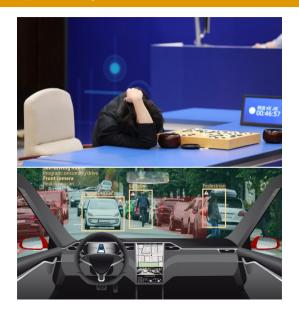
# **Introduction to Deep Learning**

Deep Learning Workshop at MBL

http://funkey.science/deep\_learning\_mbl.pdf

May 11, 2019

# Deep Learning



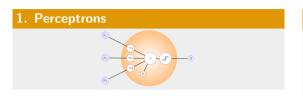


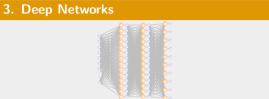




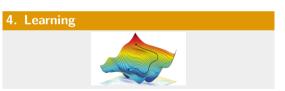


## Outline

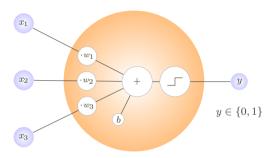






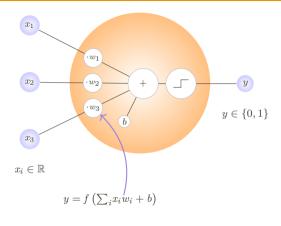




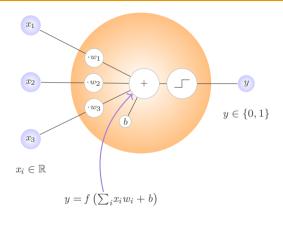


 $x_i \in \mathbb{R}$ 

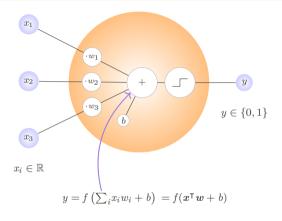
- invented by McCulloch and Pitts in 1943
- termed "perceptron" by Rosenblatt in 1958
- also known as: Threshold Logic Unit, Linear Threshold Unit, McCulloch-Pitts model



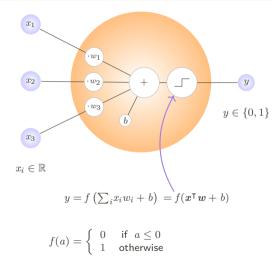
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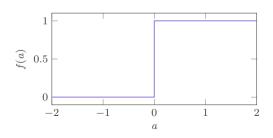
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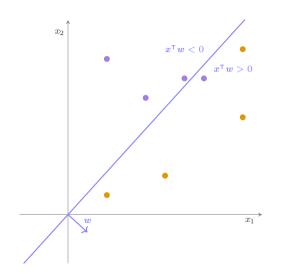
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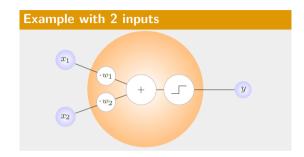


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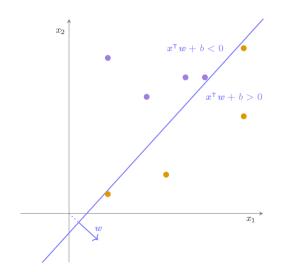


