Big data science Day 3

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https://github.com/leggerf/MLCourse-2022

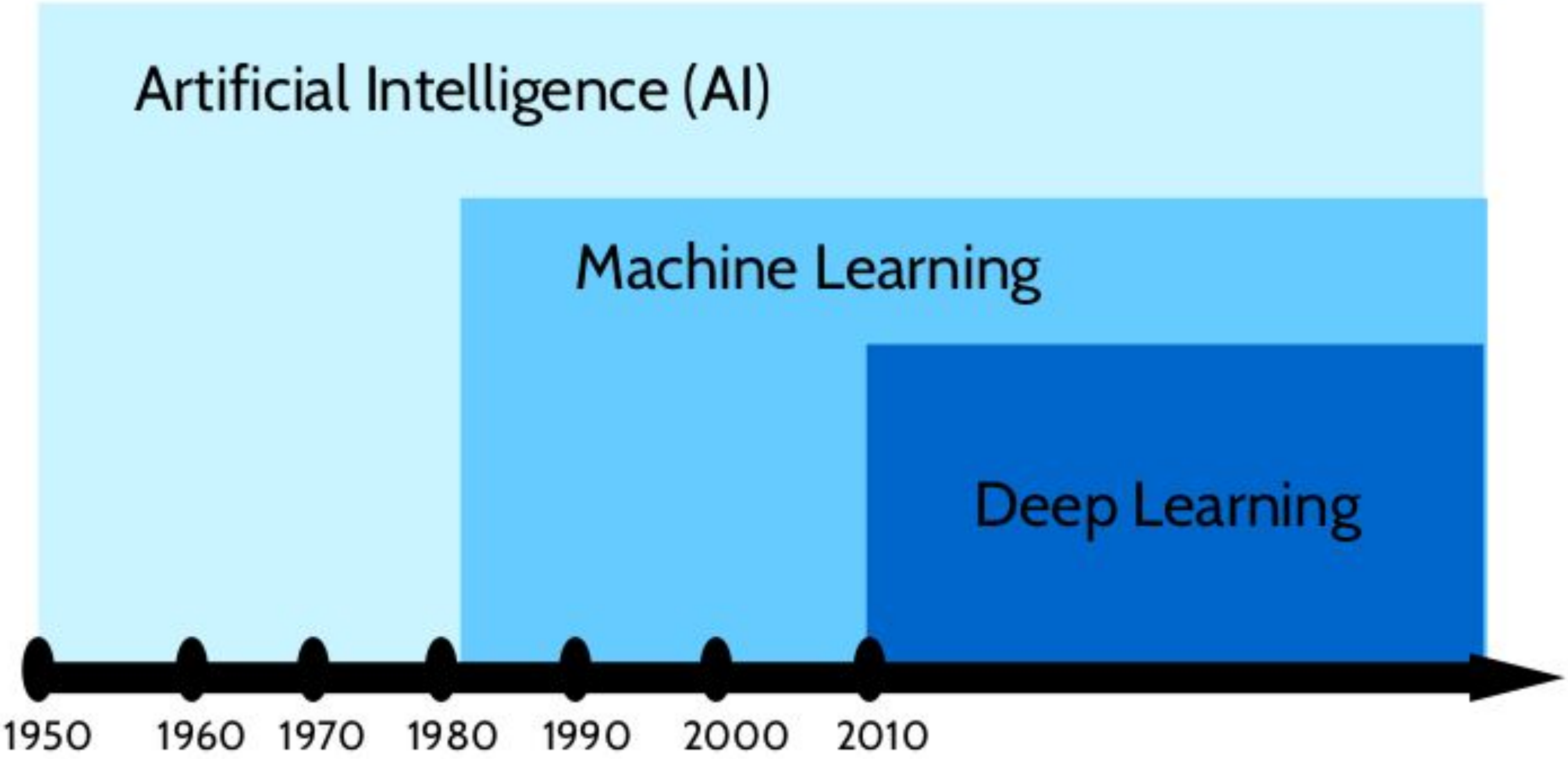
We learned

- Big data
- Analytics
- Machine learning

Today

- **Deep learning**
- Parallelisation
- Heterogeneous architectures
- Future directions

Deep Learning is a subfield of ML concerned with algorithms inspired by the structure and function of the brain called artificial neural networks [Jason Brownlee]

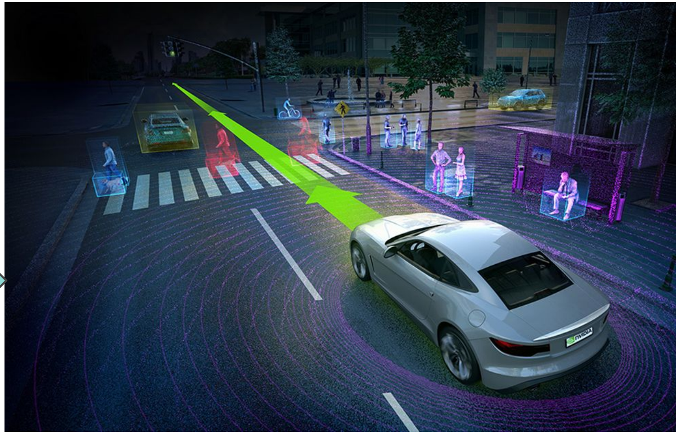


Machine translation
Real-time translation into
Mandarin Chinese (2012)

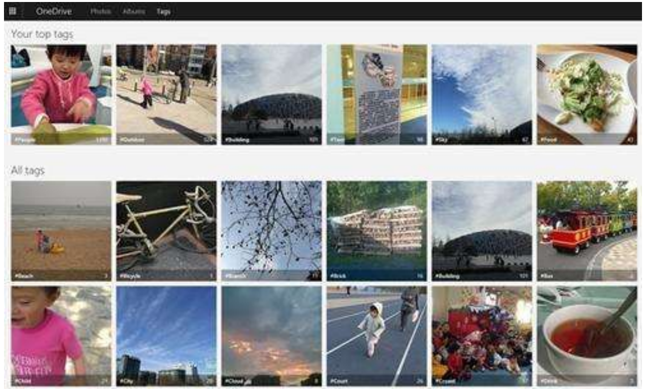
Strategy games
DeepMind beats Go
world champion (2017)

