Introduction to Deep Learning

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  "Data is the New Oil" - Clive Humby, 2006
- Artificial intelligence
  "AI is the New Electricity" - Andrew Ng, 2016

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  - Image classification

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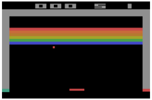

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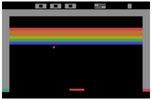

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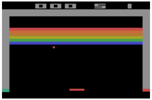

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Starcraft II

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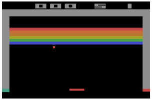

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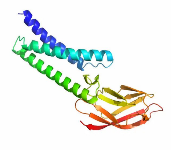
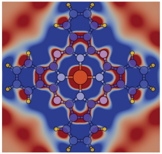
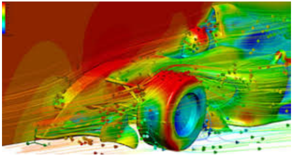
  - Natural sciences and engineering



Protein folding



Quantum physics



Computational fluid dynamics

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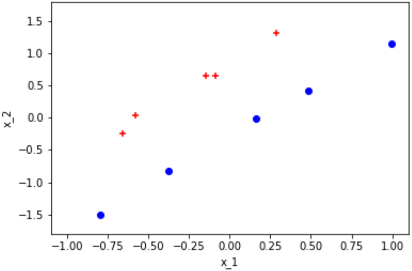
      "AI is whatever hasn't been done yet" - Larry Tesler

Example

- Training set:

x_1	x_2	y
1.00	1.15	False
-0.58	0.04	True
-0.38	-0.82	False
0.16	-0.01	False
0.29	1.31	True
-0.66	-0.24	True
-0.80	-1.50	False
-0.14	0.66	True
-0.09	0.66	True
0.48	0.41	False



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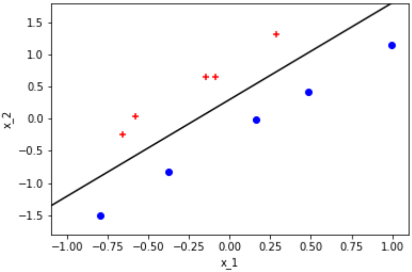

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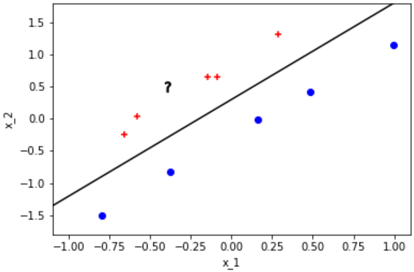

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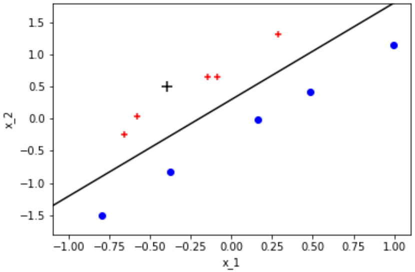
- Make a prediction



Supervised learning

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  - Outputs y
    - Discrete labels: **classification problem**
    - Continuous values: **regression problem**

Supervised learning

- In the previous example
  - Inputs x: 2D vectors
  - Outputs y: binary classes
  - Linear model
    $f_\theta(x) = (w_1 \cdot x_1 + w_2 \cdot x_2 + b \geq 0)$
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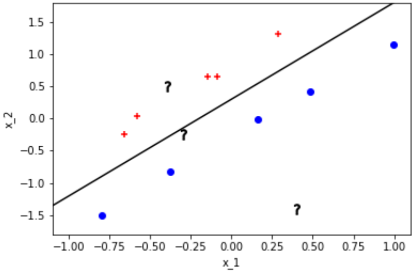

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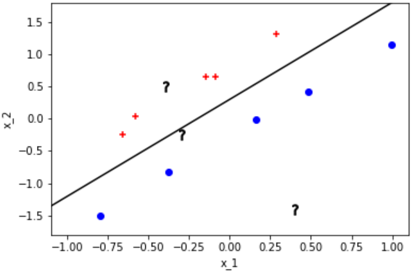

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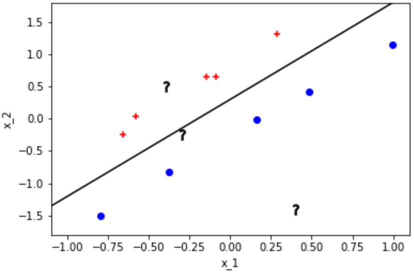

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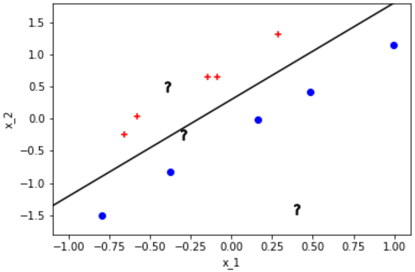

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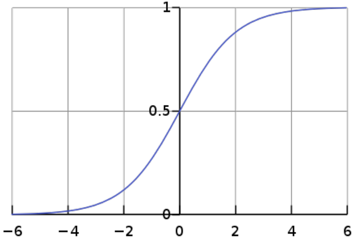

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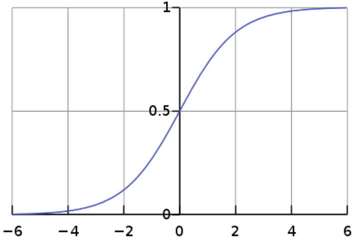

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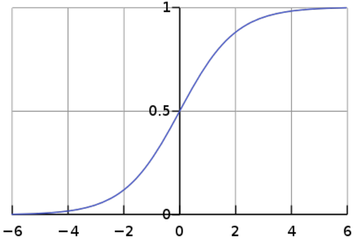

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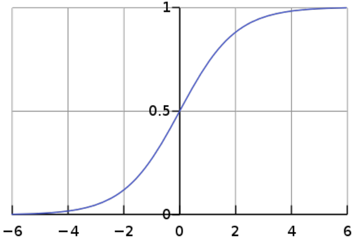

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  - For more complicated deep learning models there are many stationary points

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- If the learning rate is small enough, the algorithm converges close to a local minimum
- A global minimum in this case

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  - $\theta :=$ initial guess (e.g. random or all zeros)
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    - $B :=$ random subset of training data of size N_B
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    - $\theta := \theta - \alpha \cdot \nabla_\theta \tilde{F}(\theta, B)$
- $\nabla_\theta \tilde{F}(\theta, B)$ is an unbiased estimator of $\nabla_\theta F(\theta)$
- Converges with probability 1

Multi-class classification

- What if the output are in more than two classes?