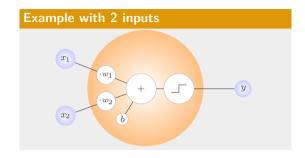
## Just a Linear Classifier



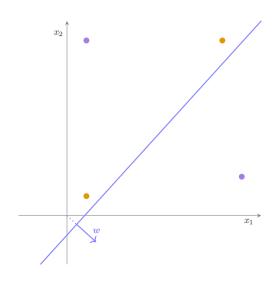


## Just a Linear Classifier

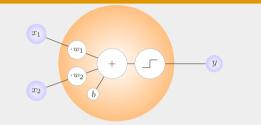




### Just a Linear Classifier



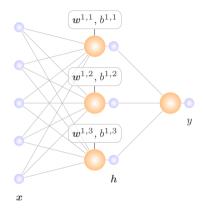
## **Example with 2 inputs**



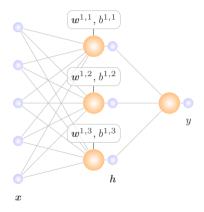
#### The XOR Affair and Al Winter

- "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

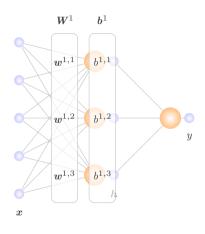




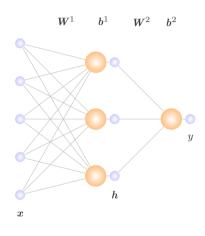
$$\boldsymbol{h} = \left( f(\boldsymbol{w^{1,1}} \boldsymbol{x} + b^{1,1}), f(\boldsymbol{w^{1,2}} \boldsymbol{x} + b^{1,2}), f(\boldsymbol{w^{1,3}} \boldsymbol{x} + b^{1,3}) \right)$$



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

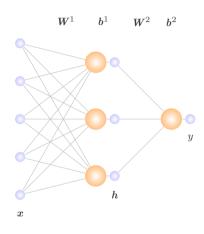


$$\begin{split} h &= \left( f(\boldsymbol{w^{1,1}} x + b^{1,1}), f(\boldsymbol{w^{1,2}} x + b^{1,2}), f(\boldsymbol{w^{1,3}} x + b^{1,3}) \right) \\ &= f\left( (\boldsymbol{w^{1,1}} x + b^{1,1}, \boldsymbol{w^{1,2}} x + b^{1,2}, \boldsymbol{w^{1,3}} x + b^{1,3}) \right) \\ &= f(\boldsymbol{W^{1}} x +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



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

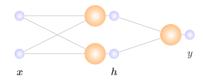


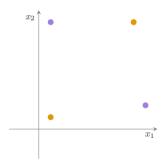
### Output Function with one Hidden Layer

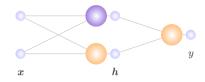
$$\begin{split} h &= \left( f(\boldsymbol{w^{1,1}}x + b^{1,1}), f(\boldsymbol{w^{1,2}}x + b^{1,2}), f(\boldsymbol{w^{1,3}}x + b^{1,3}) \right) \\ &= f\left( (\boldsymbol{w^{1,1}}x + b^{1,1}, \boldsymbol{w^{1,2}}x + b^{1,2}, \boldsymbol{w^{1,3}}x + b^{1,3}) \right) \\ &= f(\boldsymbol{W^{1}}x + b^{1})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

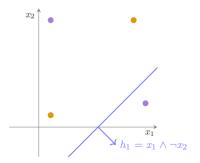
$$y = f(\boldsymbol{W}^2\boldsymbol{h} + \boldsymbol{b}^2) = f(\boldsymbol{W}^2f(\boldsymbol{W}^1\boldsymbol{x} + \boldsymbol{b}^1) + \boldsymbol{b}^2)$$

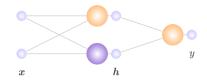
• just matrix multiplications and element-wise non-linearities

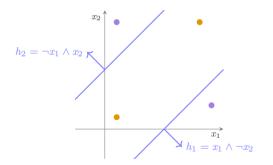


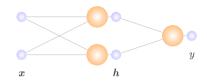


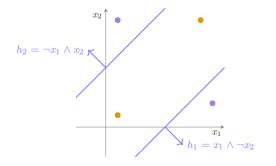


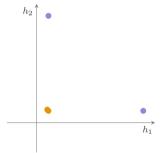


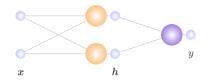


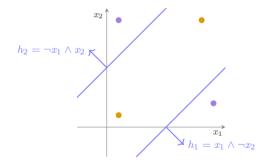


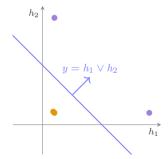












## How many layers do we need?

#### Theoretically...

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

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

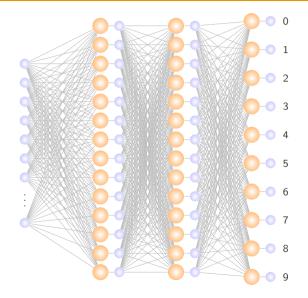


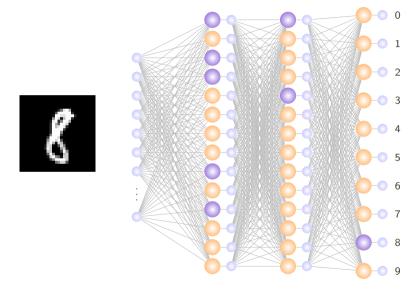
[3]