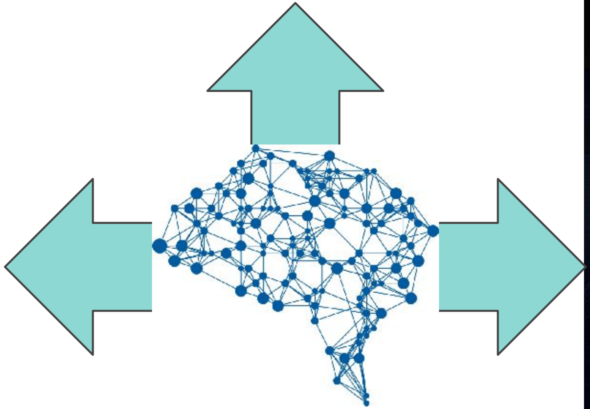
Creativity

Self driving cars

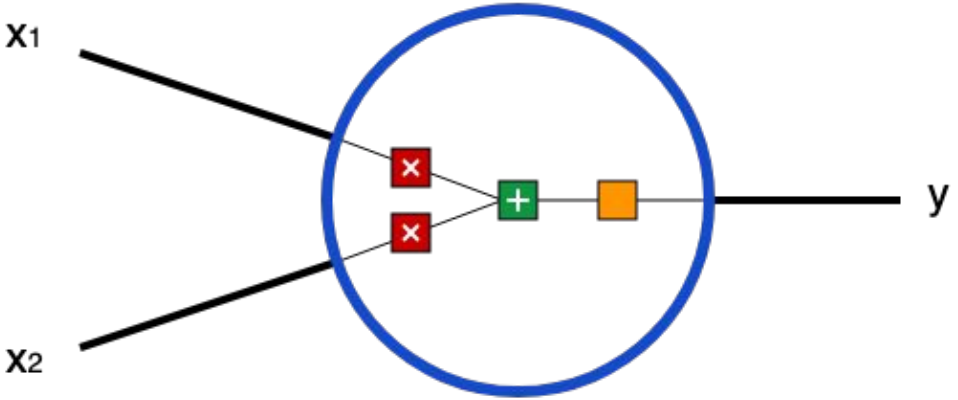


Visual recognition





Short recap: Neuron



- each **input x** is multiplied by a **weight w**

$$x_1 \rightarrow x_1 * w_1$$

$$x_2 \rightarrow x_2 * w_2$$

- all the weighted inputs are added together with a **bias *b***

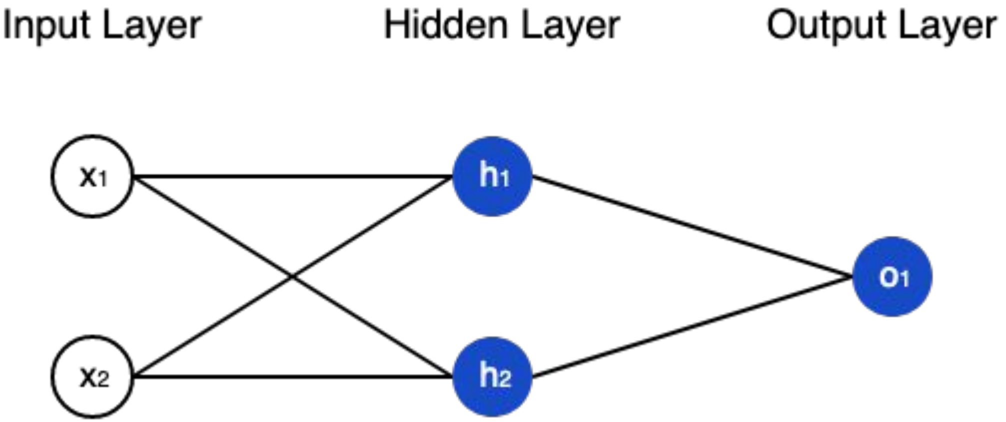
$$(x_1 * w_1) + (x_2 * w_2) + b$$

- the sum is passed through an **activation function f**

$$y = f(x_1 * w_1 + x_2 * w_2 + b)$$

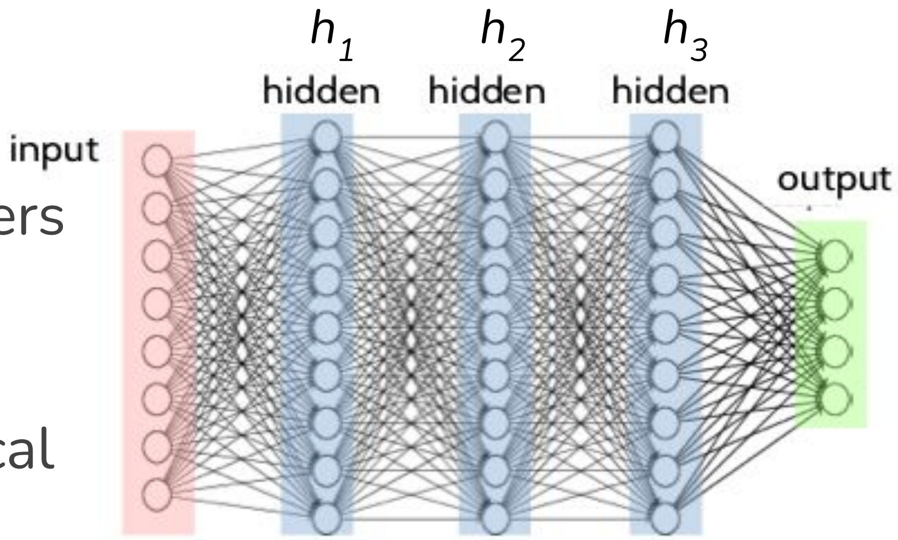
Neural network

- Combining more neurons
- A **hidden layer** is any layer between the input (first) layer and output (last) layer
  - There can be multiple hidden layers
- **Feedforward**: process of passing inputs forward to get an output



This network has:
- one **input** layer with 2 inputs
- one **hidden** layer with 2 neurons
- one **output** layer with 1 neuron

Deep Learning



- Neural network with several layers
  - Deep vs shallow
- A family of parametric models which learn non-linear hierarchical representations:

$$a_L(\mathbf{x};\boldsymbol{\Theta}) = h_L(h_{L-1}(\ldots(h_1(\mathbf{x},\boldsymbol{\theta}_1),\boldsymbol{\theta}_{L-1}),\boldsymbol{\theta}_L)$$