Multi-class classification

- What if the output are in more than two classes?
- C : number of classes
- output y is one-hot
  $y \in \{0, 1\}^C$ s.t. $\sum_j y_j = 1$

Multi-class classification

- What if the output are in more than two classes?
- C : number of classes
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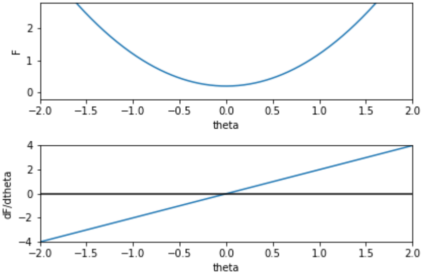
- Normalize probabilities: softmax
  $p(y_j|z) = \frac{\exp z_j}{\sum_{j'} \exp z_{j'}}$
- Loss function: categorical cross-entropy
  $L(y, p_\theta(.|x)) = -\sum_j \log p_\theta(y_j|x)$

Gradient descent example

- Example
  $F(\theta) = \theta^2 + 0.2$
  $\nabla_\theta F(\theta) = \theta$



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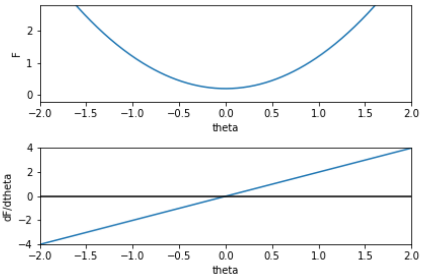

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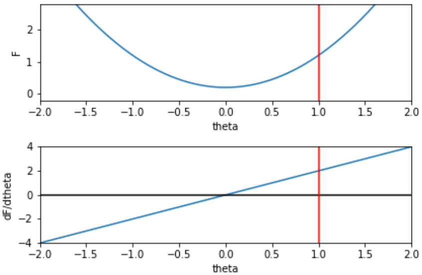
- Iterations:

θ	$\nabla_\theta F(\theta)$
1.0	2.0



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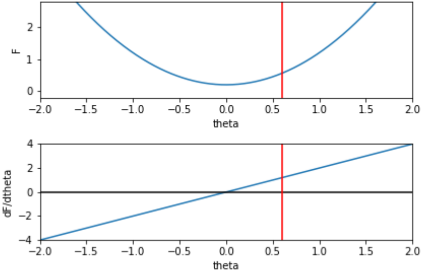
1.0	2.0
0.6	1.2



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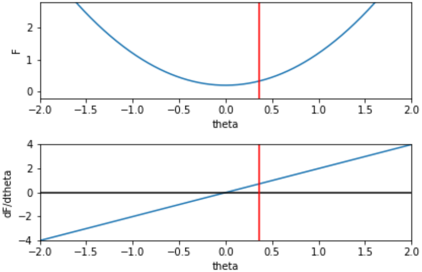
1.0	2.0
0.6	1.2
0.36	0.72



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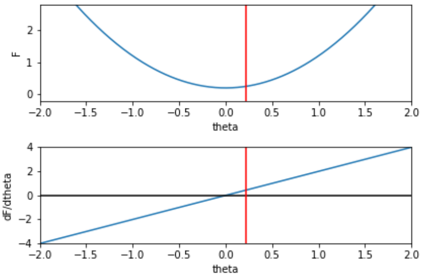

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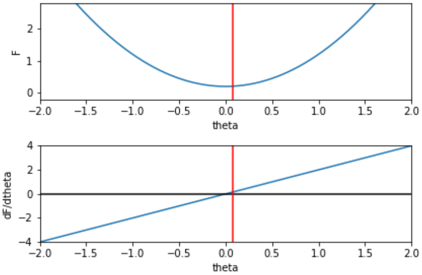
0.13	0.26



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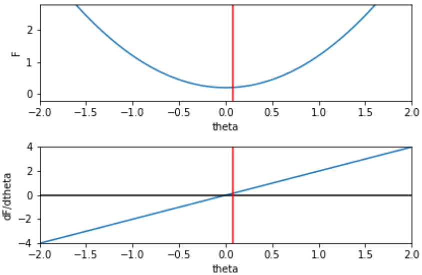
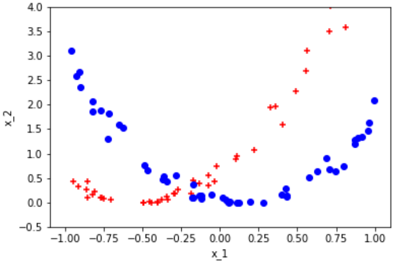
0.13	0.26
0.08	0.16



Limitations of linear models

- Sometimes the data is not linearly separable



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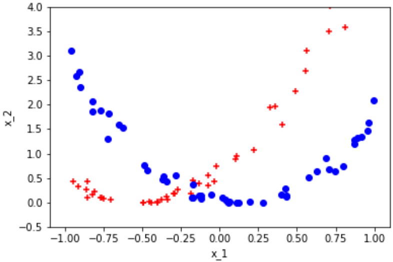

