

Machine Learning for Networks: Neural Networks

Andrea Araldo

September 29, 2025



	ML task	Linear Regression	Logistic Regression	Tree-based learning	Neural Networks	k -Nearest Neighbors
Supervised	Regression Classification	x	x	x	x	
Unsupervised	Clustering Dimensionality reduction Anomaly detection			x	x	x
	Recommender Systems				x	

- Structure of NNs
- Training (backpropagation)
- Design choices and hyper-parameters

Section 1

Introduction

BULLETIN OF
MATHEMATICAL BIOPHYSICS
VOLUME 5, 1943

A LOGICAL CALCULUS OF THE IDEAS IMMANENT IN NERVOUS ACTIVITY

WARREN S. MCCULLOCH AND WALTER PITTS

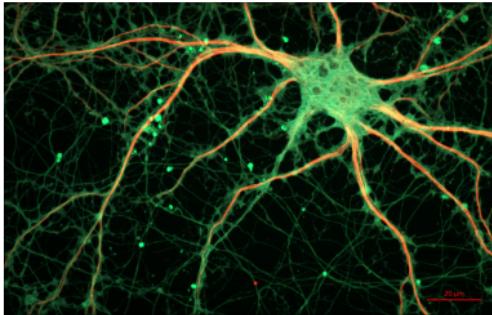
FROM THE UNIVERSITY OF ILLINOIS, COLLEGE OF MEDICINE,
DEPARTMENT OF PSYCHIATRY AT THE ILLINOIS NEUROPSYCHIATRIC INSTITUTE,
AND THE UNIVERSITY OF CHICAGO

18K citations!

Because of the "all-or-none" character of nervous activity, neural events and the relations among them can be treated by means of propositional logic. It is found that the behavior of every net can be described in these terms, with the addition of more complicated logical means for nets containing circles; and that for any logical expression satisfying certain conditions, one can find a net behaving in the fashion it describes. It is shown that many particular choices among possible neurophysiological assumptions are equivalent, in the sense that for every net behaving under one assumption, there exists another net which behaves under the other and gives the same results, although perhaps not in the same time. Various applications of the calculus are discussed.

Neural Network - Human brain

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- By ZEISS Microscopy from Germany (Cultured Rat Hippocampal Neuron) [CC BY 2.0 (<http://creativecommons.org/licenses/by/2.0/>)], via Wikimedia Commons

- <https://pixabay.com/en/neurons-brain-cells-brain-structure-1739997/>



- *Walter Pitts*: logician

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- *Warren McCulloch*: neurophysiologist



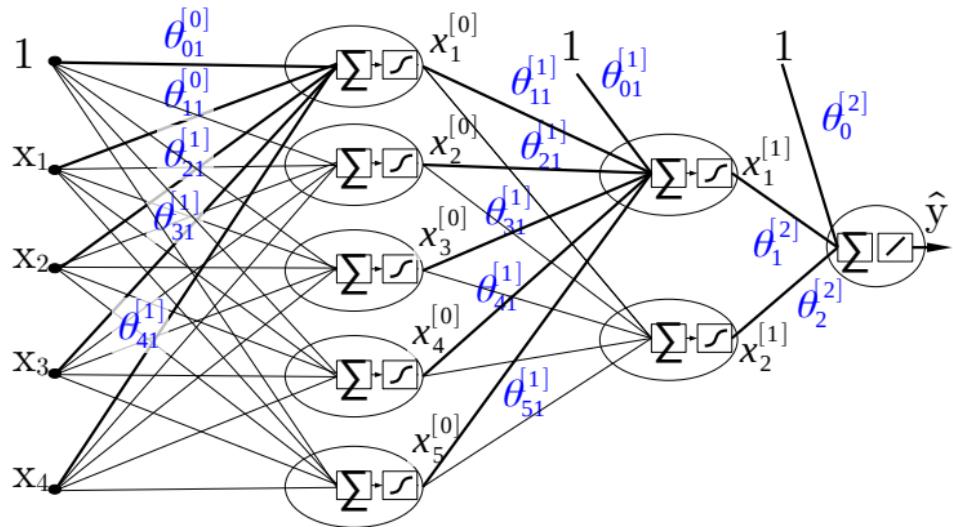
Walter Pitts:

- When he was 12, he criticized Principia Mathematica from Bertrand Russel.
- Russel invited him to Cambridge University and Pitts refused.

source: Wikipedia

Neural Network - Multi-Layer Perceptron (MLP)

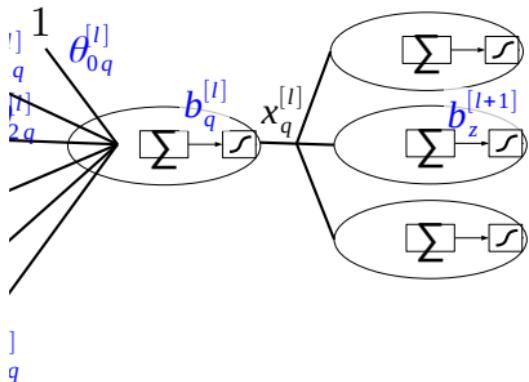
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Neural Network - Single neuron

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Let us look at the q -th neuron in the l -layer.
Do you recognize it?



- Output from the previous layer:

$$\mathbf{x}^{[l-1]} = (1, x_1^{[l-1]}, x_2^{[l-1]}, \dots)$$

- Weights:

$$\theta_q^{[l]} = (\theta_{0q}^{[l]}, \theta_{1q}^{[l]}, \dots)$$

- Weighted input

$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]}$$

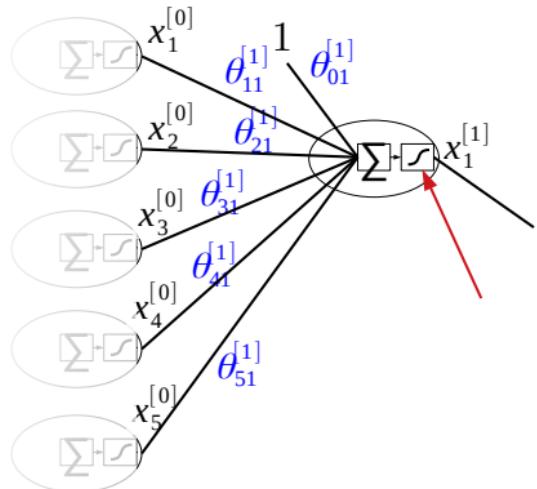
- Activation function $\sigma(\cdot)$
- Output:

$$x_q^{[l]} = \sigma(b_q^{[l]})$$

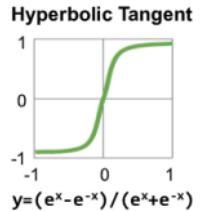
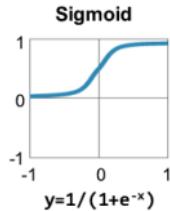
This can be fed to further neurons.

Activation Functions

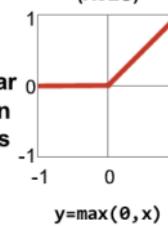
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Traditional
Non-Linear
Activation
Functions

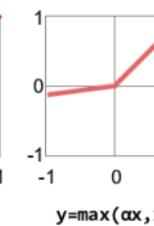


Rectified Linear Unit
(ReLU)



Modern
Non-Linear
Activation
Functions

Leaky ReLU



Exponential LU

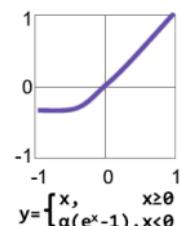
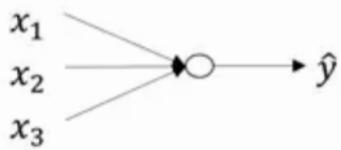


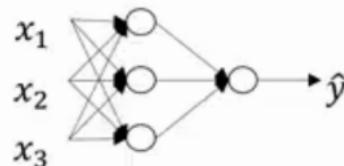
Figure from [SCYE17].

Depth of a NN

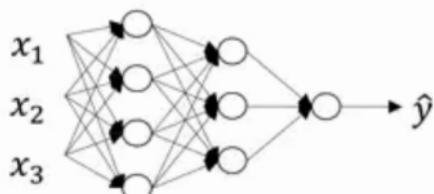
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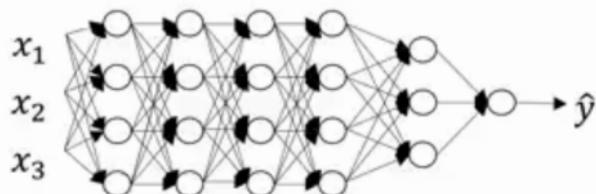
logistic regression



1 hidden layer



2 hidden layers



5 hidden layers

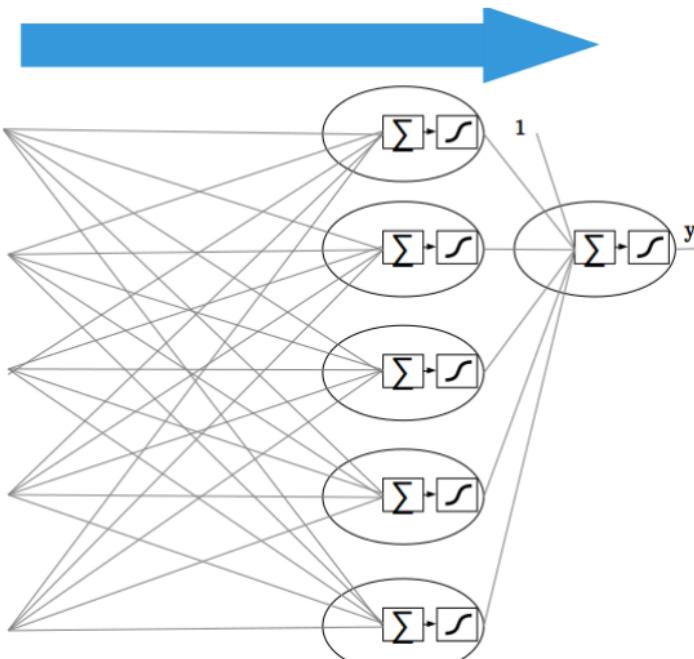
Andrew Ng

Source: Andrew Ng, Deep Neural Networks (see also Fig.10-7 of [Ger19])

Deep NN: NN with many hidden layers.

