Big data science Day 4

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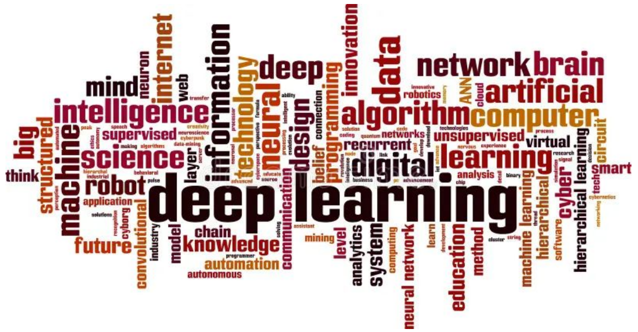
https://github.com/Course-bigDataAndML/MLCourse-2425

- So long, and thanks for all the images!
  - *Taken freely from the web*
  - *Credits go to original creators*

We learned

- Big data, analytics
- Distributed computing
- ML
  - Supervised and unsupervised models
  - Evaluate performances

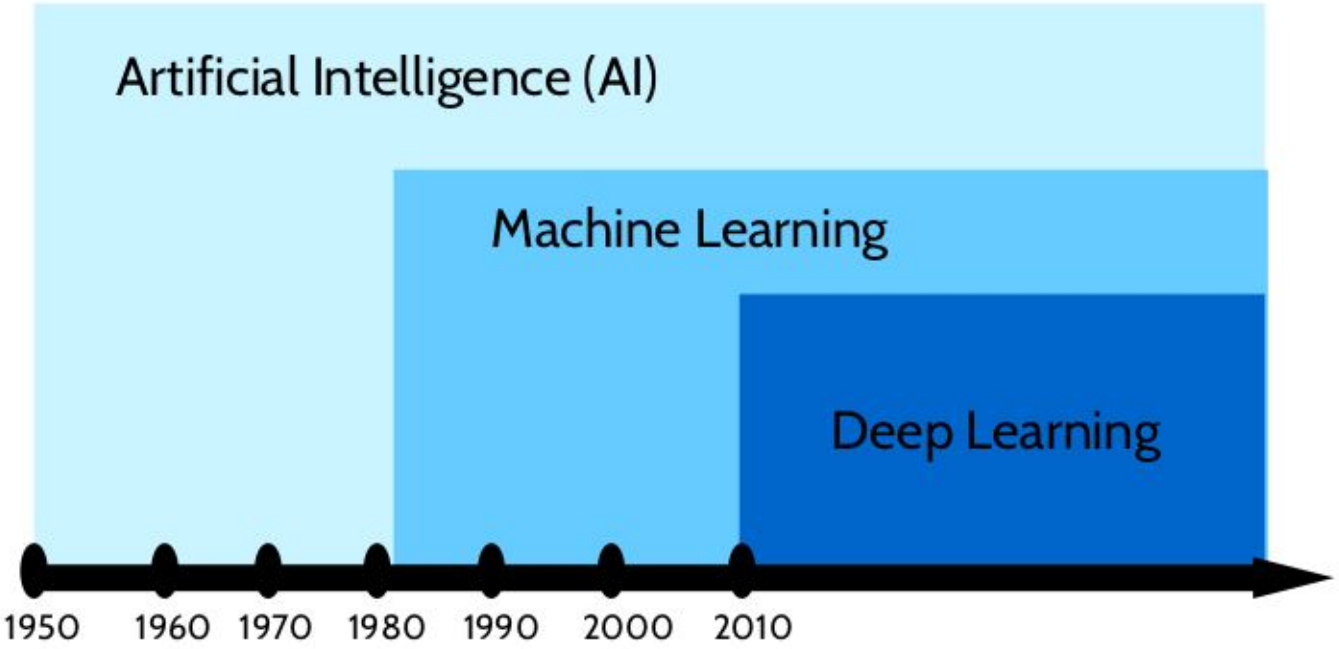
Today



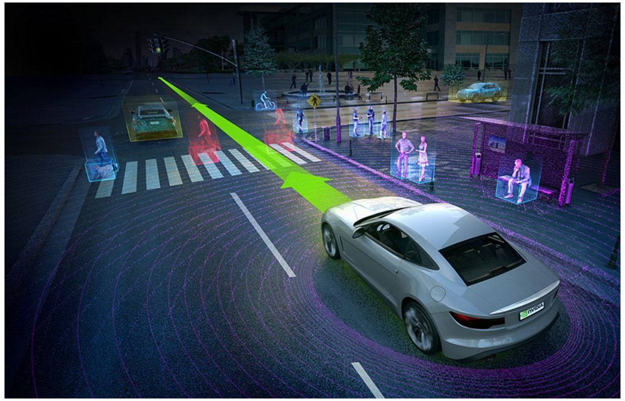
- **Deep learning**
  - neural networks
  - brief history
  - main architectures
  - how to train

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]

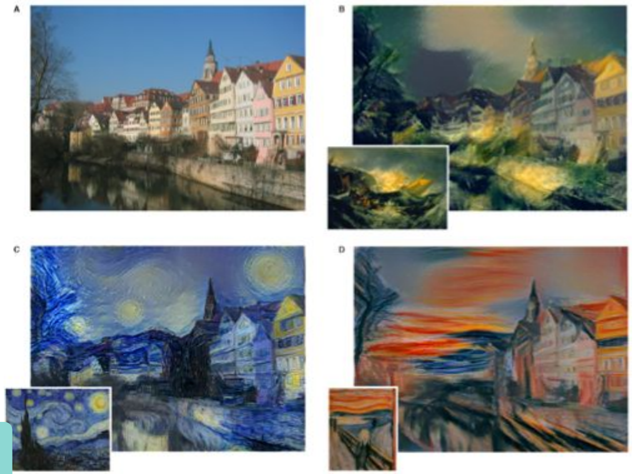


Machine translation
Real-time translation into Mandarin Chinese (2012)

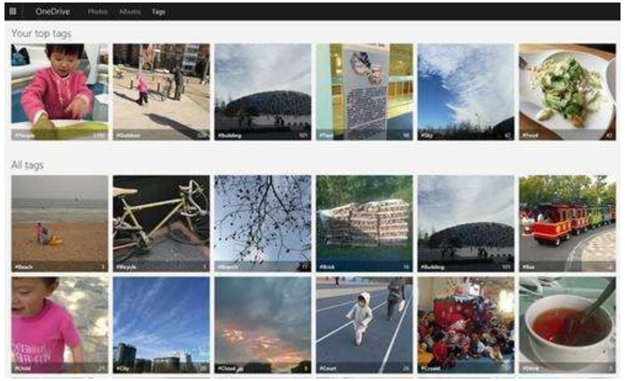


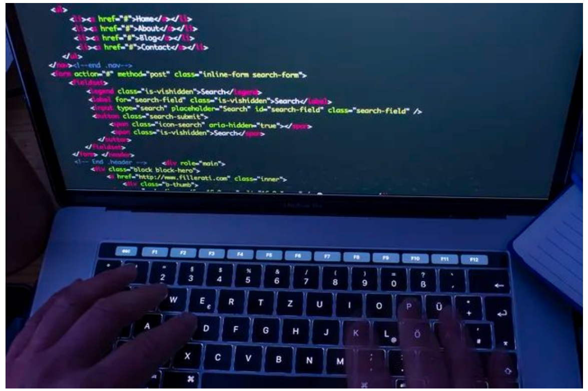
Self driving cars, Tesla autopilot (2014)

Creativity
NST (2015), GAN (2014)



Visual recognition, ResNet better than humans (2015)





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    <li><a href="#">Home</a></li>
    <li><a href="#">About</a></li>
    <li><a href="#">Blog</a></li>
    <li><a href="#">Contact</a></li>
  </ul>
</nav><!--end .nav-->
<form action="#" method="post" class="inline-form search-form">
    <fieldset>
        <legend class="is-vishidden">Search</legend>
        <label for="search-field" class="is-vishidden">Search</label>
        <input type="search" placeholder="Search" id="search-field" class="search-field" />
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            <span class="icon-search" aria-hidden="true"></span>
            <span class="is-vishidden">Search</span>
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    </fieldset>
</form> </header>
<!-- End .header -->    <div role="main">
    <div class="block block-hero">
        <a href="http://www.fillerati.com" class="inner">
            <div class="b-thumb">
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Chatbots, ChatGPT (2022)

Strategy games DeepMind beats Go world champion (2017)

And the winner is…

- The Nobel Prize in **Physics 2024** was awarded jointly to **John J. Hopfield** (Princeton) and **Geoffrey E. Hinton** (U. Toronto) *"for foundational discoveries and inventions that enable machine learning with artificial neural networks"*
- The Nobel Prize in **Chemistry 2024** was divided, one half awarded to **David Baker** (U. Washington) *"for computational protein design"*, the other half jointly to **Demis Hassabis** (Google DeepMind) and **John Jumper** (Google DeepMind) *"for protein structure prediction"*