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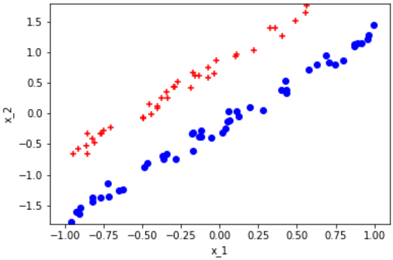

Limitations of linear models

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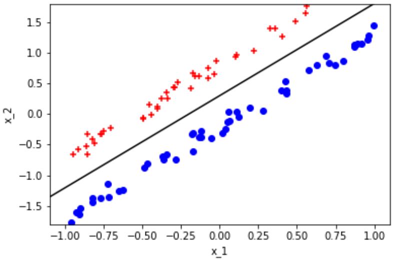
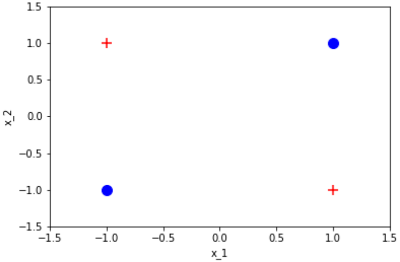
  - Find a preprocessing transformation that makes the data linearly separable
  - For example $x_2 := \sqrt{x_2}$
  - Now we can find a decision hyperplane



Limitations of linear models

- XOR problem

x_1	x_2	y
-1.0	-1.0	False
-1.0	1.0	True
1.0	-1.0	True
1.0	1.0	False



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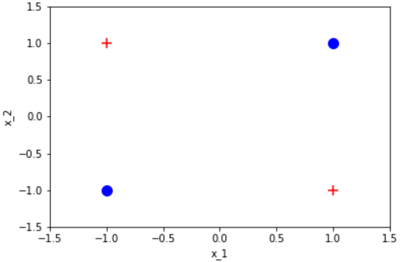

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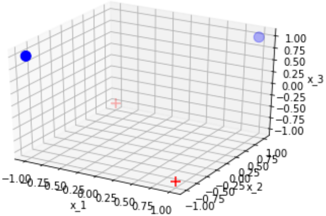

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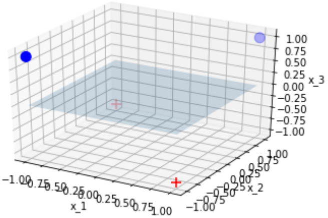

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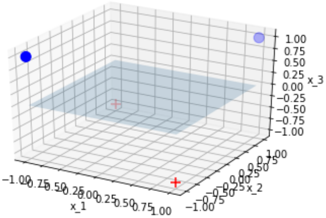
- Not linearly separable
- But becomes trivial if we define $x_3 = x_1 x_2$
- Solution: ignore x_1 and x_2 and use the sign of x_3
- The XOR problem caused research in neural networks to be abandoned from the 70s to the mid 80s



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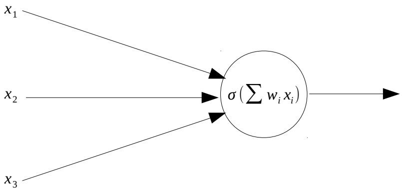

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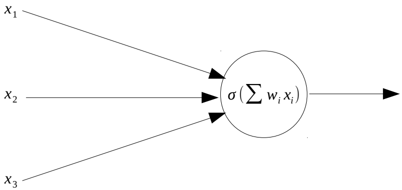

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- Images
  - Edge features
  - Corner feature
  - ...

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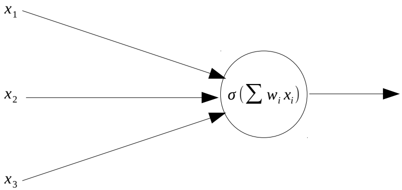

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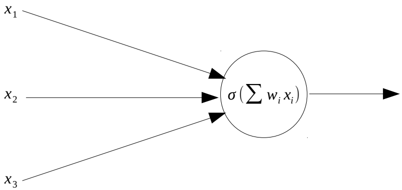

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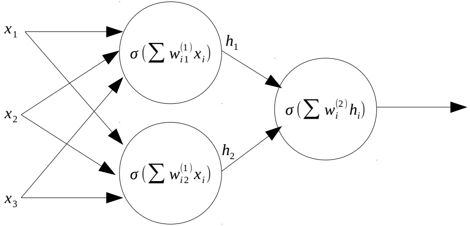
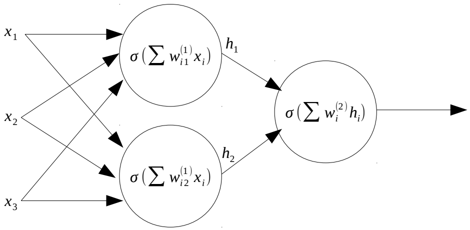
  - ...
- Can we learn non-linear features automatically?

Multi-layer perceptron



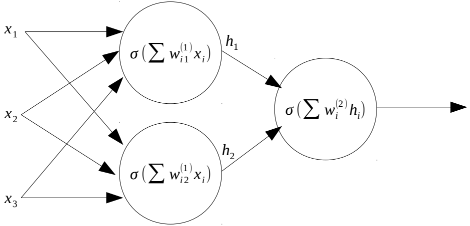
- Simplest deep feed-forward neural network

Multi-layer perceptron



- Simplest deep feed-forward neural network
- Hidden layer(s) computes non-linear features

Multi-layer perceptron



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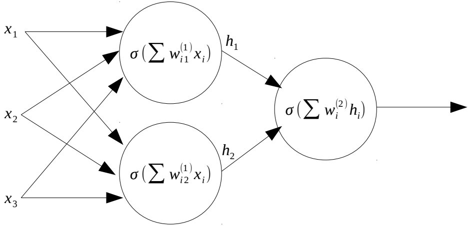