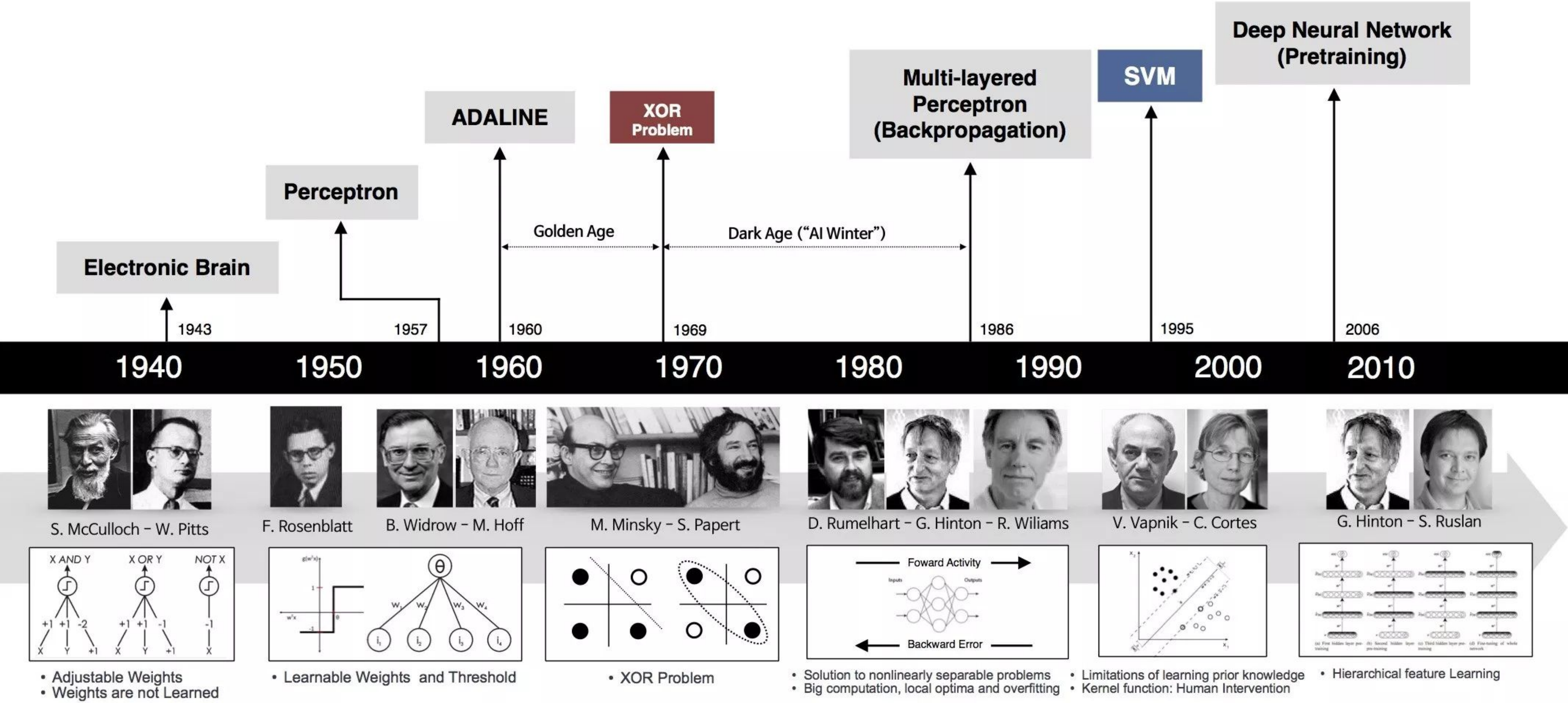
input

parameters of the network

non-linear activation function

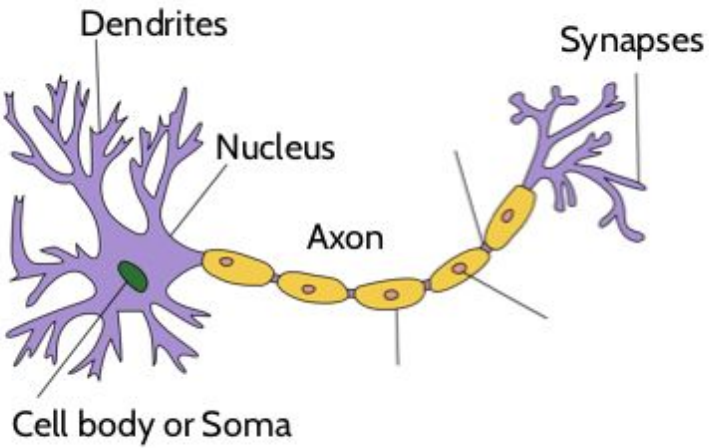
parameters of layer *L*

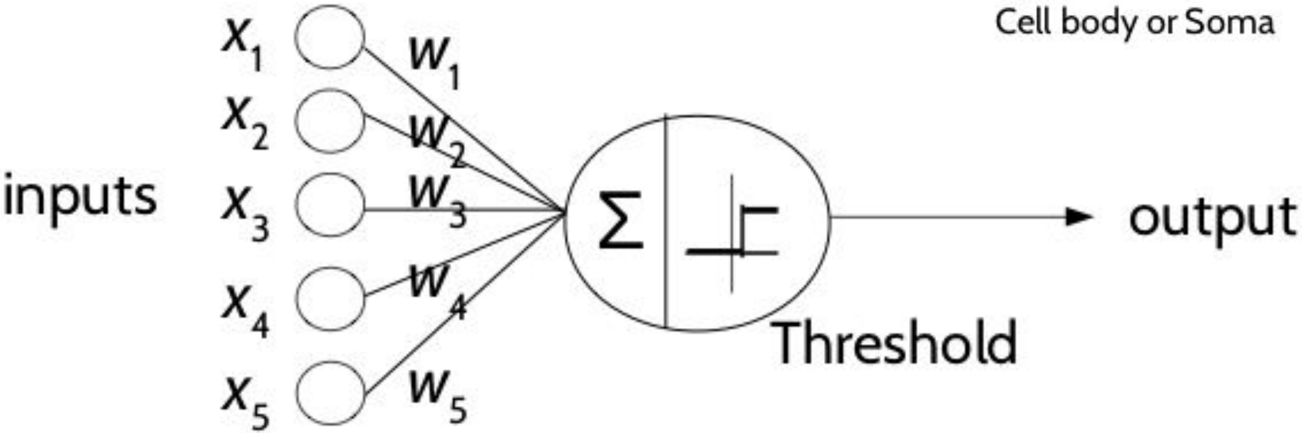
Brief history of neural networks



1943 – McCulloch & Pitts Model

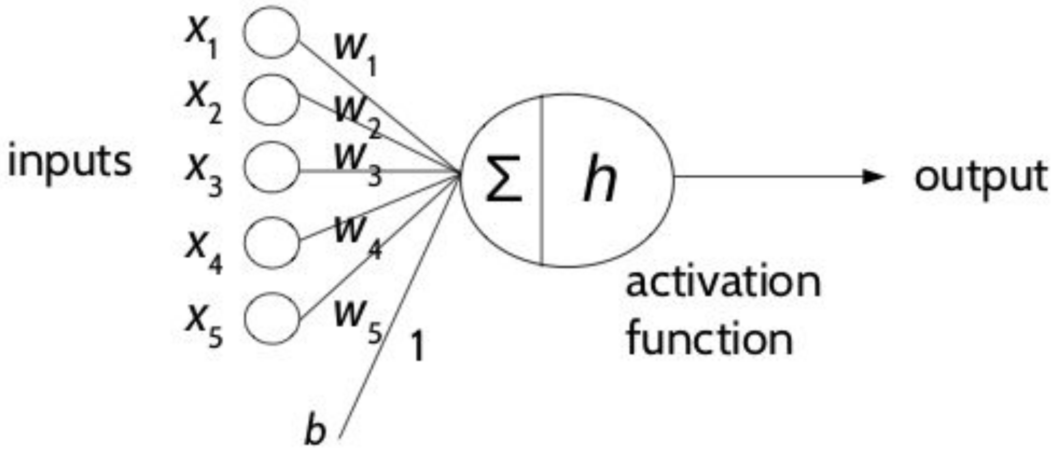
- Early model of artificial neuron
- Generates a binary output
- The weights values are fixed

