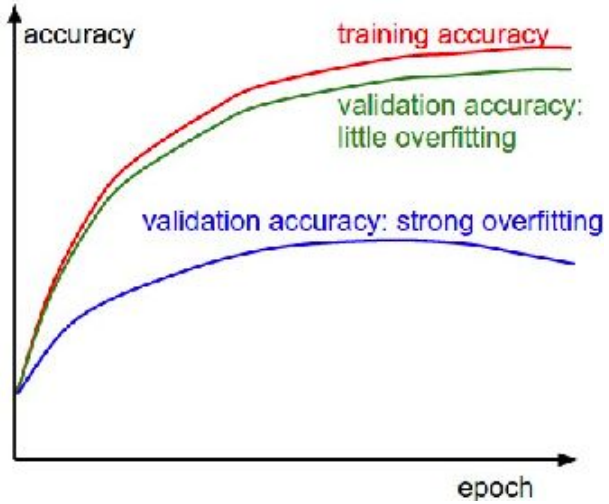

Loss
Epoch
0.0
0.5
1.0
1.5
2.0
2.5
0
20
40
60
80
100


9.5
10.0
10.5
11.0
11.5
12.0
12.5
0
50
100
150
200
250
300


Training Loss
Loss
Epoch
0.40
0.45
0.50
0.55
0.60
0.65
0.70
0
10
20
30
40
50

Training and overfitting

- As discussed previously if the capacity is large enough the network could “overfit” on the training dataset
- Have a separate, stat independent, validation/generalization sample
- Evaluate performance (with “loss” or with other metrics) on the validation sample
- Training results depends on many choices
  - Size of batches (amount of “noise”)
  - Learning rate (how much you move along the gradient at each iteration)
  - Gradient Descent algorithm
  - Capacity of the network



Neural Networks, computers and mathematics

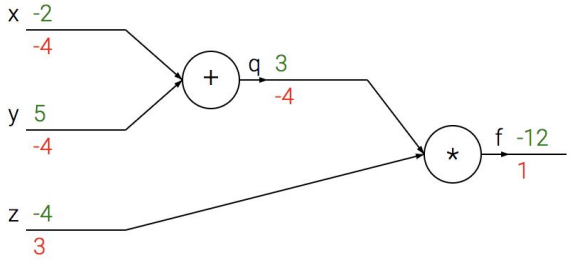
- ANN use a fairly limited and simple set of operations
  - Many operation are simply represented with linear algebra
  - Non linear function are typically applied, repeated, to multiple inputs (hence can be “vectorized”)
  - Gradient Descent works by knowing the derivatives of the functions involved in the NN calculations (weights, activations) and in the loss
- Datasets are represented as multidimensional tensors
  - The number of indices and the length per index is usually called “shape” and is a tuple with dimension of each index
  - The first index is the one running the “number of sample in the dataset”, and is sometimes omitted when describing a neural network
- Classification with multiple category is often converted in the “categorical” representation
  - I.e. rather than labelling with a scalar “y” (with 0=horse, 1=dog, 2=cat, 3=bird, …) a vector **y** is used with as many components as the category (with [1,0,0,0]=horse, [0,1,0,0]=dog, etc..)
- Tools exist to describe mathematically the network structure that are optimized for fast computations on CPU/GPU/TPU

Back-propagation

Calculating the gradient in complex networks could be computationally expensive:

- Some expression appear repeated, hence we should avoid recomputing them
- Back-propagation method allow to efficiently compute the derivatives wrt each of the weights
  - Start from the last node and apply derivative chain rule going backward
  - At each step the computation depends only on the already computed derivative and the values of the node outputs (computed already in the NN evaluation, aka forward pass)

$$f(x, y, z) = (x + y)z$$



$$q = x + y \qquad f = qz$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x} \qquad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1 \qquad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$