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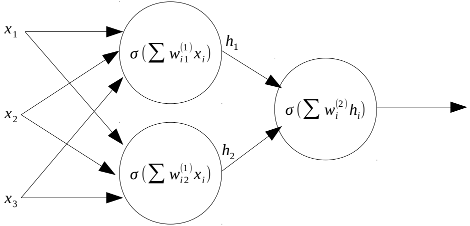
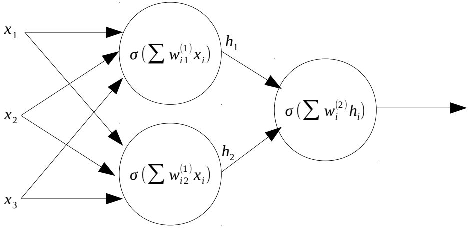


- Simplest deep feed-forward neural network
- Hidden layer(s) computes non-linear features
  - Activation function σ provides non-linearity
  - Deep linear models collapse to shallow linear models
- Fully connected

Multi-layer perceptron

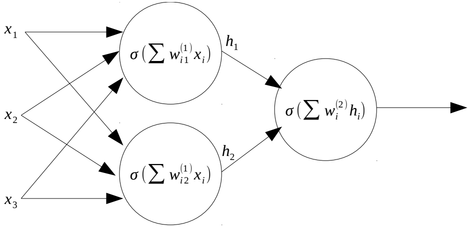


- Equations

$$h^{(0)} = x$$
$$h^{(k)} = \sigma_h(W^{(k)} \cdot h^{(k-1)} + b^{(k)})$$
$$p(y) = \sigma_{out}(W^{out} \cdot h^{(K)} + b^{out})$$

- K hidden layers of width $d^{(k)}$, $W(k) \in \mathcal{R}^{d^{(k-1)} \times d^{(k)}}$

Multi-layer perceptron



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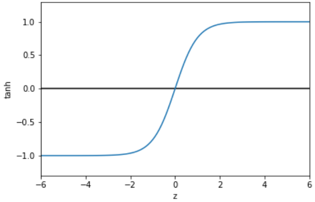
- Usually the output activation function σ_{out} and the hidden activation function σ_h are different

Activation functions

- Hyperbolic tangent
  $\tanh(z) = \frac{\exp(2z)-1}{\exp(2z)+1}$



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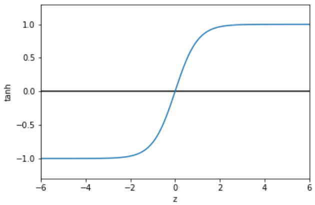

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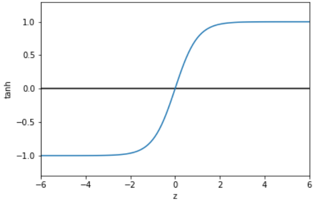

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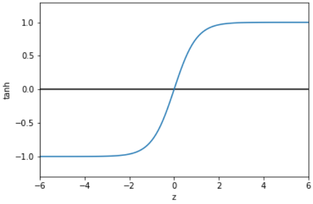

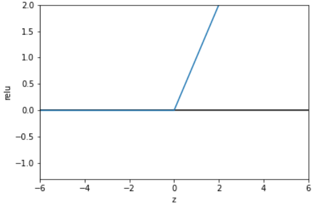

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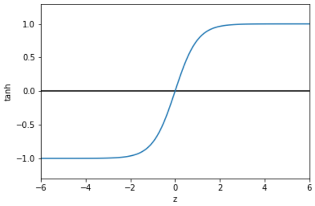
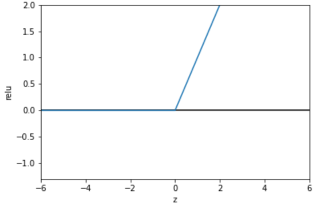
  - Differentiable **almost** everywhere





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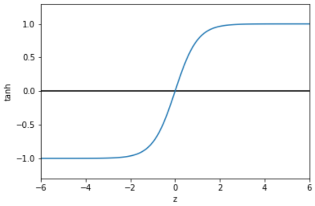
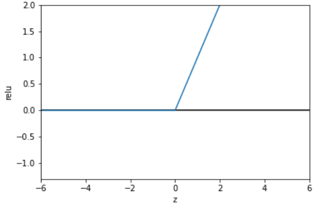
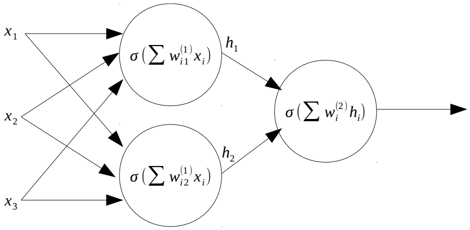


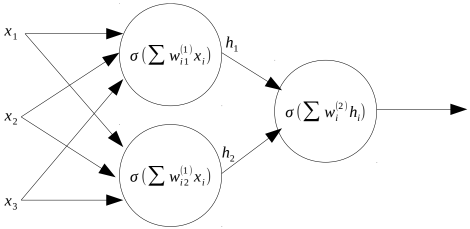


Multi-layer perceptron



- How many layers, and how big?

Multi-layer perceptron



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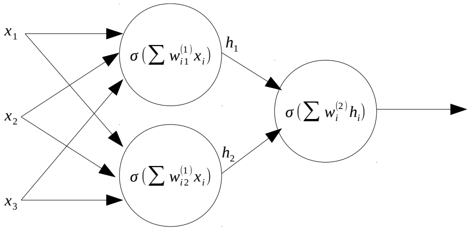

- How many layers, and how big?
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- Do we need more than one hidden layer?