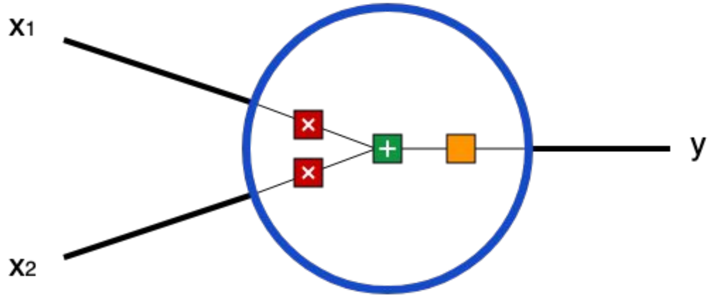
Short recap: Neuron

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

$$x_1 \rightarrow x_1 * w_1$$

$$x_2 \rightarrow x_2 * w_2$$

X



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

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

+

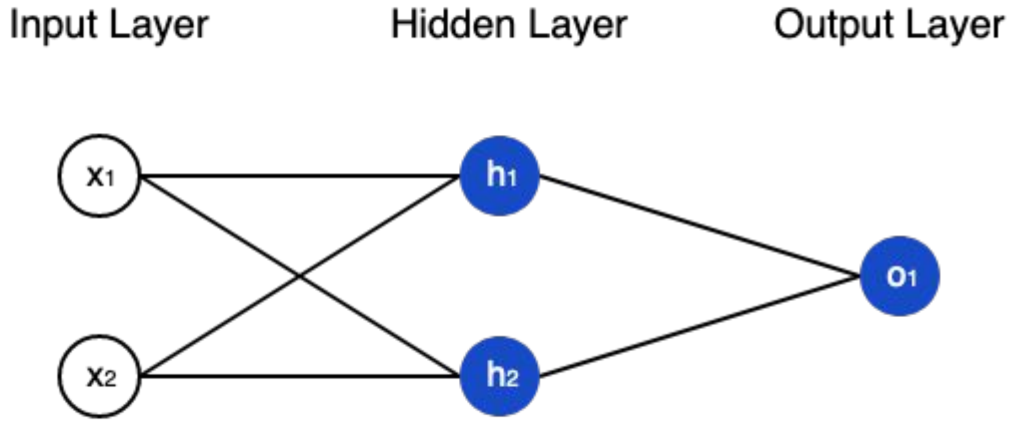
- the sum is passed through an **activation function f**

🟨

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

Neural network

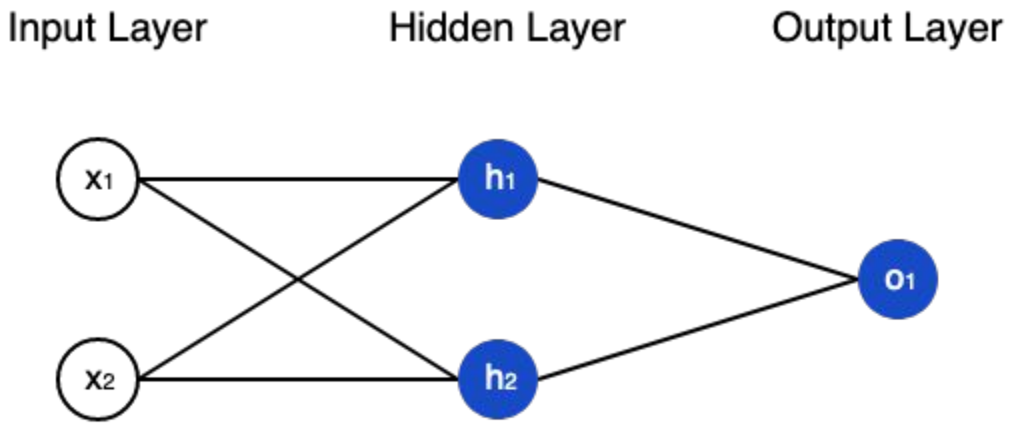
- built by combining neurons into layers
- a **hidden layer** is any layer between the **input** (first) layer and **output** (last) layer
    - there can be multiple hidden layers
- **Feedforward**: process of passing inputs forward to get an output



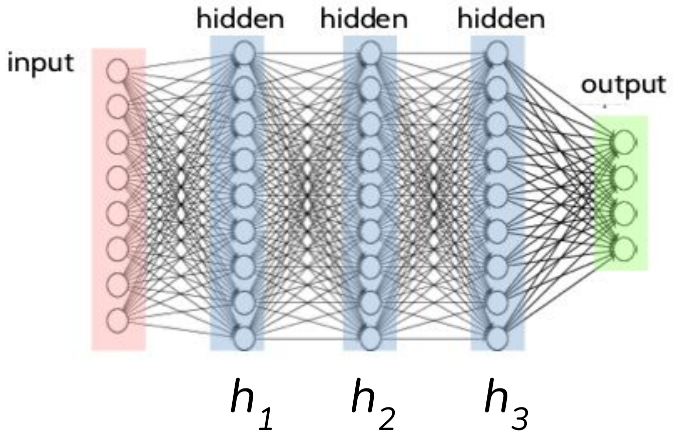
Neural network

This network has:

- one **input** layer with 2 inputs
- one **hidden** layer with 2 neurons
- one **output** layer with 1 neuron