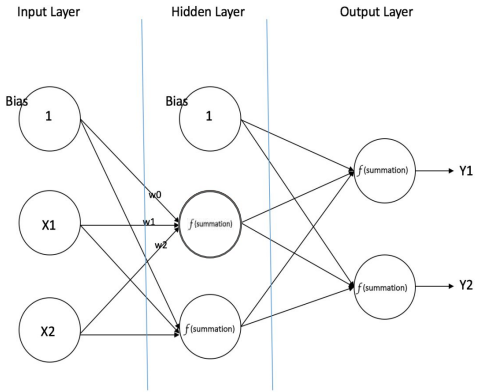
Deep networks

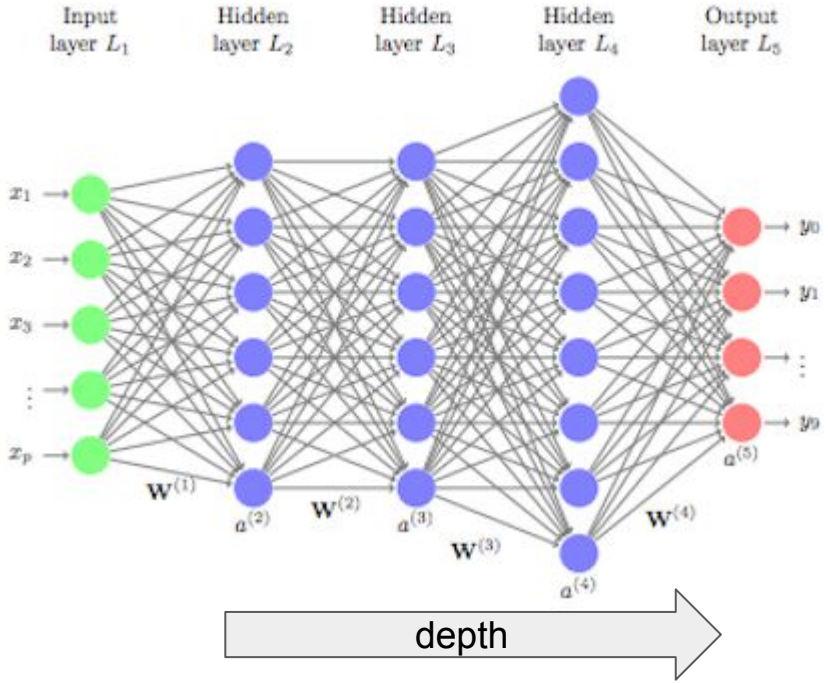
Deep Feed Forward networks

The simplest extension to the MLP is to just add more hidden layers

Other names of this network architecture

- Deep Feed Forward network
- Deep Dense network, i.e. made (only) of **Dense**(ly) connected layers





Why going deeper?

Hold on… wasn’t there a theorem saying that MLP is good enough ? Yes but…

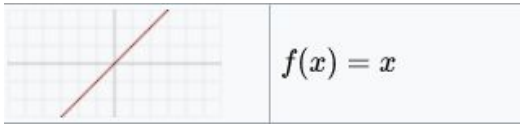
- Amount of nodes to represent complex functions can be too high
- Learning the weights on finite samples could be too difficult

Advantages of Deep architectures

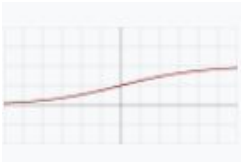
- Hierarchical structure can allow easier “abstraction” by the network with early layers computing low level features and deeper layers representing more abstract properties
- Number of neurons and connections needed to represent the same function highly reduced in many realistic cases

Activation functions

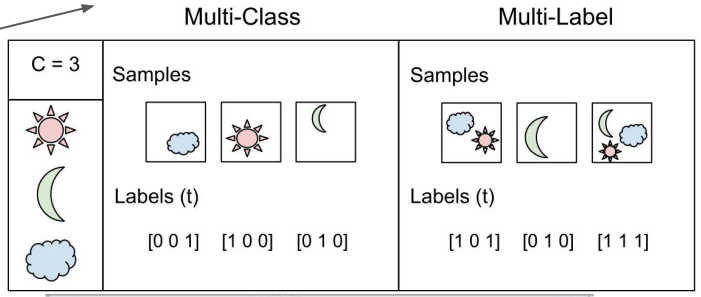
- Linear:
  - Cannot be used in hidden layer has the derivative is constant (does not depend on the inputs, cannot perform gradient descent)
  - Useful for output nodes in **regression** problems
- Sigmoid:
  - Used in the past in the hidden layer (leads to vanishing gradient problem)
  - Useful in **classification** problem with a single output or **multi-label** classifiers
- Softmax:
  - Useful in **classification** problems with one-hot encoded **multi-class**
- Rectified Linear Unit (ReLU)
  - The workhorse for hidden layers activations
  - Variants: Leaky-ReLU, Swish