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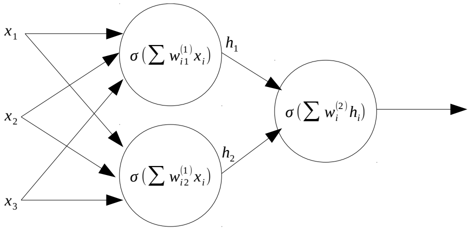

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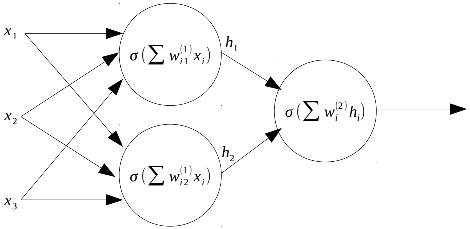

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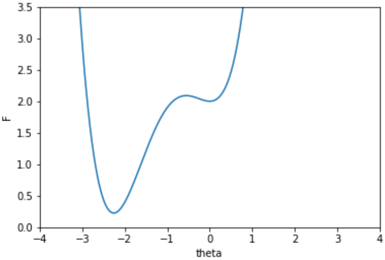
Training

- Stochastic Gradient Descent



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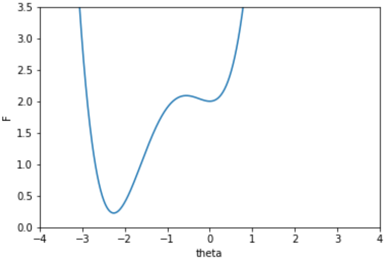
- Non-convex optimization
  - Multiple local minima
  - Local maxima
  - Saddle points



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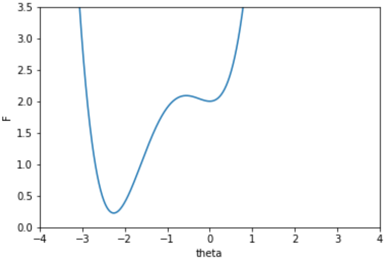

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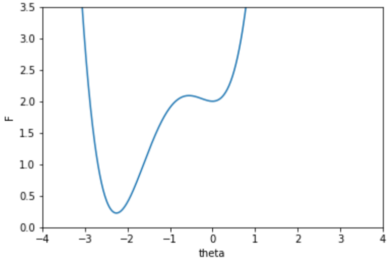
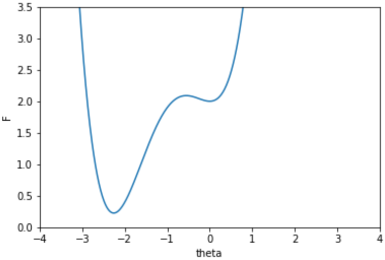
- Larger depth: **harder** optimization
  - Vanishing gradients (bad stationary points)
  - Exploding gradients (numerical divergences)



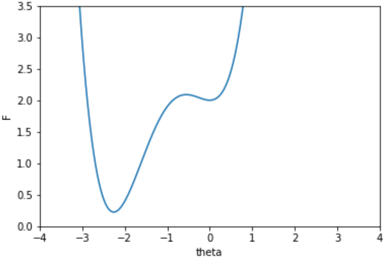
Training

- Deep neural networks can be trained effectively



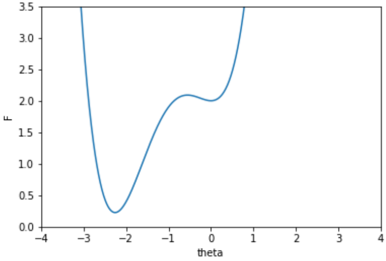
Training

- Deep neural networks can be trained effectively
- as long as we are careful
    - Optimizers
    - Initialization
    - Residual trick
    - Normalization layers
    - . . .

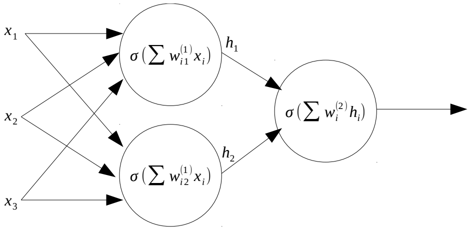


SGD with Momentum

- Add a velocity to the updates
- Algorithm:
  - $\alpha :=$ learning rate
  - $\beta :=$ momentum rate
  - $N_B :=$ batch size
  - $\theta :=$ initial guess (e.g. random or all zeros)
  - $\Delta\theta := 0$
  - while not converged
    - $B :=$ random subset of training data of size N_B
    - $\Delta\theta := -\alpha \cdot \nabla_\theta \tilde{F}(\theta, B) + \beta \cdot \Delta\theta$
    - $\theta := \theta + \Delta\theta$



Parameter initalization



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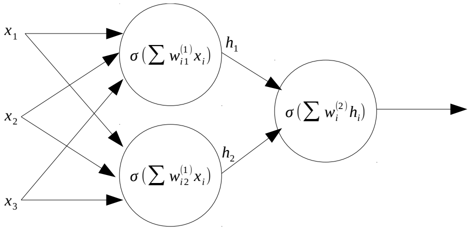

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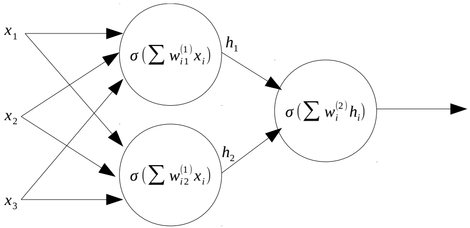

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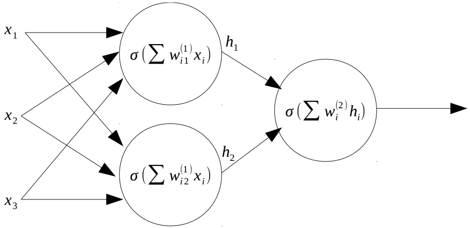
- No, we need a random initialization
- Glorot / He initializations
  - biases initialized to 0
  - For RELU layers (He)
    $W \sim N(0, 2/d^{(k-1)})$
  - For tanh or output layers (Glorot)
    $W \sim N(0, 1/d^{(k-1)})$