Prediction with neural networks

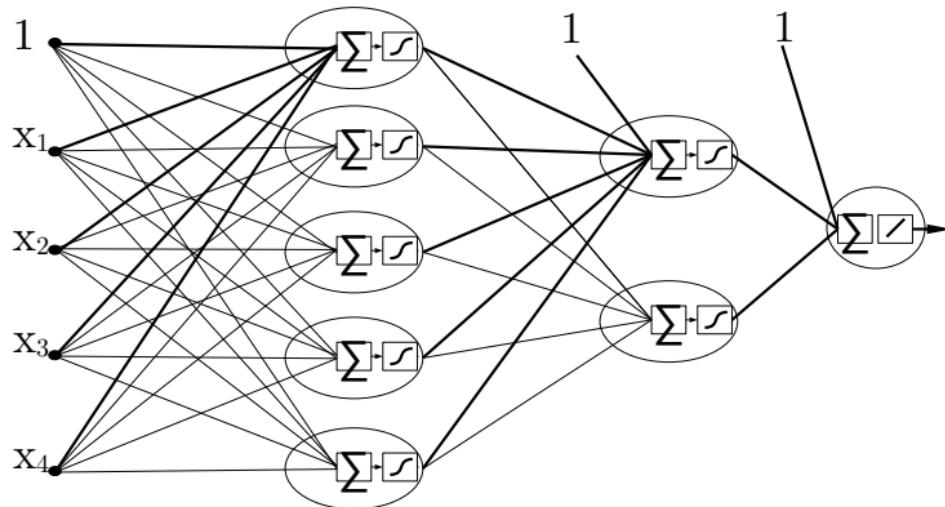
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Information is processed from left to right (forward propagation)

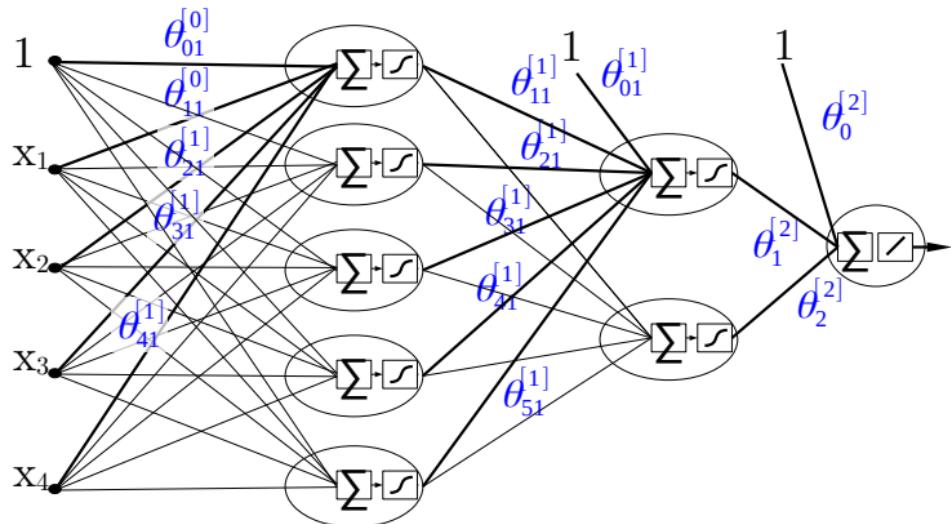
NN for regression

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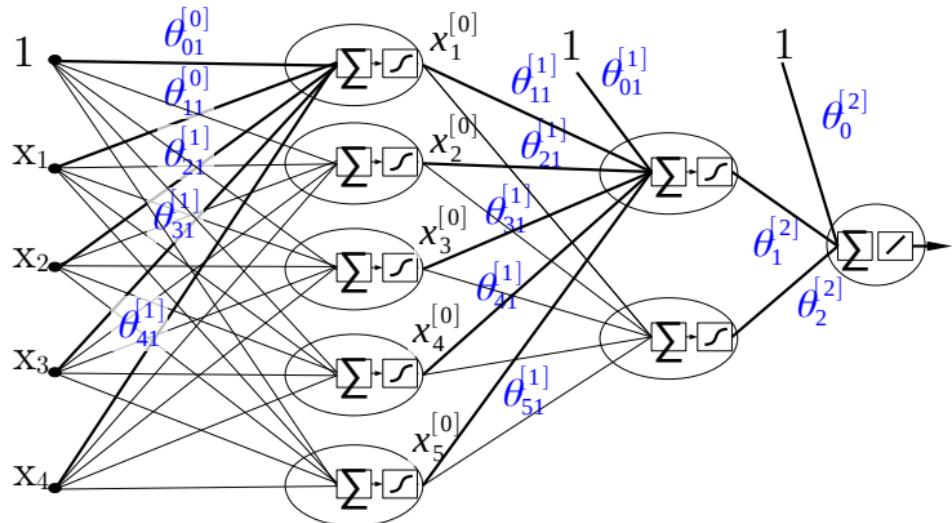
NN for regression

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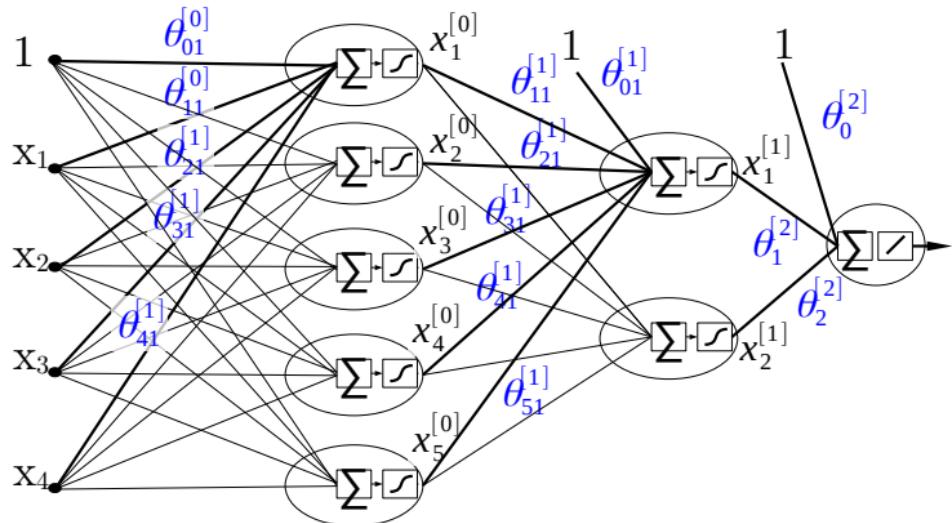
NN for regression

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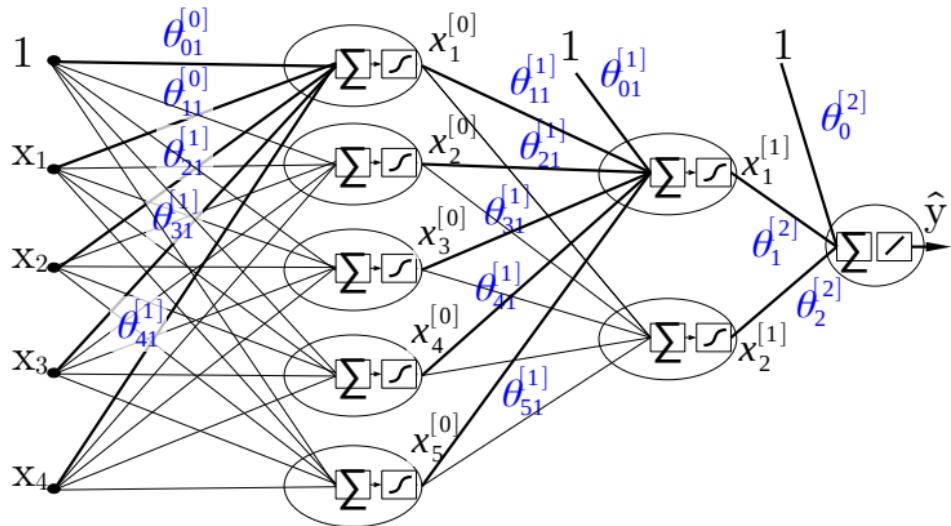
NN for regression

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NN for regression

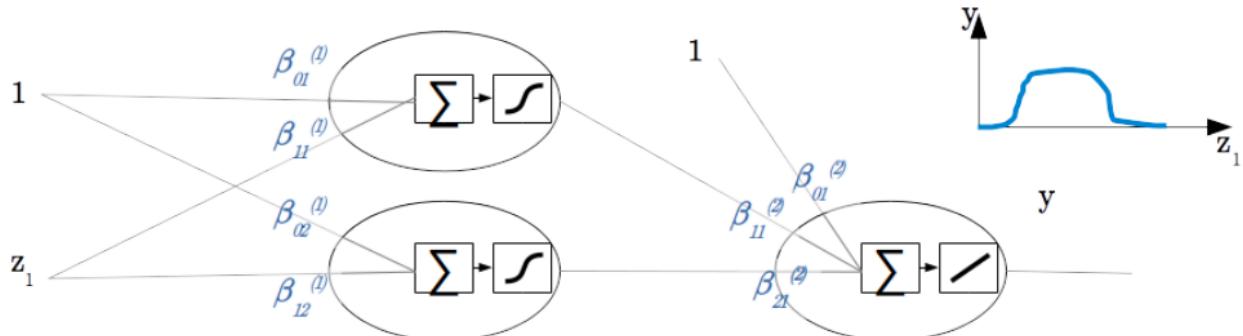
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$$\hat{y} = h_{\theta}(\mathbf{x})$$

Universal Approximator

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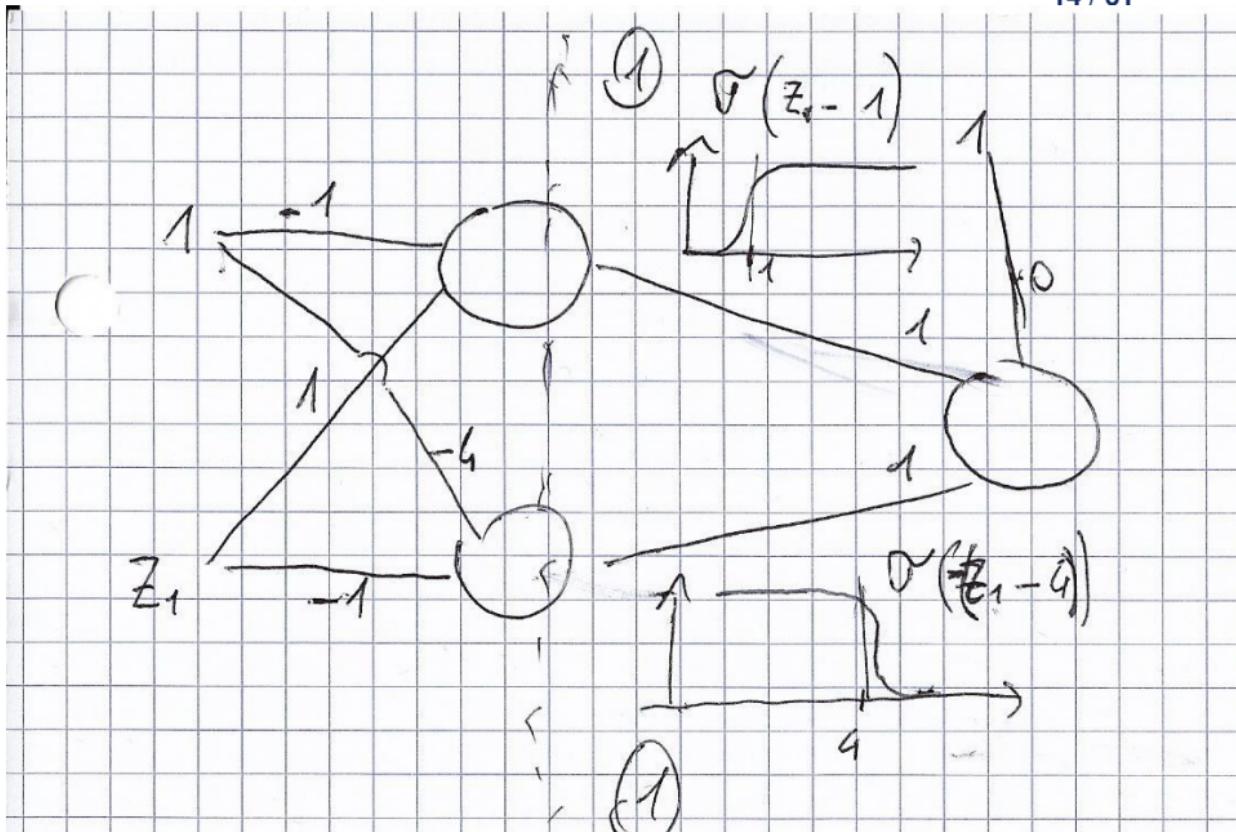


A single hidden layer neural network is a *universal approximator*: any continuous function can be approximated to arbitrary accuracy, provided that there are enough neurons.