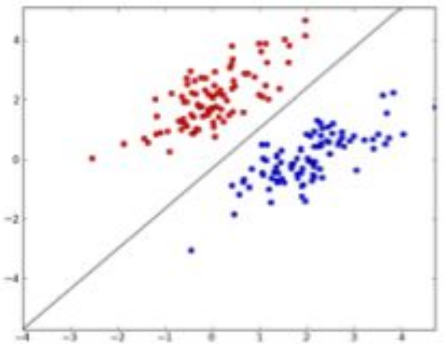




1958 – Perceptron by Rosemblatt

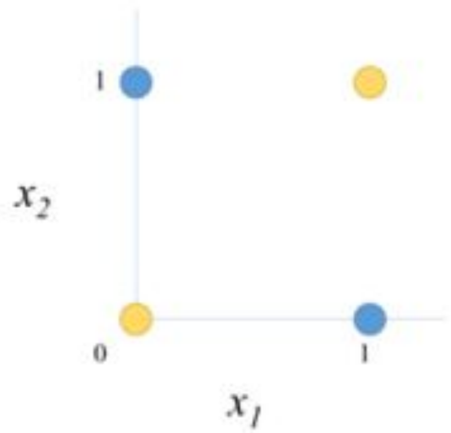
- Perceptron as a machine for linear classification
- Main idea: Learn the weights and consider bias.
  - One weight per input
  - Multiply weights with respective inputs and add bias
  - If result larger than **threshold** return 1, otherwise 0

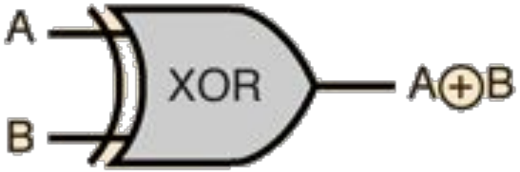




First NN winter

- 1970- Minsky. The XOR cannot be solved by perceptrons.
- Neural models cannot be applied to complex tasks.



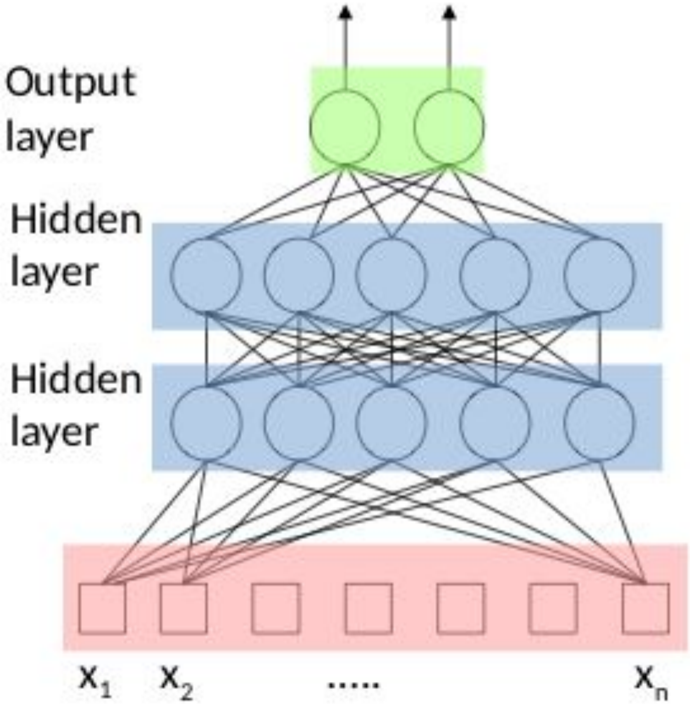


A	B	Out
0	0	0
0	1	1
1	0	1
1	1	0

Multi-layer Feed Forward Neural Network

- 1980s. Multi-layer Perceptrons (MLP) can solve XOR.

- ML Feed Forward Neural Networks:
  - Densely connect artificial neurons to realize compositions of non-linear functions
  - The information is propagated from the inputs to the outputs
  - The input data are usually *n*-dimensional feature vectors
  - Tasks: Classification, Regression



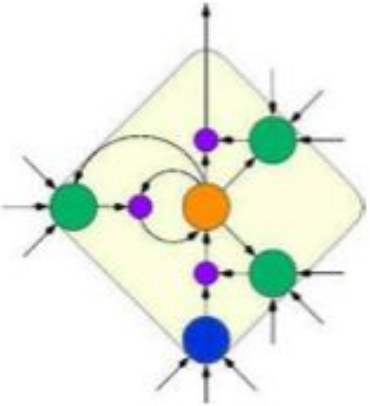
How to train it?

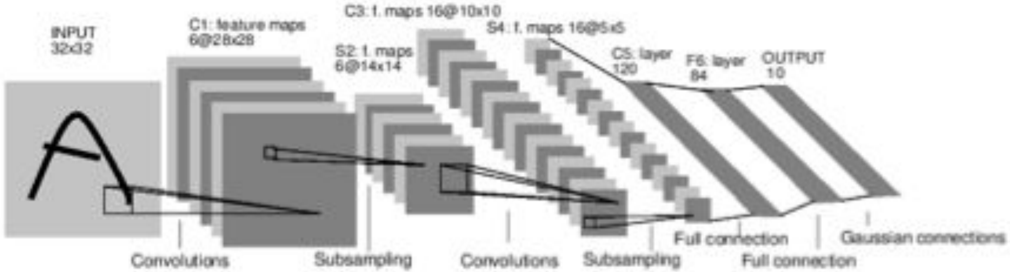
- Rosenblatt algorithm* not applicable, as it expects to know the desired target
  - For hidden layers we cannot know the desired target
- Learning MLP for complicated functions can be solved with **Back propagation (1980)**
  - efficient algorithm for complex NN which processes large training sets

* Remember? Rosenblatt developed a method to train a single neuron

1990s - CNN and LSTM

- Important advances in the field:
  - Backpropagation
  - Recurrent Long-Short Term Memory Networks (Schmidhuber, 1997)
  - Convolutional Neural Networks - LeNet: OCR solved before 2000s (LeCun, 1998).

