Neural Networks: History and foundation

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Course Intro

- Symbolic AI
- Neural Networks
- Computer Vision
- NLP
- Audio
- DL & Neuroscience

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- **Symbolic AI**
  - History and Foundations
- **Neural Networks**
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- **Computer Vision**
  - Image Classification
  - Unsupervised learning
  - Detection Segmentation
  - Visual Reasoning
- **NLP**
  - Basics
  - RNNs for NLP
  - Attention Transformers
- **Audio**
  - Sound & Speech Processing
- **DL & Neuroscience**
  - CNNs & brains
  - Spiking NNs
  - Brain Decoding

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Outline

Session 1

- History of neural networks
- Artificial neurons - Perceptrons
- Multi-layer perceptrons (MLPs)
- Optimization and objective functions
- Gradient descent and Back-propagation

Session 2

- How to design neural networks
- Choosing the architecture (CNN, RNN)
- Choosing the loss function
- Training a neural network
- Practical examples

Neural networks milestones

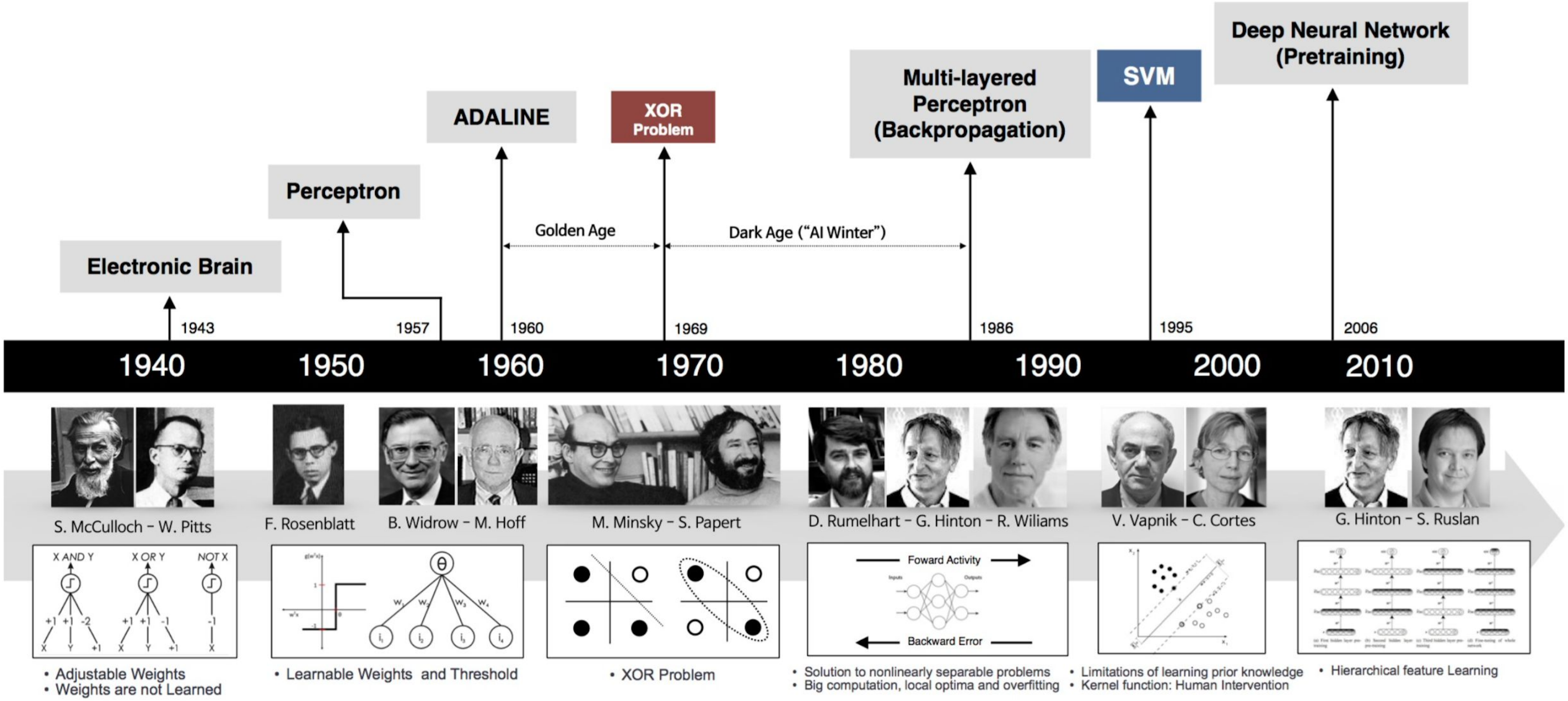
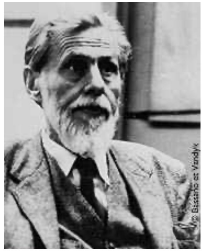


Image source: http://beamlab.org/deeplearning/2017/02/23/deep_learning_101_part1.

The beginning of Neural nets (1940s-1960s)

Artificial neuron: McCulloch & Pitt's neuron model (1943)



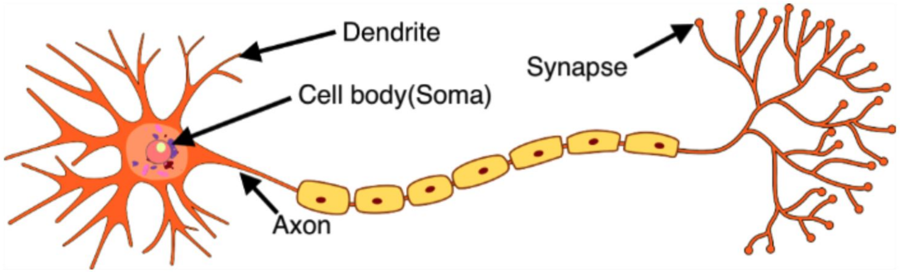
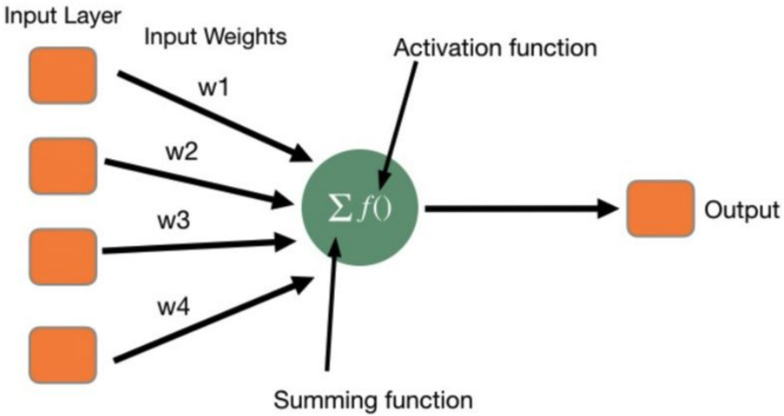


Image source: Wikimedia Commons

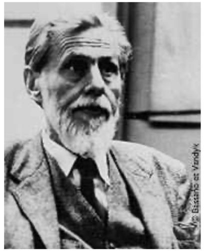
Schematic of a biological neuron



Model of an artificial neuron

The beginning of Neural nets (1940s-1960s)

Artificial neuron: McCulloch & Pitt's neuron model (1943)



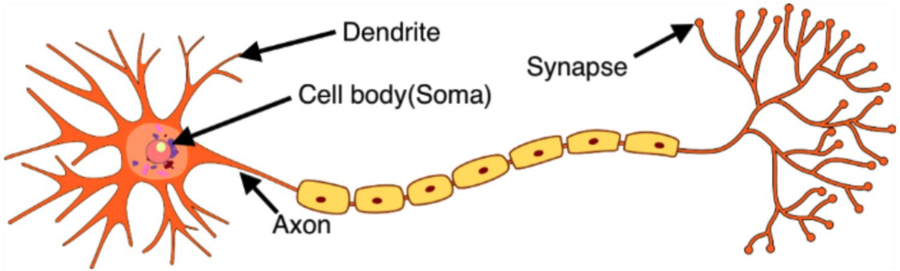
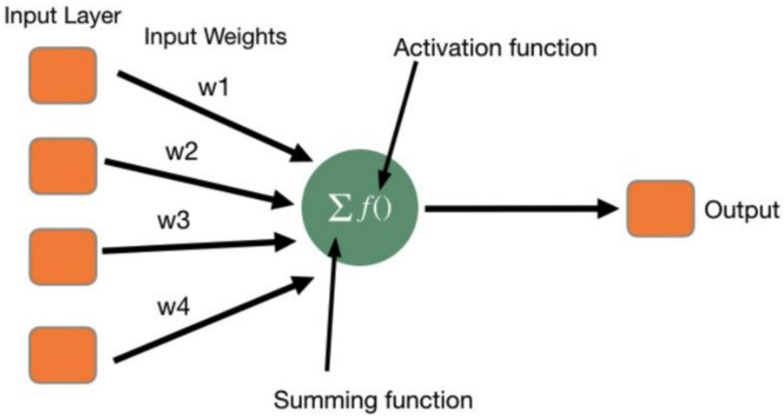


Image source: Wikimedia Commons

Schematic of a biological neuron



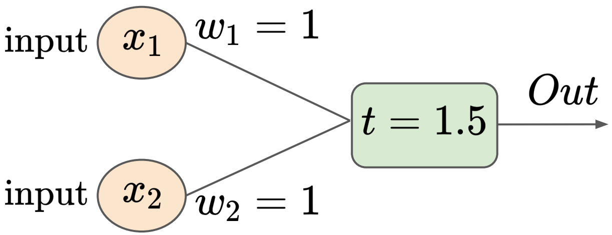
$$\text{output} = \begin{cases} 0 \quad if \quad t > \sum_{i=0}^{n} w_i x_i \\ 1 \; otherwise \end{cases}$$