Let's write the weights to approximate the function above

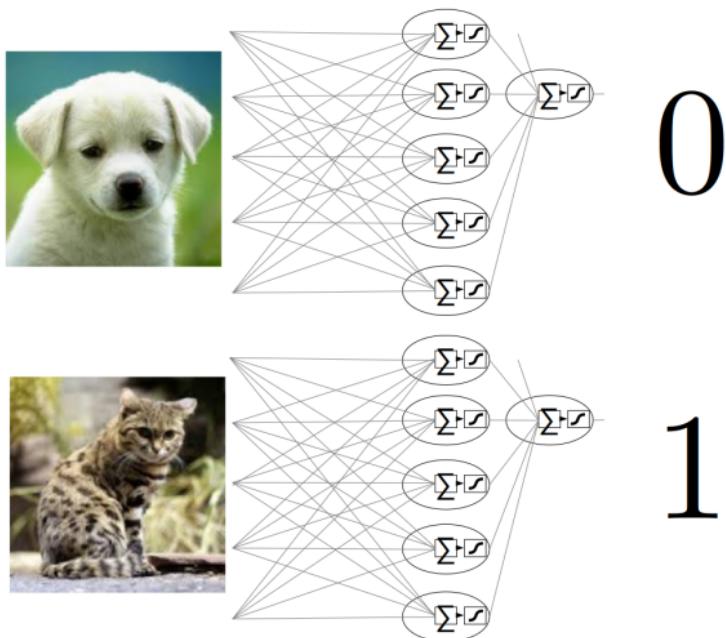
Solution

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Binary Classification: Desiderata

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Source: Google

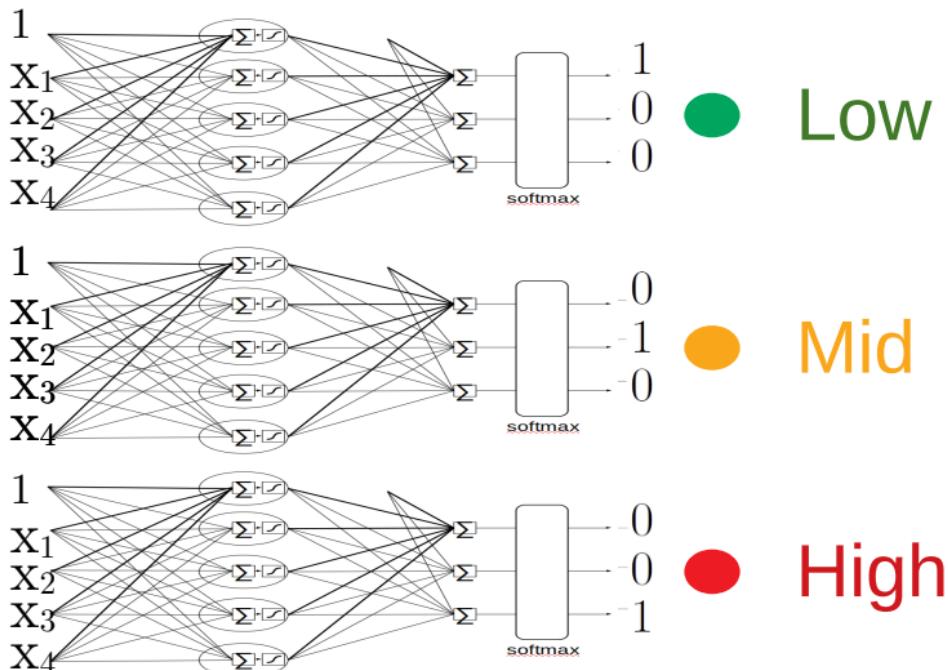
Multiclass Classification: Desiderata

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Ex.: **Telstra Kaggle Competition** [Tai17]:

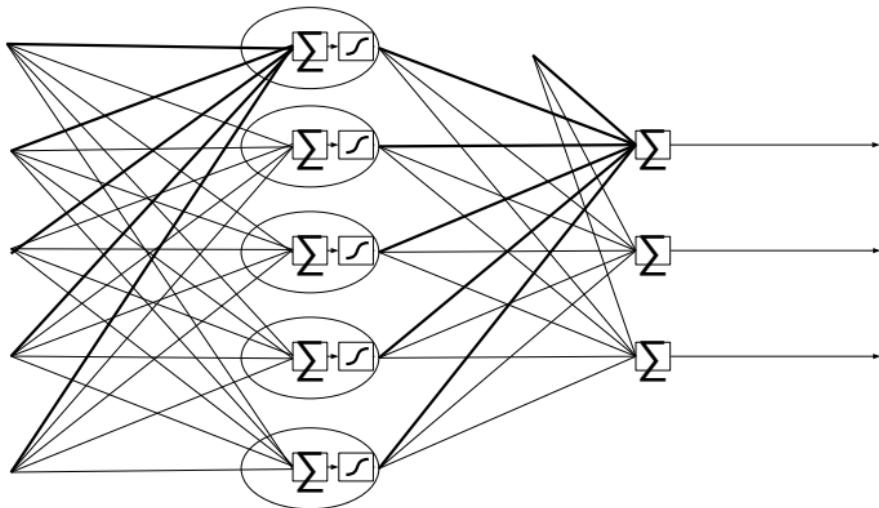
- Features: description of events (location, resource involved, type of event)
- Predict: the severity of fault



A class is *coded* in a string with one 1.

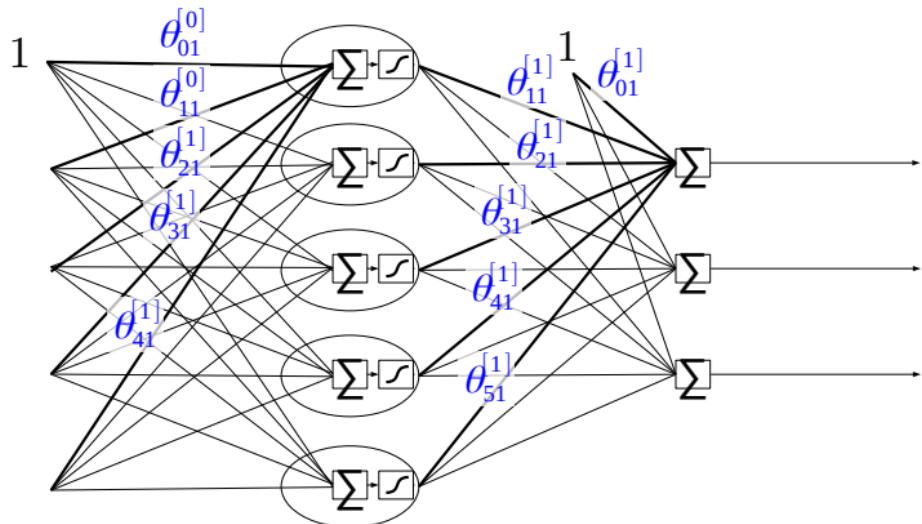
NN for classification

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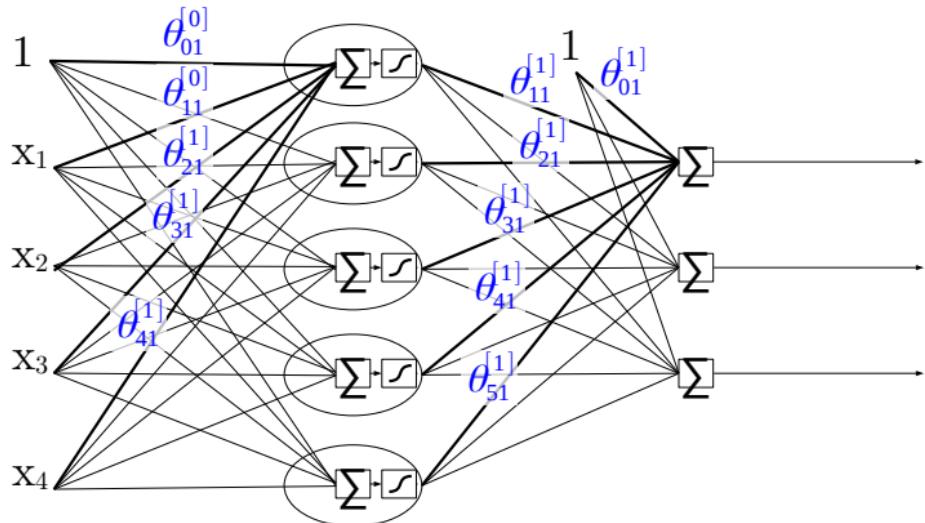
NN for classification

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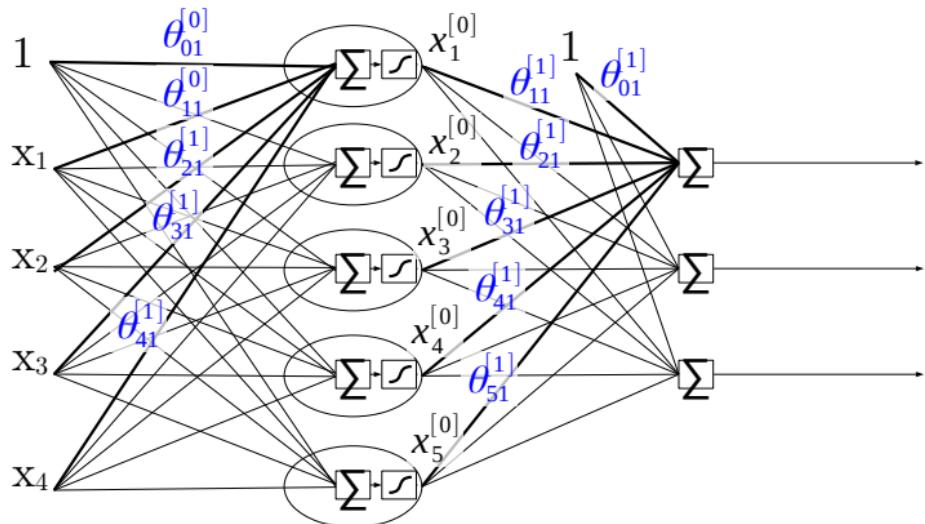
NN for classification

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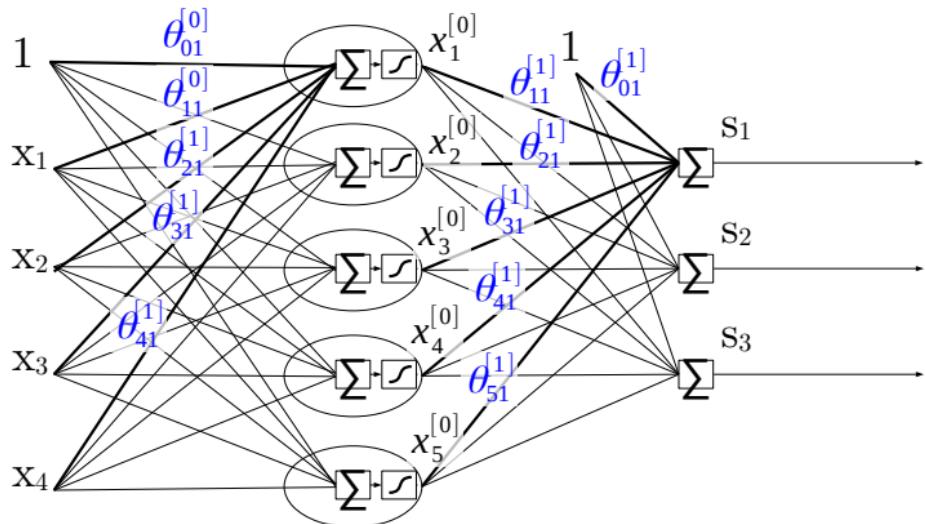
NN for classification