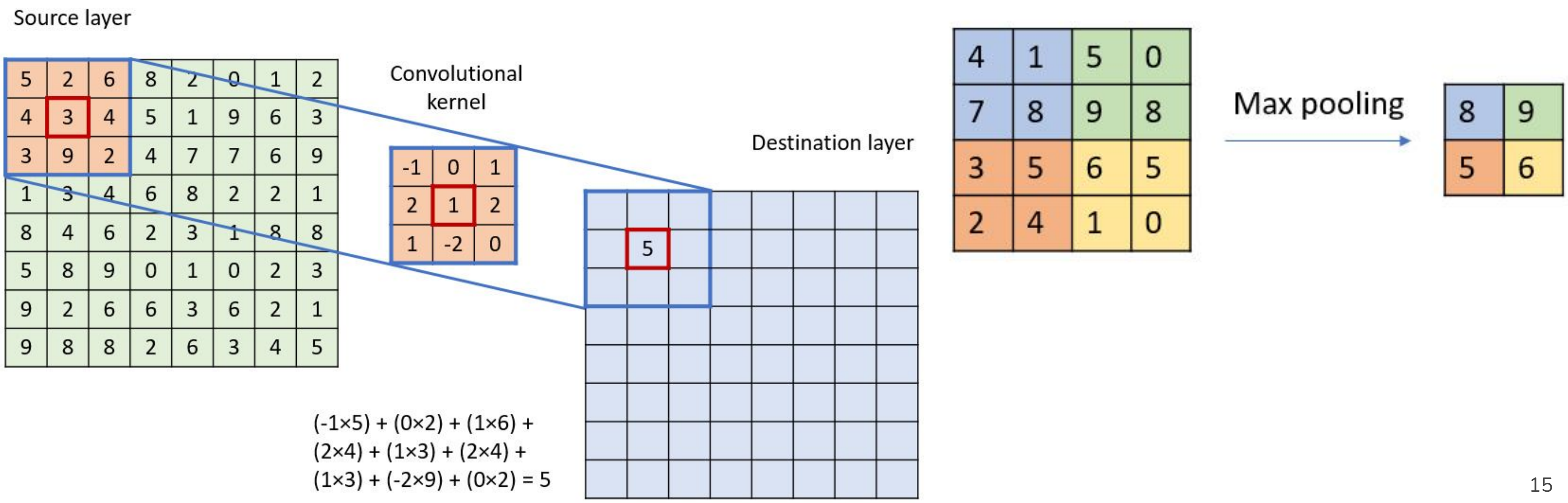




OCR: Optical character recognition

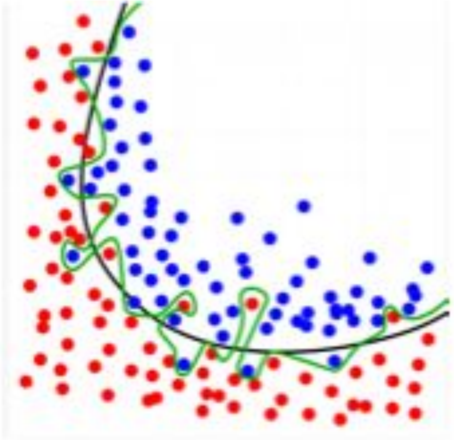
Convolutional Neural Networks (CNN)

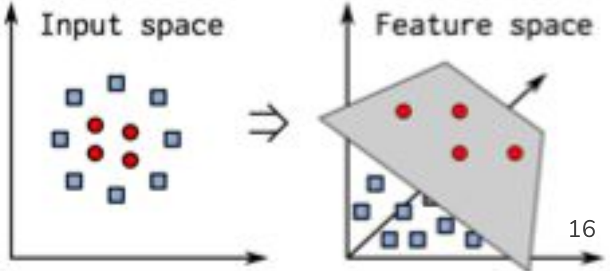
- **Convolutional** layer: two functions produce a third that describes how the shape of one is changed by the other
- **pooling** layer: reduce dimensionality



Second NN Winter

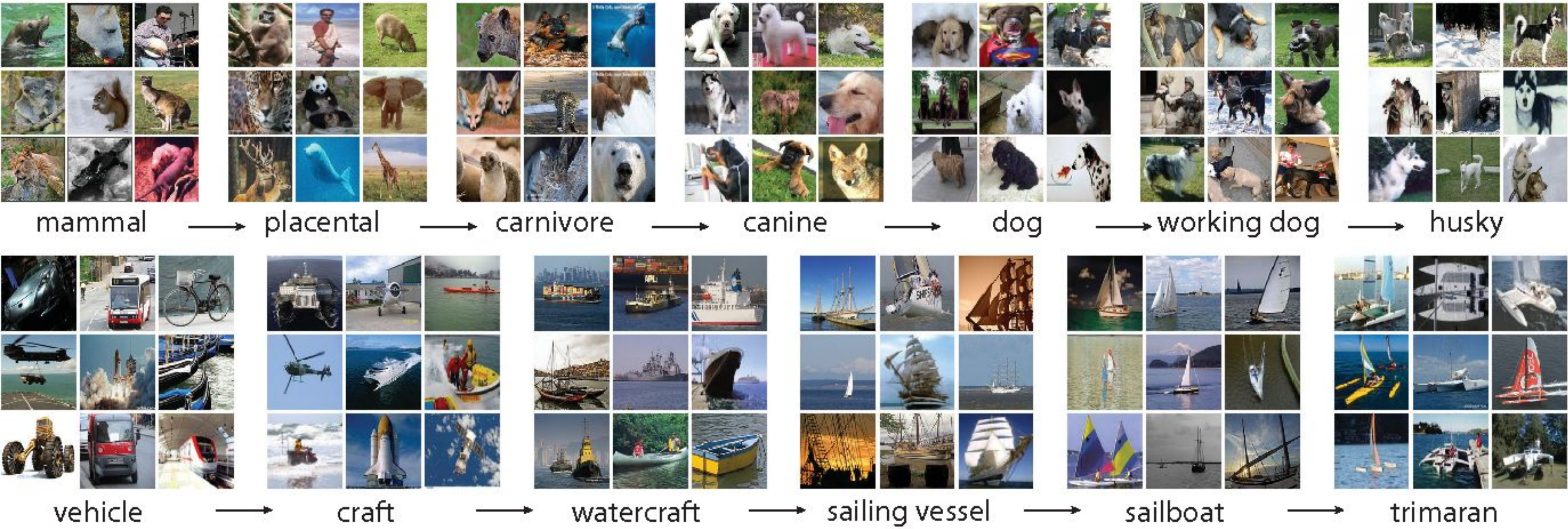
- NN cannot exploit many layers
  - Overfitting
  - Vanishing gradient (with NN training you need to multiply several small numbers → they become smaller and smaller)
- Lack of processing power (no GPUs)
- Lack of data (no large annotated datasets)
- Kernel Machines (e.g. SVMs) suddenly become very popular





ImageNet

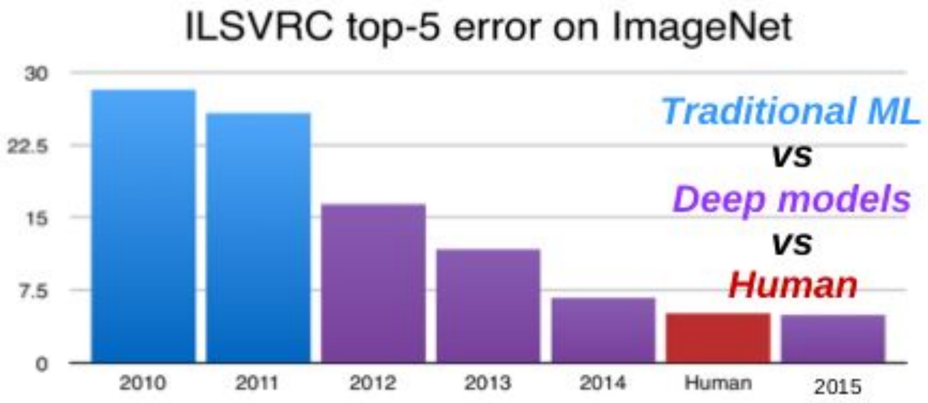
A Large-Scale Hierarchical Image Database (2009)