Single-layer neuron examples

- An artificial neuron could solve **linear** logical problems: AND, OR, NOT

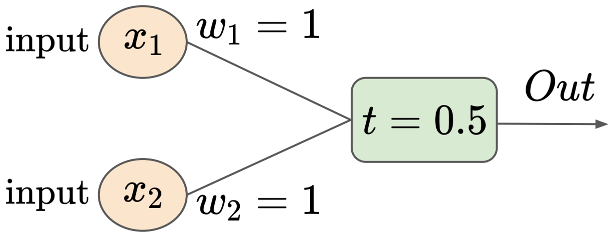
AND

x_1	x_2	Out
0	0	0
0	1	0
1	0	0
1	1	1



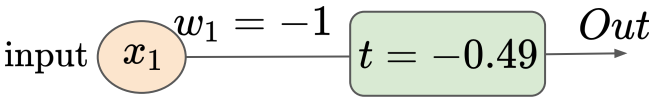
OR

x_1	x_2	Out
0	0	0
0	1	1
1	0	1
1	1	1

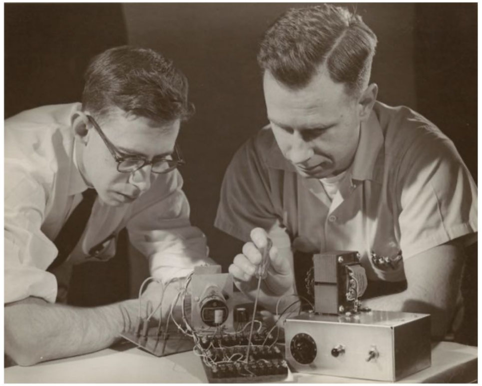


NOT

x_1	Out
0	1
1	0

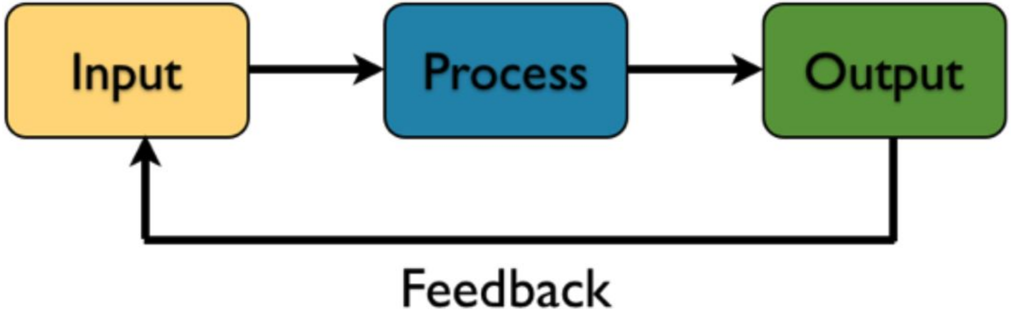


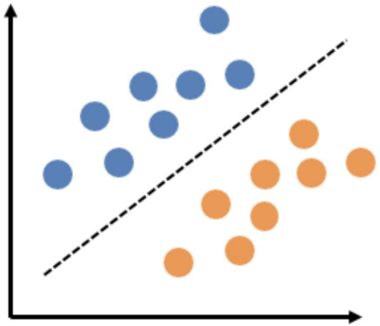
Perceptron: A learning algorithm for the neuron model



Rosenblatt, F. (1957). *The perceptron, a perceiving and recognizing automaton Project Para*.

- Automatic learning of weights
- Supervised learning of binary classifiers
- Could recognize letters and numbers





The Perceptron Learning Algorithm

$$Let\ D = (\langle x_1, y_1\rangle, \langle x_2, y_2\rangle, \ldots, \langle x_n, y_n\rangle) \in (\mathbb{R}^m \times \{0, 1\})^n$$

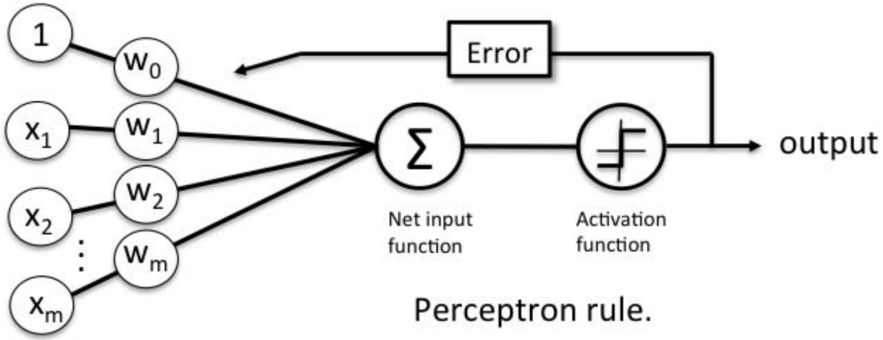
1. Initialise w_i *with random small values*
2. For every training epoch:

   For every sample $\langle x_i,\ y_i\rangle \in D$:

   (a) $\hat{y} := \sigma(x_i \times w)$ ← Compute output (prediction)

   (b) $err := (y_i - \hat{y}_i)$ ← Compute error

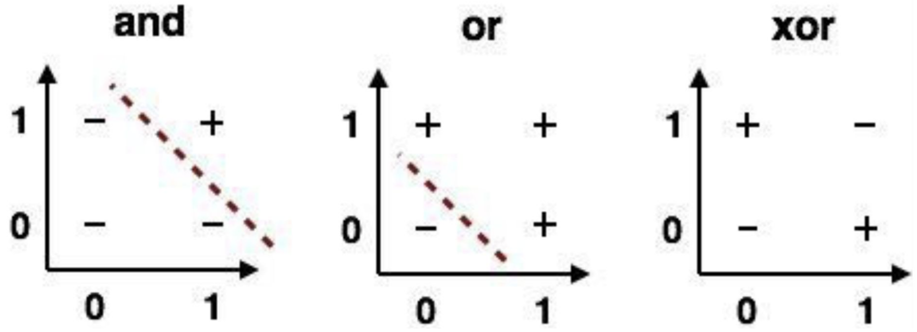
   (c) $w := w + err \times x_i$ ← Update parameters

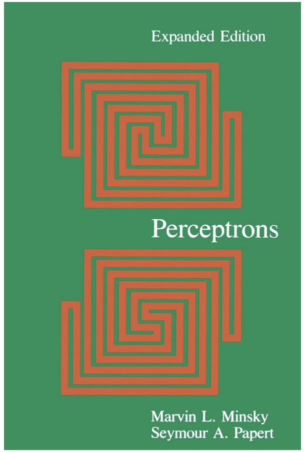


Perceptron rule.

The first AI winter

Minsky and Papert (1969) show that the perceptron can't even solve the XOR problem



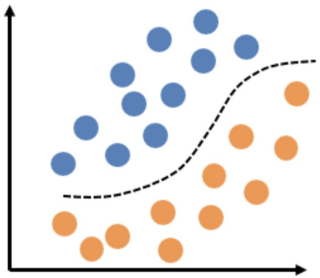


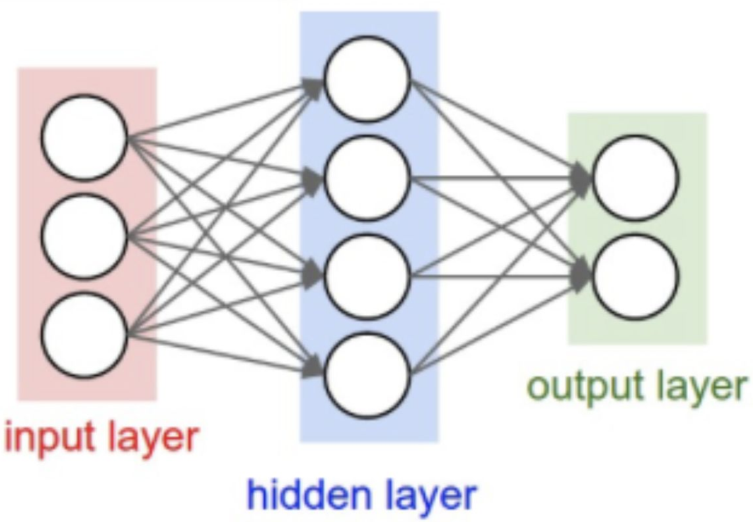
$\Rightarrow$ Kills research on neural nets for the next 15-20 years

Multilayer perceptrons (1980's)

Solution to the XOR problem: **Multilayer perceptrons**

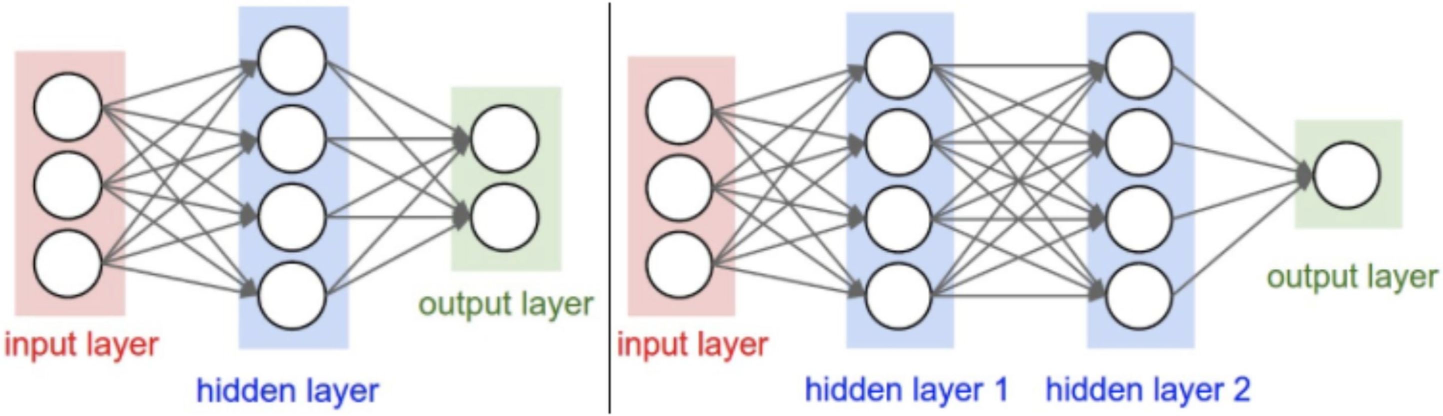
- Composed of: **input** layer, **hidden** layer(s) and an **output** layer.
- Each node (of hidden and output layers) is a neuron that uses a **nonlinear** activation function.
- It can distinguish data that is **not linearly** sep





Multilayer perceptrons (1980's)

Can add more layers to increase capacity of the network



- <u>New problem:</u> MLPs are hard to train!