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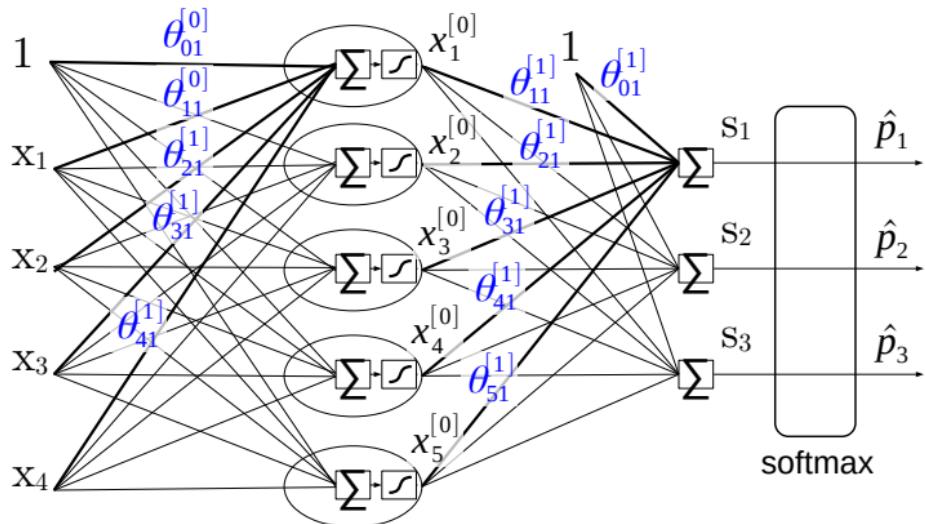
NN for classification

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NN for classification

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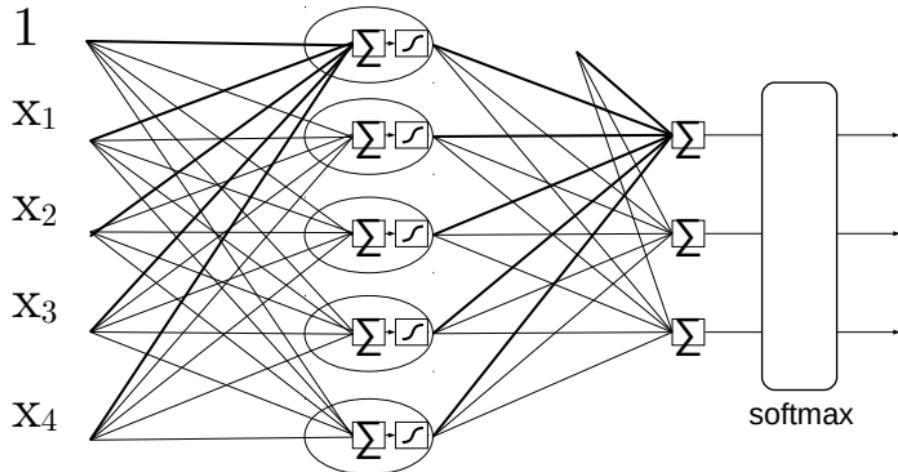


$$\hat{p}_k^{(i)} = \text{softmax}(s_k(\mathbf{x})) = \frac{\exp s_k(\mathbf{x})}{\sum_{z=1}^K \exp s_z}$$

$$k^* = \arg \max_k \hat{p}_k^{(i)}$$

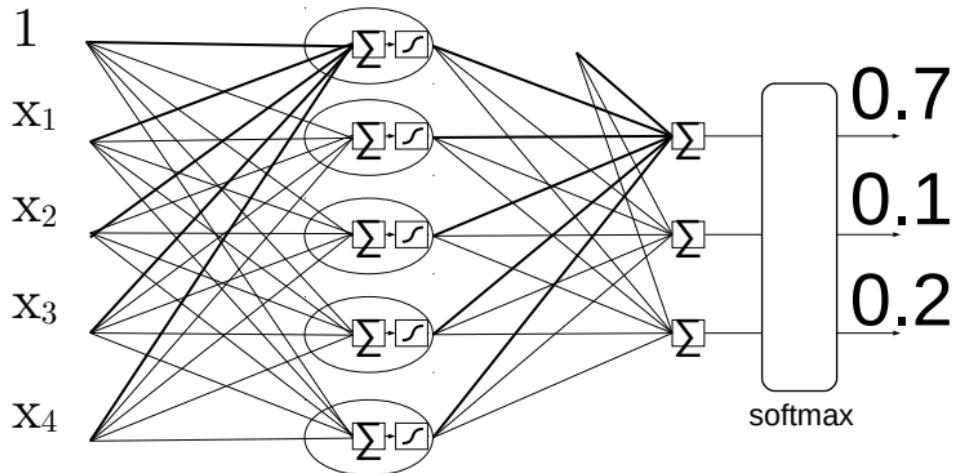
Multiclass Classification: Prediction

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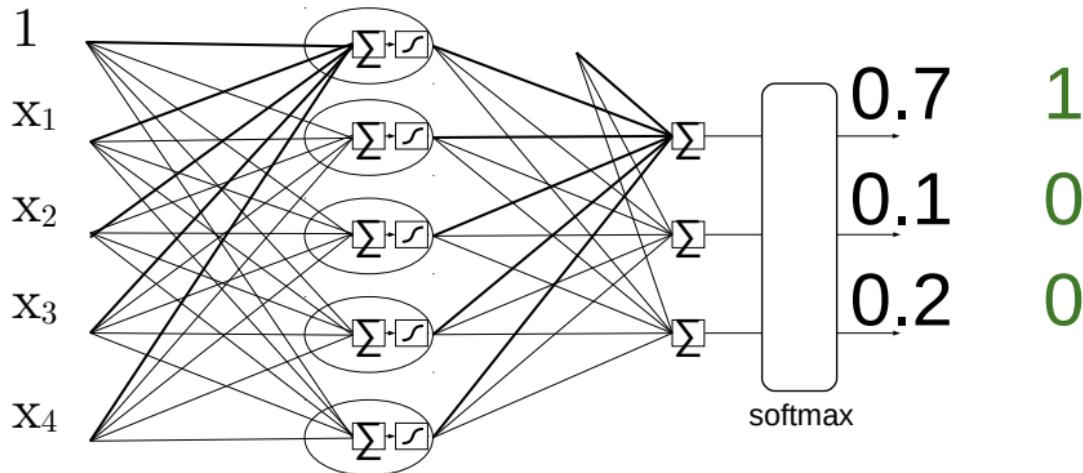
Multiclass Classification: Prediction

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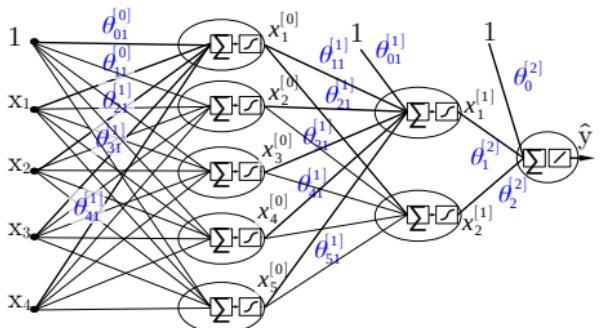
Multiclass Classification: Prediction

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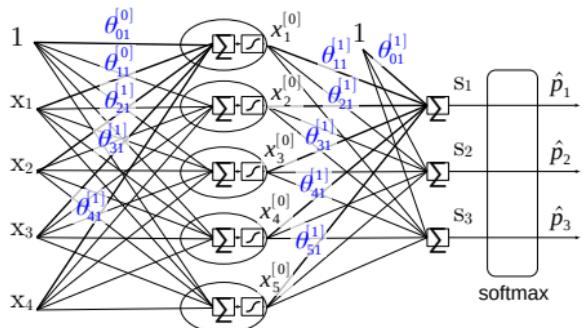


Activation functions in the output layer

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Regression: no activation function



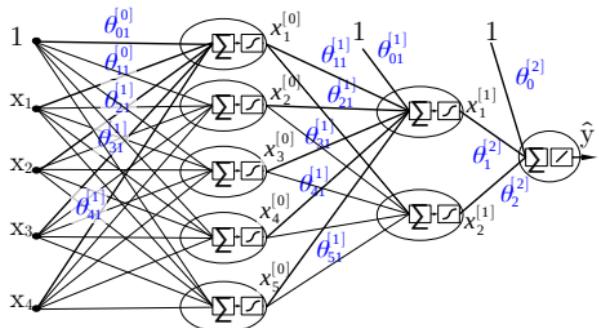
Classification: softmax

Section 2

Training (backpropagation)

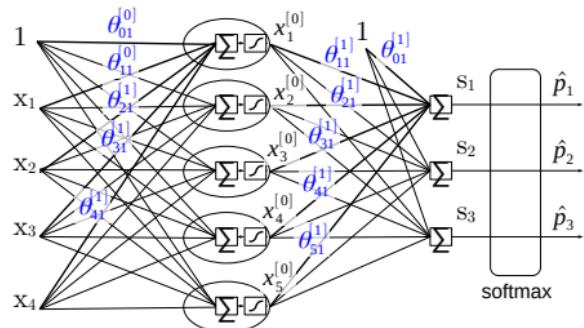
- A NN is completely specified by the weight matrix Θ
- Training: Given a training set of $(\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}})$, find the “best” matrix

$$\Theta^* \triangleq \arg \min_{\Theta} J(\Theta, \mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}) = \arg \min_{\Theta} \sum_i J(\Theta, \mathbf{x}^{(i)}, y^{(i)})$$



Regression:

$$J(\Theta, \mathbf{x}^{(i)}, y^{(i)}) = (y^{(i)} - \hat{y}^{(i)})^2$$



Classification:

$$J(\Theta, \mathbf{x}^{(i)}, y^{(i)}) = \text{cross-entropy} = -\ln \hat{p}_{y^{(i)}}^{(i)}$$

- Objective: $\min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$
 - where (\mathbf{X}, \mathbf{y}) is the training dataset.
- Initialize θ randomly
 - ... but wisely (see page 333-4 of [Ge19] for initialization techniques)
- Gradient Descent: at each iteration

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

- η : learning rate
- Gradient: $\nabla J(\theta, \mathbf{X}, \mathbf{y}) \triangleq \left(\frac{\partial}{\partial \theta_{qv}^{[l]}} J(\theta, \mathbf{X}, \mathbf{y}) \right)_{qvl}$
 - $\theta_{qv}^{[l]}$: weight of layer l connecting neuron q to neuron v .

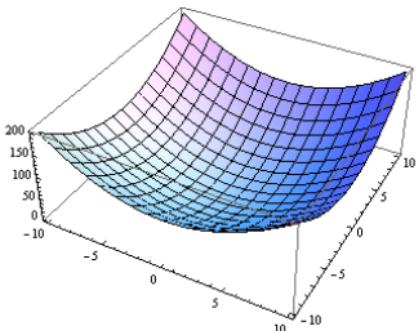
Non-convexity

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Logistic Regression:

$J(\theta, \mathbf{X}, \mathbf{y})$ derivable and convex
(unique minimum)

⇒ Convergence to minimum guaranteed.



By JackB09 [Public domain], via Wikimedia Commons

Neural Network:

$J(\theta, \mathbf{X}, \mathbf{y})$ derivable but not convex (local minima)

⇒ Gradient descent may be trapped in local minima

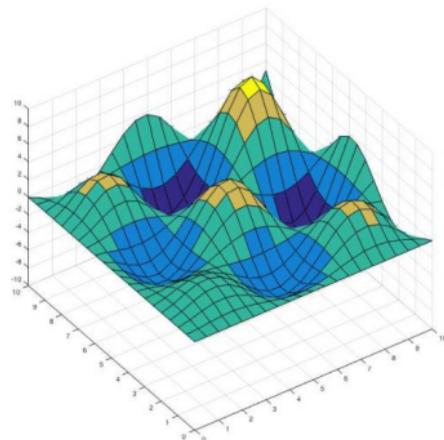


Figure from Bauso, Dario & Gao, Jian & Tembine, Hamidou. (2017). Distributionally Robust Games: f-Divergence and Learning.

Backpropagation gossip

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George Hinton, Prof. Emeritus at Toronto University (1947)



RESEARCH & INNOVATION

Geoffrey Hinton wins
2019 Honda Prize

(Photo by Nick Iwanyshyn)

George Hinton, Prof. Emeritus at Toronto University (1947)



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*“Hinton has made significant contributions
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learning, but Honda credits him for
fundamental inventions of others whom he
did not cite.”*

sources: [Univ. of Toronto](#) and [Medium](#).