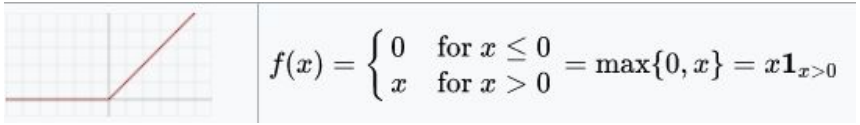
$$f(x) = x$$



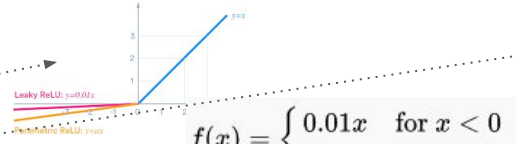
$$f(x) = \sigma(x) = \frac{1}{1+e^{-x}}$$ [1]



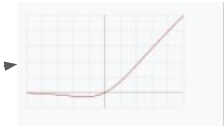
$$f_i(\vec{x}) = \frac{e^{x_i}}{\sum_{j=1}^{J} e^{x_j}} \quad \text{for } i = 1, \ldots, J$$



$$f(x) = \begin{cases} 0 & \text{for } x \leq 0 \\ x & \text{for } x > 0 \end{cases} = \max\{0, x\} = x\mathbf{1}_{x>0}$$