https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=5206848&tag=1

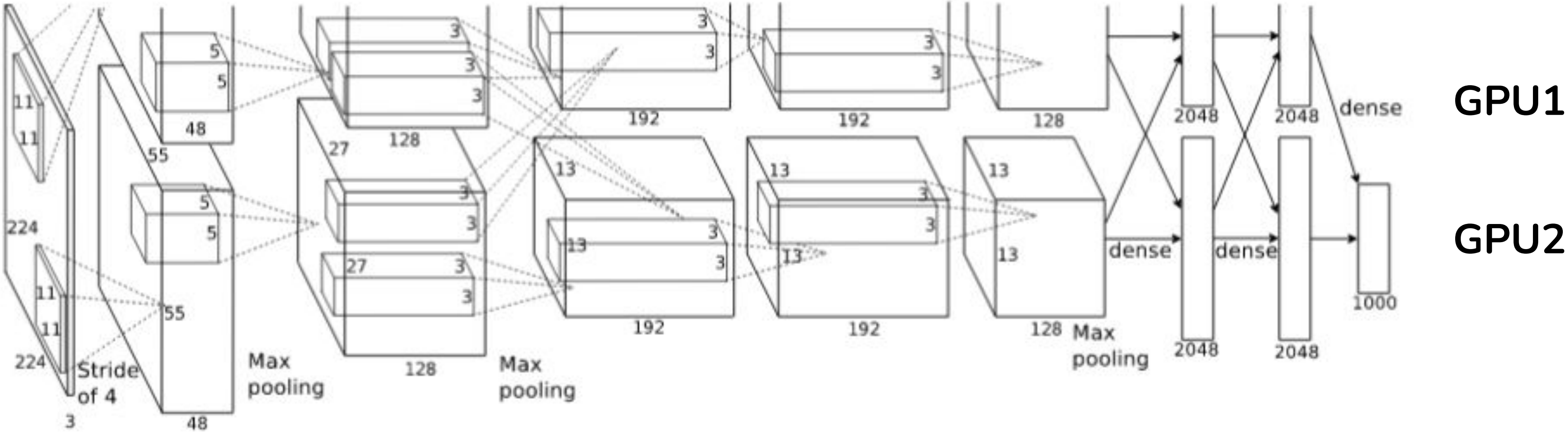
2012 - AlexNet

- Hinton's group implemented a CNN similar to LeNet [LeCun1998] but...
  - Trained on ImageNet (1.4M images, 1K categories)
  - With 2 GPUs
  - Other technical improvements (ReLU, dropout, data augmentation)



https://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks.pdf

AlexNet



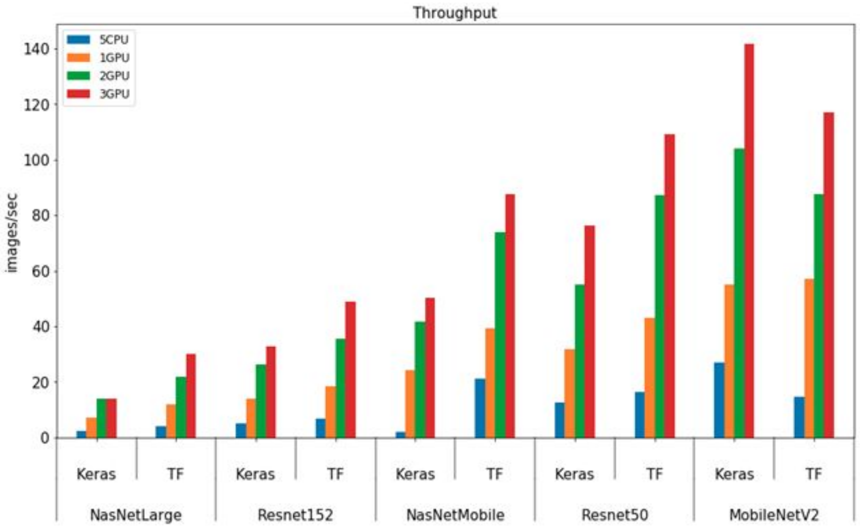
- 60M parameters
- Limited information exchange between GPUs

https://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks.pdf

Why Deep Learning now?

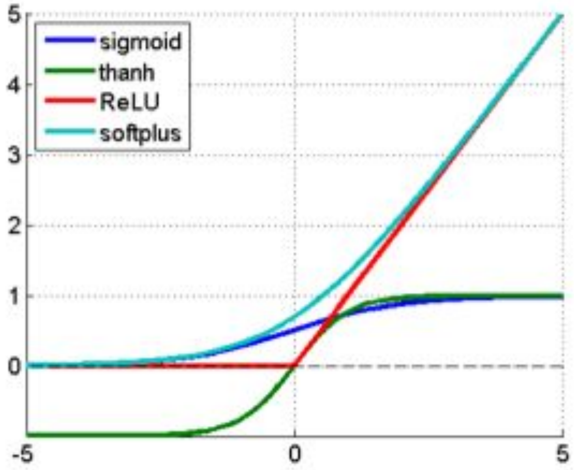
- Three main factors:
  - Better hardware
  - Big data
  - Technical advances:
    - Layer-wise pretraining
    - Optimization (e.g. Adam, batch normalization)
    - Regularization (e.g. dropout)

    ....



Rectified Linear Units - Activation function (2010)

$$f(x) = \max(0, x)$$

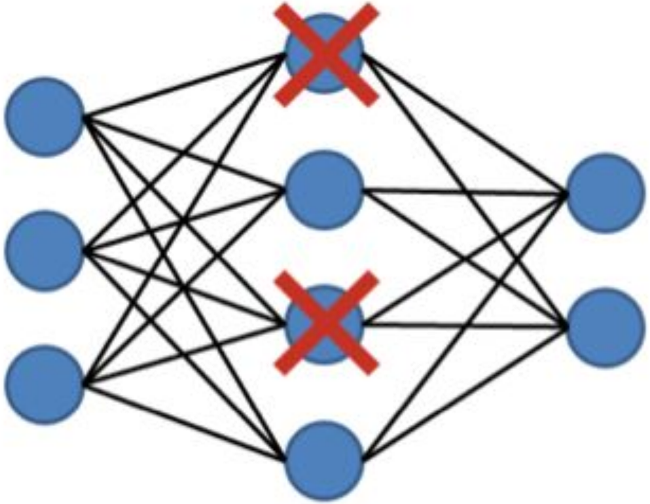


- More efficient gradient propagation: (derivative is 0 or constant)
- More efficient computation: (only comparison, addition and multiplication).
- Sparse activation: e.g. in a randomly initialized networks, only about 50% of hidden units are activated (having a non-zero output)