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(Photo by Nick Iwanyshyn)

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Reddit post from George Hinton:

geoftinton Google Brain 177 points · 22 hours ago

Having a public debate with Schmidhuber about academic credit is not advisable because it just encourages him and there is no limit to the time and effort that he is willing to put into trying to discredit his perceived rivals. He has even resorted to tricks like having multiple aliases in Wikipedia to make it look as if other people are agreeing with what he says. The page on his

am going to respond once and only once. I have never claimed that I invented backpropagation. David Rumelhart invented it independently long after people in other fields had invented it. It is

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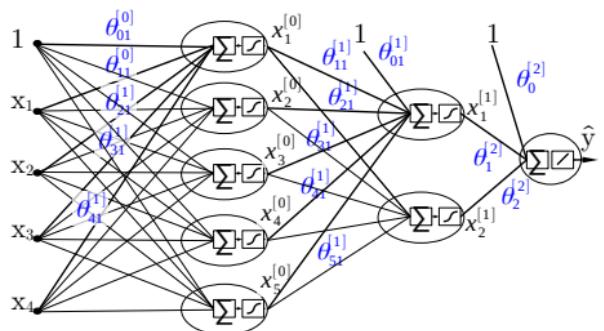
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... but backpropagation already
appears in the MSc thesis of
Seppo Ilmari Linnainmaa (1945-)
(based on [Wikipedia](#))



sources: [Univ. of Toronto](#) and [Medium](#).

Derivatives in the last layer L

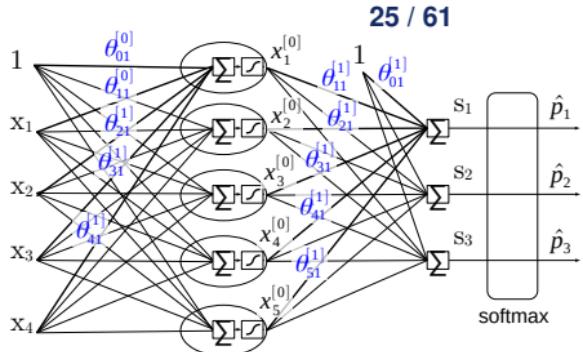


Regression:

$$J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = (y^{(i)} - \hat{y}^{(i)})^2$$

$$= \left(y^{(i)} - \underbrace{\sum_q \theta_q^{[L]} \cdot x_q^{(i)[L-1]}}_{\varepsilon^{(i)}} \right)^2$$

$$\Rightarrow \frac{\partial}{\partial \theta_q^{[L]}} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = -2 \cdot \varepsilon^{(i)} \cdot x_q^{(i)[L-1]}$$



Classification:

$$J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = -\ln \hat{p}_{k(i)}^{(i)}$$

$$= -\ln \frac{\exp \left(\theta_{k(i)}^{[L] T} \cdot \mathbf{x}^{(i)[L-1]} \right)}{\sum_{z=1}^K \exp \left(\theta_z^{[L] T} \cdot \mathbf{x}^{(i)[L-1]} \right)}$$

$k(i)$: true class of sample i .

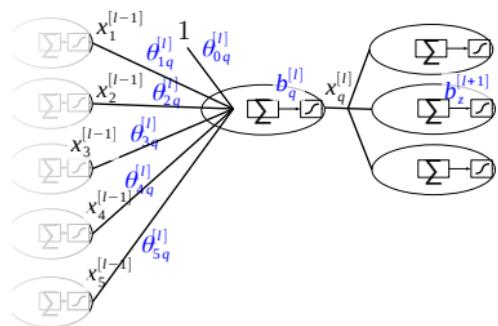
$\theta_z^{[L]}$: vector of weights of the z -th exit.

We can compute $\frac{\partial}{\partial \theta_{qz}^{[L]}} J(\theta, \mathbf{x}^{(i)}, y^{(i)})$

Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

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Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

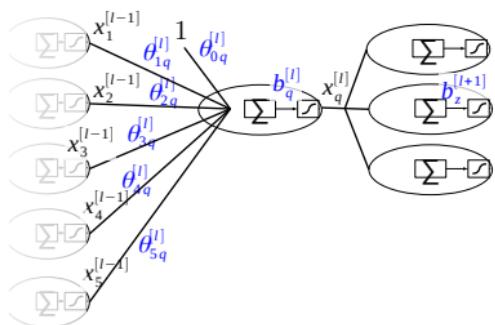


Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

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Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

- Consider the q -th neuron of intermediary layer l .



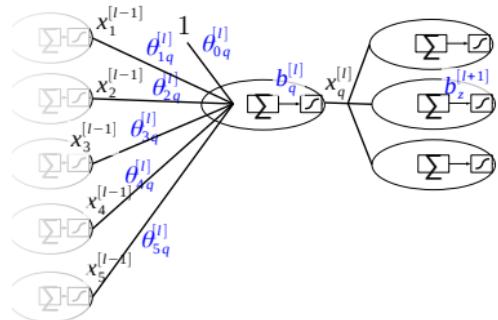
Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

26 / 61

Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

- Consider the q -th neuron of intermediary layer l .
- *Weighted input* (to the neuron):

$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]} = \sum_z \theta_{zq}^{[l]} \cdot x_z^{[l-1]}$$



Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

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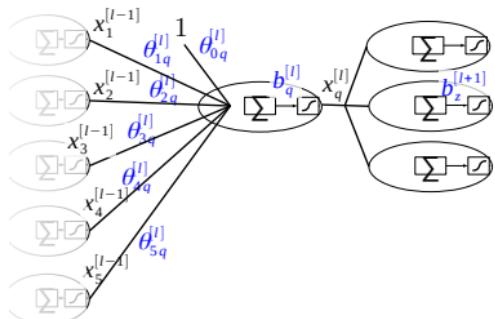
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$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]} = \sum_z \theta_{zq}^{[l]} \cdot x_z^{[l-1]}$$

$$\begin{aligned} \bullet \quad \frac{\partial J}{\partial \theta_{vq}^{[l]}} &= \underbrace{\frac{\partial J}{\partial b_q^{[l]}}} \cdot \underbrace{\frac{\partial b_q^{[l]}}{\partial \theta_{vq}^{[l]}}} = \delta_q^{[l]} \cdot x_v^{[l-1]} \\ &\triangleq \text{error } \delta_q^{[l]} \quad x_v^{[l]} \end{aligned}$$



Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

26 / 61

Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

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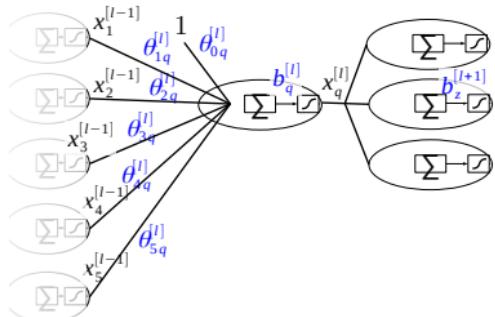
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- **Multivariable chain rule** of derivation:

$$\delta_q^{[l]} \triangleq \frac{\partial J}{\partial b_q^{[l]}} = \sum_z \frac{\partial J}{\partial b_z^{[l+1]}} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \sum_z \delta_z^{[l+1]} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}}$$



Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

26 / 61

Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

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- Weighted input* (to the neuron):

$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]} = \sum_z \theta_{zq}^{[l]} \cdot x_z^{[l-1]}$$

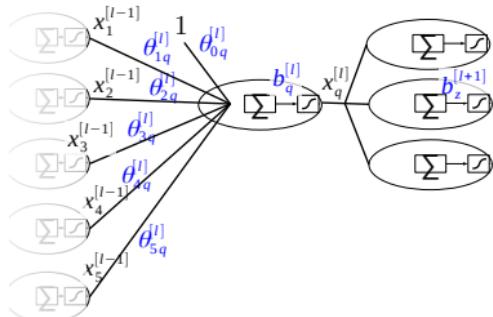
$$\begin{aligned} \bullet \quad \frac{\partial J}{\partial \theta_{vq}^{[l]}} &= \underbrace{\frac{\partial J}{\partial b_q^{[l]}}} \cdot \underbrace{\frac{\partial b_q^{[l]}}{\partial \theta_{vq}^{[l]}}} = \delta_q^{[l]} \cdot x_v^{[l-1]} \\ &\triangleq \text{error } \delta_q^{[l]} \quad x_v^{[l]} \end{aligned}$$

- Multivariable chain rule** of derivation:

$$\delta_q^{[l]} \triangleq \frac{\partial J}{\partial b_q^{[l]}} = \sum_z \frac{\partial J}{\partial b_z^{[l+1]}} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \sum_z \delta_z^{[l+1]} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}}$$

- Recall that

$$b_z^{[l+1]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot x_{z'}^{[l]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot \sigma(b_{z'}^{[l]})$$



Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

26 / 61

Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

- Consider the q -th neuron of intermediary layer l .

- Weighted input* (to the neuron):

$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]} = \sum_z \theta_{zq}^{[l]} \cdot x_z^{[l-1]}$$

$$\begin{aligned} \bullet \quad \frac{\partial J}{\partial \theta_{vq}^{[l]}} &= \underbrace{\frac{\partial J}{\partial b_q^{[l]}}} \cdot \underbrace{\frac{\partial b_q^{[l]}}{\partial \theta_{vq}^{[l]}}} = \delta_q^{[l]} \cdot x_v^{[l-1]} \\ &\triangleq \text{error } \delta_q^{[l]} \quad x_v^{[l]} \end{aligned}$$

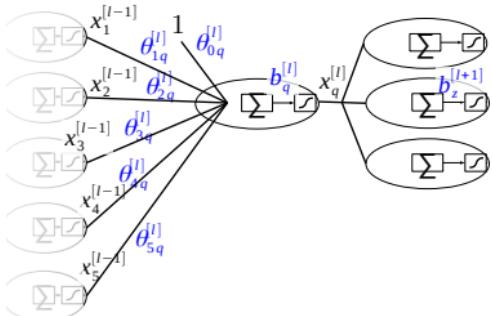
- Multivariable chain rule** of derivation:

$$\delta_q^{[l]} \triangleq \frac{\partial J}{\partial b_q^{[l]}} = \sum_z \frac{\partial J}{\partial b_z^{[l+1]}} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \sum_z \delta_z^{[l+1]} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}}$$

- Recall that

$$b_z^{[l+1]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot x_{z'}^{[l]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot \sigma(b_{z'}^{[l]})$$

$$\bullet \implies \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \theta_{qz}^{[l+1]} \cdot \sigma'(b_q^{[l]})$$



Backpropagation (i.e. $\nabla_{\theta} J()$ computation)

26 / 61

Compute $\frac{\partial J}{\partial \theta_{vq}^{[l]}}(\theta, \mathbf{x}, y)$, \forall training sample (\mathbf{x}, y) :

- Consider the q -th neuron of intermediary layer l .