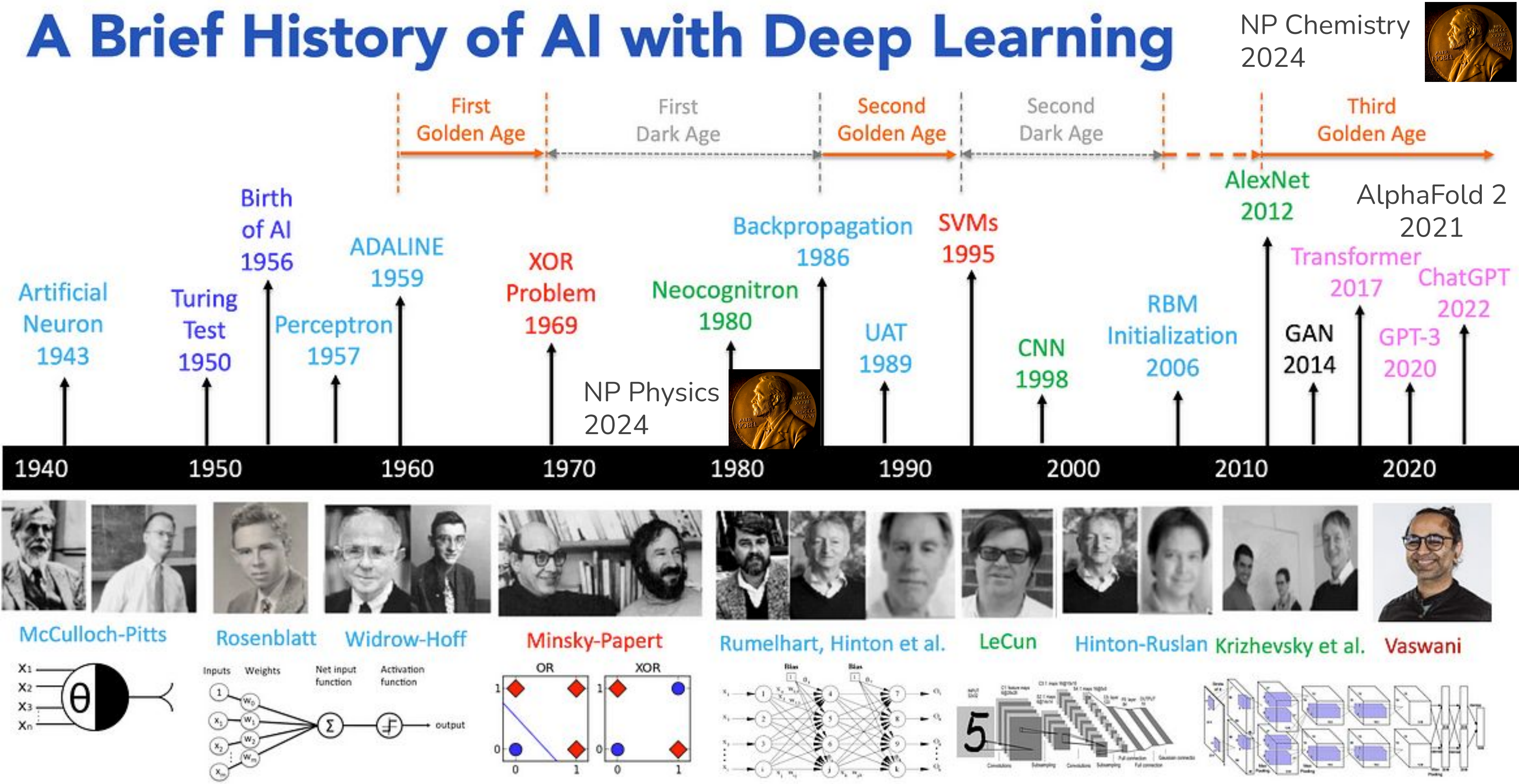
Deep Learning



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

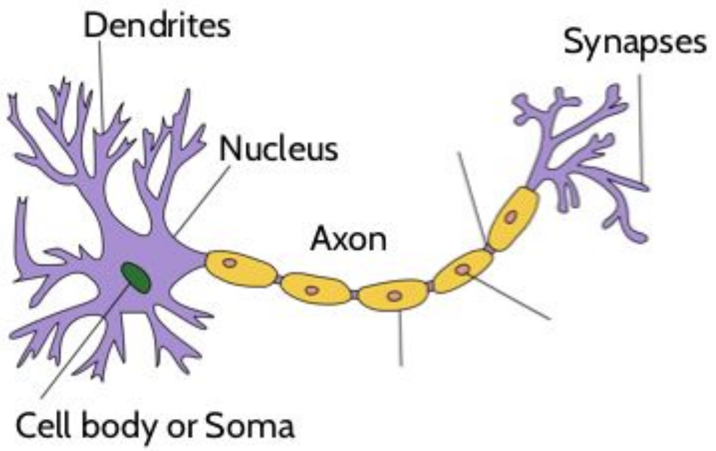
$$\underset{\text{input}}{a_L(\mathbf{x}};\underset{\text{parameters of the network}}{\boldsymbol{\Theta}}) = h_L(h_{L-1}(\ldots(\underset{\text{non-linear activation function}}{h_1}(\mathbf{x},\boldsymbol{\theta}_1),\boldsymbol{\theta}_{L-1}),\underset{\text{parameters of layer } L}{\boldsymbol{\theta}_L})$$

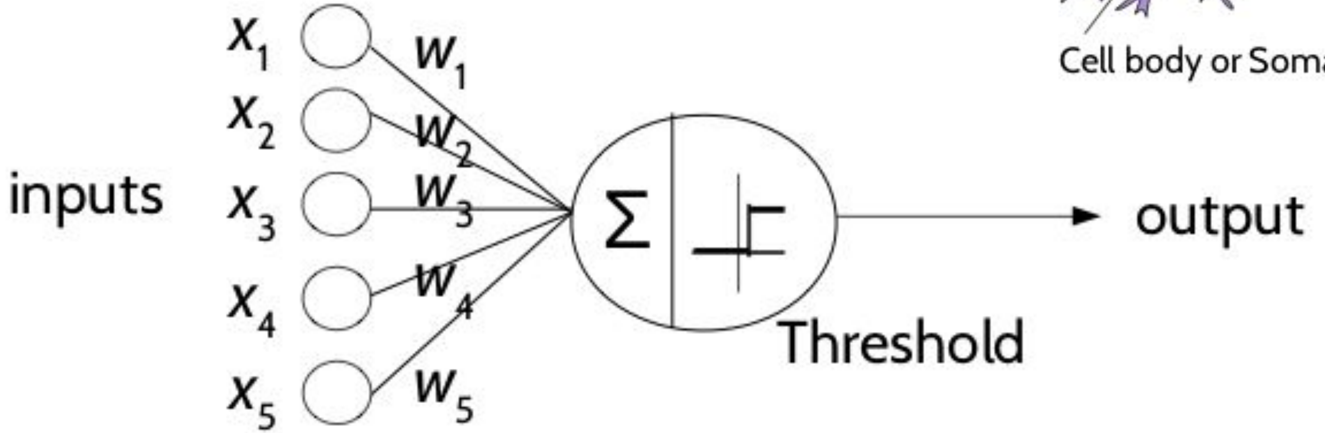
A Brief History of AI with Deep Learning



1943: McCulloch & Pitts Model

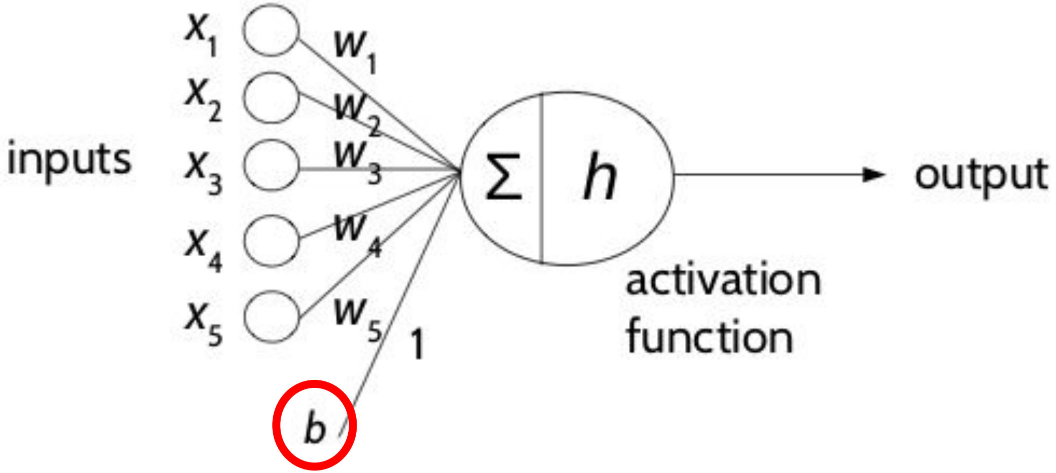
- Early model of artificial neuron
- Generates a binary output
- The weights values are fixed

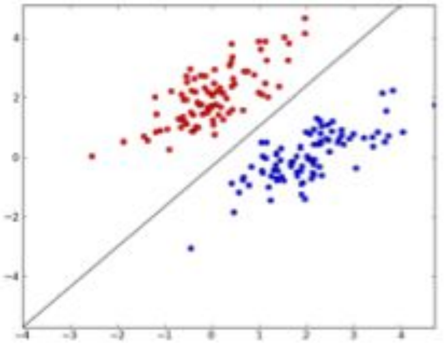




1958: Perceptron by Rosenblatt

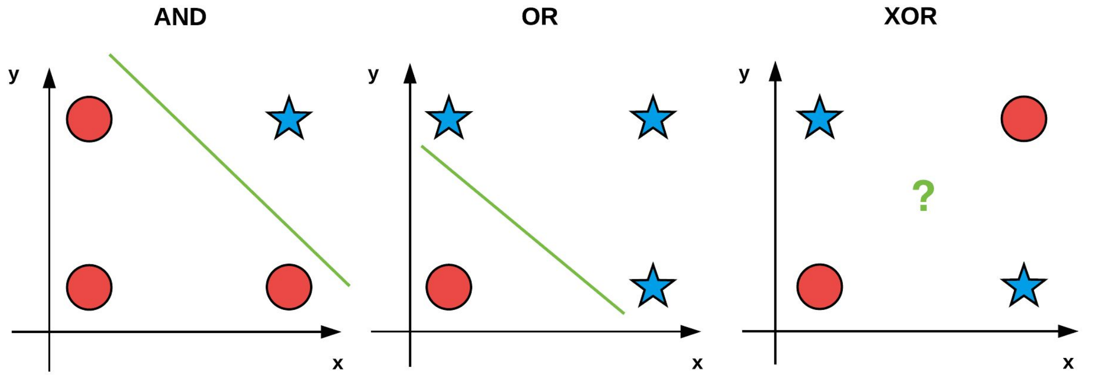
- Perceptron as a machine for linear classification
- Main idea: Learn the weights and consider bias.
  - One weight per input
  - Multiply weights with respective inputs and add bias
  - If result larger than **threshold** return 1, otherwise 0





1970: First NN winter

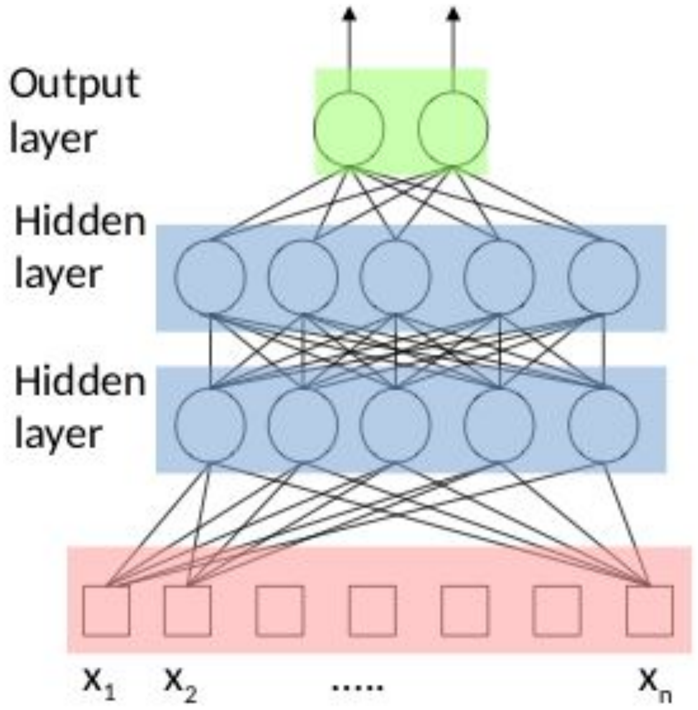
- Minsky showed that the XOR cannot be solved by perceptrons
- Single-layer perceptrons are only capable of learning linearly separable patterns
- **Neural models cannot be applied to complex tasks**



1980: Multi-layer 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?

