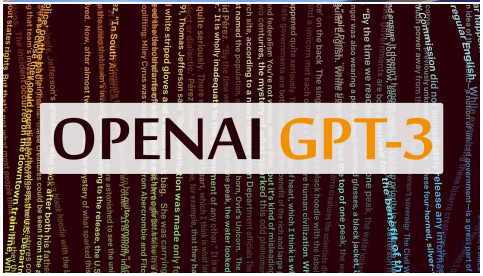
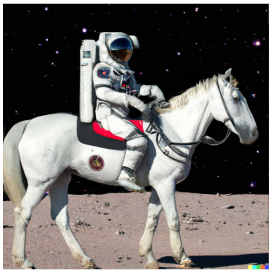
Introduction to Deep Learning

DL@MBL 2022

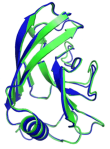
August 27, 2022

Deep Learning





T1037 / 6vr4
90.7 GDT
(RNA polymerase domain)

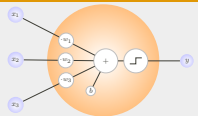


T1049 / 6y4f
93.3 GDT
(adhesin tip)

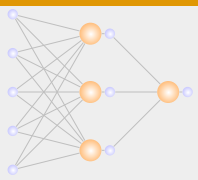
Experimental result
Computational prediction

Outline

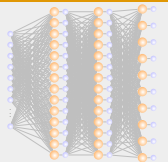
1. Perceptrons



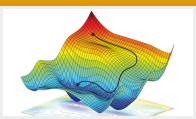
2. Networks



3. Deep Networks

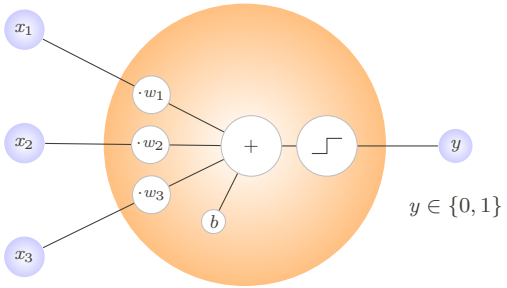


4. Learning



5. Convolutional Networks

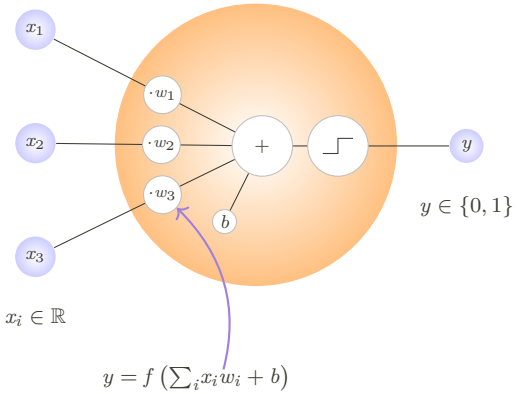
The Building Block of Neural Networks



Perceptron

- invented by McCulloch and Pitts in 1943
- termed "perceptron" by Rosenblatt in 1958
- also known as: Threshold Logic Unit, Linear Threshold Unit, McCulloch-Pitts model

The Building Block of Neural Networks



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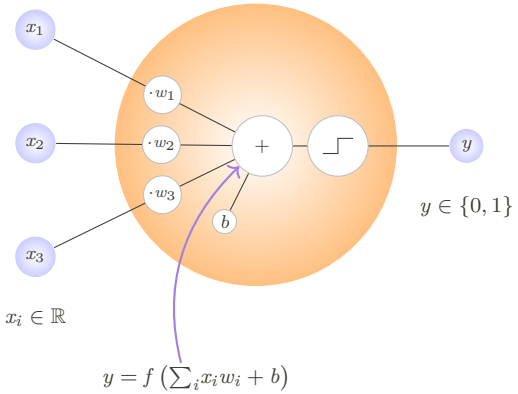

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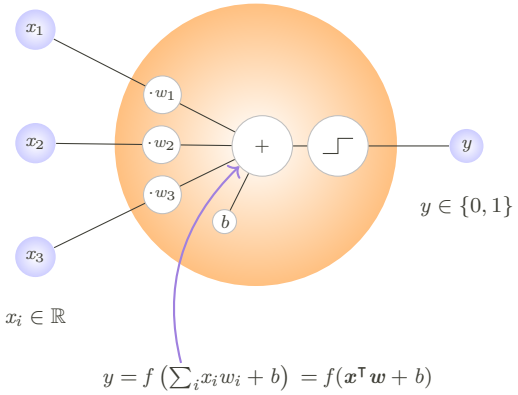

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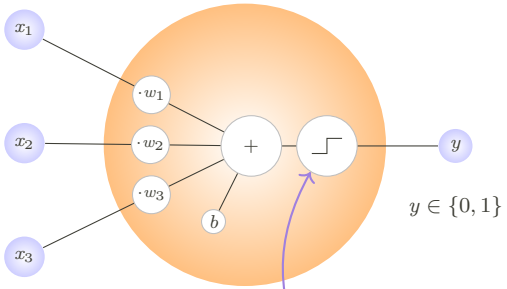

$$y = f\left(\sum_i x_i w_i + b\right) = f(\boldsymbol{x}^\intercal \boldsymbol{w} + b)$$

$$f(a) = \begin{cases} 0 & \text{if } a \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