- Weighted input* (to the neuron):

$$b_q^{[l]} = \theta_q^{[l]T} \cdot \mathbf{x}^{[l-1]} = \sum_z \theta_{zq}^{[l]} \cdot x_z^{[l-1]}$$

- $$\frac{\partial J}{\partial \theta_{vq}^{[l]}} = \underbrace{\frac{\partial J}{\partial b_q^{[l]}}}_{\triangleq \text{error } \delta_q^{[l]}} \cdot \underbrace{\frac{\partial b_q^{[l]}}{\partial \theta_{vq}^{[l]}}}_{x_v^{[l]}} = \delta_q^{[l]} \cdot x_v^{[l-1]}$$

- Multivariable chain rule** of derivation:

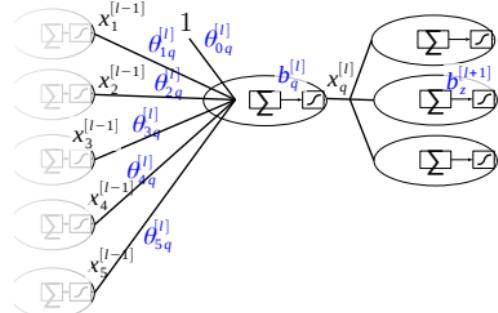
$$\delta_q^{[l]} \triangleq \frac{\partial J}{\partial b_q^{[l]}} = \sum_z \frac{\partial J}{\partial b_z^{[l+1]}} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \sum_z \delta_z^{[l+1]} \cdot \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}}$$

- Recall that

$$b_z^{[l+1]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot x_{z'}^{[l]} = \sum_{z'} \theta_{z'z}^{[l+1]} \cdot \sigma(b_{z'}^{[l]})$$

- $$\Rightarrow \frac{\partial b_z^{[l+1]}}{\partial b_q^{[l]}} = \theta_{qz}^{[l+1]} \cdot \sigma'(b_q^{[l]})$$

- $$\Rightarrow \delta_q^{[l]} = \sigma'(b_q^{[l]}) \cdot \sum_z \delta_z^{[l+1]} \cdot \theta_{qz}^{[l+1]}$$



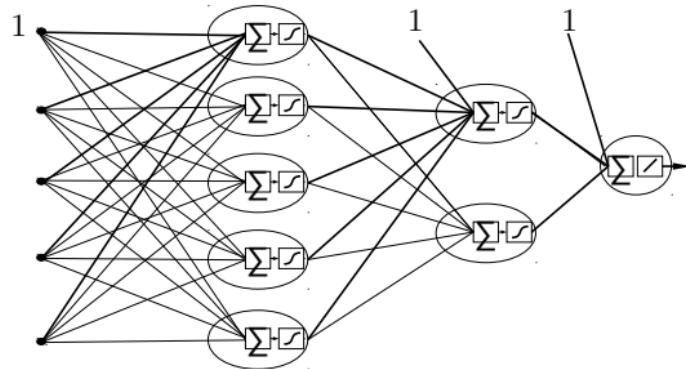
The errors $\delta_z^{[l+1]}$ propagate back to layer l .

In NN for regression, in the last layer L there is only one neuron and $\delta^{[L]} = 1$

Backpropagation explained in [Bis06, §5.3]

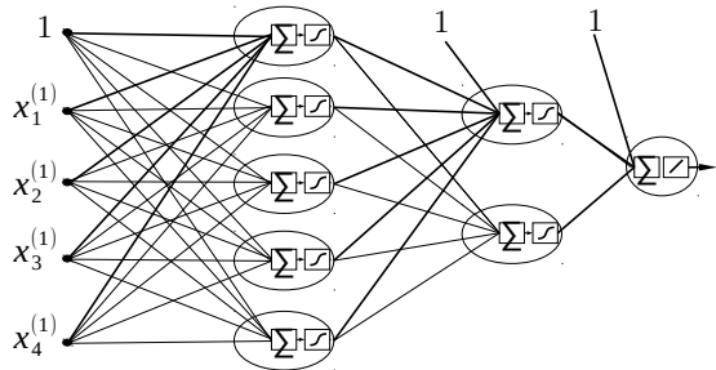
Forward and Backward Propagation

27 / 61



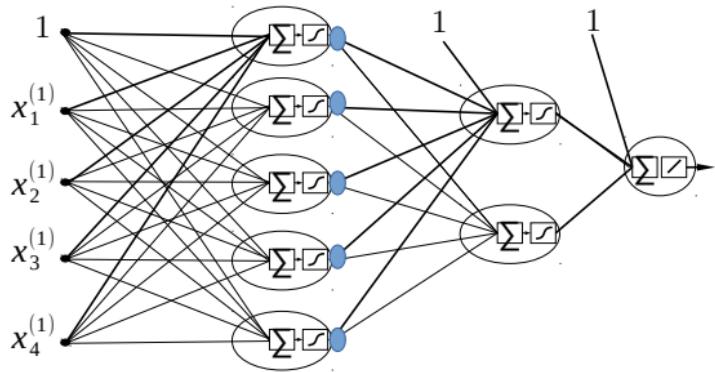
Forward and Backward Propagation

27 / 61



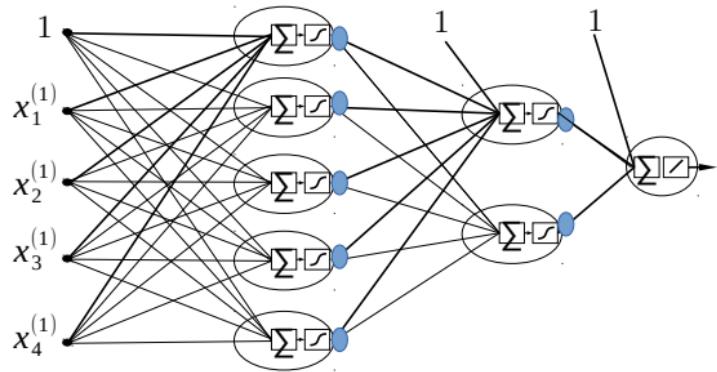
Forward and Backward Propagation

27 / 61



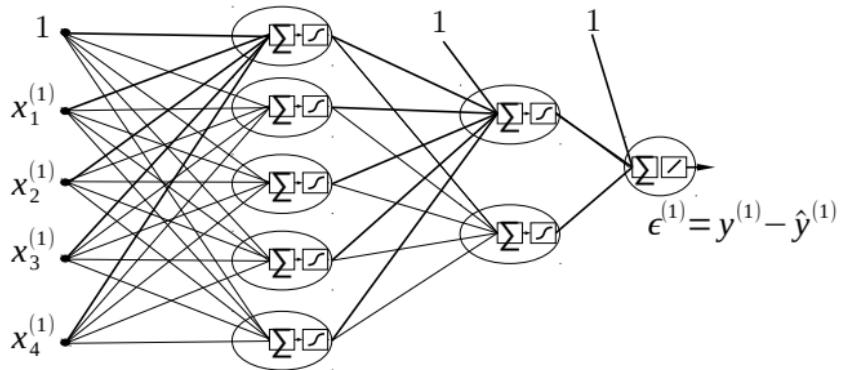
Forward and Backward Propagation

27 / 61



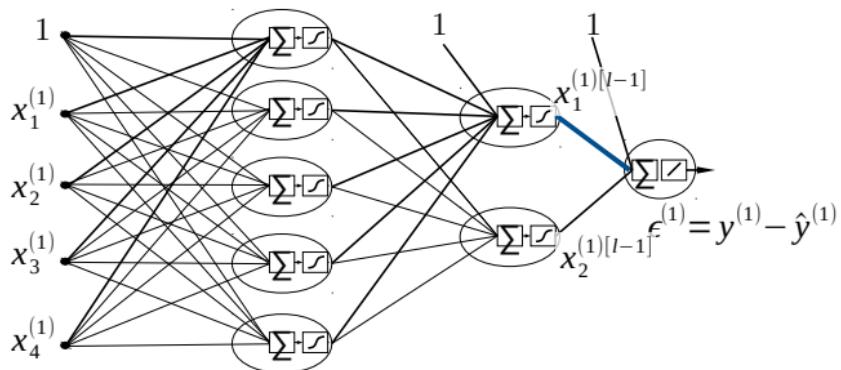
Forward and Backward Propagation

27 / 61



Forward and Backward Propagation

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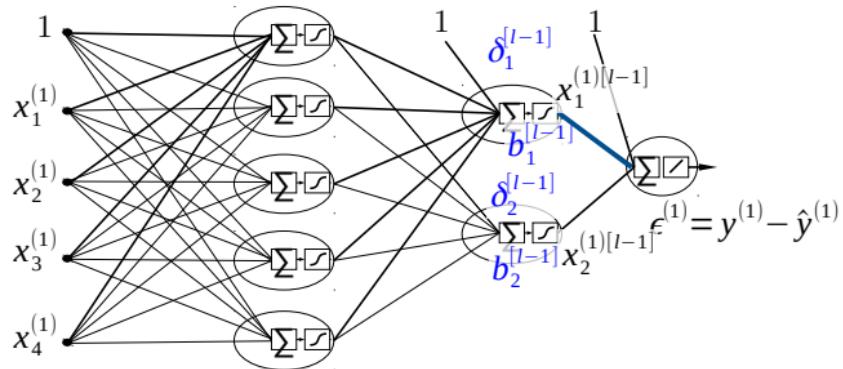
- Compute

$$\frac{\partial}{\partial \theta_q^{[L]}} J(\Theta, \mathbf{x}^{(1)}, y^{(1)}) = \epsilon^{(1)} \cdot x_q^{(1)[L-1]}$$

for all $\theta_q^{[L]}$ in the last layer

Forward and Backward Propagation

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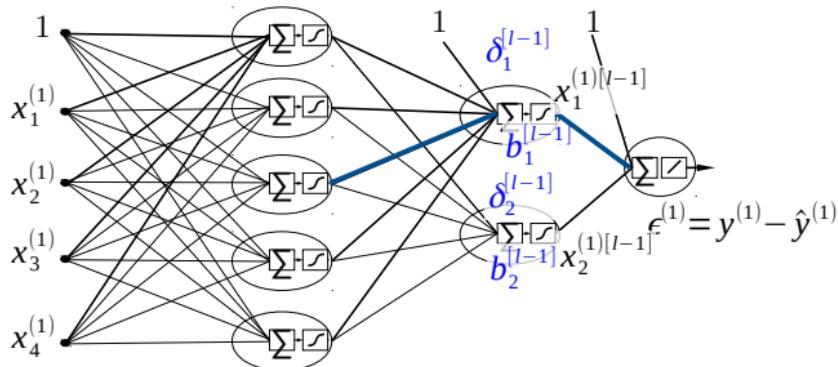


- Compute

$$\delta_q^{[l-1]} = \sigma'(b^{[l-1]}) \cdot \sum_z \delta_z^{[l]} \cdot \theta_{qz}^{[l]}$$

Forward and Backward Propagation

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- Compute

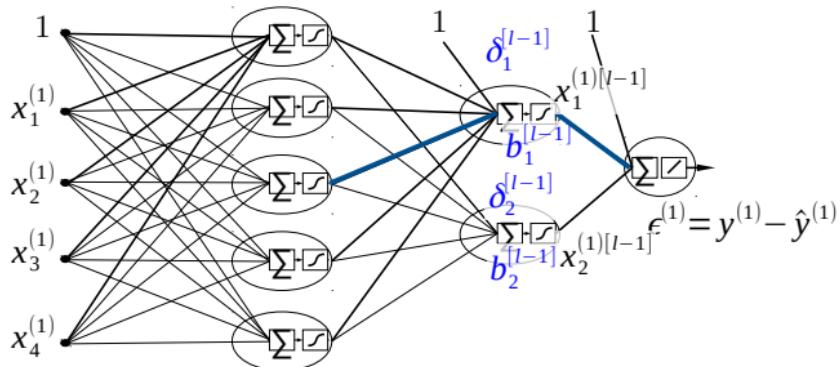
$$\delta_q^{[l-1]} = \sigma'(b^{[l-1]}) \cdot \sum_z \delta_z^{[l]} \cdot \theta_{qz}^{[l]}$$

- and

$$\frac{\partial}{\partial \theta_{vq}^{[l-1]}} J = \delta_q^{[l-1]} \cdot x_v^{(1)[l-1]}$$