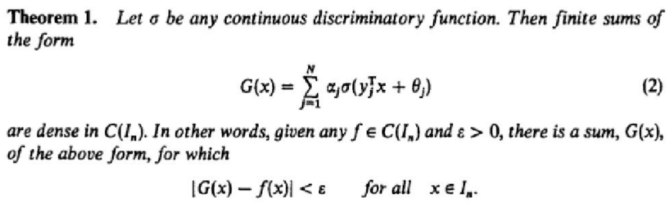
- Rosenblatt algorithm* not applicable, as it expects to know the desired target
  - For hidden layers we cannot know the desired target
- Learning MLP for complicated functions can be solved with **Back propagation** (1986)**
  - efficient algorithm for complex NN which processes large training sets

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

** later today

1989: Universal Approximation Theorem (UAT)

- A multilayered neural network with a **single hidden layer** can approximate any continuous function to any desired precision

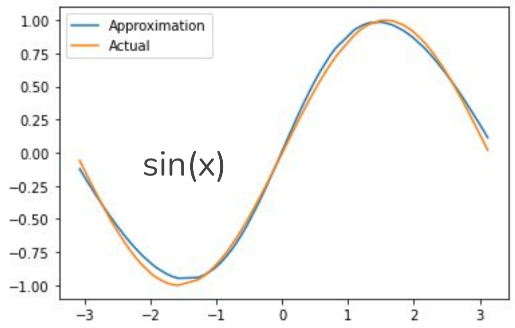


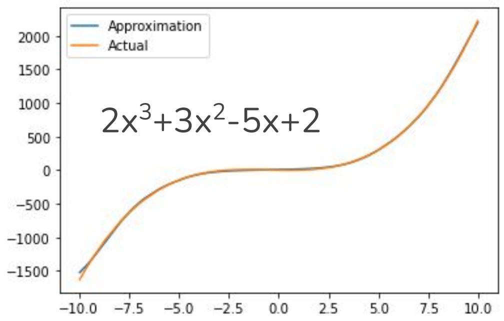
Theorem 1. *Let σ be any continuous discriminatory function. Then finite sums of the form*

$$G(x)=\sum_{j=1}^{N}\alpha_j\sigma(y_j^{T}x+\theta_j) \qquad (2)$$

are dense in $C(I_n)$. In other words, given any $f\in C(I_n)$ and $\varepsilon>0$, there is a sum, $G(x)$, of the above form, for which

$$|G(x)-f(x)|<\varepsilon \qquad \textit{for all} \quad x\in I_n.$$



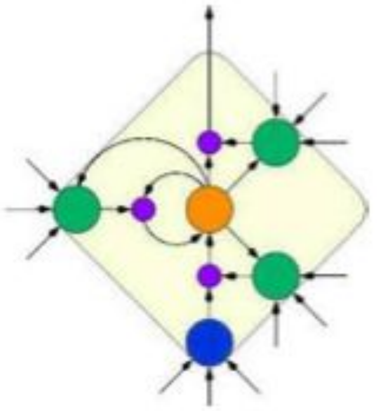


Cybenko, G. (1989). "Approximation by superpositions of a sigmoidal function". *Mathematics of Control, Signals, and Systems*. **2** (4): 303–314

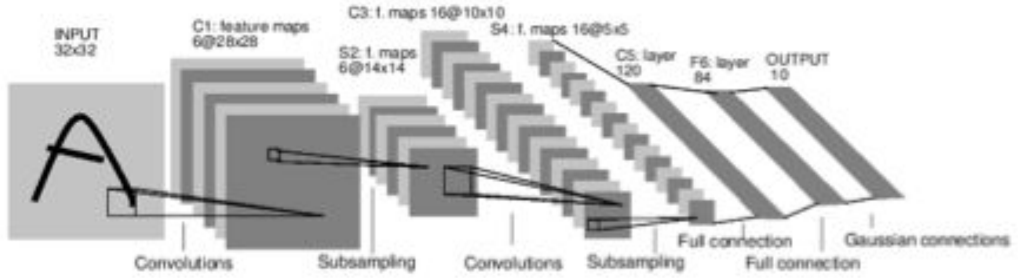
Hornik, Kurt; Stinchcombe, Maxwell; White, Halbert (January 1989). "Multilayer feedforward networks are universal approximators". *Neural Networks*. **2** (5): 359–366

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).

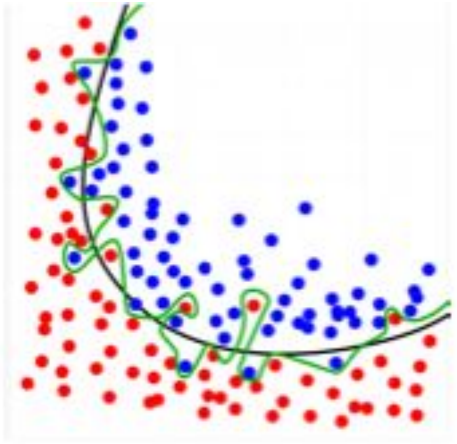


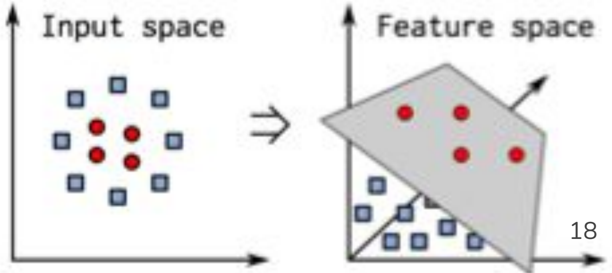
OCR: Optical character recognition



Second NN Winter

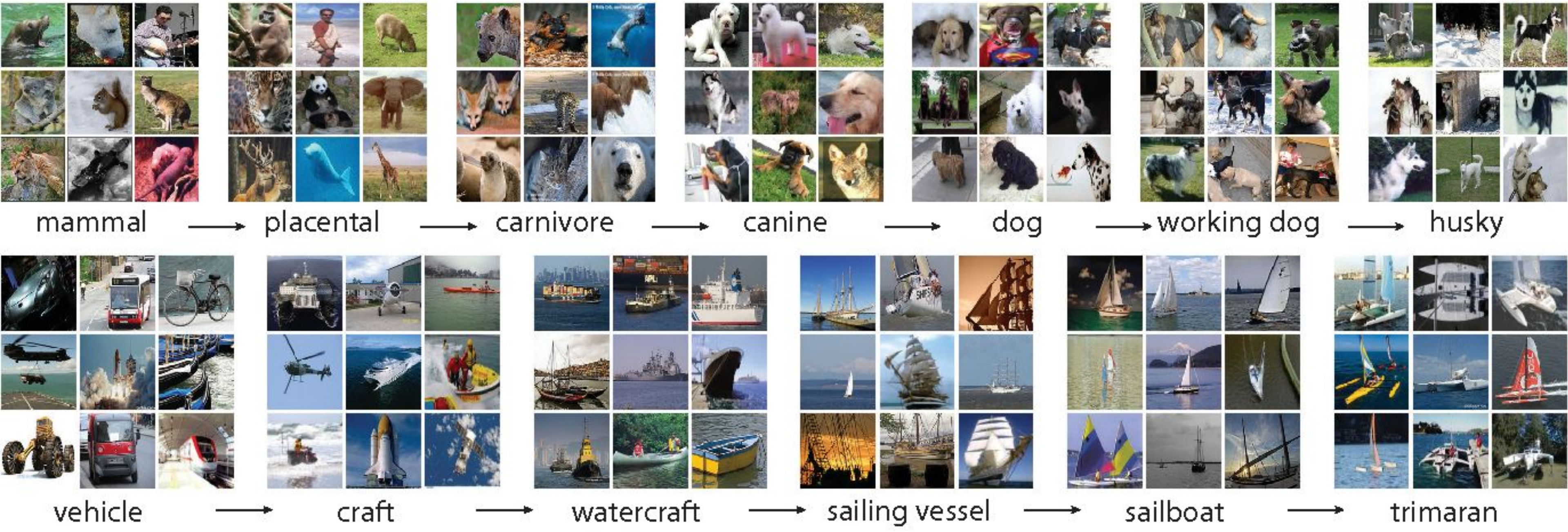
- NN cannot exploit many layers
  - Overfitting
  - Vanishing gradient (with NN training you need to multiply several small numbers → they become smaller and smaller)
- Lack of processing power (no GPUs)
- Lack of data (no large annotated datasets)
- Kernel Machines (e.g. SVMs) suddenly become very popular