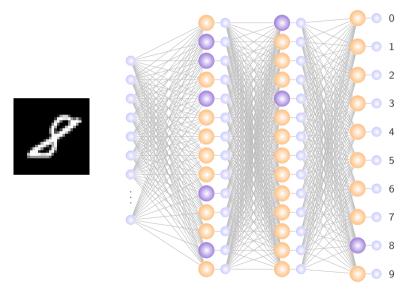
#### Practically...

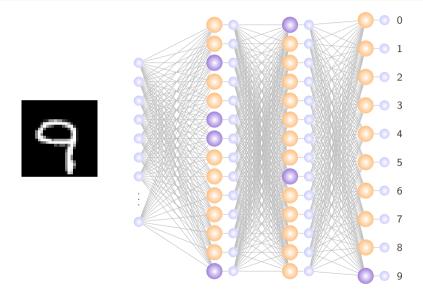
...more than one layer will be more efficient:











### Model

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

#### Data

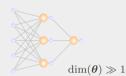
- $\bullet \ T = \left\{ \boldsymbol{x}^{i}, \boldsymbol{y}^{i} \right\}_{i=1,...,k}$
- ullet input x
- ullet desired output y

## Objective

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

### Model

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

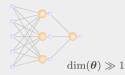
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### Data

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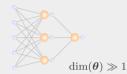
lots of it

## **Objective**

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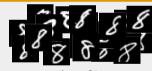
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#### Data

- $T = \left\{ \boldsymbol{x}^i, \boldsymbol{y}^i \right\}_{i=1,\dots,k}$
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lots of it

## **Objective**

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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**

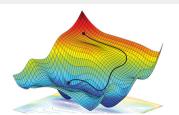
Learning objective:

$$\theta^* = \underset{\theta}{\operatorname{arg\,min}} L(\theta)$$

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

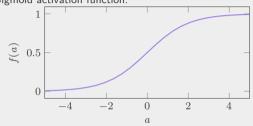
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta})$$

fallback to gradient descent

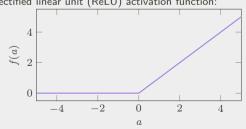


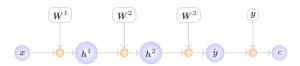
#### **Differentiable Non-linearities**

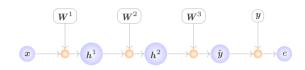
Sigmoid activation function:



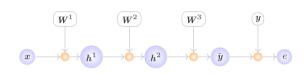
Rectified linear unit (ReLU) activation function:







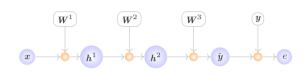
$$\begin{split} \hat{y} &= M_{\theta}(x) \ \, (\text{with } \theta = \textbf{\textit{W}}^1, \textbf{\textit{W}}^2, \textbf{\textit{W}}^3) \\ &= f(\textbf{\textit{W}}^3 \textbf{\textit{h}}^2) \\ &= f(\textbf{\textit{W}}^3 f(\textbf{\textit{W}}^2 \textbf{\textit{h}}^1)) \\ &= f(\textbf{\textit{W}}^3 f(\textbf{\textit{W}}^2 f(\textbf{\textit{W}}^1 \textbf{\textit{x}}))) \\ e &= L(\theta) = \frac{1}{k} \sum_{i=1}^k l(\hat{y}, y) \end{split}$$



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#### Chain Rule

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

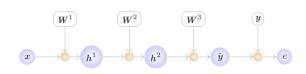


$$\begin{split} \hat{y} &= M_{\theta}(x) \ \, (\text{with } \theta = \textbf{\textit{W}}^1, \, \textbf{\textit{W}}^2, \, \textbf{\textit{W}}^3) \\ &= f(\textbf{\textit{W}}^3 \textbf{\textit{h}}^2) \\ &= f(\textbf{\textit{W}}^3 f(\textbf{\textit{W}}^2 \textbf{\textit{h}}^1)) \\ &= f(\textbf{\textit{W}}^3 f(\textbf{\textit{W}}^2 f(\textbf{\textit{W}}^1 \textbf{\textit{x}}))) \\ e &= L(\theta) = \frac{1}{k} \sum_{i=1}^k l(\hat{\textbf{\textit{y}}}, \textbf{\textit{y}}) \end{split}$$