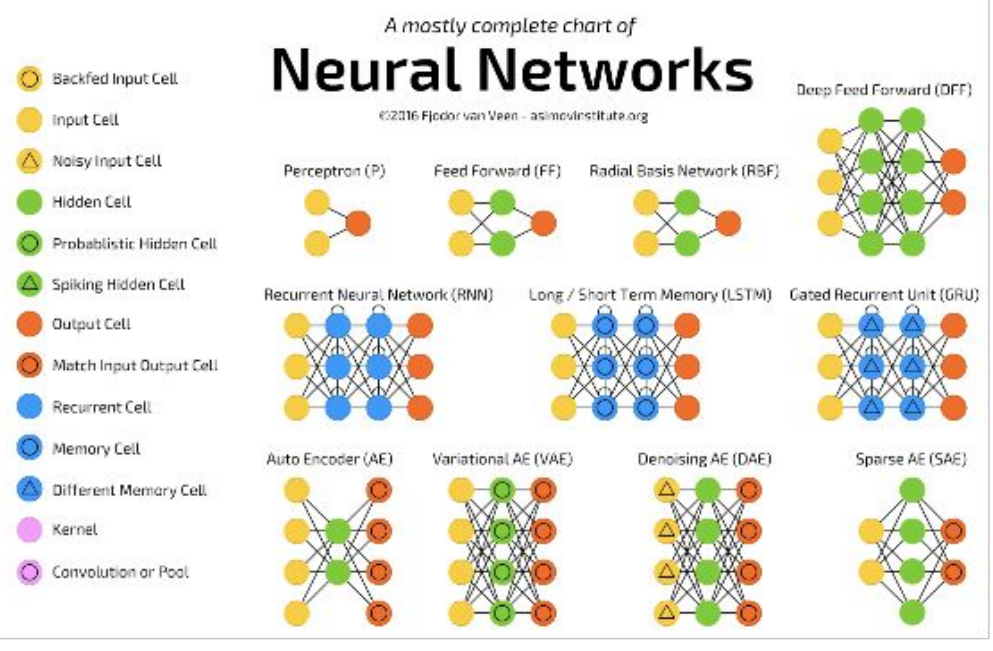


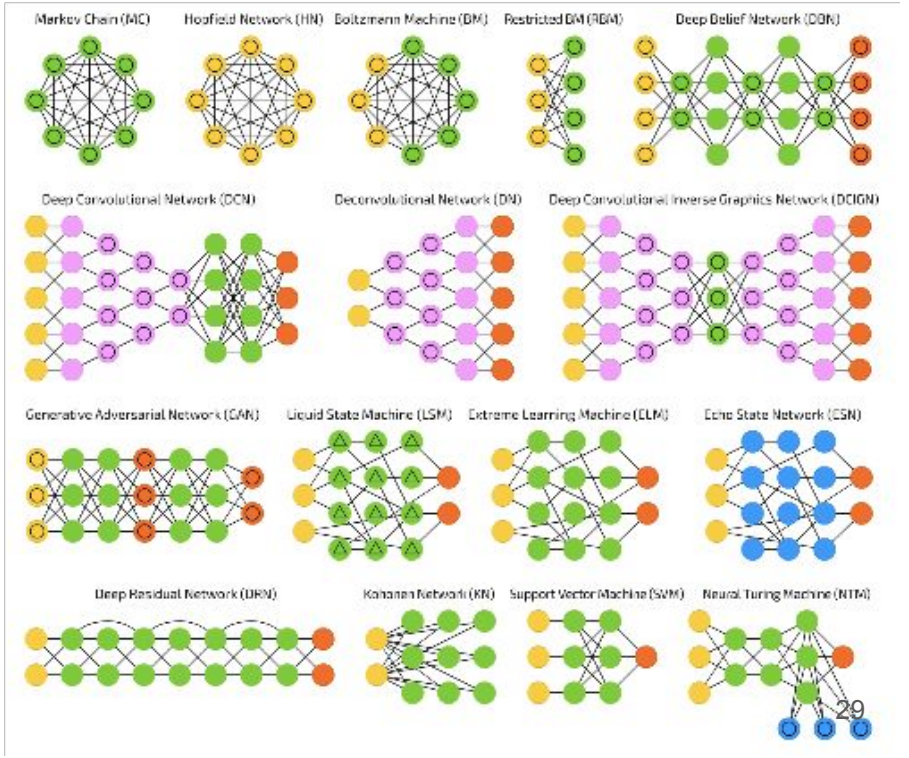
$$f(x) = \begin{cases} 0.01x & \text{for } x < 0 \\ x & \text{for } x \geq 0 \end{cases}$$



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

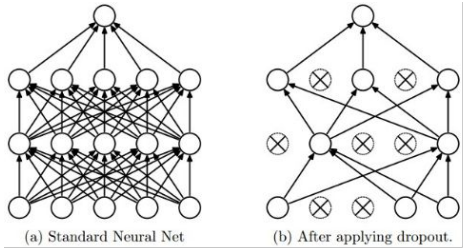
Deep architectures

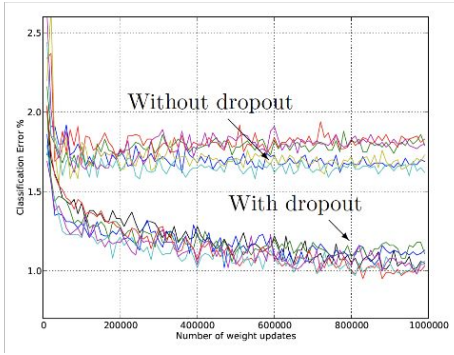




Dropout and regularization methods

- NN training is a numerical process
- Often the number of samples is limited hence the gradient accuracy is not great
- Several regularization methods exists to avoid being dominated by stochastic effects
  - Caps to the weights (so that individual nodes cannot be worth more than some amount)
  - **Dropout** techniques: during the training a fraction of nodes is discarded, randomly, at each iteration
    - NN more robust to noise
    - Effectively “augmenting” the input dataset