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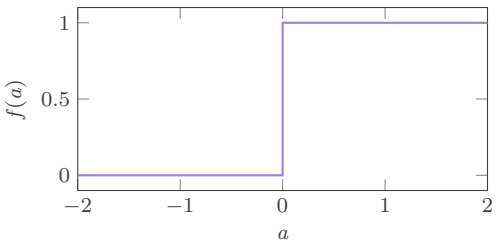
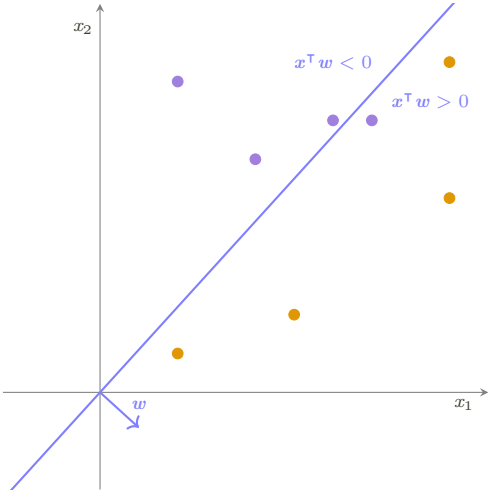
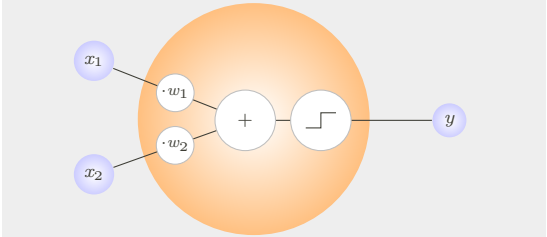


Just a Linear Classifier



Example with 2 inputs



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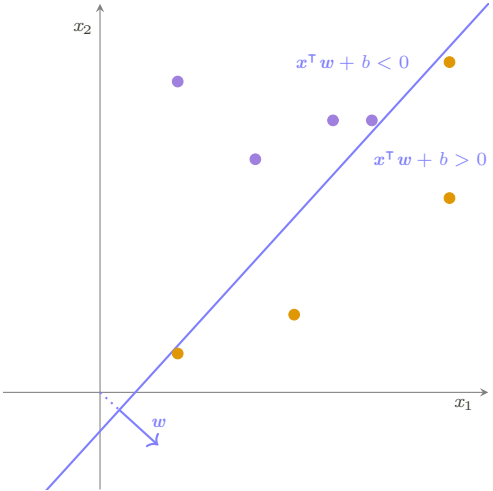

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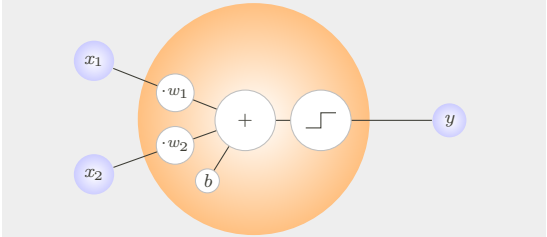

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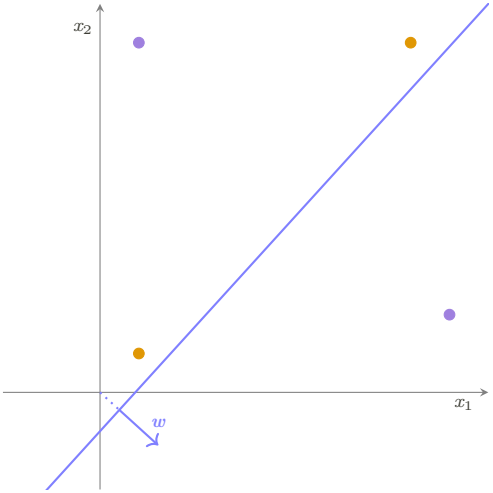

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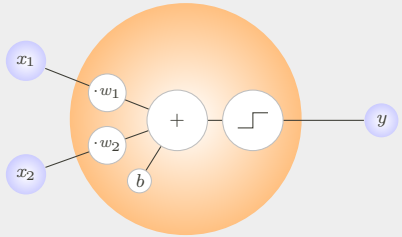
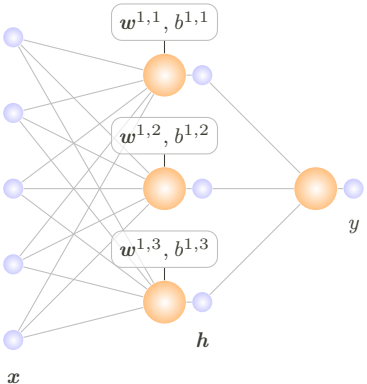


The XOR Affair and AI Winter

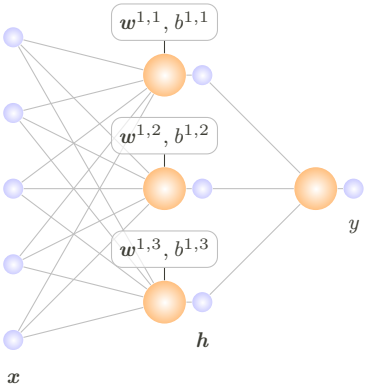
- "The perceptron may eventually be able to learn, make decisions, and translate languages." –Rosenblatt, 1958
- "Some functions are tricky." –Minsky/Papert, 1969
- interest in neural networks declined until the 80s

[1]