Residual trick



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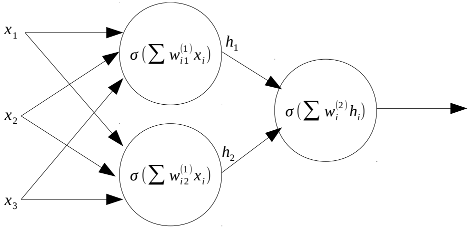

- How to train very very deep networks (hundreds of layers)?
- Add a skip connection to the layers

$$
\begin{aligned}
h^{(0)} &= x \\
h^{(1)} &= \sigma_h(W^{(1)} \cdot h^{(0)} + b^{(1)}) \\
h^{(k)} &= h^{(k-1)} + \sigma_h(W^{(k)} \cdot h^{(k-1)} + b^{(k)}) \\
p(y) &= \sigma_{out}(W^{out} \cdot h^{(K)} + b^{out})
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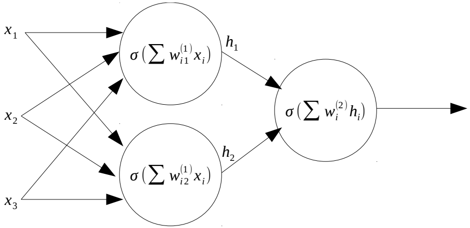

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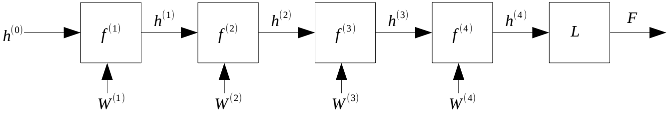
- Hidden layers must have the same size

Backpropagation algorithm



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$$h^{(k)} = f^{(k)}(h^{(k-1)}, W^{(k)})$$
$$F = L(h^{(K)})$$

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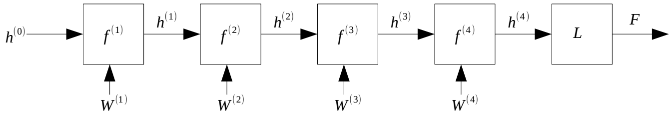

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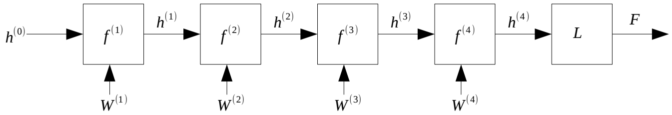

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- Assume that the derviative of any $f^{(k)}$ w.r.t. any of its inputs is efficiently computable given the other input

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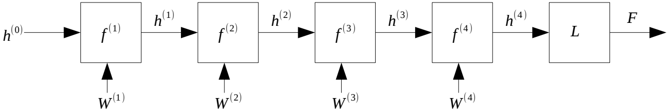

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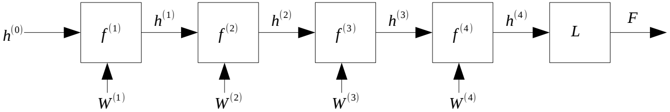

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- And so on ...
- Each $\frac{\mathrm{d}F}{\mathrm{d}W^{(k)}}$ can be computed locally from
  - The saved activation: $h^{(k-1)}$
  - The **adjoint**: $\frac{\mathrm{d}L}{\mathrm{d}h^{(K)}} \cdot \frac{\mathrm{d}h^{(K)}}{\mathrm{d}h^{(K-1)}} \cdot \ldots \cdot \frac{\mathrm{d}h^{(k+1)}}{\mathrm{d}h^{(k)}}$

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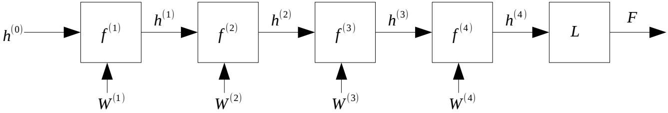

- Forward pass:
  - For k in range $[1, K]$
    - Store in memory $h^{(k-1)}$
    - $h^{(k)} := f^{(k)}(h^{(k-1)}, W^{(k)})$
  - Store in memory $h^{(K)}$
  - Return $L(h^{(K)})$

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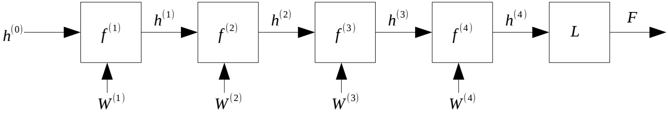

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- Backward pass:
  - $h^{(K)}$:= retrive from memory
  - adjoint $:= \frac{\mathrm{d}L}{\mathrm{d}h^{(K)}}$
  - For k in range $[K, 1]$
    - $h^{(k-1)}$:= retrive from memory
    - $\frac{\mathrm{d}F}{\mathrm{d}W^{(k)}} :=$ adjoint $\cdot \frac{\mathrm{d}}{\mathrm{d}W^{(k)}} f^{(k)}(h^{(k-1)}, W^{(k)})$
    - adjoint := adjoint $\cdot \frac{\mathrm{d}}{\mathrm{d}h^{(k-1)}} f^{(k)}(h^{(k-1)}, W^{(k)})$
  - Return $\frac{\mathrm{d}F}{\mathrm{d}W^{(k)}}$ for all k

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  - For each node, add the **adjoints** coming from all its outgoing edges

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    - Used to be more important in the past

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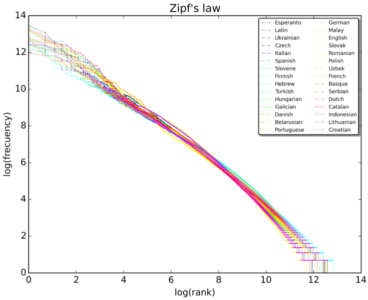

From Wikipedia

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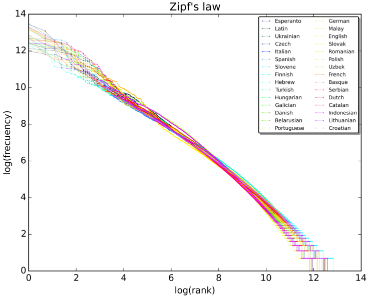