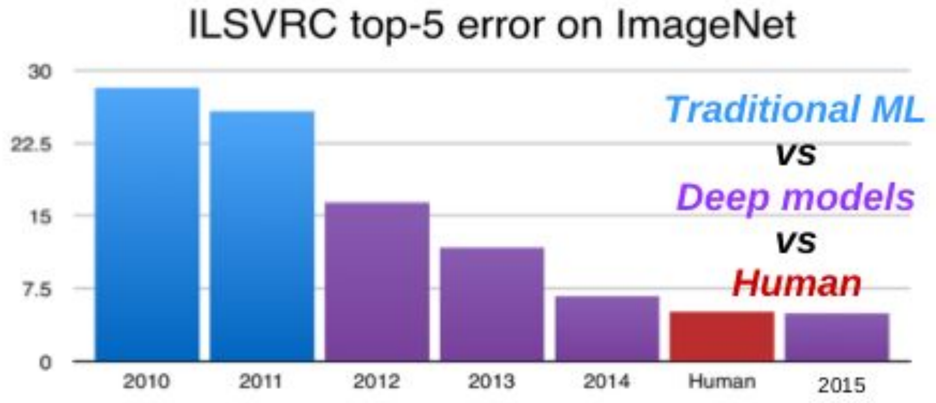
2009: ImageNet

A Large-Scale Hierarchical Image Database


mammal → placental → carnivore → canine → dog → working dog → husky
vehicle → craft → watercraft → sailing vessel → sailboat → trimaran

2012: AlexNet

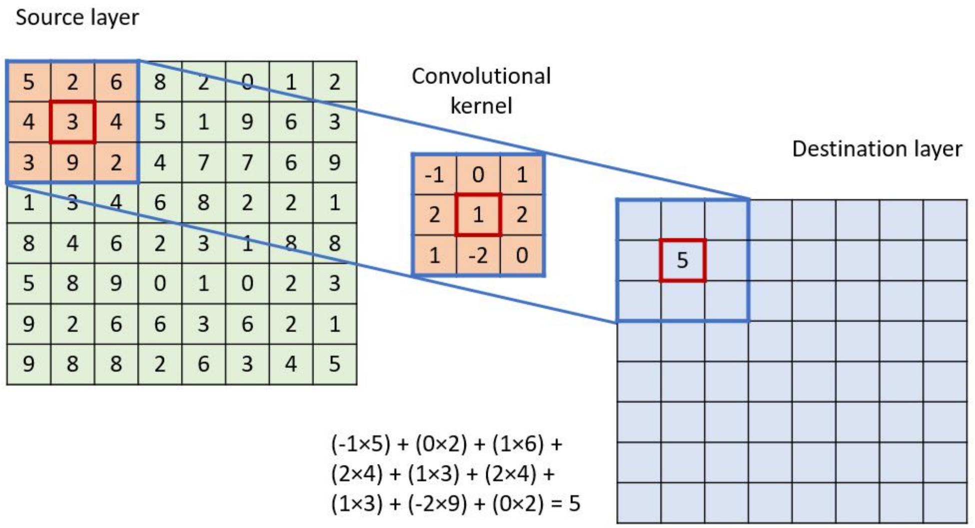
- Hinton's group implemented a CNN similar to LeNet [LeCun1998] but...
  - Trained on ImageNet (1.4M images, 1K categories)
  - With 2 GPUs
  - Other technical improvements (ReLU, dropout, data augmentation)

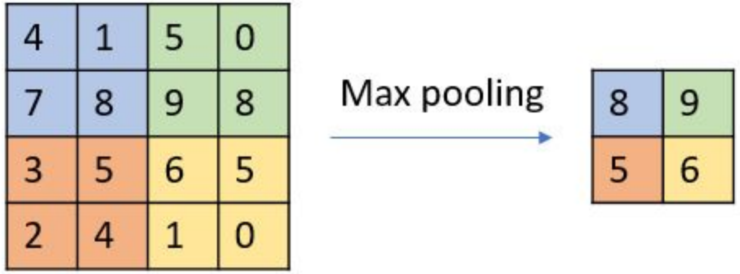


https://papers.nips.cc/paper/4824-imagenet-classification-with-deep-convolutional-neural-networks.pdf

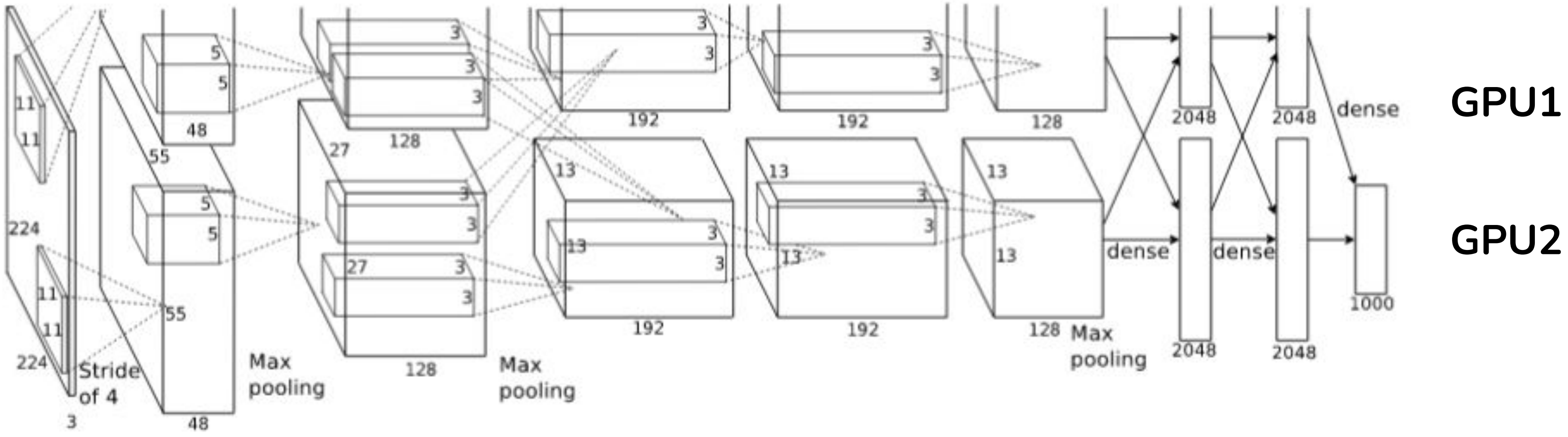
Convolutional NN (CNN)

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





AlexNet

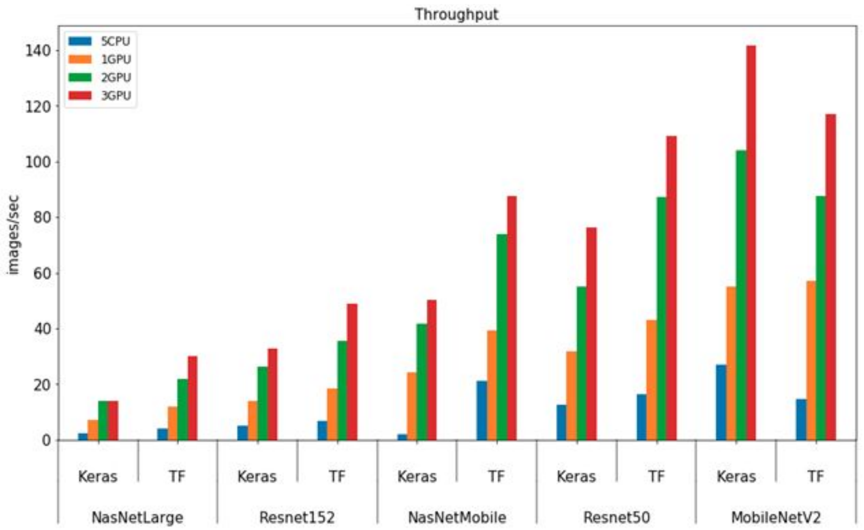


- 60M parameters
- Limited information exchange between GPUs

Why DL now?