Output Function with one Hidden Layer

$$\boldsymbol{h} = \big(f(\boldsymbol{w}^{\mathbf{1,1}}\boldsymbol{x} + b^{1,1}), f(\boldsymbol{w}^{\mathbf{1,2}}\boldsymbol{x} + b^{1,2}), f(\boldsymbol{w}^{\mathbf{1,3}}\boldsymbol{x} + b^{1,3})\big)$$



Output Function with one Hidden Layer

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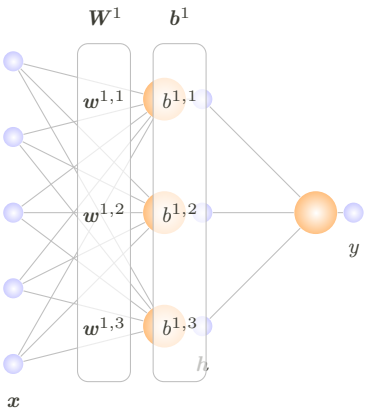

Output Function with one Hidden Layer

$$
\begin{aligned}
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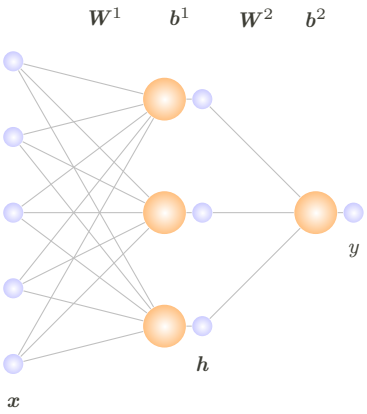
&= f\left((\boldsymbol{w}^{\mathbf{1,1}}\boldsymbol{x} + b^{1,1}, \boldsymbol{w}^{\mathbf{1,2}}\boldsymbol{x} + b^{1,2}, \boldsymbol{w}^{\mathbf{1,3}}\boldsymbol{x} + b^{1,3})\right) \\
&= f(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1)
\end{aligned}
$$



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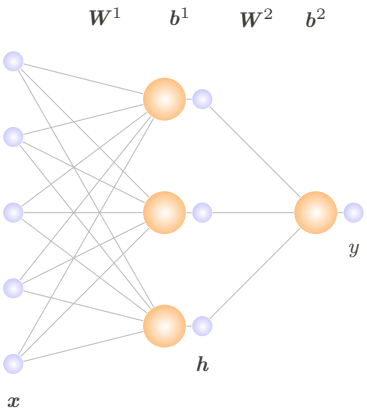
\end{aligned}
$$

$$
y = f(\boldsymbol{W^2h} + \boldsymbol{b^2}) = f(\boldsymbol{W^2}f(\boldsymbol{W^1x} + \boldsymbol{b^1}) + \boldsymbol{b^2})
$$



Output Function with one Hidden Layer

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\boldsymbol{h} &= \big(f(\boldsymbol{w^{1,1}}\boldsymbol{x} + b^{1,1}), f(\boldsymbol{w^{1,2}}\boldsymbol{x} + b^{1,2}), f(\boldsymbol{w^{1,3}}\boldsymbol{x} + b^{1,3})\big) \\
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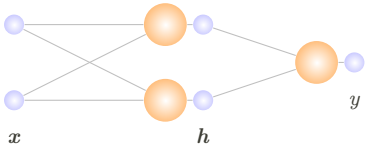
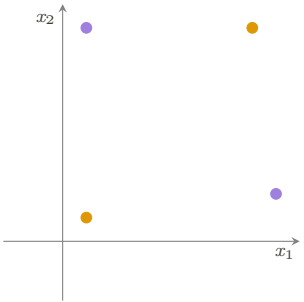
\end{aligned}
$$

$$
y = f(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2) = f(\boldsymbol{W}^2 f(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) + \boldsymbol{b}^2)
$$

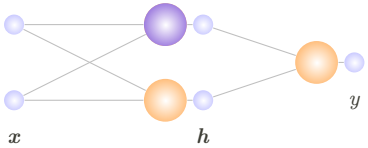
- just matrix multiplications and element-wise non-linearities

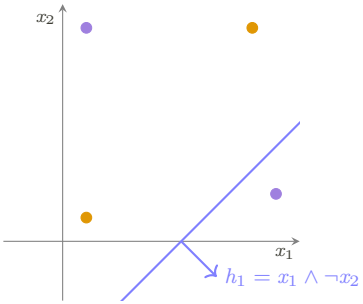
XOR Revisited



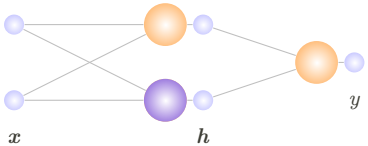


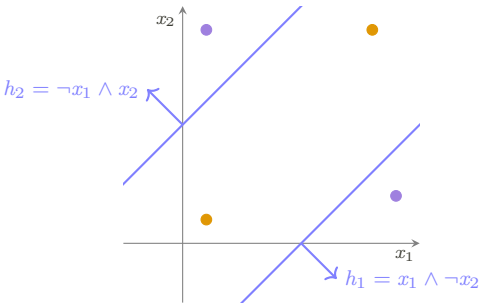
XOR Revisited





XOR Revisited





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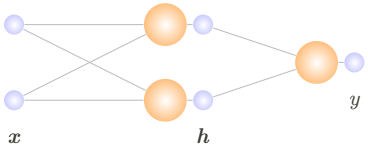