Forward and Backward Propagation

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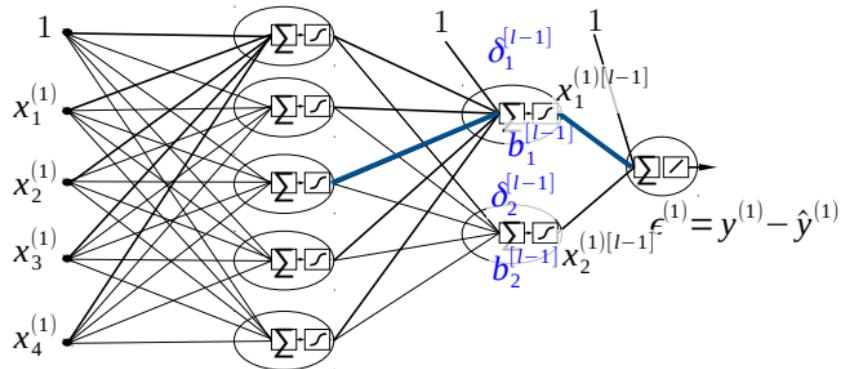
- Do the same for all the weights, backward, to compute

$$\frac{\partial}{\partial \theta_{vq}^{[l-1]}} J = \delta_q^{[l-1]} \cdot x_v^{(1)[l-1]}$$

for all weights $\theta_{vq}^{[l]}$

Forward and Backward Propagation

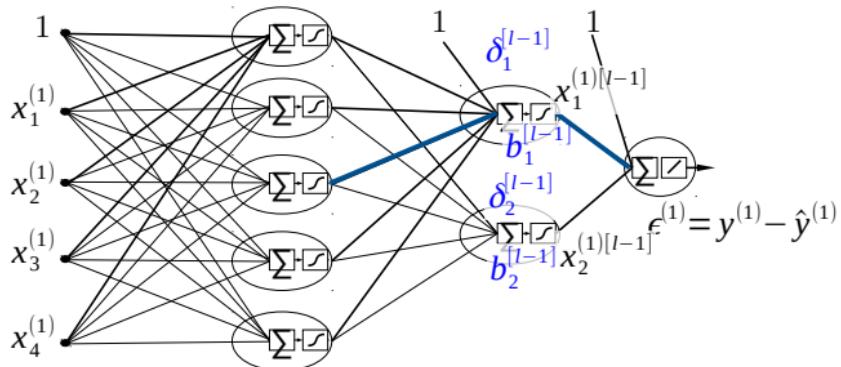
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- We thus obtain $\nabla J(\Theta, \mathbf{x}^{(i)}, y^{(i)})$

Forward and Backward Propagation

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- Do the same for all the samples
- Finally

$$\nabla J(\theta, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \nabla J(\theta, \mathbf{x}^{(i)}, y^{(i)})$$

And update

$$\theta := \theta - \eta \cdot \nabla J(\theta, \mathbf{X}, \mathbf{y})$$

1. Full Gradient Descent

- Predict $\hat{y}^{(i)}$ for all $\mathbf{x}^{(i)}$ in $\mathcal{D}^{\text{train}}$
- $\nabla J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \nabla J(\boldsymbol{\theta}, \mathbf{x}^{(i)}, y^{(i)})$
- Update weights $\boldsymbol{\theta} := \boldsymbol{\theta} - \eta \cdot \nabla J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y})$

2. Stochastic Gradient Descent

(update parameters at each sample)

- For each sample $\mathbf{x}^{(i)}$
 - Predict $\hat{y}^{(i)}$
 - Compute $J(\boldsymbol{\theta}, \mathbf{x}^{(i)}, y^{(i)})$
 - Assume $\nabla J(\boldsymbol{\theta}, \mathbf{x}^{(i)}, y^{(i)}) \simeq \nabla J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y})$
 - Update weights
$$\boldsymbol{\theta} := \boldsymbol{\theta} - \eta \cdot \nabla J(\boldsymbol{\theta}, \mathbf{x}^{(i)}, y^{(i)})$$

3. Batch Gradient Descent

- Divide $\mathcal{D}^{\text{train}}$ in batches
- Update the parameters after predicting each batch.

- **Epoch:** Sequence of predictions on the entire $\mathcal{D}^{\text{train}}$
- How many parameter updates per-epoch (using the 3 strategies)?
- Usually **many epochs** are needed

Multi-Layer Perceptron Implementation

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On the right: weights θ (potentiometers adjust via motors)

$$\theta := \theta - \eta \cdot \nabla J(\theta, \mathbf{x}^{(i)}, y^{(i)})$$

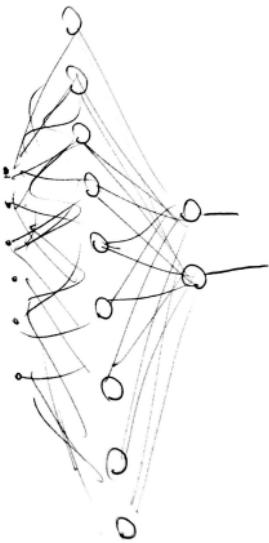
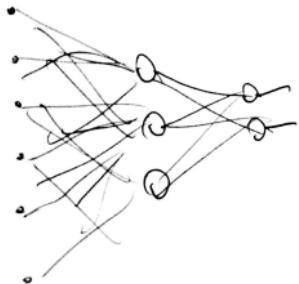
Figure from [Bis06]

Section 3

Design of NNs

Neural Network - Dimensionality

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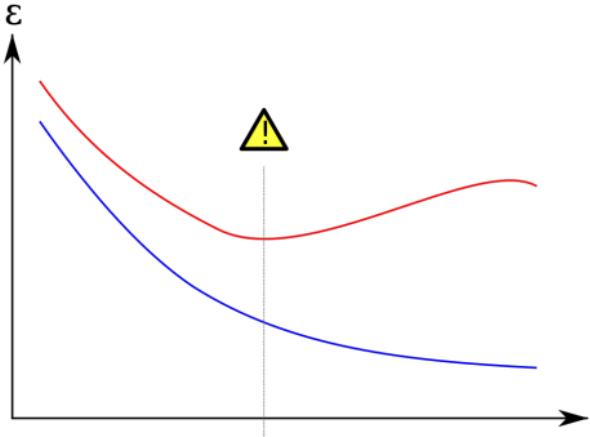
Compression vs. Augmentation.

Some authors use the same number of neurons per layer - pag. 324 of [Ger19]

Model complexity and Overfitting

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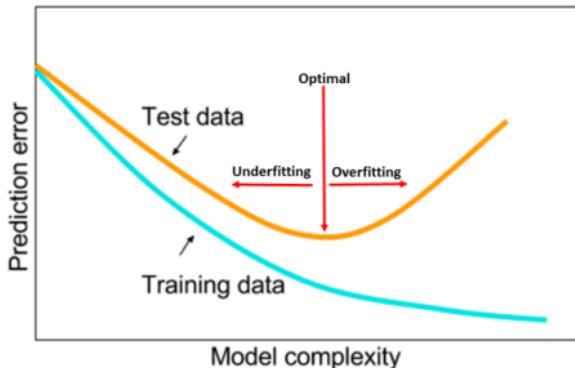
Overfitting



From User:Gringer, Wikipedia

Solution:

- Use smaller architectures
- Regularize
- Early Stopping:
stop training when the test error
does not improve for some
consecutive epochs



From [Smi18]

- NN with many parameters are **too flexible**: they can approximate weird functions
- To avoid **overfitting** the training data, we must reduce their flexibility
- **Regularization**
- The loss function to minimize during training is
 - For regression

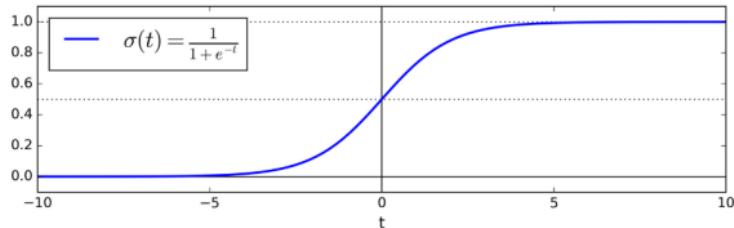
$$J(\theta, \mathbf{X}, \mathbf{y}) = \underbrace{\frac{1}{M} \sum_{i=1}^M (y^{(i)} - \hat{y}^{(i)})^2}_{\text{Error term}} + \underbrace{\alpha \|\theta\|^2}_{\text{Regularization term}}$$

- For classification

$$J(\theta, \mathbf{X}, \mathbf{y}) = \underbrace{-\frac{1}{M} \sum_{i=1}^M \ln \hat{p}_{y^{(i)}}^{(i)}}_{\text{Error term}} + \underbrace{\alpha \|\theta\|^2}_{\text{Regularization term}}$$

where $y^{(i)}$ is the true class of sample i

- Activation functions like sigmoids are intended to get values in a small range, otherwise they *saturate*.



Ex. If we enter to the neuron 8, 10 the output is practically the same.

- Scaling is also needed because we regularize NNs
- ⇒ Always scale the dataset (StandardScaler)

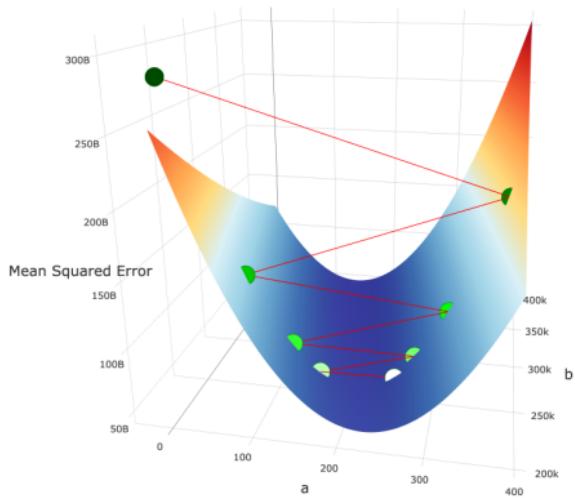
- Hyper-parameters:
 - Architecture
 - Layers? (start with few, increase if needed)
 - Neurons per layer?
 - Learning rate η : too high: noise; too low: slow to converge.
 - How many epochs?
 - Regularization weight α
 - Weight initialization.
 - Batch size.
 - Activation Functions.
- Strategies for tuning
 - Grid search (time consuming)
 - Random search, Bayesian Optimization, Design Space Exploration (time consuming) - see pagg.320-323 of [Ger19]
 - Trial and error, experience (people with less money need to be smarter)

Fixed learning rate

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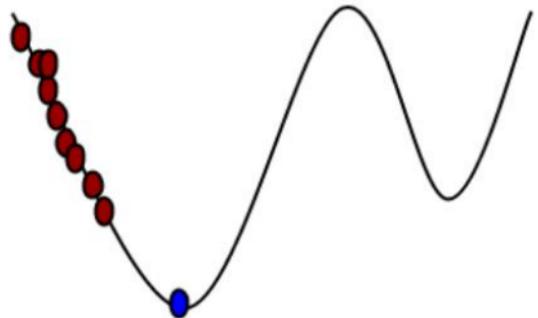
$$\theta := \theta - \eta \cdot \nabla J(\theta, \mathbf{X}, \mathbf{y})$$

η too large

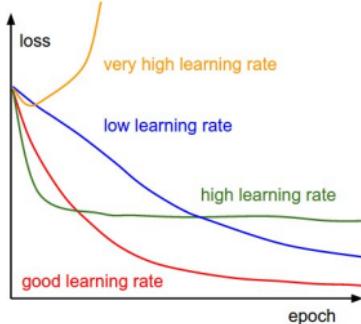


From S. Harrington [blog](#)

η too small

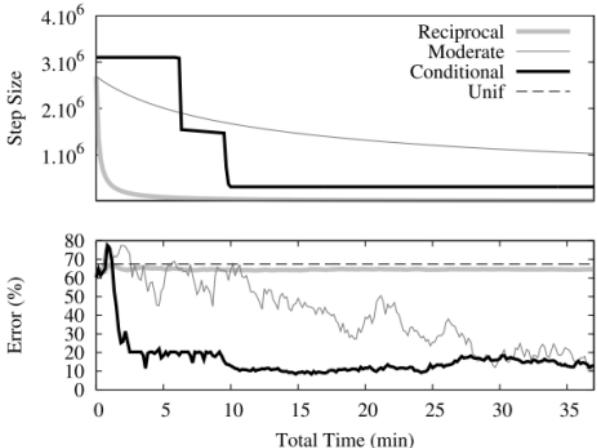
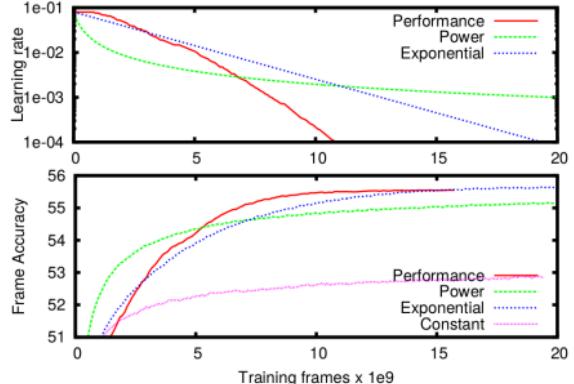


From ProgrammerSought [blog](#).