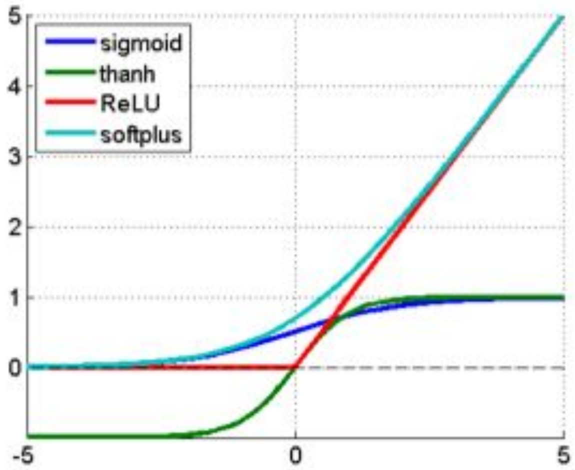
- Three main factors:
  - Better hardware
  - Big data
  - Technical advances:
    - Layer-wise pretraining
    - Optimization (e.g. Adam, batch normalization)
    - Regularization (e.g. dropout)

    ....



2010: Rectified Linear Units (ReLU)

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



Activation function

- 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)

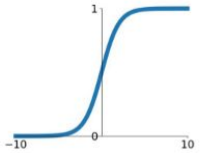
https://www.cs.toronto.edu/~fritz/absps/reluICML.pdf

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

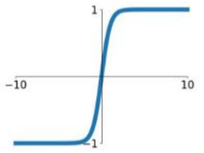
Sigmoid

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



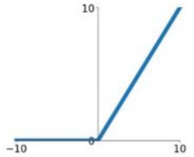
tanh

$\tanh(x)$



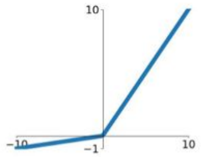
ReLU

$\max(0, x)$



Leaky ReLU

$\max(0.1x, x)$

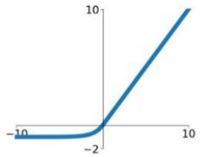


Maxout

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

ELU

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



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

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

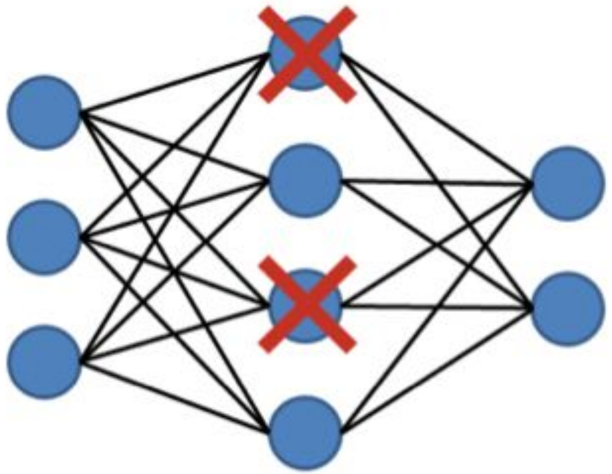
  - **L2** or Ridge regularization adds a penalty which is the sum of the squared values of weights
    - L2+MSE

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

- **Early Stopping** is a time regularization technique which stops training based on given criteria

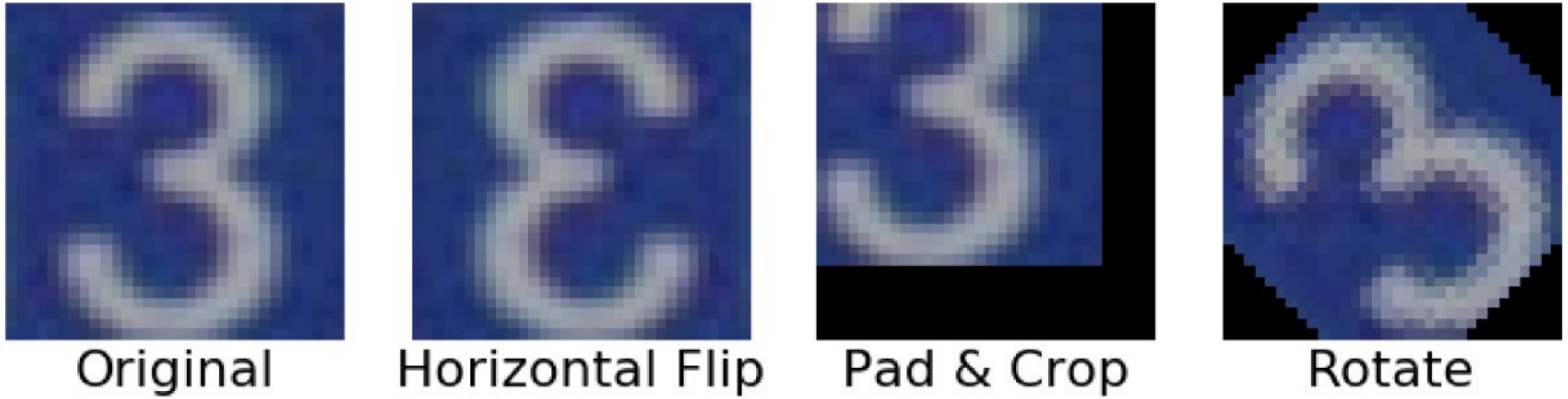
Dropout

- 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

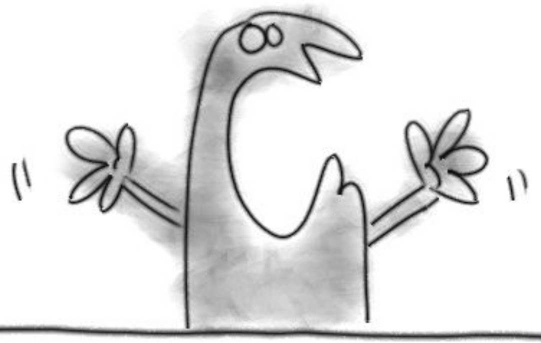


Data augmentation

- 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

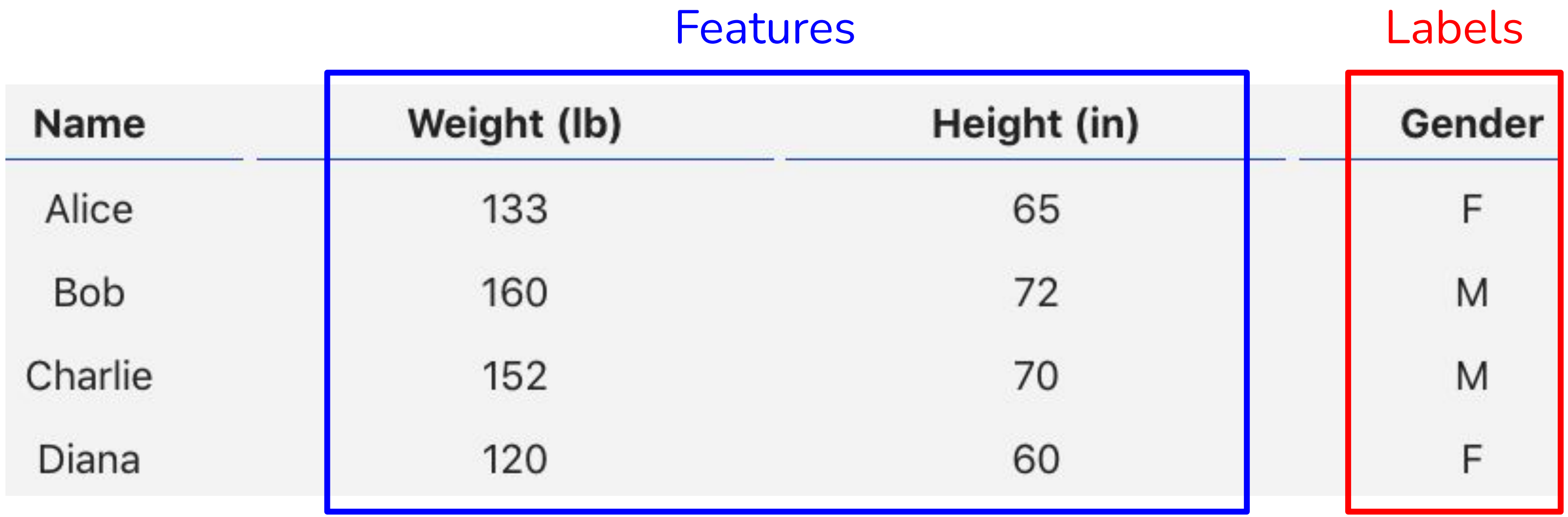


Now What?!!