Multilayer perceptrons (1980's)

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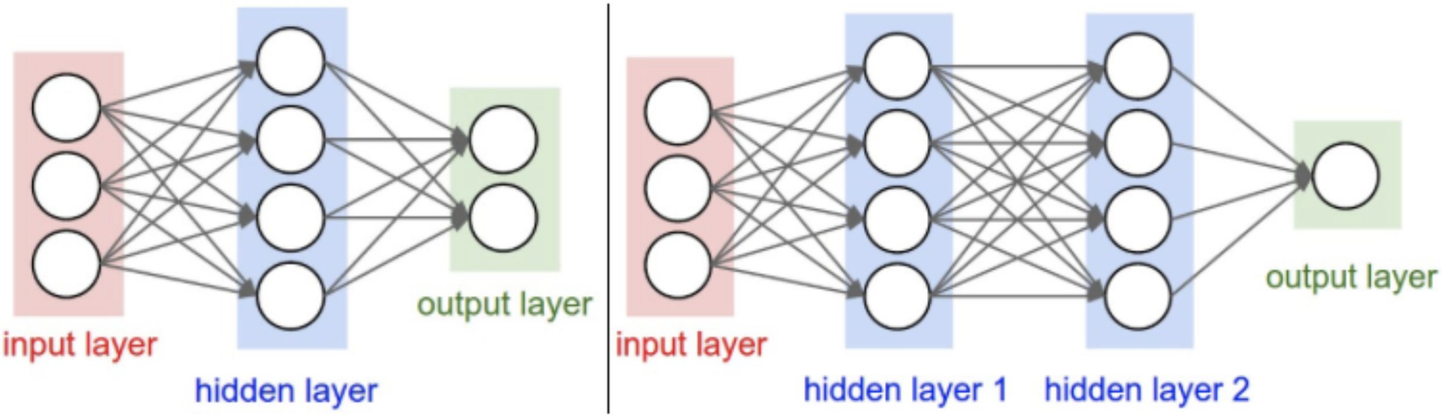


- <u>New problem:</u> MLPs are hard to train!

⇒ Solution: The **Backpropagation** algorithm

The Backpropagation algorithm

Learning representations by back-propagating errors

David E. Rumelhart*, Geoffrey E. Hinton† & Ronald J. Williams*

* Institute for Cognitive Science, C-015, University of California, San Diego, La Jolla, California 92093, USA
† Department of Computer Science, Carnegie-Mellon University, Pittsburgh, Philadelphia 15213, USA

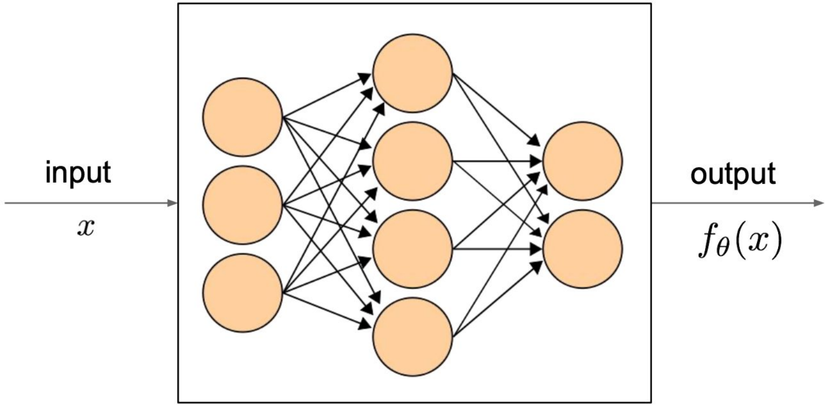
We describe a new learning procedure, back-propagation, for networks of neurone-like units. The procedure repeatedly adjusts the weights of the connections in the network so as to minimize a measure of the difference between the actual output vector of the net and the desired output vector. As a result of the weight adjustments, internal 'hidden' units which are not part of the input or output come to represent important features of the task domain, and the regularities in the task are captured by the interactions of these units. The ability to create useful new features distinguishes back-propagation from earlier, simpler methods such as the perceptron-convergence procedure[1].

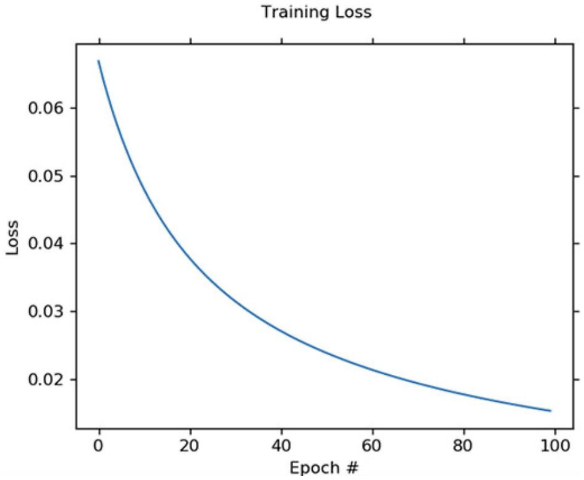
Rumelhart, Hinton, and Williams (1986) introduced Backpropagation to train MLPs

Principle: Computing the <u>gradient</u> of the <u>cost function</u> w.r.t the weights of the network

Neural Network learning as optimization

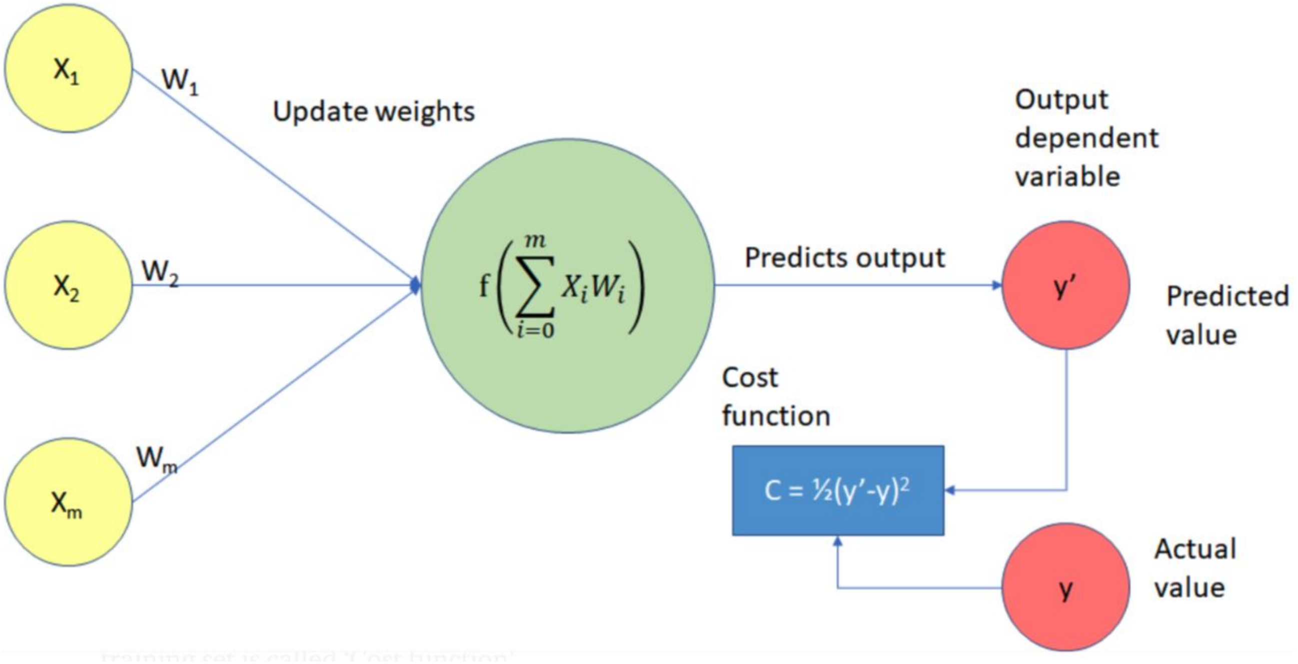
- Mapping a set of inputs to a set of outputs from training data
- Learning is cast as an **optimization** problem to make good enough predictions
- Training with **gradient descent**





Cost functions

- A cost function is a measure of error between predictions and true values



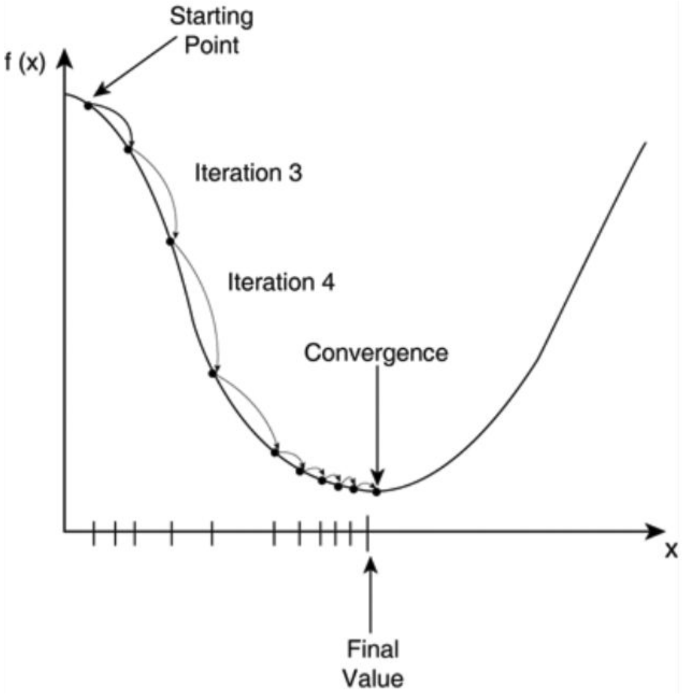
Cost functions

- A cost function is a measure of error between predictions and true values
- Guides the training process to find a set of weights that minimizes its value

<u>Some examples:</u>

$$\mathrm{MAE} = \underbrace{\frac{1}{n}\sum_{i=1}^{n}}_{\text{test set}} \left|\underbrace{y_i}_{\text{predicted vaue}} - \underbrace{\hat{y}_i}_{\text{actual value}}\right|$$