https://www.cs.toronto.edu/~fritz/absps/reluICML.pdf

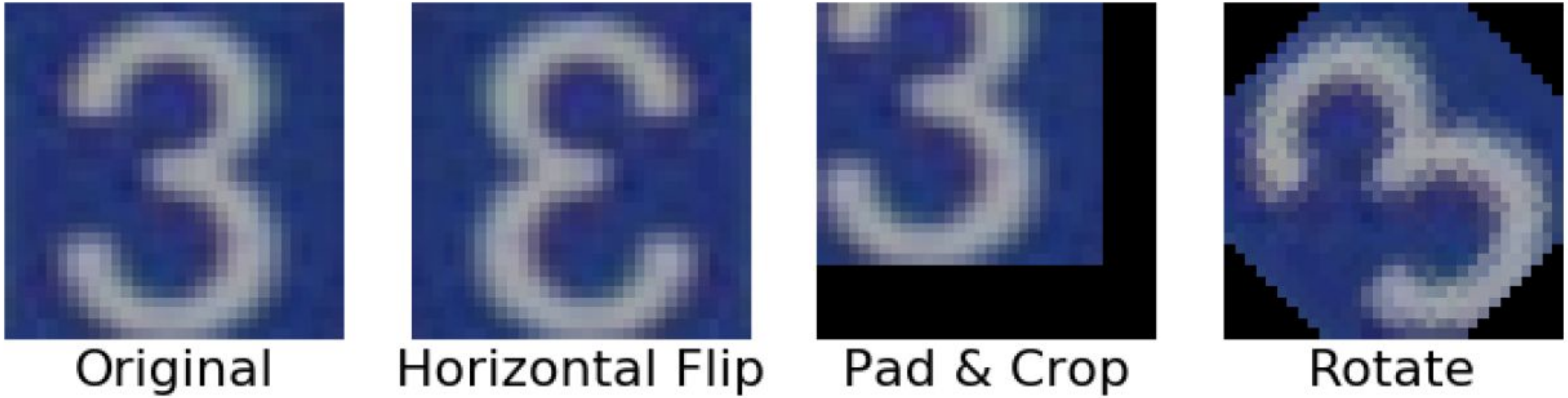
Regularization - Dropout

- For each instance drop a node (hidden or input) and its connections with probability *p* and train
- Final net just has all averaged weights (actually scaled by 1-*p*)
- As if ensembling 2^n different network substructures



Data augmentation

- Techniques to significantly increase the diversity of data available for training models, without actually collecting new data
- Data augmentation techniques such as cropping, padding, and horizontal flipping are commonly used to train large neural networks



Training a neural network

Name	Weight (lb)	Height (in)	Gender
Alice	133	65	F
Bob	160	72	M
Charlie	152	70	M
Diana	120	60	F

- Predict gender from weight and height

Feature engineering

- Symmetrize numeric values
- Category -> numbers

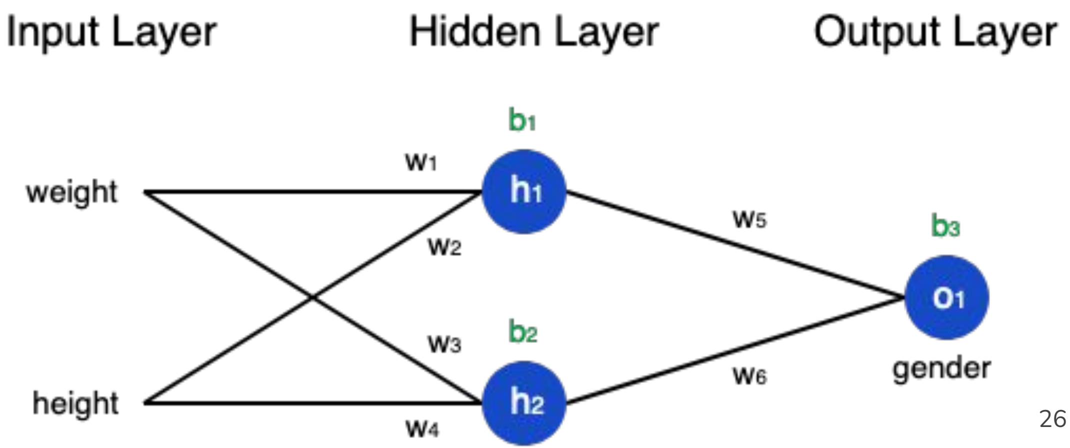
Name	Weight (lb)	Height (in)	Gender
Alice	133	65	F
Bob	160	72	M
Charlie	152	70	M
Diana	120	60	F

Name	Weight (minus 135)	Height (minus 66)	Gender
Alice	-2	-1	1
Bob	25	6	0
Charlie	17	4	0
Diana	-15	-6	1

Ingredients

- **n** : 4, number of samples (Alice, Bob, Charlie, Diana)
- **y** : variable being predicted (Gender)
- $\mathbf{y_{true}}$: true value of y, $\mathbf{y_{pred}}$: predicted value of y = **o**
- Loss function **L: MSE**
- Activation function **f**
- Outputs of the hidden layer **h**
- Unknown parameters: weights **w** and biases **b**

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_{true} - y_{pred})^2$$



Back propagation

- **Training the network == trying to minimize its loss**
  - Find weights **w** and biases **b**
  - $L(w_1, w_2, w_3, w_4, w_5, w_6, b_1, b_2, b_3)$
- Minimization taking partial derivatives (**back propagation**)

$$\boxed{\frac{\partial L}{\partial w_1} = \frac{\partial L}{\partial y_{pred}} * \frac{\partial y_{pred}}{\partial h_1} * \frac{\partial h_1}{\partial w_1}}$$

For very simple case: with only Alice in the dataset, n=1

$$L = (1 - y_{pred})^2$$

$$\frac{\partial L}{\partial y_{pred}} = \frac{\partial (1 - y_{pred})^2}{\partial y_{pred}}$$

$$y_{pred} = o_1 = f(w_5 h_1 + w_6 h_2 + b_3)$$

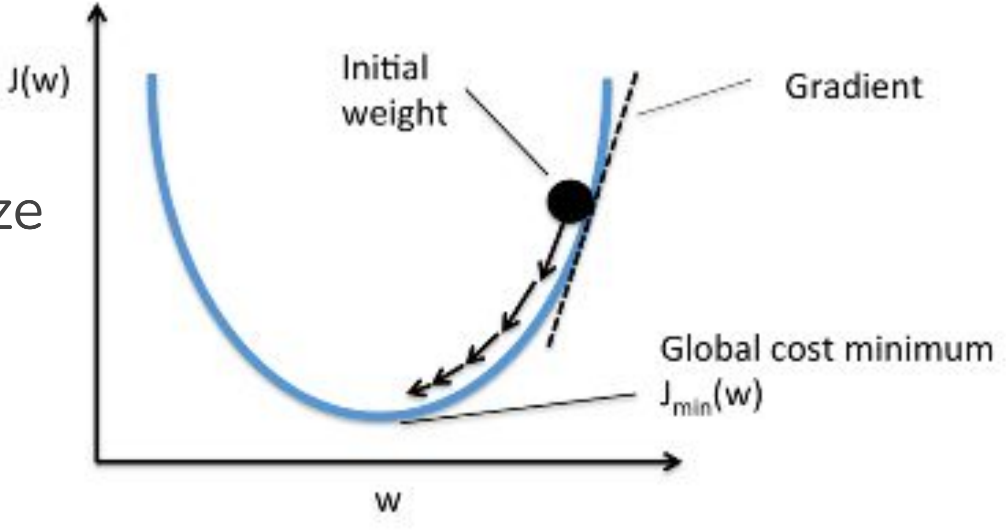
$$\frac{\partial y_{pred}}{\partial h_1} = \boxed{w_5 * f'(w_5 h_1 + w_6 h_2 + b_3)}$$

$$h_1 = f(w_1 x_1 + w_2 x_2 + b_1)$$

$$\frac{\partial h_1}{\partial w_1} = \boxed{x_1 * f'(w_1 x_1 + w_2 x_2 + b_1)}$$

Gradient Descent

- optimization algorithm to find weights and biases to minimize loss
- **update equation**:



$$w_1 \leftarrow w_1 - \eta \frac{\partial L}{\partial w_1}$$

- **η (learning rate)** is a constant that controls how fast we train

- If $\frac{\partial L}{\partial w_1}$ is positive, w_1 will decrease, which makes L decrease.
- If $\frac{\partial L}{\partial w_1}$ is negative, w_1 will increase, which makes L decrease.