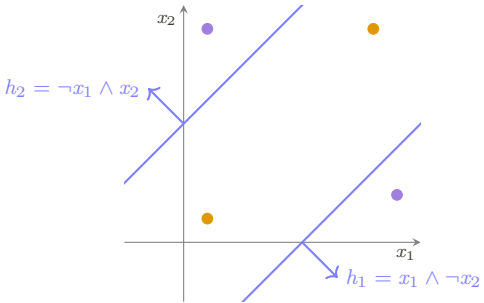

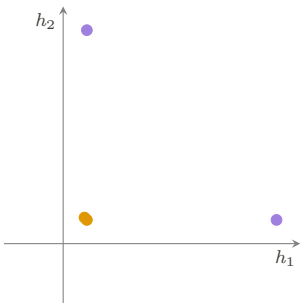

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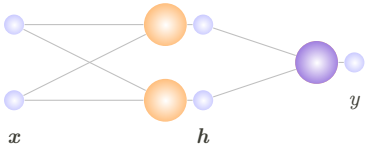
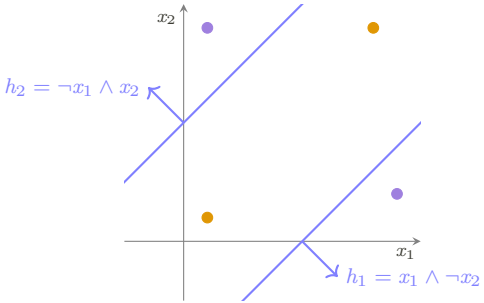
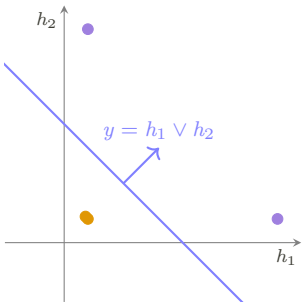






How many layers do we need?

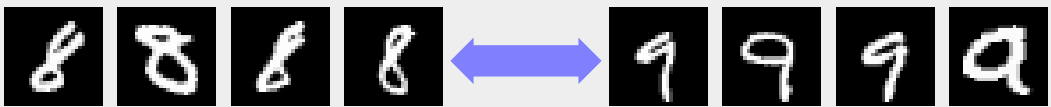
Theoretically...

...one hidden layer is sufficient to model any function:

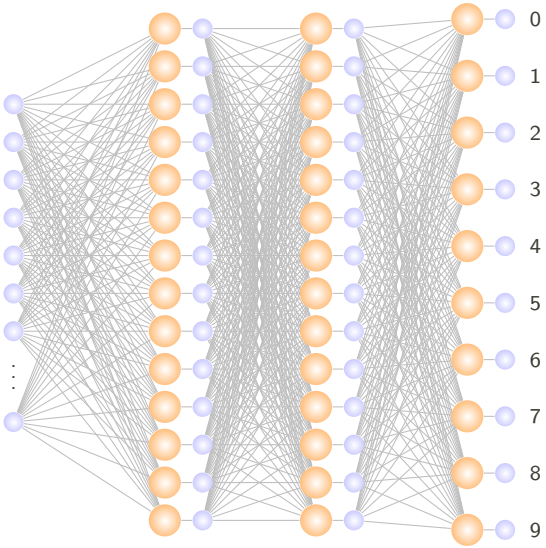
- every boolean function can be transformed into disjunctive normal form [2]
- every continuous function can be approximated with one hidden layer [3]

Practically...

...more than one layer will be more efficient:

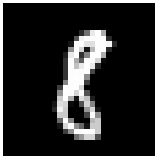


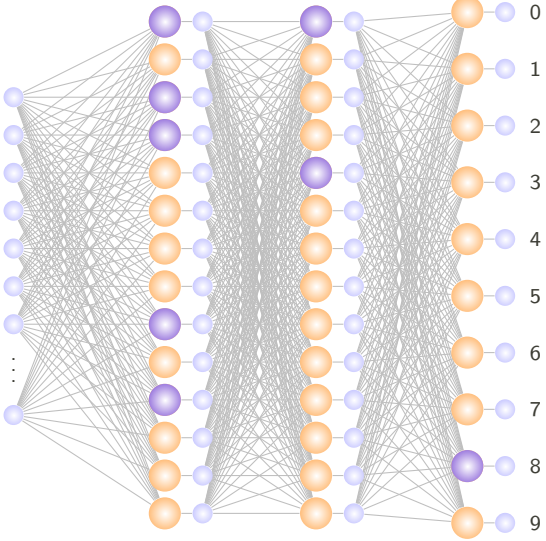
Example: Digit Recognition



[4]

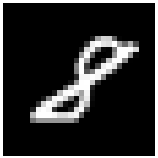
Example: Digit Recognition

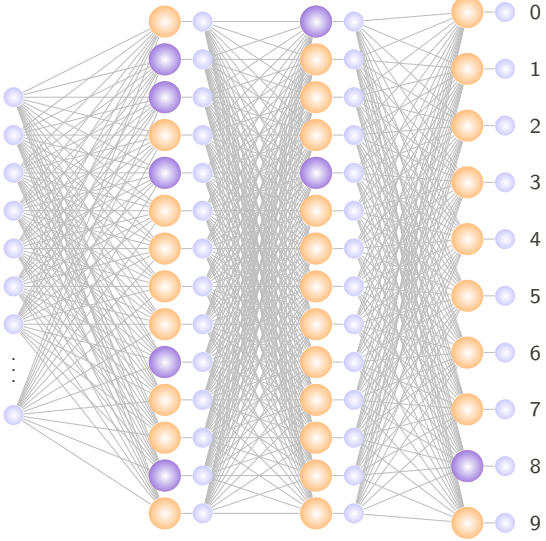




[4]