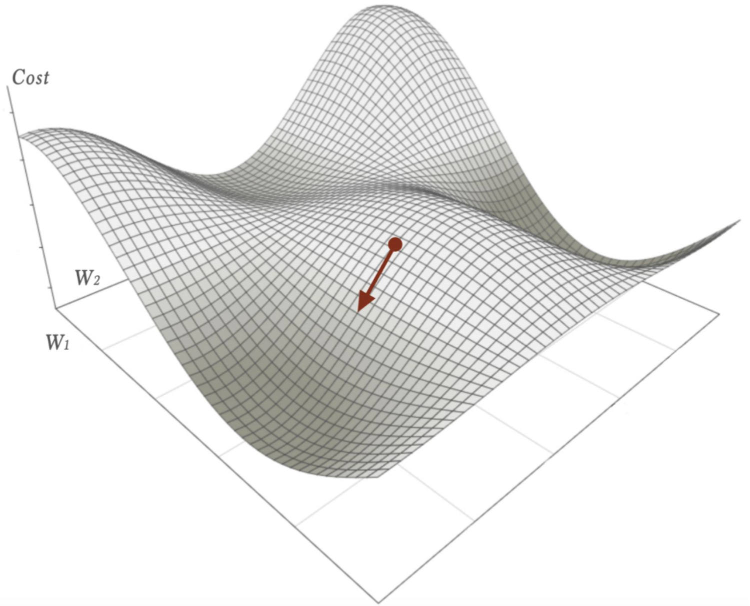
$$\mathrm{MSE} = \underbrace{\frac{1}{n}\sum_{i=1}^{n}}_{\text{test set}} \left(\underbrace{y_i}_{\text{predicted vaue}} - \underbrace{\hat{y}_i}_{\text{actual value}}\right)^2$$



Gradient Descent

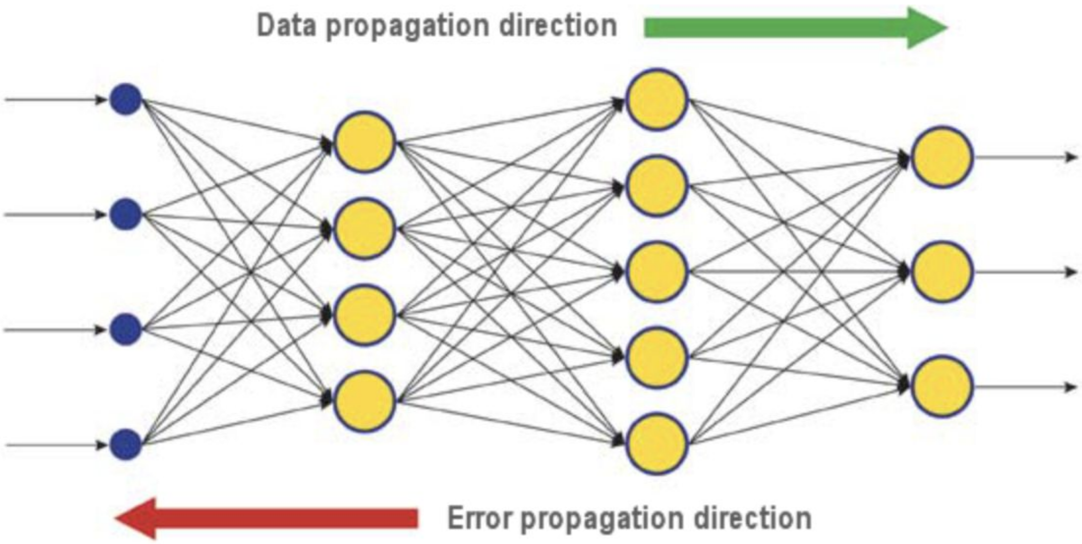
- Finding minimum of the cost function C
- Negative gradient $-\nabla C$ points in the direction where the function decreases most rapidly
- Calculate new weights: $W^+ = W - \eta \, \nabla C$

$$\begin{bmatrix} w_1^+ \\ w_2^+ \\ \vdots \\ w_n^+ \end{bmatrix} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} - \eta \begin{bmatrix} \frac{\partial C}{\partial w_1} \\ \frac{\partial C}{\partial w_2} \\ \vdots \\ \frac{\partial C}{\partial w_n} \end{bmatrix}$$



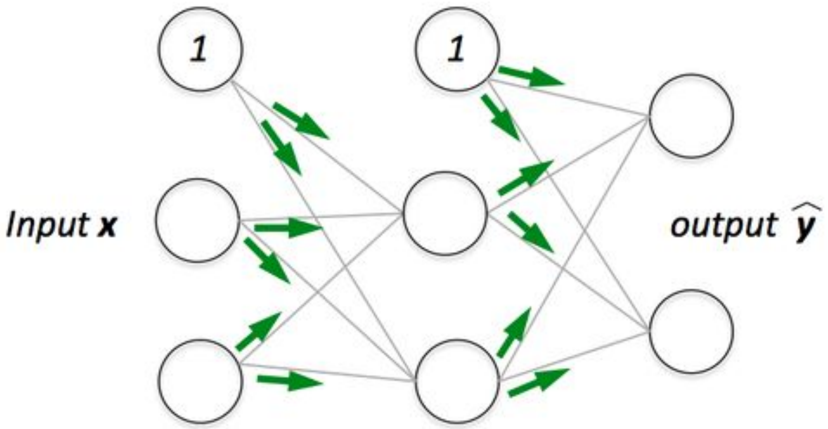
How Backpropagation works

- **Minimization** through **gradient descent** requires computing the gradient
- Backpropagation: way to compute the gradient by applying the **chain rule**



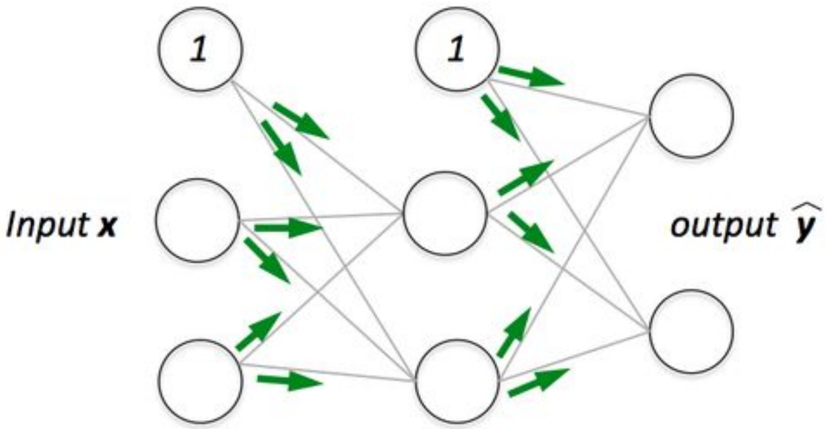
How Backpropagation works

1) Forward pass: propagate data through the network to get predictions



How Backpropagation works

1) Forward pass: propagate data through the network to get predictions
2) Calculate the total error w.r.t desired outputs

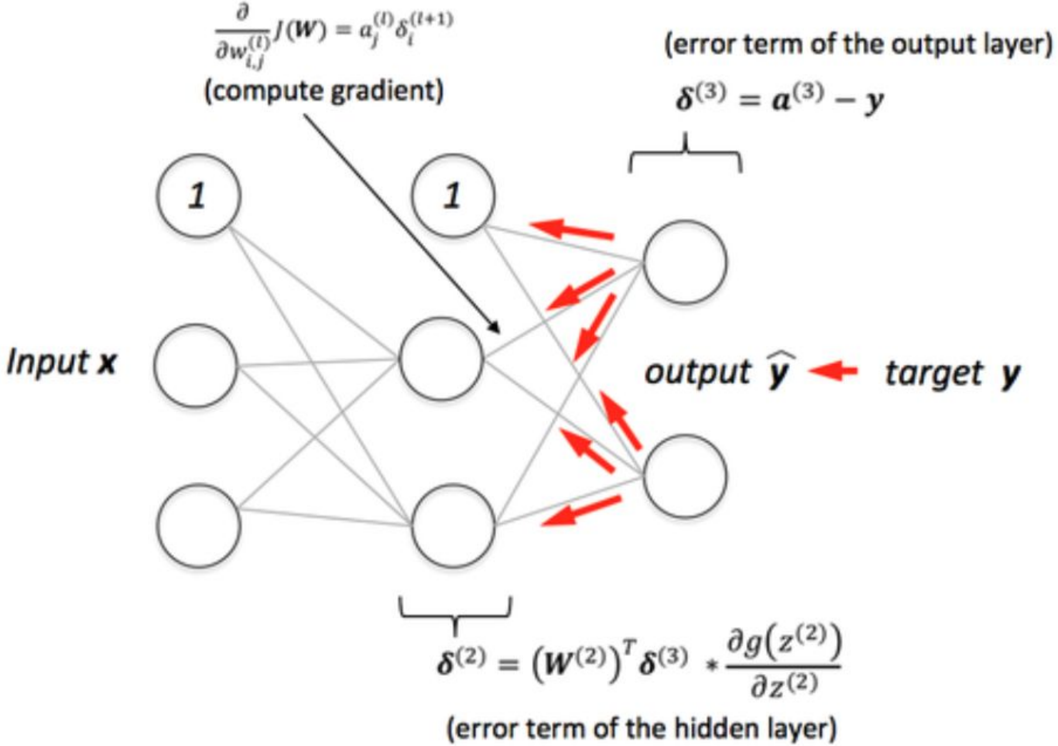


How Backpropagation works

1) <u>Forward pass:</u> propagate data through the network to get predictions
2) Calculate the total error w.r.t desired outputs
3) <u>Backward pass:</u>

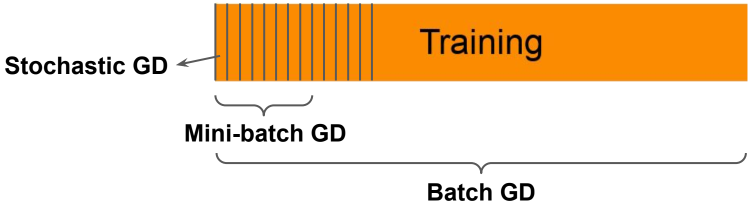
   a) Compute partial derivatives of the error w.r.t each weight $\frac{\mathrm{d}E}{\mathrm{d}w_{ij}}$ by applying the **<u>chain rule</u>**