Training a neural network

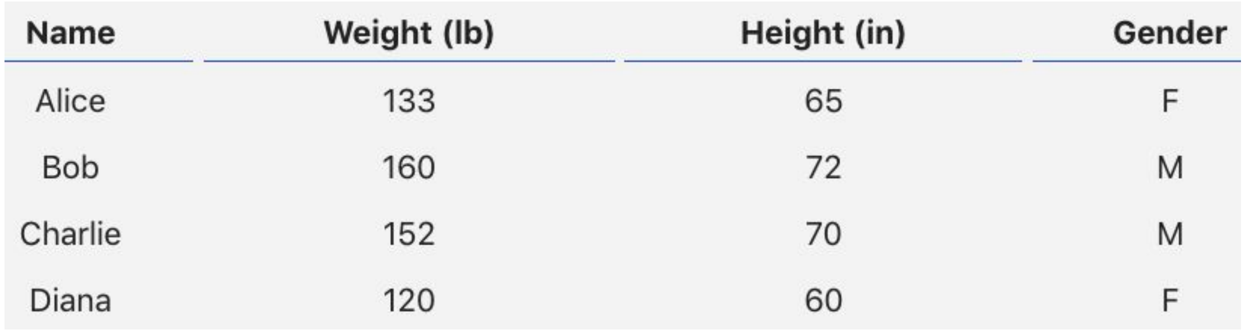
- **Problem:** Predict gender from weight and height
- **Input Dataset:**


Features
Labels

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

1. Feature engineering

- Symmetrize numeric values
- Category -> numbers



Name	Weight (lb)	Height (in)	Gender
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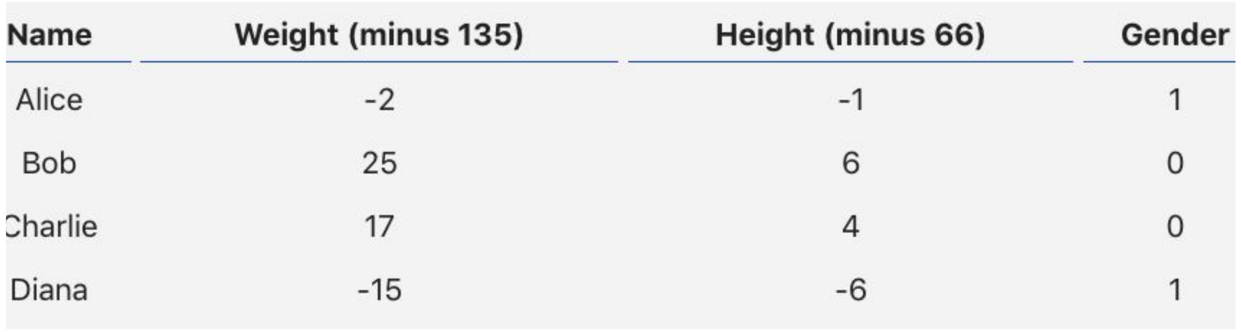
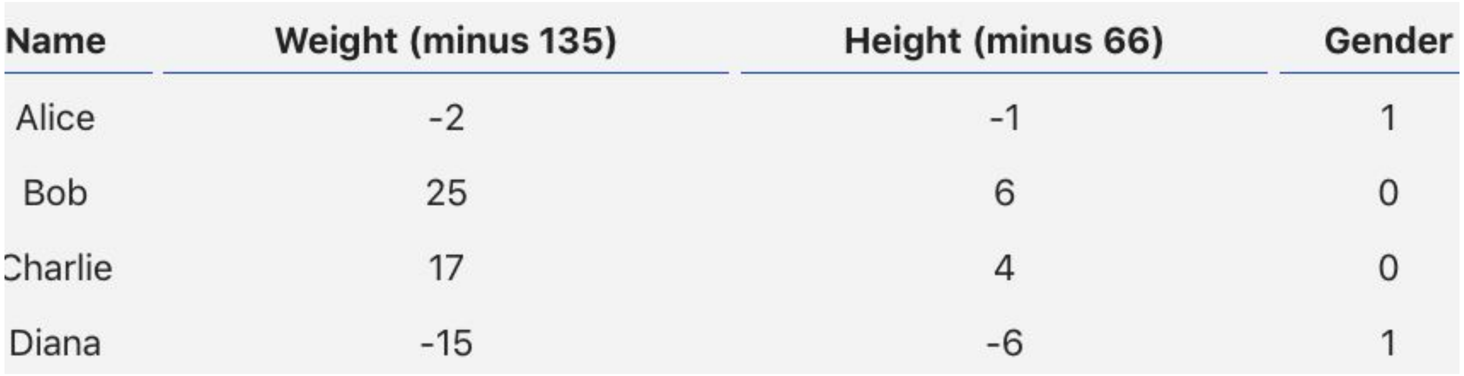
Diana	120	60	F



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

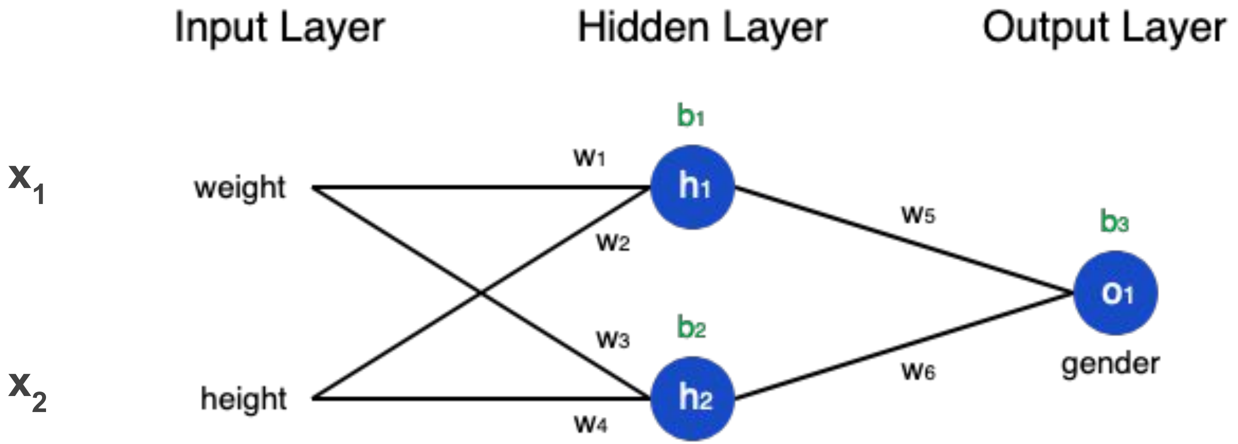
- **n** : 4, number of samples (Alice, Bob, Charlie, Diana)
- **Inputs: X**, dimension = 2
  - weights **(X_1)** and heights **(X_2)**
- **Features: $x = (x_1, x_2)$**, transformed inputs
- **y** : variable being predicted (Gender)
- **y_{true}** : true value of y



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

2. Model

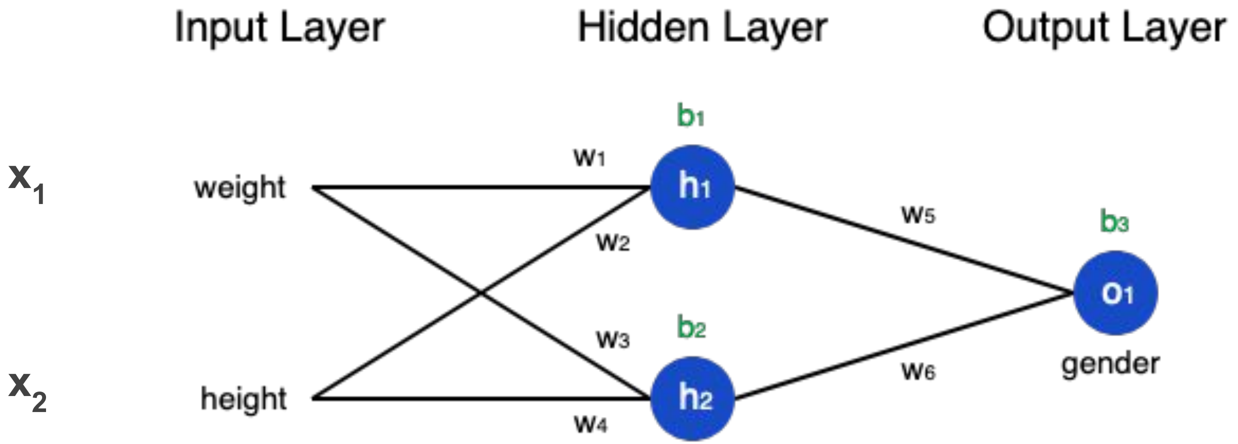
- $\mathbf{y_{pred}}$: predicted value of y = **o**
- Neural network: with 1 hidden layer with 2 neurons
- Outputs of the hidden layer: **h**
- Unknown parameters: weights **w** and biases **b**