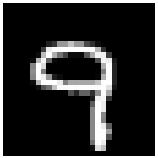
Example: Digit Recognition

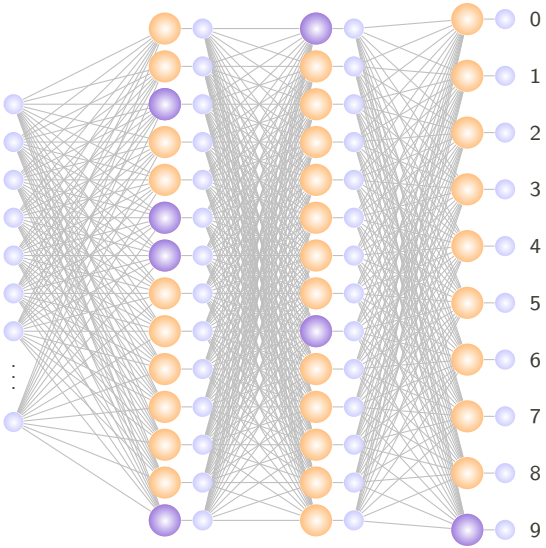




[4]

Example: Digit Recognition





[4]

Supervised Learning

Model

- function $M_{\boldsymbol{\theta}} : \mathbb{R}^n \mapsto \mathbb{R}^m$, $\hat{\boldsymbol{y}} = M_{\boldsymbol{\theta}}(x)$
- parameterized by $\boldsymbol{\theta}$

Data

- $T = \left\{\boldsymbol{x}^i, \boldsymbol{y}^i\right\}_{i=1,\ldots,k}$
- input $\boldsymbol{x}$
- desired output $\boldsymbol{y}$

Objective

- $l : \mathbb{R}^m \times \mathbb{R}^m \mapsto \mathbb{R}$, e.g., $l(\hat{\boldsymbol{y}}, \boldsymbol{y}) = \frac{1}{2}|\hat{\boldsymbol{y}} - \boldsymbol{y}|^2$
- $L(\boldsymbol{\theta}) = \frac{1}{k}\sum_{i=1}^{k} l(\hat{\boldsymbol{y}}^i, \boldsymbol{y}^i)$

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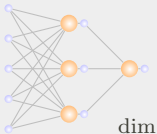

$\dim(\boldsymbol{\theta}) \gg 1$

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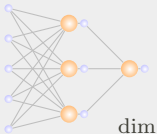

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lots of it

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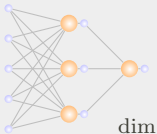

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- $L(\boldsymbol{\theta}) = \frac{1}{k}\sum_{i=1}^{k} l(\hat{\boldsymbol{y}}^i, \boldsymbol{y}^i)$

smooth, differentiable

Learning by Gradient Descent

Optimization Problem

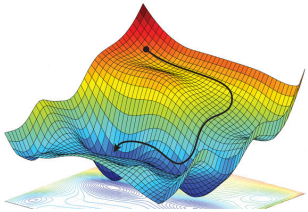
Learning objective:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \; L(\theta)$$

- in general no closed-from solution
- probably not even wanted

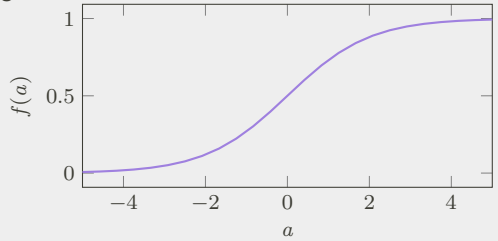
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

- fallback to gradient descent

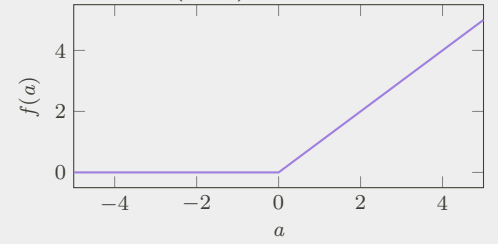


Differentiable Non-linearities

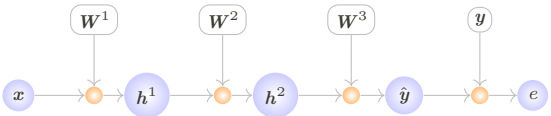
Sigmoid activation function:



Rectified linear unit (ReLU) activation function:



Error Back Propagation



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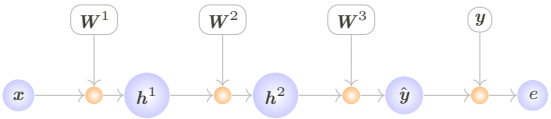

$$
\begin{aligned}
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&= f(\boldsymbol{W}^3 \boldsymbol{h}^2) \\
&= f(\boldsymbol{W}^3 f(\boldsymbol{W}^2 \boldsymbol{h}^1)) \\
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\end{aligned}
$$

$$
e = L(\boldsymbol{\theta}) = \frac{1}{k} \sum_{i=1}^{k} l(\hat{\boldsymbol{y}}, \boldsymbol{y})
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How to compute $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) = \frac{\mathrm{d}e}{\mathrm{d}\boldsymbol{\theta}}$?