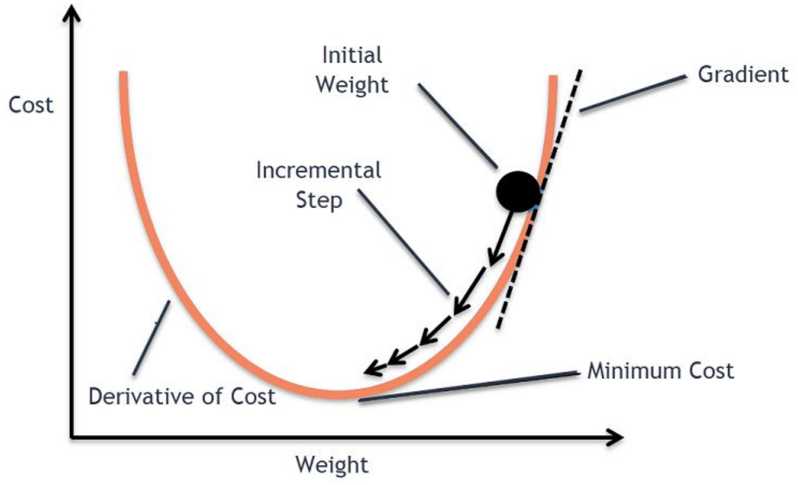
   b) Update weights:
   $$w_i = w_i - \eta \frac{\mathrm{d}E}{\mathrm{d}w_{ij}}$$



Training with Gradient descent and BP

- **batch** GD, **stochastic**, or **mini-batch**?
- **SGD** in DL generally refers to mini-batch GD





Some useful resources

http://neuralnetworksanddeeplearning.com/chap1.html

https://towardsdatascience.com/part-2-gradient-descent-and-backpropagation-bf90932c066a

https://towardsdatascience.com/a-concise-history-of-neural-networks-2070655d3fec#.ekc89166m

https://people.idsia.ch//~juergen/who-invented-backpropagation.html

Training a neural network

Data

Data Samples and Labels

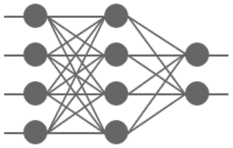
$$\{(x_1, y_1), (x_2, y_2), ...\}$$

Task

Input and output

$$x_i \rightarrow y_i$$

Architecture



Loss function

$$loss = diff(prediction, label)$$

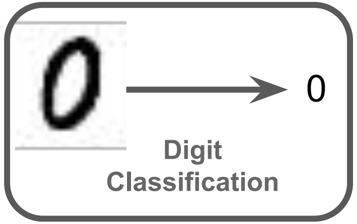
Optimization

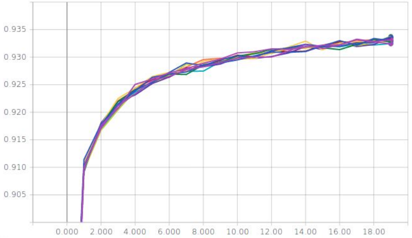
prediction → backpropagation → gradient descent → prediction

Training a neural network

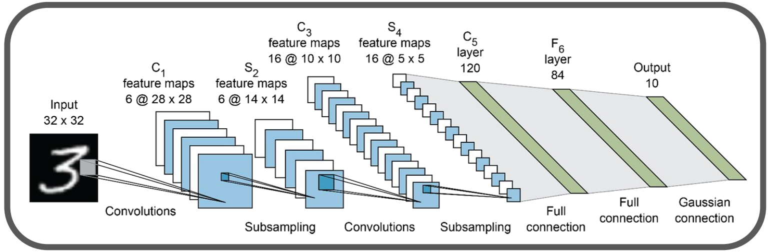
Data

Task

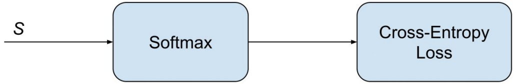




Architecture

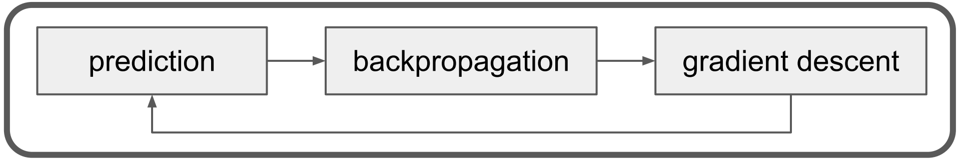


Loss function

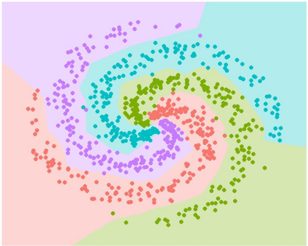


$$f(s)_i = \frac{e^{s_i}}{\sum_j^C e^{s_j}} \qquad CE = -\sum_i^C t_i log(f(s)_i)$$

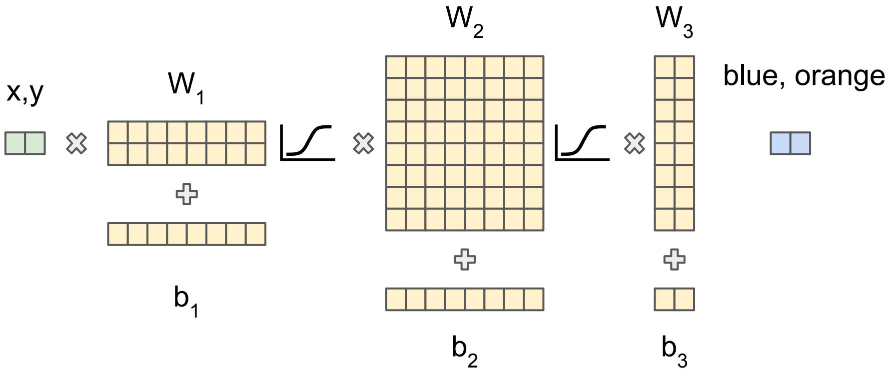
Optimization

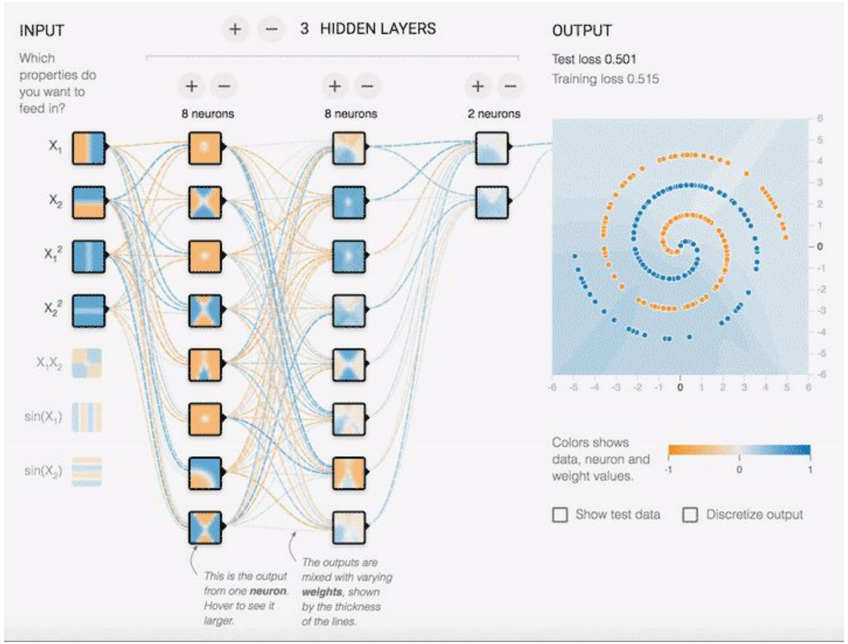


How to choose the architecture



Multi-layer perceptrons **MLPs** are the standard solution for data with simple structure (ex. tabular data).



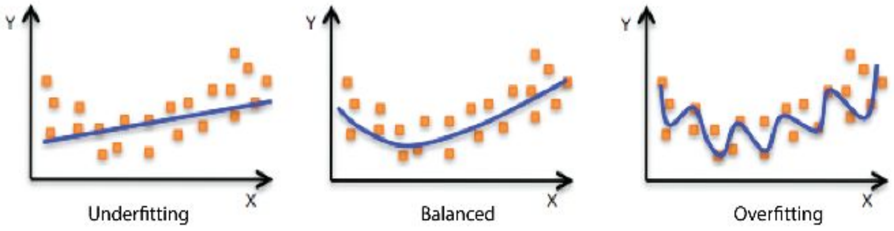


Source: playground.tensorflow.org

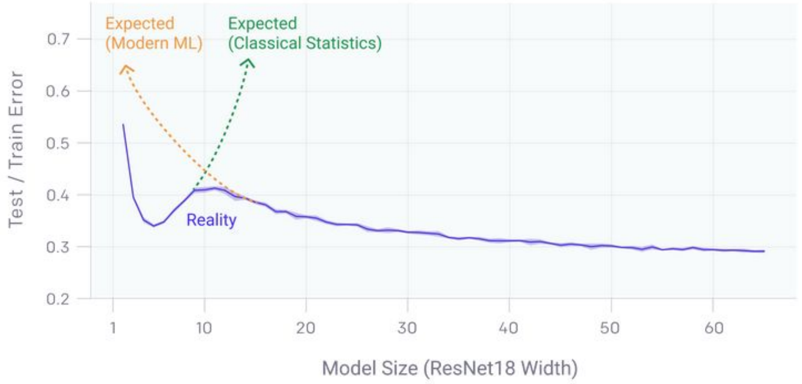
How to choose the architecture

What's important ?

- Generalization
  - Fitting the data distribution
  - Fitting unseen examples



- Efficiency
  - Memory (how large is the model ?)
  - Time (how long does it take to train ?)
  - Data (how many training samples does it need ?)