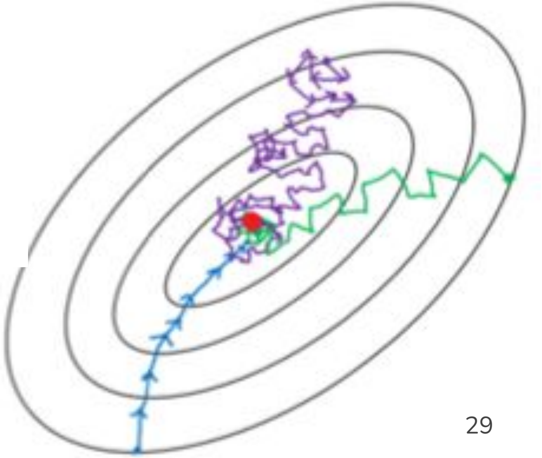
Stochastic gradient descent (SDG)

- **Stochastic** -> the parameters are updated using only a single training instance (usually randomly selected) in each iteration

- Use mini-batch **sampled** in the dataset for gradient estimate.

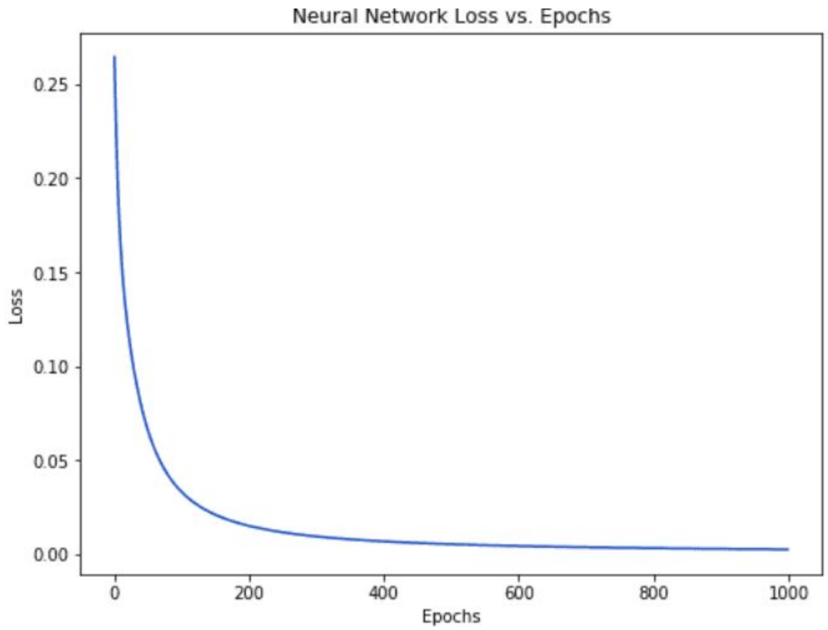
$$\Theta^{t+1} = \Theta^{t} - \frac{\eta_t}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} \nabla_{\Theta} \mathcal{L}_i$$

- Sometimes helps to escape from local minima
- Noisy gradients act as regularization
- Variance of gradients increases when batch size decreases
- Not clear how many sample per batch



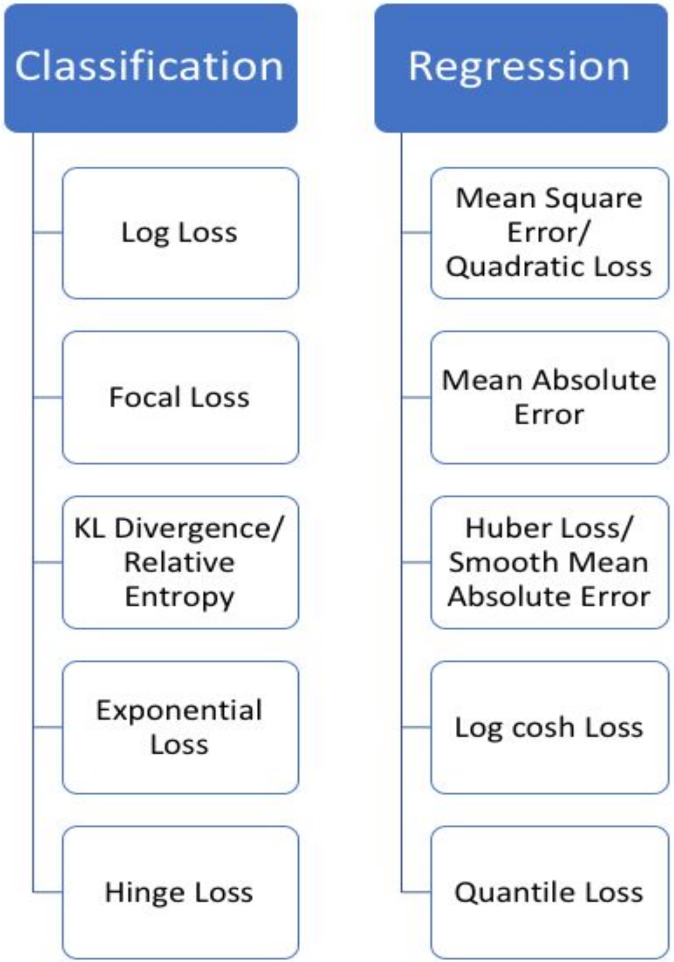
Training the network

- Choose one sample from our dataset
  - This is what makes it stochastic gradient descent - only operate on one sample at a time
- Calculate all the partial derivatives of loss with respect to weights or biases
- Use the update equation to update each weight and bias
- Iterate



Loss functions

- https://heartbeat.fritz.ai/5-regression-loss-functions-all-machine-learners-should-know-4fb140e9d4b0
- https://www.wikiwand.com/en/Loss_functions_for_classification



Regularization

- One of the major aspects of training the model is overfitting -> the ML model captures the noise in your training dataset
- The **regularization** term is an addition to the loss function which helps generalize the model
    - **L1** or Lasso regularization adds a penalty which is the sum of the absolute values of the weights
        - L1+MSE

$$Min(\sum_{i=1}^{n}(y_i - w_i x_i)^2 + p\sum_{i=1}^{n}|w_i|)$$

    - **L2** or Ridge regularization adds a penalty which is the sum of the squared values of weights
        - L2+MSE

$$Min(\sum_{i=1}^{n}(y_i - w_i x_i)^2 + p\sum_{i=1}^{n}(w_i)^2)$$

- **Dropout** in NN context: hidden nodes are dropped randomly
- **Early Stopping** is a time regularization technique which stops training based on given criteria

Activation functions

- Classification: sigmoid functions
  - sigmoids and tanh functions are sometimes avoided due to the vanishing gradient problem
- **ReLU** function is a general activation function
- dead neurons in our networks -> the leaky ReLU
- ReLU function should only be used in the hidden layers
- As a rule of thumb, start with ReLU