#### Chain Rule

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

$$\frac{\mathrm{d}e}{\mathrm{d}\mathbf{W}^3} = \frac{\mathrm{d}e}{\mathrm{d}\hat{\mathbf{y}}} \frac{\mathrm{d}\hat{\mathbf{y}}}{\mathrm{d}\mathbf{W}^3} = \frac{\mathrm{d}e}{\mathrm{d}\hat{\mathbf{y}}} f'(\mathbf{W}^3 \mathbf{h}^2) \mathbf{h}^2$$



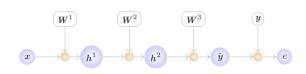
$$\begin{split} \hat{y} &= M_{\theta}(x) \ \, (\text{with } \theta = W^1, \, W^2, \, W^3) \\ &= f(\, W^3 h^2) \\ &= f(\, W^3 f(\, W^2 h^1)) \\ &= f(\, W^3 f(\, W^2 f(\, W^1 x))) \\ e &= L(\theta) = \frac{1}{k} \sum_{i=1}^k l(\hat{y}, y) \end{split}$$

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$$\frac{\mathrm{d}e}{\mathrm{d}\mathbf{W}^2} = \frac{\mathrm{d}e}{\mathrm{d}\hat{\mathbf{y}}} \frac{\mathrm{d}\hat{\mathbf{y}}}{\mathrm{d}\mathbf{h}^2} \frac{\mathrm{d}\mathbf{h}^2}{\mathrm{d}\mathbf{W}^2}$$

# Error Back Propagation



$$\begin{split} \hat{y} &= M_{\theta}(x) \ \, (\text{with } \theta = \textit{\textbf{W}}^1, \, \textit{\textbf{W}}^2, \, \textit{\textbf{W}}^3) \\ &= f(\, \textit{\textbf{W}}^3 \textit{\textbf{h}}^2) \\ &= f(\, \textit{\textbf{W}}^3 f(\, \textit{\textbf{W}}^2 \textit{\textbf{h}}^1)) \\ &= f(\, \textit{\textbf{W}}^3 f(\, \textit{\textbf{W}}^2 f(\, \textit{\textbf{W}}^1 \textit{\textbf{x}}))) \\ e &= L(\theta) = \frac{1}{k} \sum_{i=1}^k l(\hat{y}, \textit{\textbf{y}}) \end{split}$$

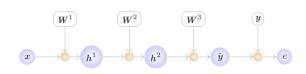
### Chain Rule

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

$$\begin{split} \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^3} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\,\boldsymbol{W}^3} = \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} f'(\boldsymbol{W}^3\boldsymbol{h}^2)\boldsymbol{h}^2 \\ \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^2} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\boldsymbol{h}^2} \frac{\mathrm{d}\boldsymbol{h}^2}{\mathrm{d}\,\boldsymbol{W}^2} \\ \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^1} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\boldsymbol{h}^2} \frac{\mathrm{d}\boldsymbol{h}^2}{\mathrm{d}\boldsymbol{h}^1} \frac{\mathrm{d}\boldsymbol{h}^1}{\mathrm{d}\,\boldsymbol{W}^1} \end{split}$$

How to compute  $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) = \frac{\mathrm{d}e}{\mathrm{d}\boldsymbol{\theta}}$ ?

# Error Back Propagation



$$\begin{split} \hat{y} &= M_{\theta}(x) \ \, (\text{with } \theta = \textit{\textbf{W}}^1, \, \textit{\textbf{W}}^2, \, \textit{\textbf{W}}^3) \\ &= f(\, \textit{\textbf{W}}^3 \textit{\textbf{h}}^2) \\ &= f(\, \textit{\textbf{W}}^3 f(\, \textit{\textbf{W}}^2 \textit{\textbf{h}}^1)) \\ &= f(\, \textit{\textbf{W}}^3 f(\, \textit{\textbf{W}}^2 f(\, \textit{\textbf{W}}^1 \textit{\textbf{x}}))) \\ e &= L(\theta) = \frac{1}{k} \sum_{i=1}^k l(\hat{\textit{\textbf{y}}}, \textit{\textbf{y}}) \end{split}$$