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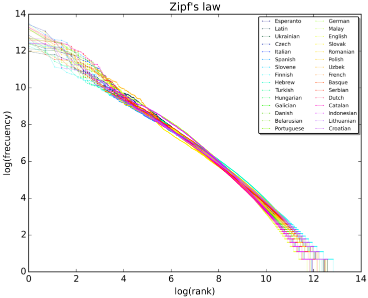

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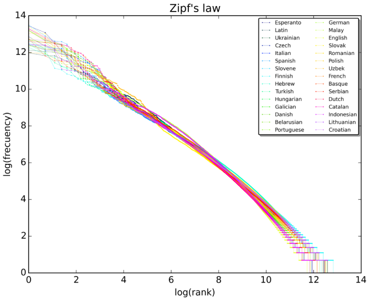
- Replace all other words with a special symbol "**<unk>**"



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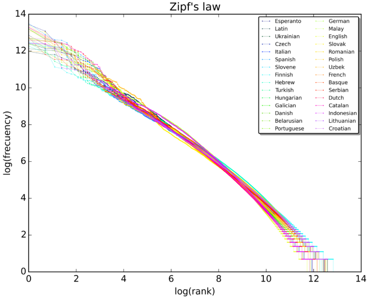

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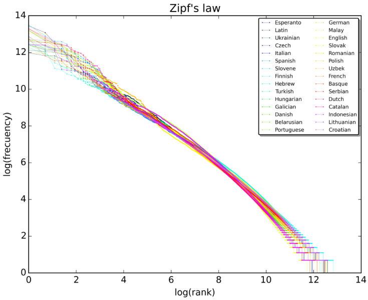
- Map to one-hot vectors $e_i \in \{0, 1\}^V$
  $e_{i,j} = 1$ if $t_i = j$, 0 otherwise
- Multiply by an embedding matrix $W \in \mathcal{R}^{d_{emb} \times V}$
  $h_i^{(0)} = W \cdot e_i$



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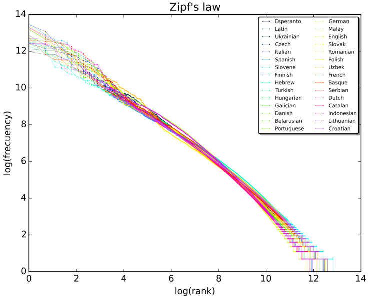
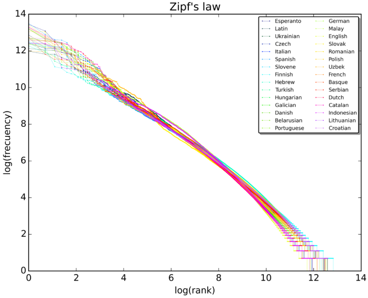


From Wikipedia

Word vectorization

- Input: sequence of M integer token ids $[t_1, t_2, \ldots, t_M]$
- Map to one-hot vectors $e_i \in \{0, 1\}^V$ $e_{i,j} = 1$ if $t_i = j$, 0 otherwise
- Multiply by an embedding matrix $W \in \mathcal{R}^{d_{emb} \times V}$ $h_i^{(0)} = W \cdot e_i$
  - This is equivalent of just selecting the j-th row of W
  - Can be done efficiently with an **Embedding** layer



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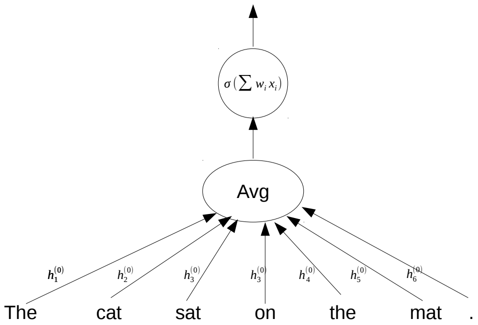
Bag-of-words classification model

- Simple linear model

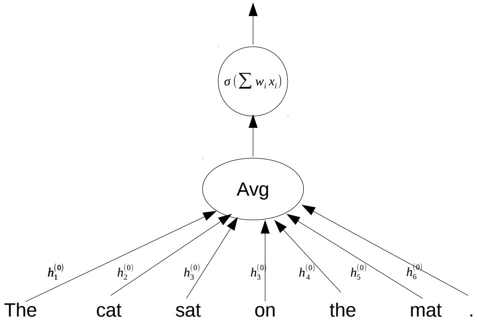


Bag-of-words classification model

- Simple linear model

$$h^{(1)} = \frac{1}{M} \sum_{i=1}^{M} h_i^{(0)}$$

$$p(y) = \text{softmax}(W^{out} \cdot h^{(1)} + b^{out})$$



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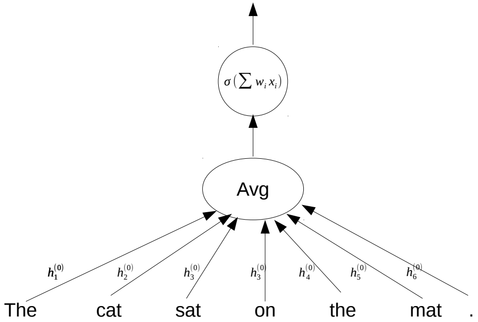

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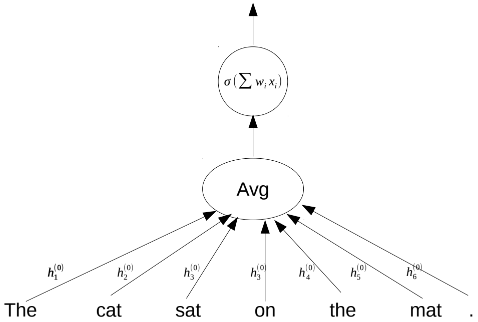