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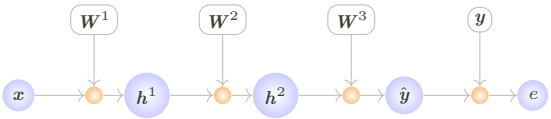

Chain Rule

$$\frac{\mathrm{d}f(g(x))}{\mathrm{d}x} = \frac{\mathrm{d}f(g(x))}{\mathrm{d}g(x)} \frac{\mathrm{d}g(x)}{\mathrm{d}x}$$

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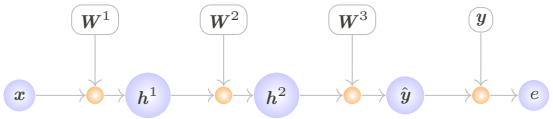

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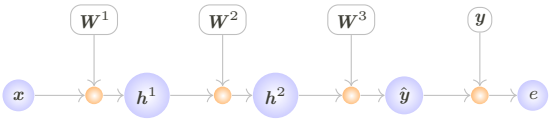

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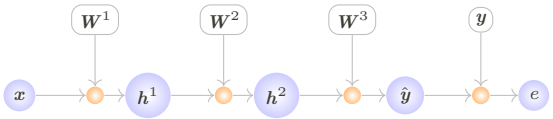

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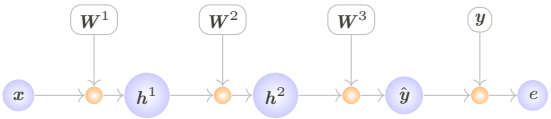

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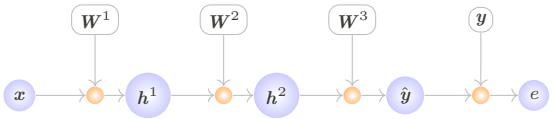

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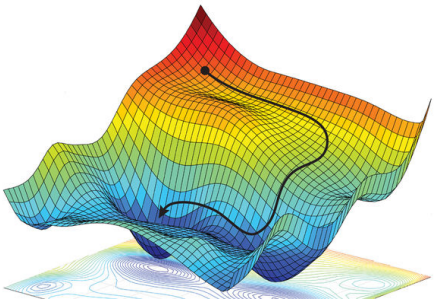
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$



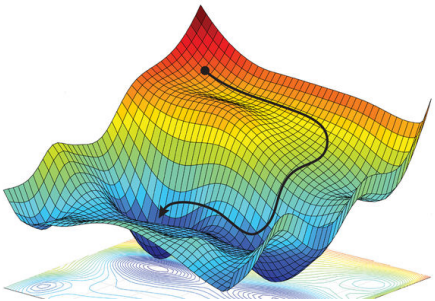
Gradient Descent

$$L(\boldsymbol{\theta}) = \frac{1}{k} \sum_{i=1}^{k} l(\hat{\boldsymbol{y}}, \boldsymbol{y})$$

- impractical for large k

Sampling Strategies

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$



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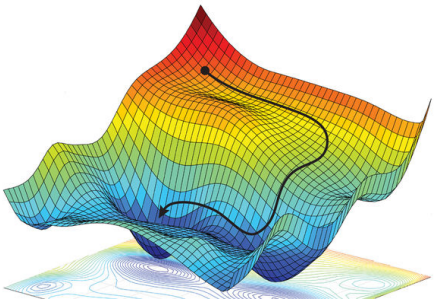
Stochastic Gradient Descent

$$L(\boldsymbol{\theta}) = l(\hat{\boldsymbol{y}}^{i}, \boldsymbol{y}^{i}) \text{ with } i \text{ random in } [1, \ldots, k]$$

- randomly sampled training example

Sampling Strategies

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$



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- randomly sampled training example

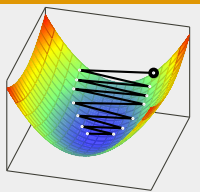
Batch Gradient Descent

$$L(\boldsymbol{\theta}) = \frac{1}{b} \sum_{i=1}^{b} l(\hat{\boldsymbol{y}}^{p_i}, \boldsymbol{y}^{p_i}) \text{ with } p_i \text{ random in } [1, \ldots, k]$$

- randomly sampled set of training examples

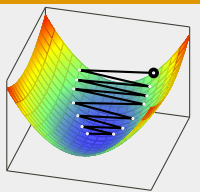
Plain Gradient Descent

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^{t} - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{t})$$



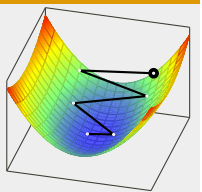
Plain Gradient Descent

$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t)$$



Gradient Descent with Momemtum

$$\boldsymbol{\delta}^t = \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t) + \beta \boldsymbol{\delta}^{t-1}$$
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \boldsymbol{\delta}^t$$



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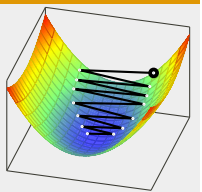

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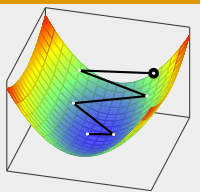
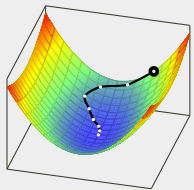