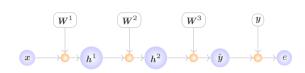
### Chain Rule

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

$$\begin{split} \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^3} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\,\boldsymbol{W}^3} = \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} f'(\boldsymbol{W}^3\boldsymbol{h}^2)\boldsymbol{h}^2 \\ \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^2} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\boldsymbol{h}^2} \frac{\mathrm{d}\boldsymbol{h}^2}{\mathrm{d}\,\boldsymbol{W}^2} \\ \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^1} &= \frac{\mathrm{d}e}{\mathrm{d}\hat{\boldsymbol{y}}} \frac{\mathrm{d}\hat{\boldsymbol{y}}}{\mathrm{d}\boldsymbol{h}^2} \frac{\mathrm{d}\boldsymbol{h}^2}{\mathrm{d}\boldsymbol{h}^1} \frac{\mathrm{d}\boldsymbol{h}^1}{\mathrm{d}\,\boldsymbol{W}^1} \\ \\ \frac{\mathrm{d}e}{\mathrm{d}\,\boldsymbol{W}^i} &= \frac{\mathrm{d}e}{\mathrm{d}\boldsymbol{h}^i} f'(\boldsymbol{W}^i\boldsymbol{h}^{i-1})\boldsymbol{h}^{i-1} \end{split}$$

How to compute  $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}) = \frac{\mathrm{d}e}{\mathrm{d}\boldsymbol{\theta}}$ ?

# Error Back Propagation



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#### Chain Rule

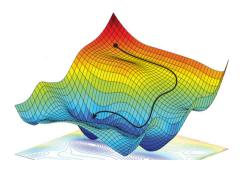
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# Sampling Strategies

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



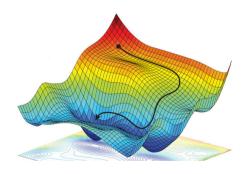
## **Gradient Descent**

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

ullet impractical for large k

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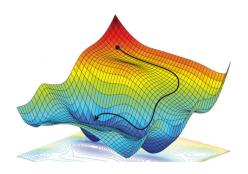
### Stochastic Gradient Descent

$$L(oldsymbol{ heta}) = l(\hat{oldsymbol{y}}^i, oldsymbol{y}^i)$$
 with  $i$  random in  $[1, \dots, k]$ 

• randomly sampled training example

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### **Batch Gradient Descent**

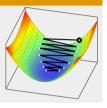
$$L(oldsymbol{ heta}) = rac{1}{b} \sum_{i=1}^b l(\hat{oldsymbol{y}}^{p_i}, oldsymbol{y}^{p_i}) \;\; ext{with} \; p_i \; ext{random in} \; [1, \dots, k]$$

randomly sampled set of training examples

# Optimization Algorithms

### Plain Gradient Descent

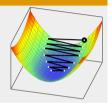
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t)$$



# Optimization Algorithms

### Plain Gradient Descent

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## **Gradient Descent with Momemtum**

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

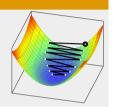
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \boldsymbol{\delta}^t$$



# **Optimization Algorithms**

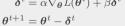
#### **Plain Gradient Descent**

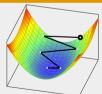
$$\boldsymbol{\theta}^{t+1} = \boldsymbol{\theta}^t - \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t)$$



### **Gradient Descent with Momemtum**

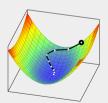
$$\boldsymbol{\delta}^t = \alpha \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^t) + \beta \boldsymbol{\delta}^{t-1}$$

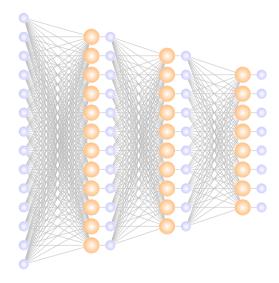


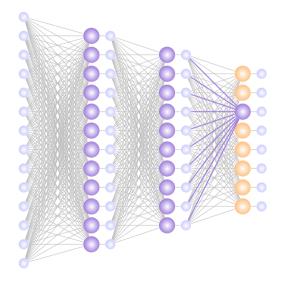


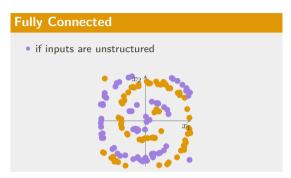
### **Adaptive Moment Estimation (Adam)**