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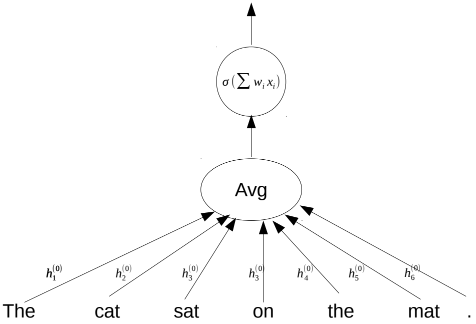
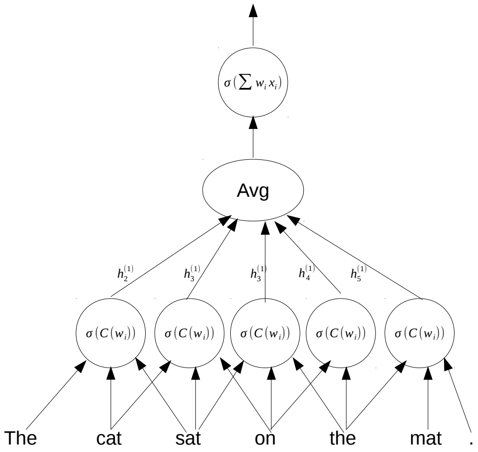


Convolutional classification model

- Deep neural network



Convolutional classification model

- Deep neural network

$$h_i^{(1)} = \mathrm{ReLU}(\sum_{y=-s}^{s} W_y^{(1)} \cdot h_{y+i}^{(0)} + b^{(1)})$$

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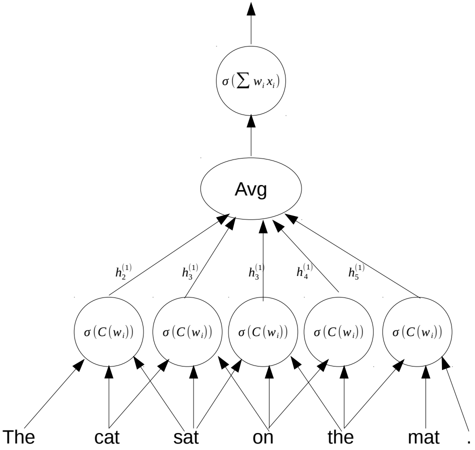
- Kernel size: $2s + 1$ (e.g. 3)



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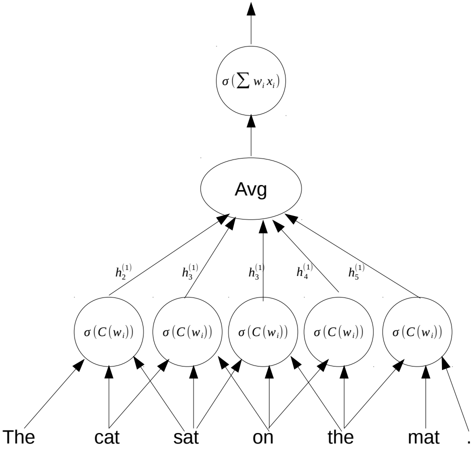

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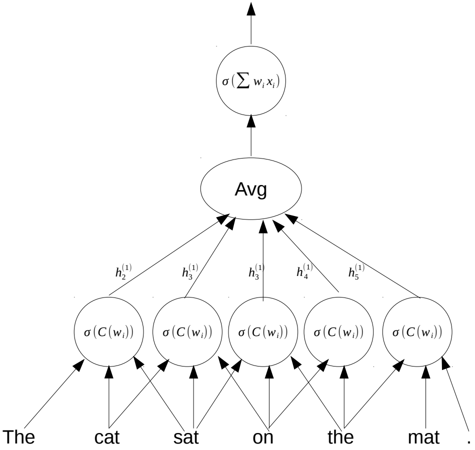

Convolutional classification model

- More concretely, ignoring ReLUs and biases

$$h_2^{(1)} = W_{-1}^{(1)} \cdot \text{"The"} + W_0^{(1)} \cdot \text{"cat"} + W_{+1}^{(1)} \cdot \text{"sat"}$$
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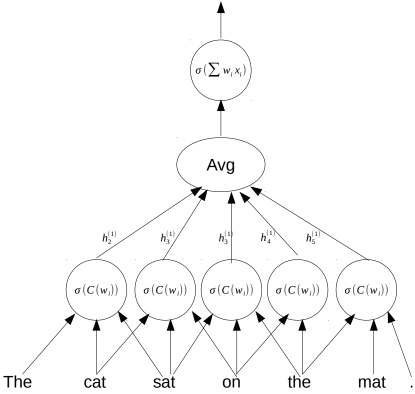

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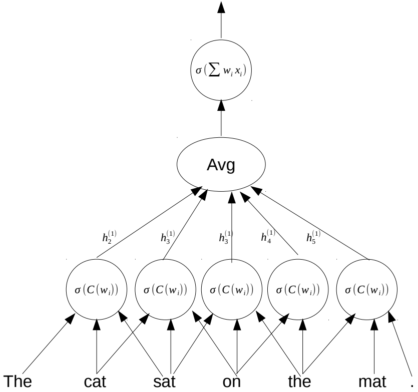

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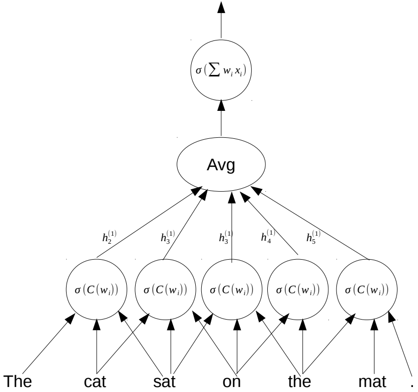
- Captures word n-grams
- We can have multiple layers, of course



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Thanks for your attention

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Course material: `https://github.com/Avmb/IntroDeepLearning`