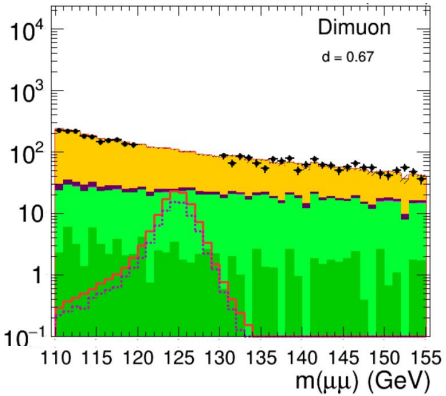


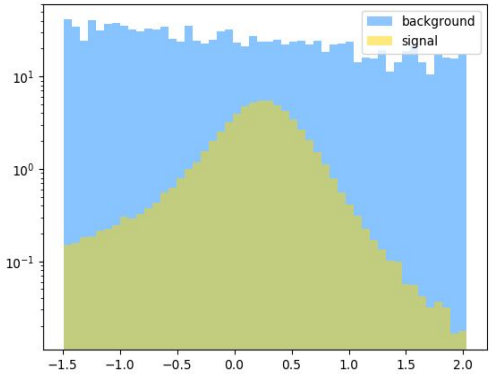


(Batch) normalization

- Input features have typically different ranges, means, variance
- It is generally useful to “normalize” the input distribution
  - Mean zero
  - Variance 1
- Often it could be practical to compute the normalization on individual batches rather than full sample
  - Batch vs full sample ? may depend on your use case

A typical observable, e.g. the invariant mass of a pairs of leptons



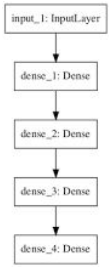


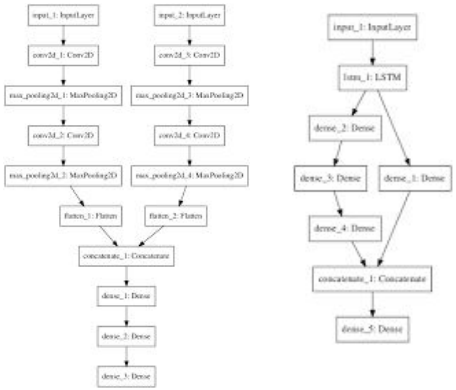
Normalized version

DNN Tools

Keras

- Keras is a python library that allow to build, train and evaluate NN with many modern technologies
- Keras supports multiple backends for actual calculations
- Two different syntax are usable to build the network architecture
  - Sequential: simple linear “stack” of layers
  - Model (functional API): create more complex topologies
- Multiple type of “Layers” are supported
  - Dense: the classic fully connected layer of a FF network
  - Convolutional layers
  - Recurrent layers
- Multiple type of activation functions
- Various optimizers and gradient descent techniques





Other common tools

Common alternative to keras

- Pytorch (trending up!)
- Sonnet
- Direct usage of TensorFlow (or other backends, e.g. Theano)
  - Need to write yourself some of the basics of NN training
  - Especially useful to develop new ideas (e.g. a new descent technique, a new type of basic unit/layer)

Keras Sequential example

```
# first neural network with keras tutorial
from numpy import loadtxt
from keras.models import Sequential
from keras.layers import Dense
# load the dataset
dataset = loadtxt('pima-indians-diabetes.csv', delimiter=',')
# split into input (X) and output (y) variables
X = dataset[:,0:8]
y = dataset[:,8]
# define the keras model
model = Sequential()
model.add(Dense(12, input_dim=8, activation='relu'))
model.add(Dense(8, activation='relu'))
model.add(Dense(1, activation='sigmoid'))
# compile the keras model
model.compile(loss='binary_crossentropy', optimizer='adam', metrics=['accuracy'])
# fit the keras model on the dataset
model.fit(X, y, epochs=150, batch_size=10)
# evaluate the keras model
_, accuracy = model.evaluate(X, y)
print('Accuracy: %.2f' % (accuracy*100))
```

Keras “Model” Functional API

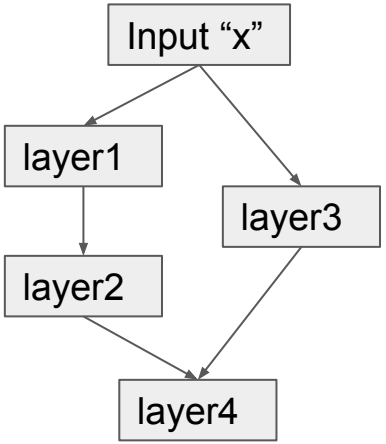
A NN can be seen as the composition of multiple functions (one per layer), e.g.

- A simple stack of layers is: $y=f_5(f_4(f_3(f_2(f_1(\boldsymbol{x})))))$
- A more complex structure could be something like

$$y=f_4(\ f_2(f_1(\boldsymbol{x})),f_3\ (\boldsymbol{x})\ )$$

- The functional API allow to express the idea that each layer is evaluate on the output of a previous layer, i.e.