Some math

- For each neuron: $y_j = b_j + \mathbf{f} \sum_i x_i w_{ij}$
- **f** is the activation function

- For the net:
    - $h_1 = f(w_1x_1+w_2x_2)+b_1$
    - $h_2 = f(w_3x_1+w_4x_2)+b_2$
    - $o_1 = f(w_5h_1+w_6h_2)+b_3$



3. Model training

- Training the network == Find weights **w** and biases **b** that minimize the loss
- Loss function **L: MSE**
- Find weights **w** and biases **b** to minimise

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

$$L(w_1, w_2, w_3, w_4, w_5, w_6, b_1, b_2, b_3)$$

- Typically, this is already implemented in ML software packages

1986: Back propagation

- Gradient descent
- Chain rule
- Layered Computation

- Minimization taking **partial derivatives**
- For very simple case: with only Alice in the dataset, n=1

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

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

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

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

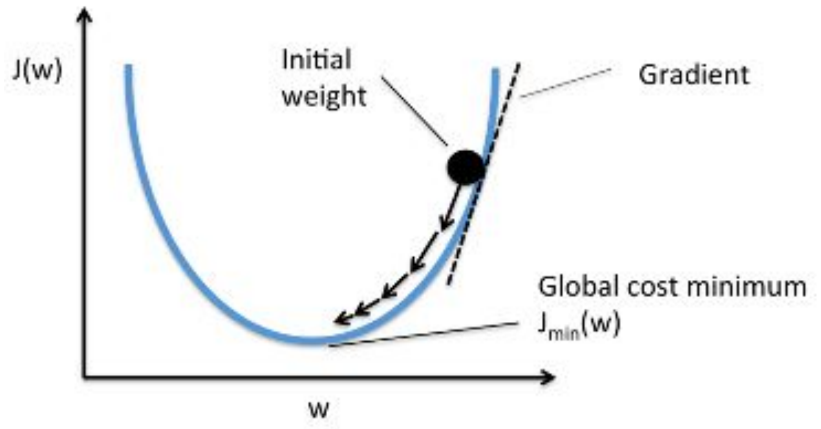
$$y_{pred} = o_1 = f(w_5 h_1 + w_6 h_2 + b_3)$$

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

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

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

Stochastic Gradient Descent (SGD)



- Start with randomly initialised weights
- **update equation**:

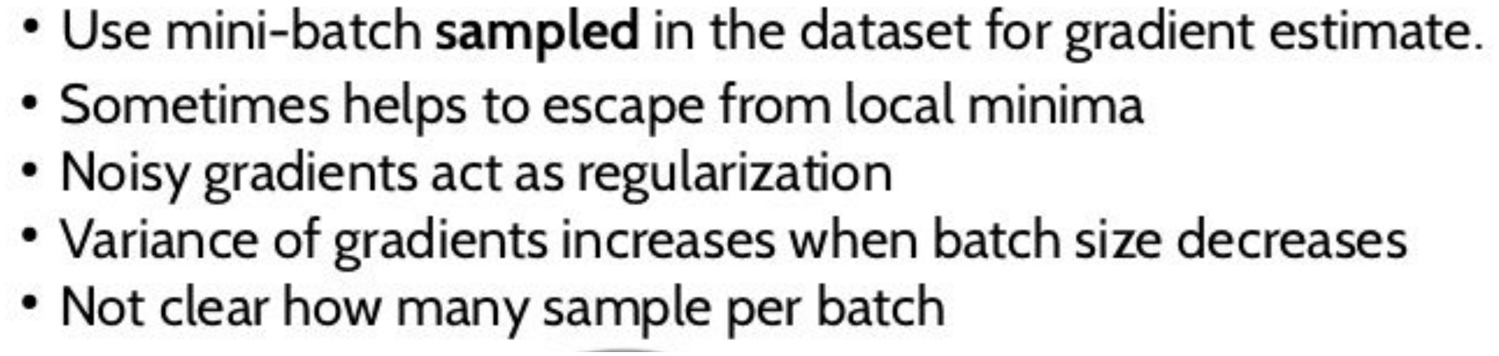
$$w_1 \leftarrow w_1 - \eta \frac{\partial L}{\partial w_1}$$

- **η** is a constant called the **learning rate** 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 vs Batch Gradient Descent (BGD) vs mini-batch

- In SVG the parameters are updated using only one single training instance (usually randomly selected) in each iteration vs the whole training set (== batch)



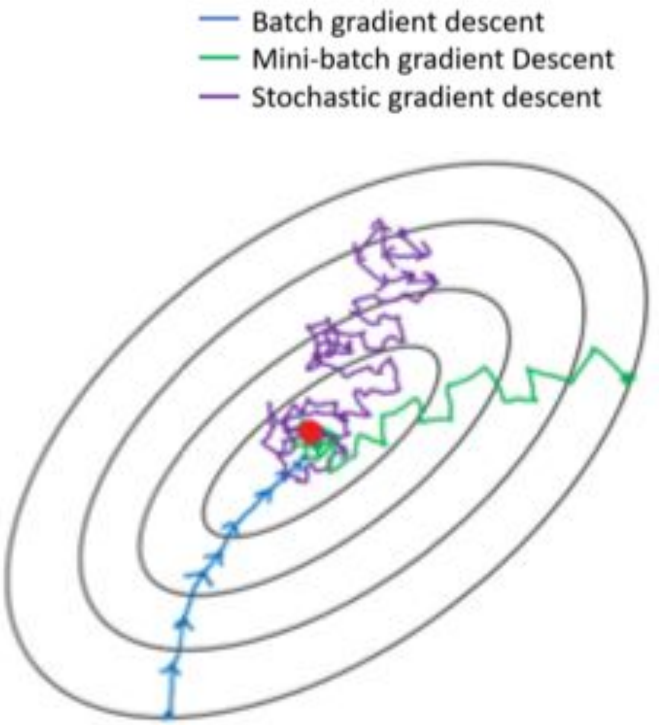
- Use mini-batch **sampled** in the dataset for gradient estimate.
- Sometimes helps to escape from local minima
- Noisy gradients act as regularization
- Variance of gradients increases when batch size decreases
- Not clear how many sample per batch

What happens in **one epoch** for SGD:

1. Take a random sample
2. Feed it to Neural Network
3. Calculate its gradient
4. Use the gradient we calculated in step 3 to update the weights
5. Repeat steps 1–4 for all the examples in training dataset

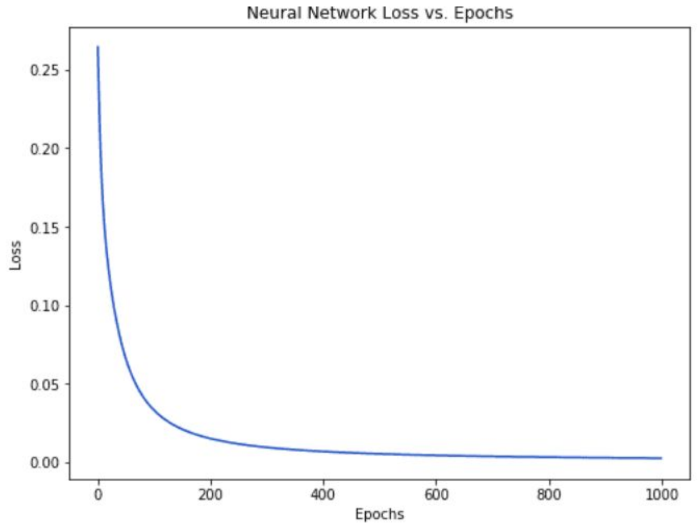
What happens in **one epoch** for Mini-BGD**:**

1. Pick a mini-batch
2. Feed it to Neural Network
3. Calculate the mean gradient of the mini-batch
4. Use the mean gradient we calculated in step 3 to update the weights
5. Repeat steps 1–4 for the mini-batches we created



Take home messages

- **Gradient descent** is an iterative learning algorithm that uses a training dataset to update a model.
    - **BGD**: Batch Size = Size of Training Set
    - **SGD**: Batch Size = 1
    - **Mini-BGD**. 1 < Batch Size < Size of Training Set
- The **batch size** is a hyperparameter of gradient descent that controls the number of training samples to work through before the model's internal parameters are updated.



- The number of **epochs** is a hyperparameter of gradient descent that controls the number of complete passes through the training dataset