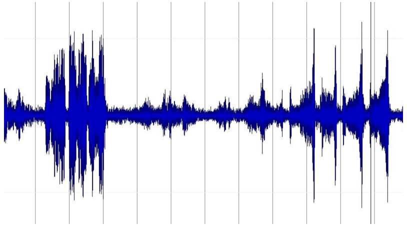
How to choose the architecture

Do MLPs work for all types of data ? Yes, but not efficiently

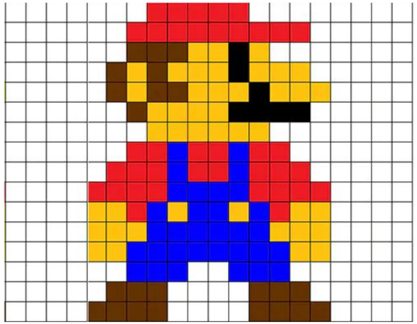
text

I am a student

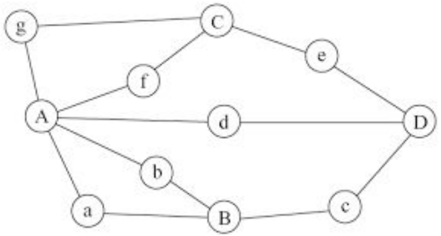
time sequences



images

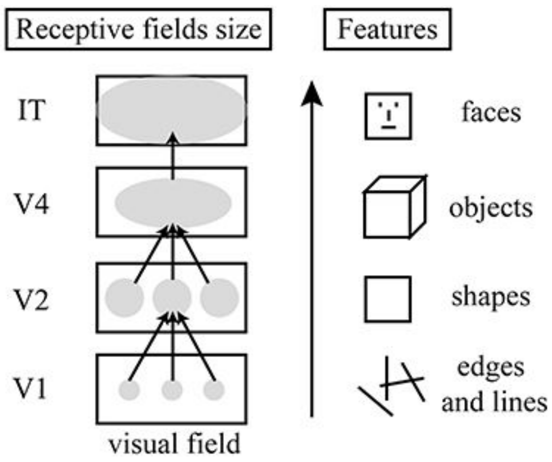


graphs



Inductive bias : an architectural assumption or constraint

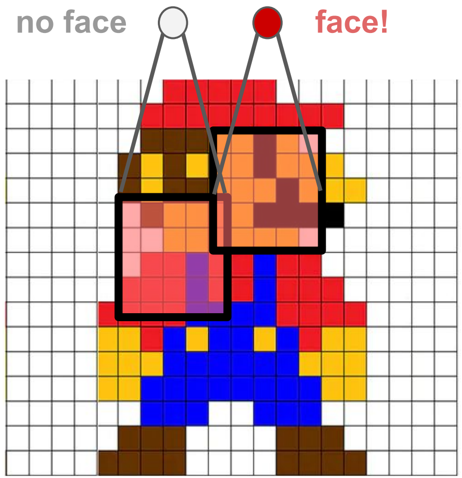
Convolutional Neural Network (CNN)



Local Connectivity

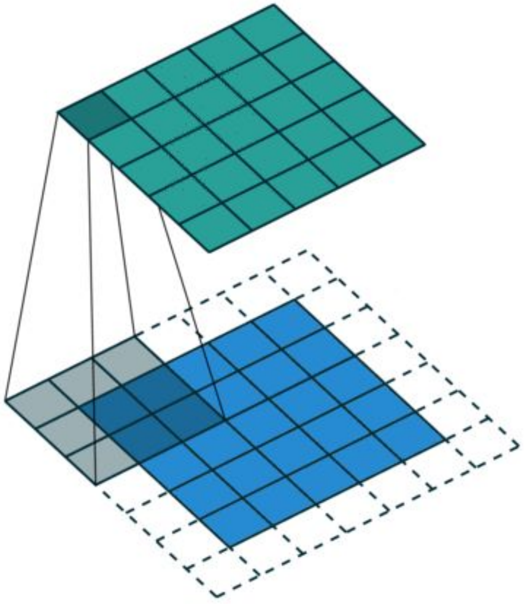
Hierarchical Processing

+



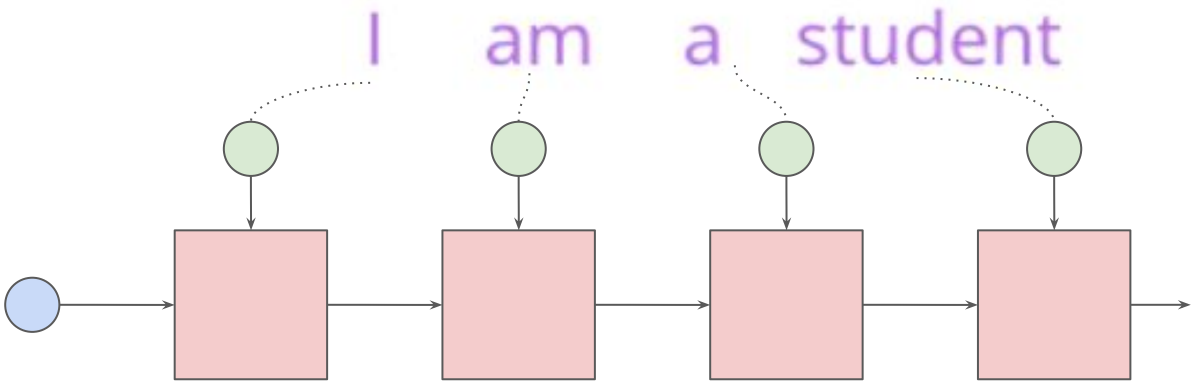
Weight sharing

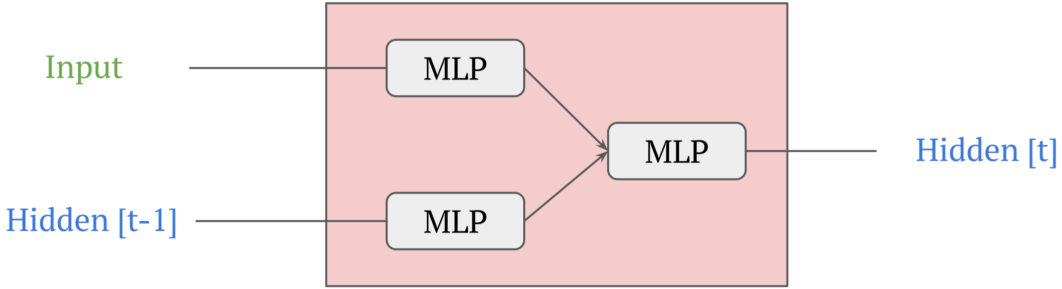
=



Convolution

Recurrent neural networks (RNN)



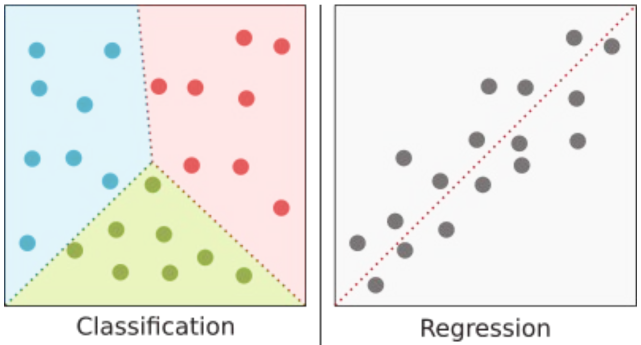


How to choose the loss

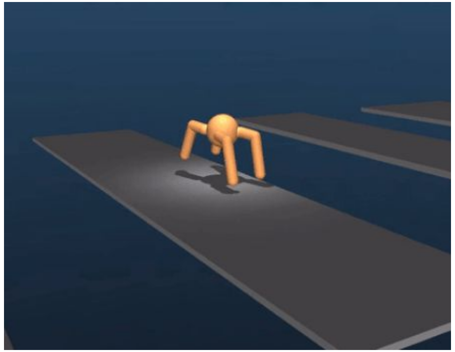
The choice of the loss is crucial !

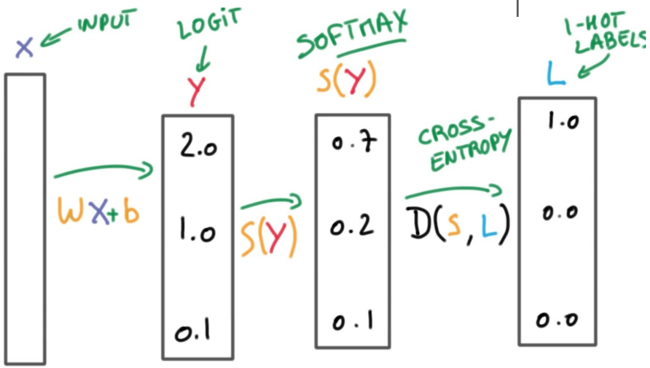
What’s important in the loss design?

- Adaptability to the problem (correlates with performance metrics)
- Continuous and differentiable
- Numerically stable



	Classification	Regression
Label :	Categorical (discrete)	Continuous
Examples :	Cross Entropy Hinge Loss	Mean Square Error (L2) Mean Absolute Error (L1)