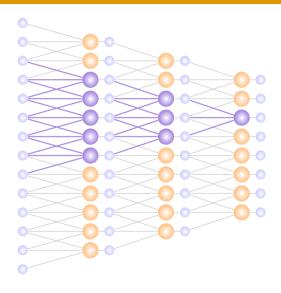
$$egin{aligned} egin{aligned} oldsymbol{g}^t &= 
abla_{oldsymbol{ heta}} L(oldsymbol{ heta}^t) \ oldsymbol{m}^t &= eta_1 oldsymbol{m}^{t-1} + (1-eta_1) oldsymbol{g}^t \odot oldsymbol{g}^t) \ oldsymbol{v}^{t+1} &= oldsymbol{ heta}^t - lpha rac{oldsymbol{m}^t}{\sqrt{oldsymbol{v}^t} + \epsilon} \end{aligned}$$





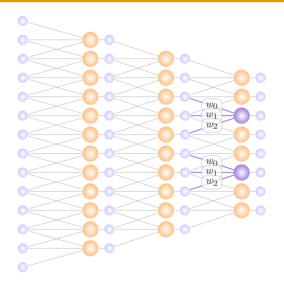






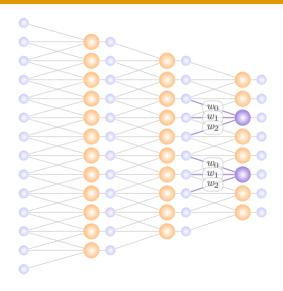
## **Locally Connected and Shared Weights**

• if inputs have spatial/temporal structure



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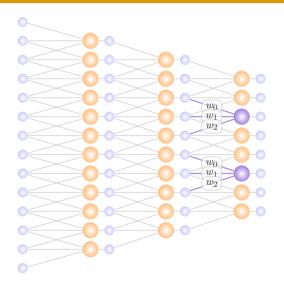
- if inputs have spatial/temporal structure
- if outputs are equivariant to inputs



## **Locally Connected and Shared Weights**

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

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



### **Locally Connected and Shared Weights**

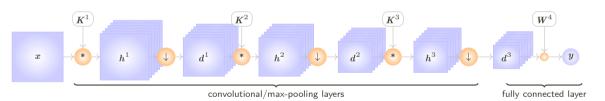
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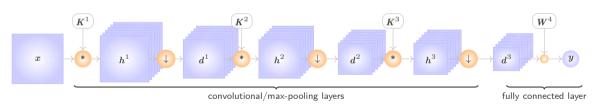
$$= f(\sum_{j=0}^2 h_{i+j}w_j + b_i)$$

$$\mathbf{y} = f(\mathbf{h} * \mathbf{k} + \mathbf{b}) \text{ with } \mathbf{k} = (w_j)_{j=0,\dots,2}$$

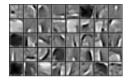
→ convolutional neural networks (CNNs)

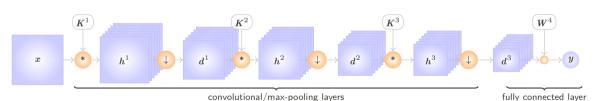


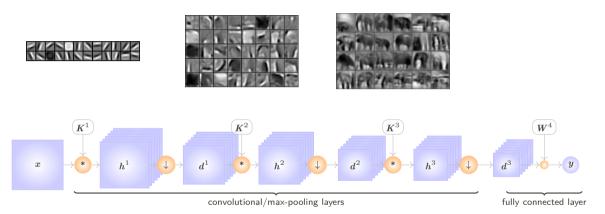




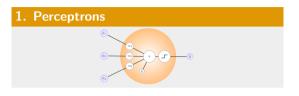


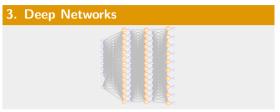




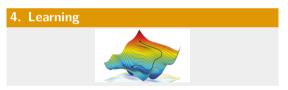


## Summary











#### References

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