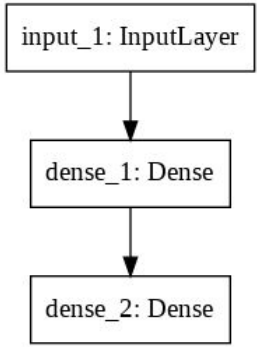
```
x = Input()
layer1=FirstLayerType(parameters) (x)
layer2=SecondLayerType(parameters) (layer1)
layer3=ThirdLayerType(parameters) (x)
layer4=FourthLayerType(parameters)([layer2,layer3])
```

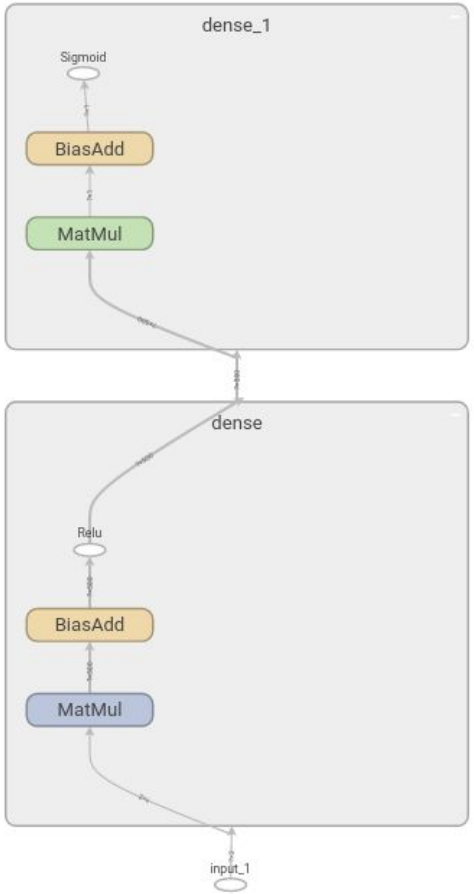


A (modernized) MLP in keras

```
from keras.models import Model
from keras.layers import Input, Dense
x = Input(shape=(32,))
hid = Dense(32, activation="relu")(x)
out = Dense(1, activation="sigmoid")(hid)
model = Model(inputs=x, outputs=out)


model.summary()
from keras.utils import plot_model
plot_model(model, to_file='model.png')
```



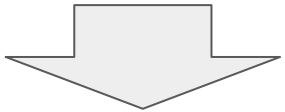



```
Model: "model_1"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
input_1 (InputLayer)         (None, 32)                0
_________________________________________________________________
dense_1 (Dense)              (None, 32)                1056
_________________________________________________________________
dense_2 (Dense)              (None, 1)                 33
=================================================================
Total params: 1,089
Trainable params: 1,089
Non-trainable params: 0
_________________________________________________________________
```

From the ~1995 to ~2010

```
from keras.models import Model
from keras.layers import Input, Dense

x = Input(shape=(32,))
hid = Dense(32, activation="sigmoid")(x)
out = Dense(1, activation="sigmoid")(hid)
model = Model(inputs=x, outputs=out)
```



```
from keras.models import Model
from keras.layers import Input, Dense

x = Input(shape=(32,))
b = Dense(32,activation="relu")(a)
c = Dense(32,activation="relu")(b)
d = Dense(32,activation="relu")(c)
e = Dense(32,,activation="sigmoid")(d)
model = Model(inputs=x, outputs=e)
```

Training a model with Keras

```
from keras.layers import Input, Dense
from keras.models import Model

# This returns a tensor
inputs = Input(shape=(784,))

# a layer instance is callable on a tensor, and returns a tensor
x = Dense(64, activation='relu')(inputs)
x = Dense(64, activation='relu')(x)
predictions = Dense(10, activation='softmax')(x)

# This creates a model that includes
# the Input layer and three Dense layers
model = Model(inputs=inputs, outputs=predictions)
model.compile(optimizer='rmsprop',
              loss='categorical_crossentropy',
              metrics=['accuracy'])
model.fit(data, labels)  # starts training
```

Those are numpy arrays with your data

Keras layers

Keras basic layers

- Basic layers
  - Inputs
  - Dense
  - Activation
  - Dropout
- Convolutional layers (for next week)
  - Conv1D/2D/3D
  - ConvTranspose or “Deconvolution”
  - UpSampling and ZeroPadding
  - MaxPooling, AveragePooling
  - Flatten
- More stuff
  - Recursive layers
  - ...check the keras docs...