Cross Entropy

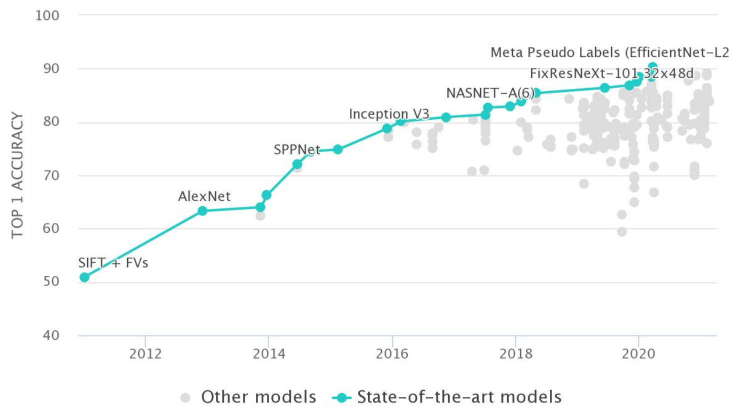
Training and Evaluation

Training: optimization of the model

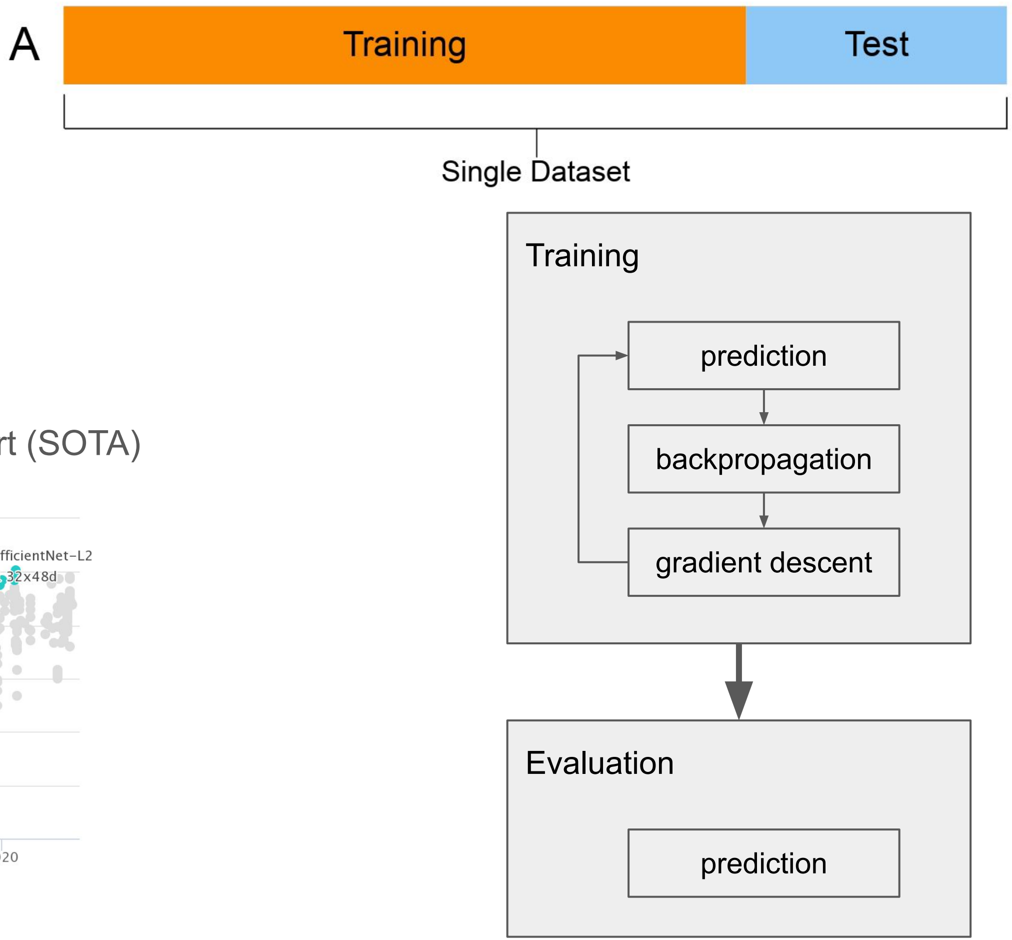
Evaluation: testing generalization

Metrics: Loss and accuracy

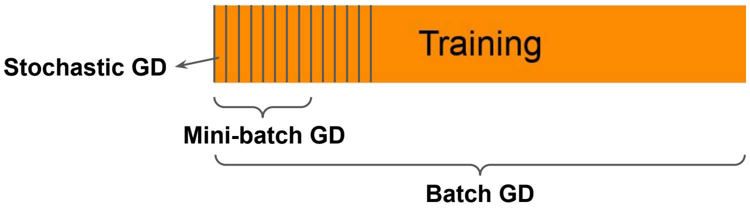
Models with the highest accuracy are state of the art (SOTA)



Imagenet Benchmark on paperswithcode.com

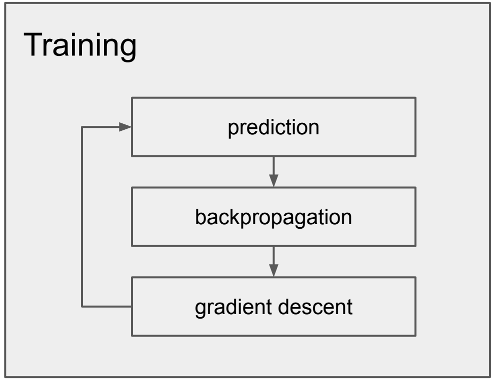


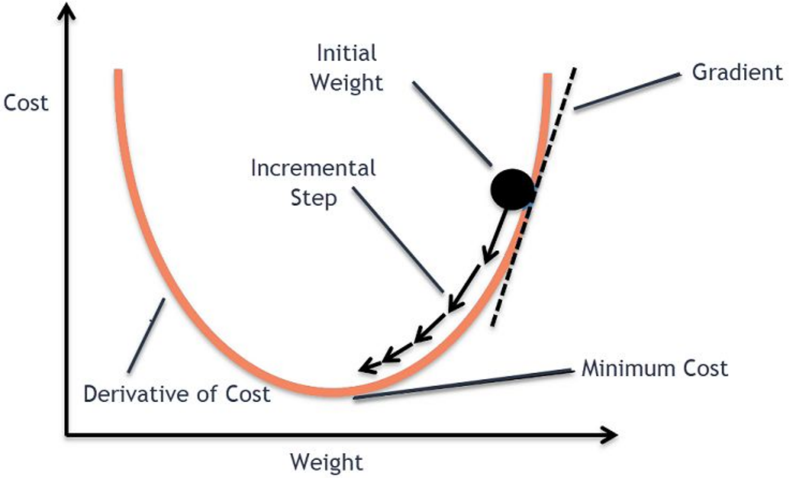
Training



SGD in DL generally refers to mini-batch GD

Epoch: one pass through the dataset



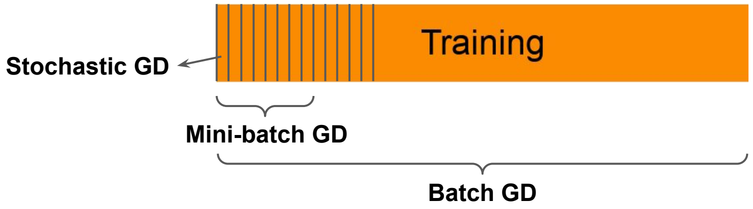


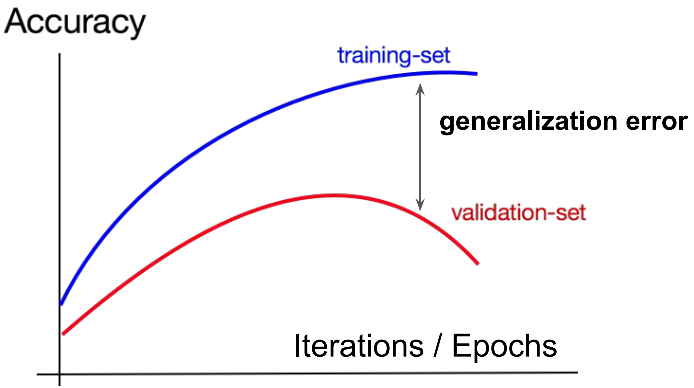
Training

How many iterations/epochs ?