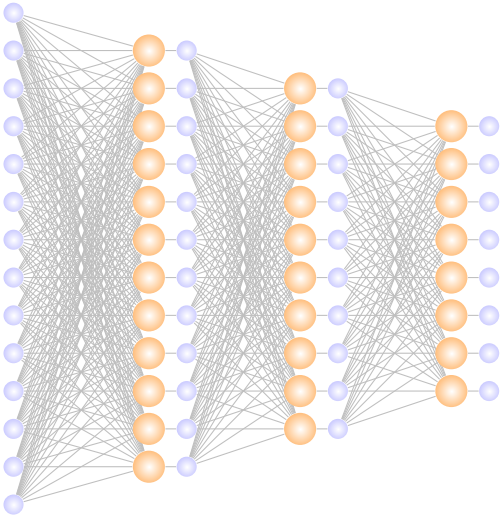
Adaptive Moment Estimation (Adam)

$$\boldsymbol{g}^t = \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t)$$
$$\boldsymbol{m}^t = \beta_1 \boldsymbol{m}^{t-1} + (1-\beta_1)\boldsymbol{g}^t$$
$$\boldsymbol{v}^t = \beta_2 \boldsymbol{v}^{t-1} + (1-\beta_2)\left(\boldsymbol{g}^t \odot \boldsymbol{g}^t\right)$$
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \frac{\boldsymbol{m}^t}{\sqrt{\boldsymbol{v}^t} + \epsilon}$$

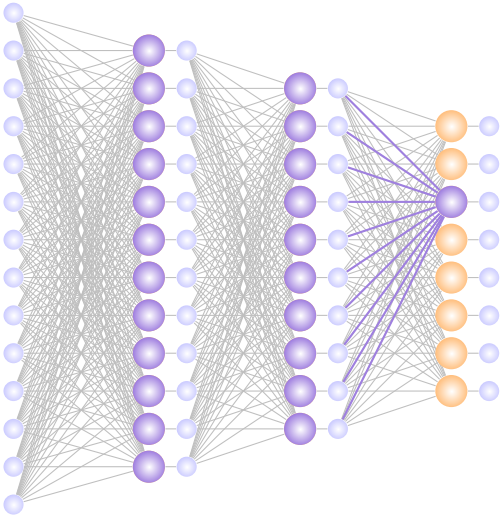


[5]

Receptive Fields

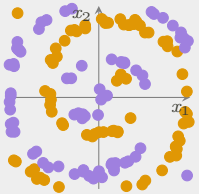


Receptive Fields

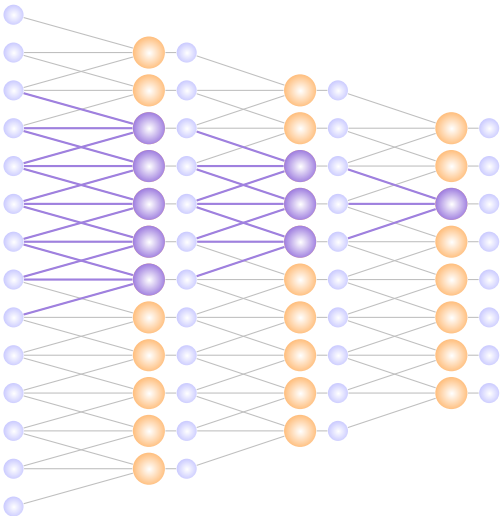


Fully Connected

- if inputs are unstructured



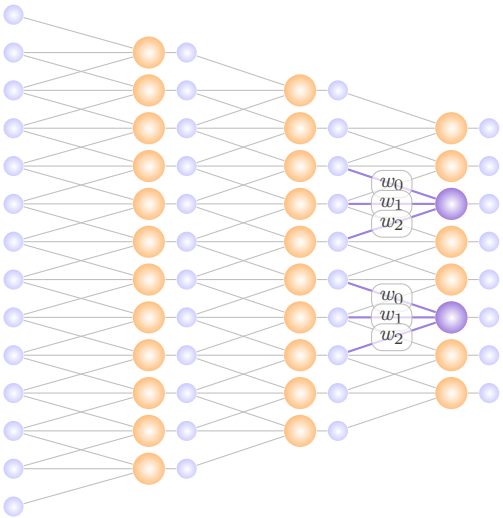
Receptive Fields



Locally Connected and Shared Weights

- if inputs have spatial/temporal structure

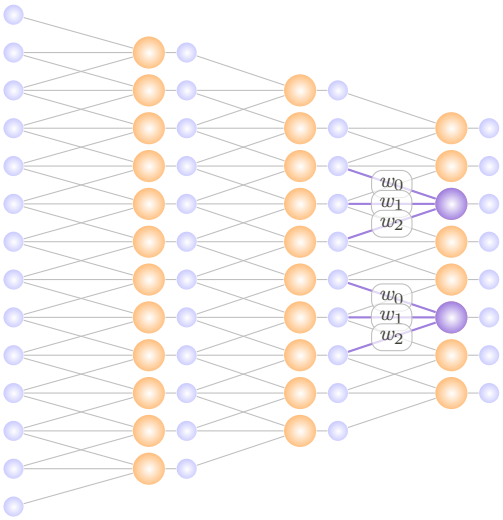
Receptive Fields



Locally Connected and Shared Weights

- if inputs have spatial/temporal structure
- if outputs are equivariant to inputs