Callbacks

- During training some “callbacks” can be passed to the fit function
  - E.g. to monitor the progress of the training
  - To adapt the training
    - Stop if no improvements in the last N epochs
    - Change learning rate (reduce) if no improvements in the last M epochs
  - Some callbacks are predefined in keras, other can be user implemented

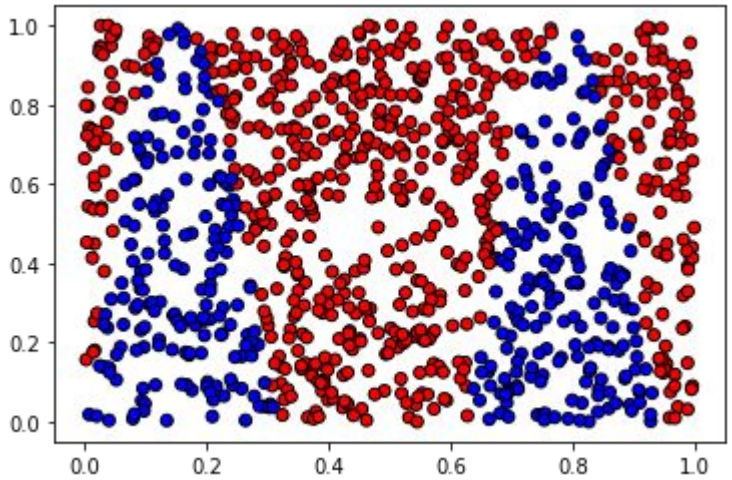
```
from keras.callbacks import EarlyStopping, ReduceLROnPlateau
# train
history = model.fit(X_train, y_train, epochs=n_epochs, batch_size=batch_size, verbose = 2,
                validation_data=(X_test, y_test),
                callbacks = [
                EarlyStopping(monitor='val_loss', patience=10, verbose=1),
                ReduceLROnPlateau(monitor='val_loss', factor=0.1, patience=2, verbose=1)
                ])
```

Assignment 1

- Partition a 2D region with a simple function that returns true vs false having x1,x2 as arguments
  - E.g. x1>x2 or x1*2>x2 or x1 > 1/x2 or … whatever...
- Generate 1000 samples
- Create a classifier with a MLP or a DNN with similar number of parameters that approximate the function above

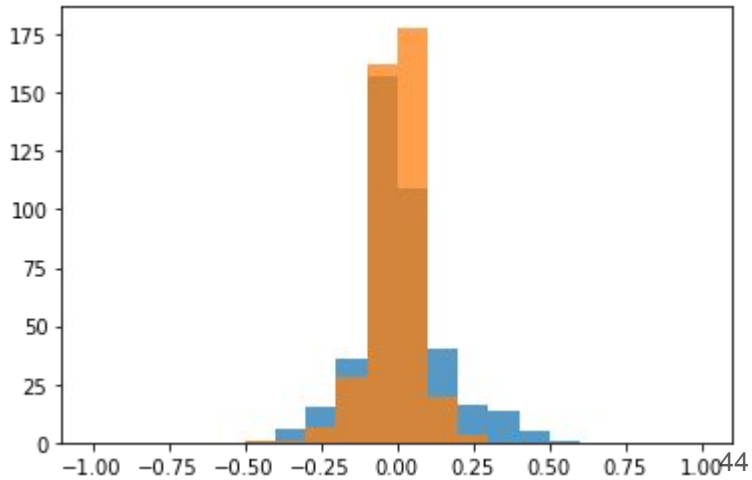
Start from this notebook:
Exercise 1

Solution



Assignment 2

- Let's try to implement a **regression** with DNN in keras
- Invent a function of x1,x2,x3,x4,x5
- Generate some data
- Create a Feed Forward model (with 1 or more hidden layers)
- What should we change compared to the classification problem?
  - What is the loss function to use?
  - Which activation function in last layer?
- Try to make a histogram of the residuals on the validation sample
  - residuals=(y_predicted - y_truth)



Start from this notebook: Exercise 2

Solution