The validation set is used for early stopping

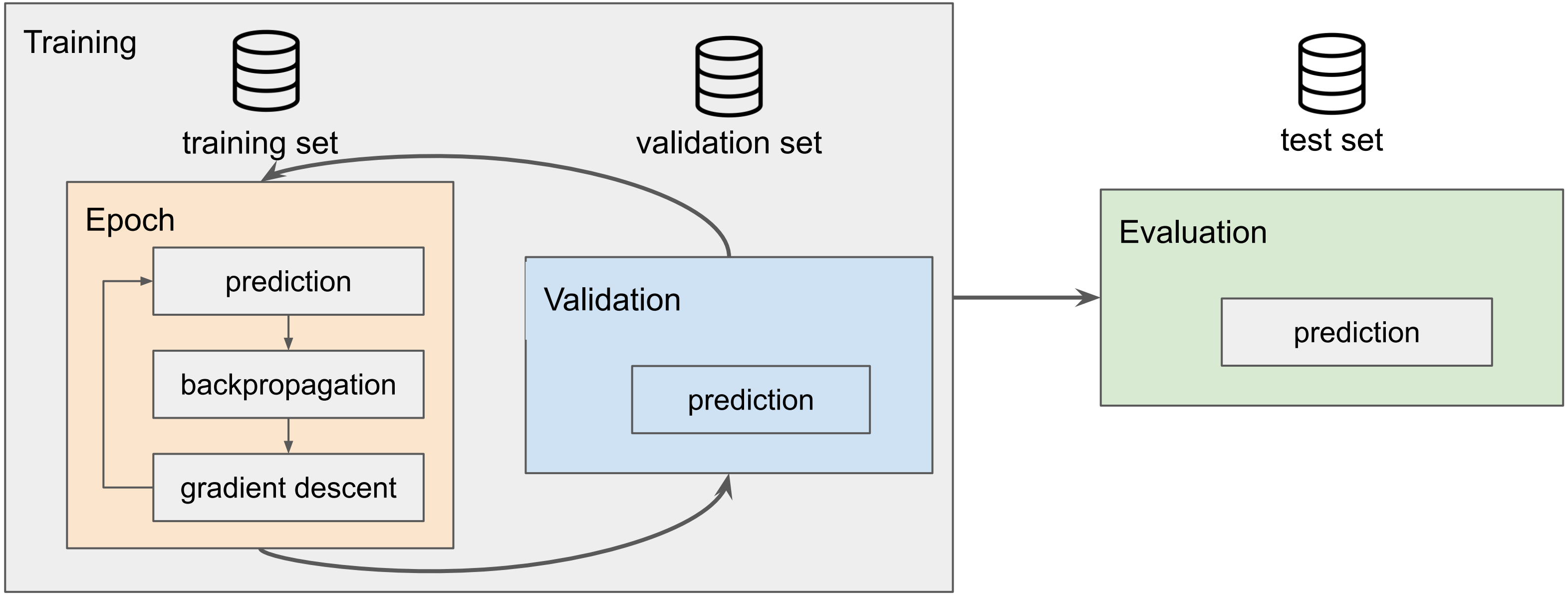
Test set ≠ validation set





Training and Evaluation

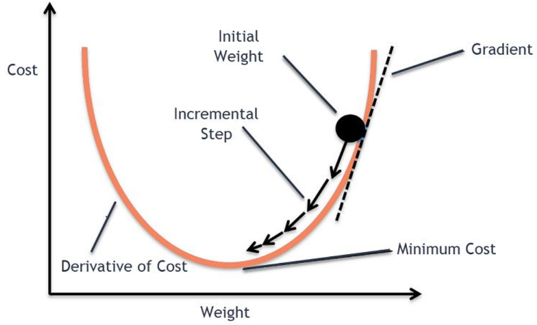
B

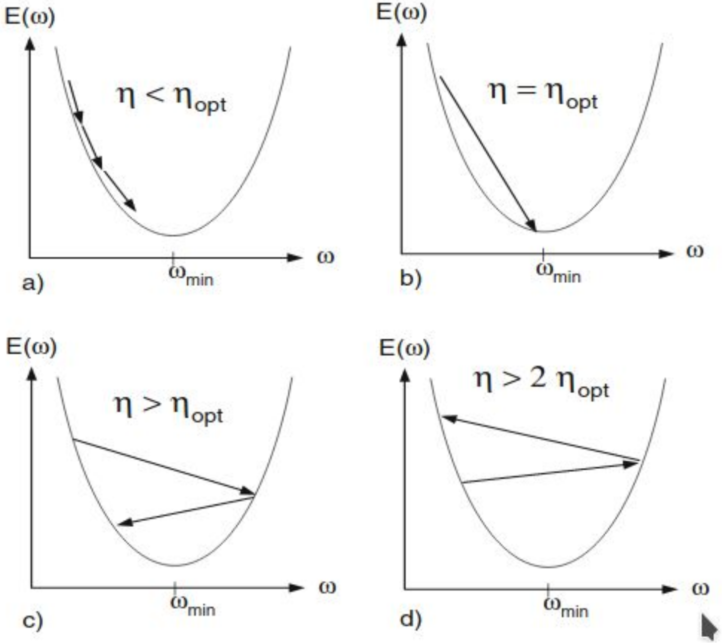


Training

How to find the learning rate ? η

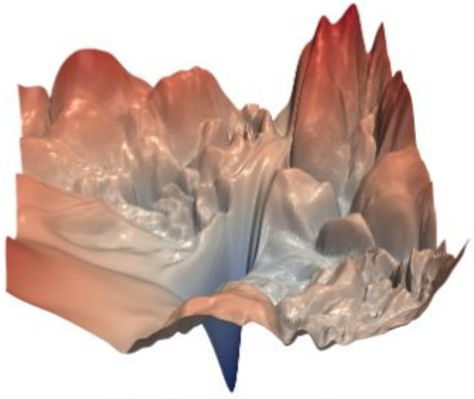
$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$





Optimizers

$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta}$$



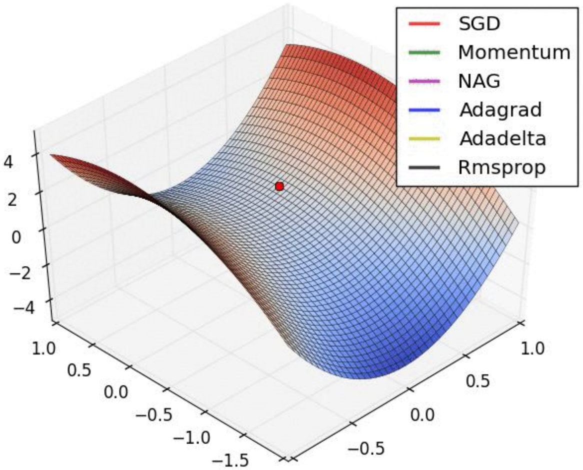
This is a 2 parameter example!
Imagine millions

Loss landscapes are not easy to navigate for optimizers

Ideas:

- Use the gradient history of previous timesteps to inform GD in future timesteps
- Adapt the learning rate to each parameter

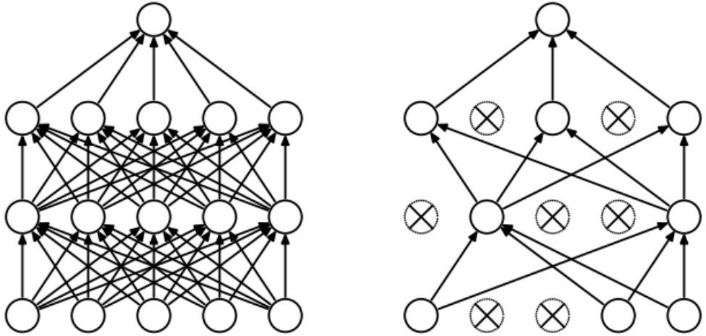
Adam optimizer is an extension of SGD which makes use of these two ideas. It is currently the most used optimizer in DL after SGD.



Regularization

Additional constraints to reduce overfitting

Dropout: stochastically dropping weights during inference

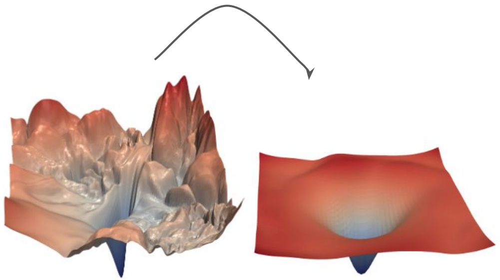


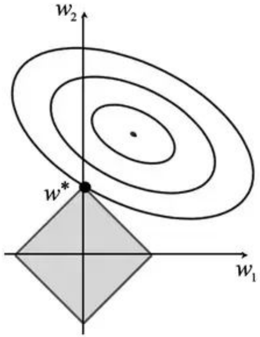
(a) Standard Neural Net (b) After applying dropout.

Early stopping: stopping the training as soon as the validation loss starts increasing

Weight penalties (weight decay): L1 norm (Lasso) / L2 norm (ridge). Terms added to the loss.

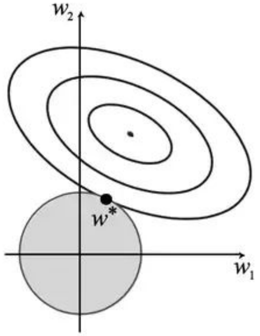
Data augmentations: artificially boosting the number of training samples





L1

Sparse weights



L2

Smaller weight values

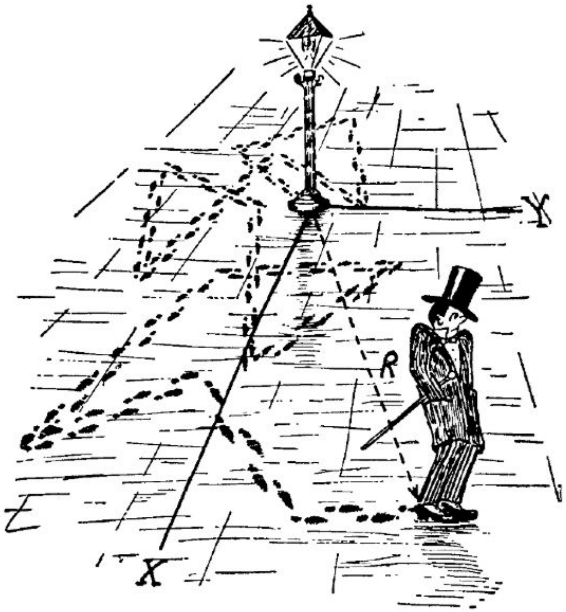
Hyperparameters

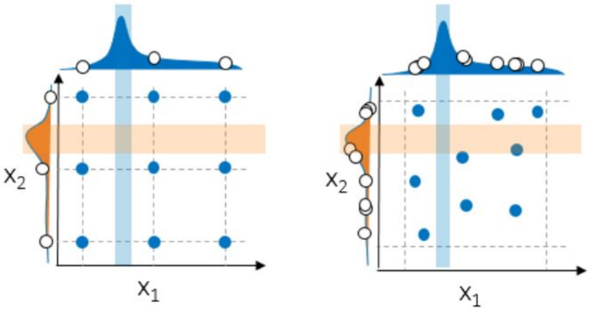
All parameters and settings that are set before training:

- Architectural choices: types and number of layers, size of each layer
- Losses/regularization: weights, additional constants
- Optimization: batch size, learning rate, iterations/epochs, schedule

Hyperparameter search. Another optimization problem ?

- Often done manually.
- When resources are available, large scale search is possible





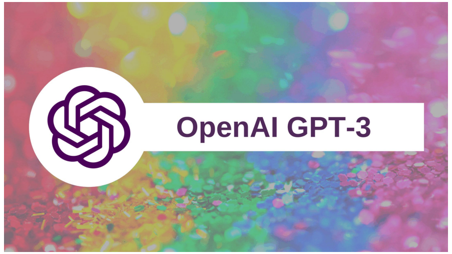
(a) Standard Grid Search (b) Random Search

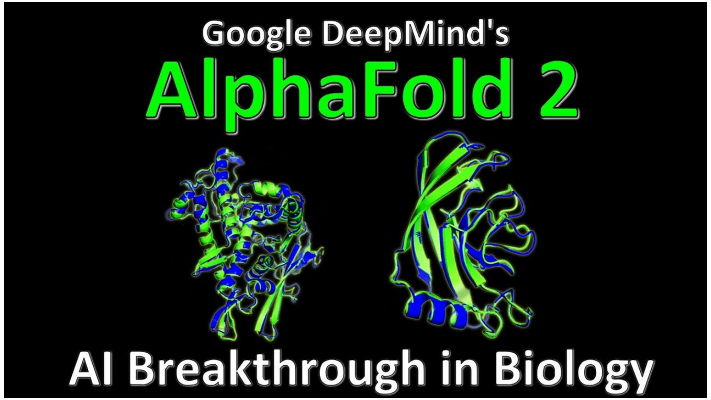
The machine learner pipeline

1. Understanding the data and the task
2. Set up the end-to-end training/evaluation skeleton
    a. a basic architecture
    b. a standard loss
    c. Standard optimization pipeline
3. Complexify one thing at a time
4. Regularize
5. Tune Hyperparameters

Practical examples

With this formula you can do all of this





This was 5 years ago

Go to notebook