Receptive Fields

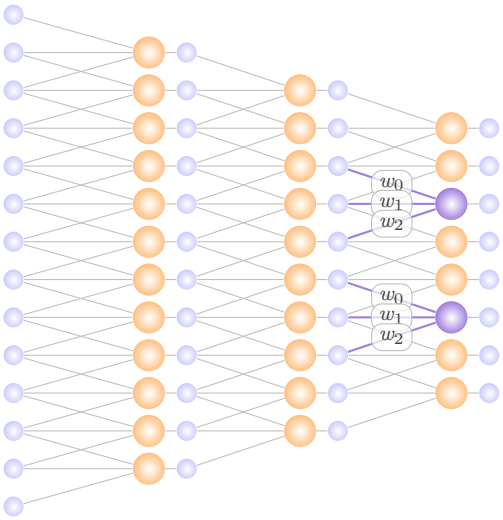


Locally Connected and Shared Weights

- if inputs have spatial/temporal structure
- if outputs are equivariant to inputs

$$y_i = f(\boldsymbol{W}\boldsymbol{h} + \boldsymbol{b})_i$$
$$= f(\sum_{j=0}^{2} h_{i+j} w_j + b_i)$$
$$\boldsymbol{y} = f(\boldsymbol{h} * \boldsymbol{k} + \boldsymbol{b}) \text{ with } \boldsymbol{k} = (w_j)_{j=0,\ldots,2}$$

Receptive Fields



Locally Connected and Shared Weights

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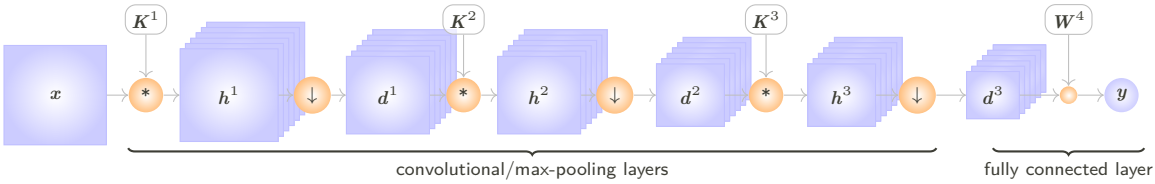
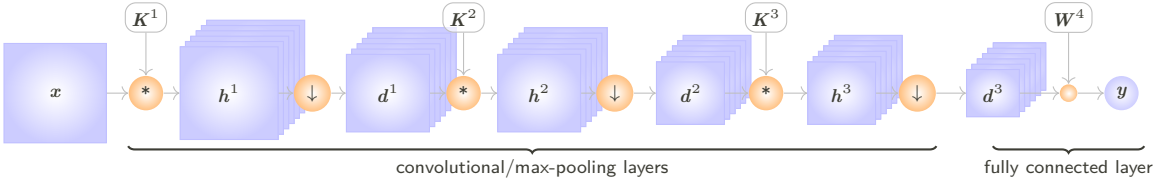
$\rightarrow$ convolutional neural networks (CNNs)

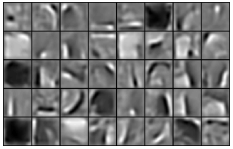
Convolutional Neural Networks

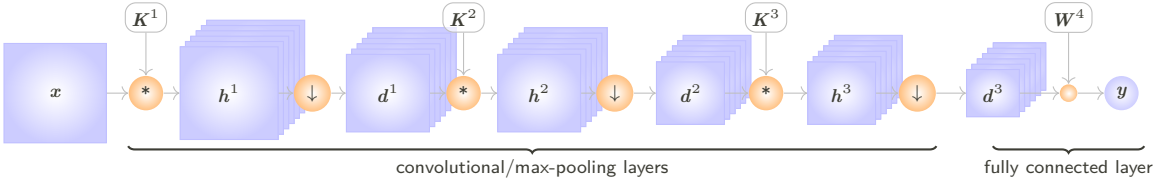


Convolutional Neural Networks

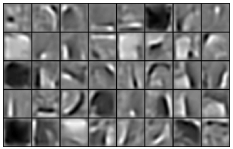


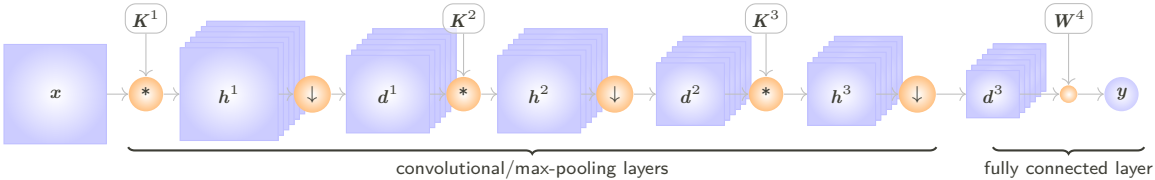
Convolutional Neural Networks





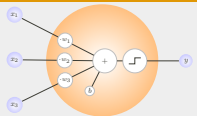
Convolutional Neural Networks



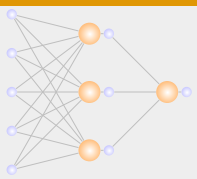


Summary

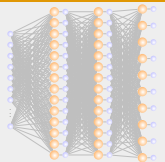
1. Perceptrons



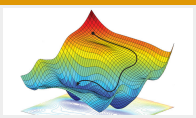
2. Networks



3. Deep Networks



4. Learning



5. Convolutional Networks

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`1412.6980`.