From CS231 [class](#) at Stanford

Start with large learning rates and reduce them after parameter updates



From [Sen13] and [ADR18]

See pagg.359-364 of [Ger19] to know more.

Gradient descent is

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

Other optimizers use a different parameter update equation, using gradient in a smarter way.

Most popular: Adaptive Moment Estimation (Adam)

[Animated comparison](#) of optimizers.

See pagg. 351-359 of [Ger19] to know more.

*“Friends, don’t let friends use
mini-batches larger than 32 ”*
Yann LeCun tweet, 2018



From Wikipedia

Yann LeCun (Facebook, New York University, ACM Turing Award)

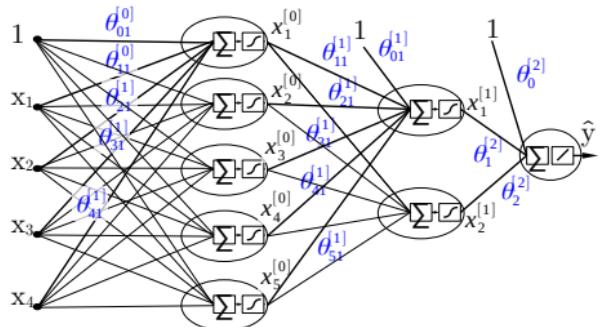
Large minibatches

- Allow to use GPU parallelization
- Risk of instability in loss minimization

Activation functions

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In the last layer



Regression: no activation function

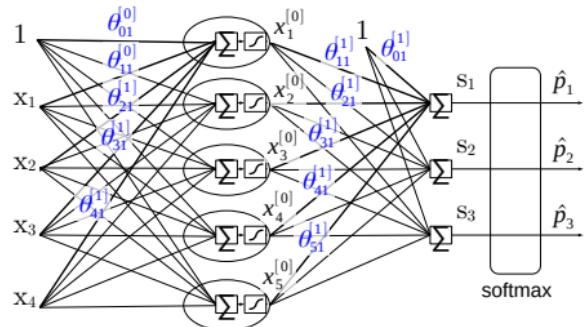
In the hidden layer: The most popular is **relu**

Sigmoid: old school, don't use it

The derivative of the sigmoid is almost zero far from zero

⇒ Vanishing gradient (p 325 of [Ger19])

Updates by gradient descent are too small



Classification: softmax

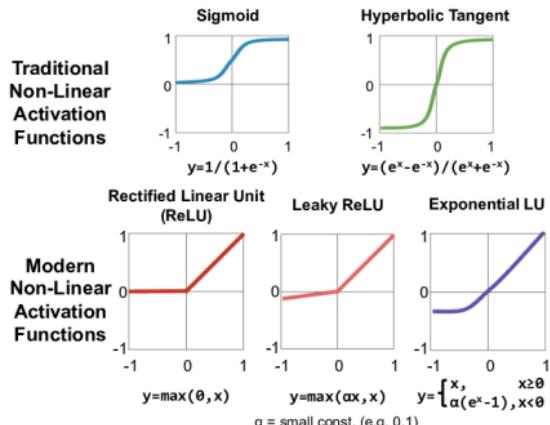
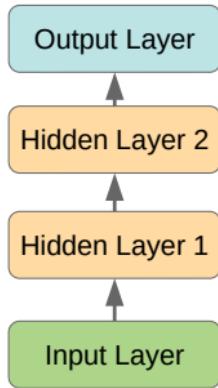


Figure from [SCYE17].

Section 4

Complex architectures

Multi-layer perceptron



Other architectures

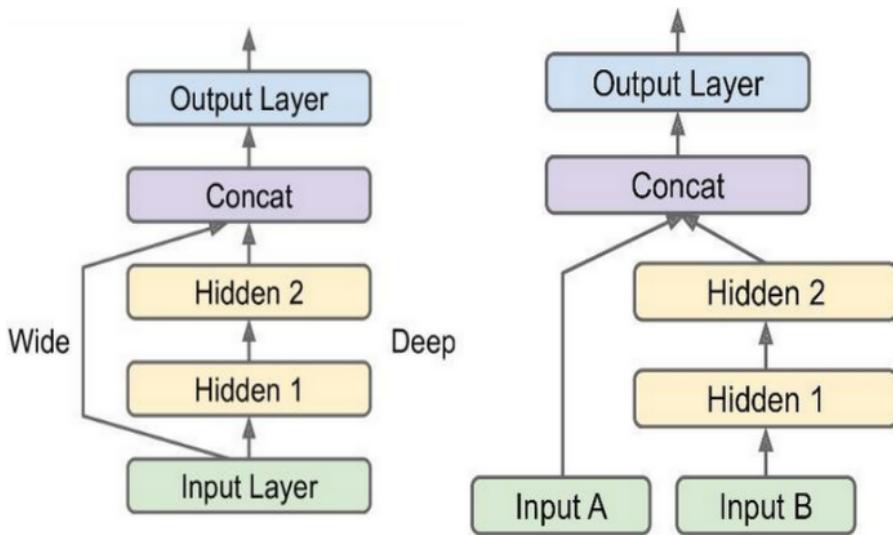


Figure from [Ger19].

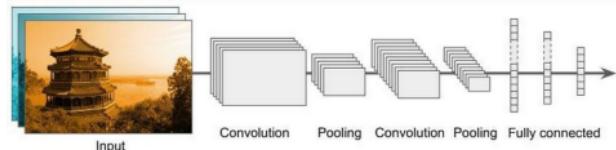
- Limit of Multi-Layer Perceptron: all input data are “deformed” by hidden layers.
- Other architectures are able to *bypass* some hidden layer
- Feel free to experiment with them in your project (pagg.308-313 of [Ger19]).

Notable deep Neural Networks

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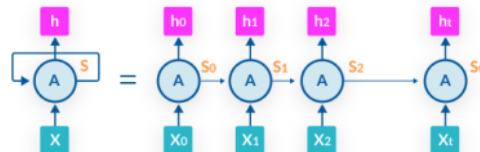
Convolutional NN:

- Image processing



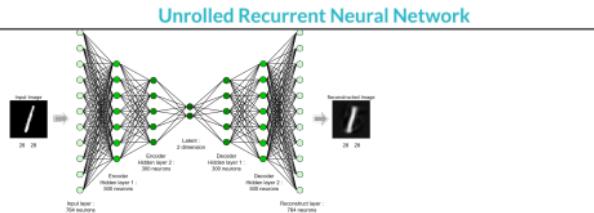
Recurrent NN:

- Time series, language modeling



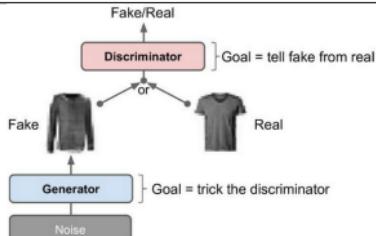
Autoencoder (AE):

- Dimensionality reduction and anomaly detection



Generative Adversarial Networks (GAN):

- To generate images or sounds



Figures from [Ger19], missinglink.ai, medium.com, [Ger19]

How to choose the right Neural Network?

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No standard procedure \Rightarrow Need for intuition, experience and, more importantly, trial and test \Rightarrow Neural Networks are an art!

However, some rough guidelines are:

- Image in input \Rightarrow Convolutional Neural Networks (slide 43)
- Time series in input \Rightarrow Recurrent Neural Networks (slide 43)
- The output layer depends on the task (regression or classification - slide 19)
- Size: start with a small neural network (few layers, few neurons per layer) and check the test result. Improve this result via Early Stopping and Regularization (slide 32). The result will be your reference baseline. Then, try with bigger architectures and compare the test error with the reference baseline (slide 43)
- Activation function and optimizers: use the latest findings from research (e.g., relu as activation function and Adam as optimizer - slide 9)
- If you have a lot of servers and a lot of time: automatically train several neural networks and get the best after some days / weeks! (grid search, randomized search)

Note that guidelines are continuously broken/replaced, as deep learning progresses!

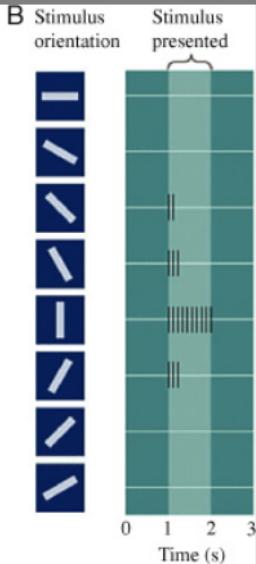
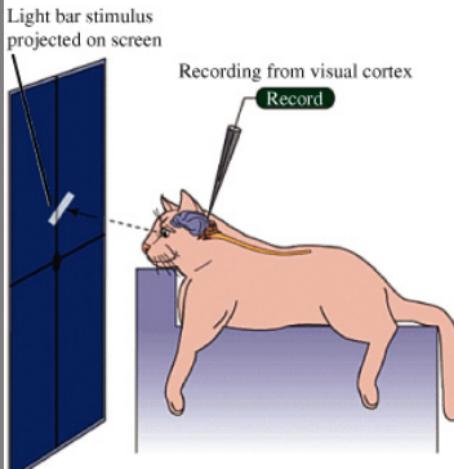


Go to notebook 04.neural-networks.ipynb

Convolutional NN

A celebrity among cats: Hubel and Wiesel (Nobel prize '81) cat (Harvard)

A Experimental setup

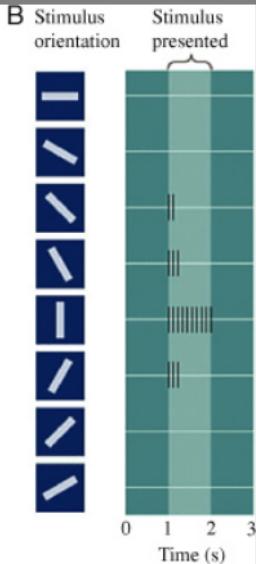
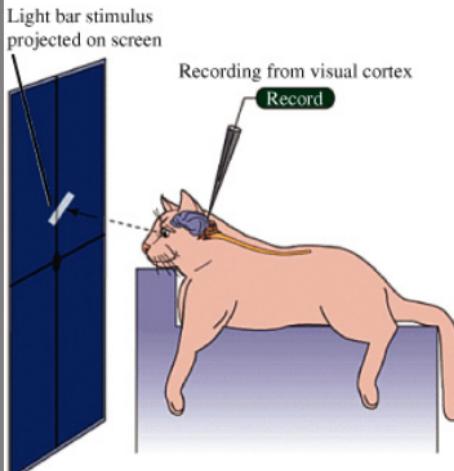


Source: Purves, Brains: How They Seem to Work

Source: youtube

A celebrity among cats: Hubel and Wiesel (Nobel prize '81) cat (Harvard)

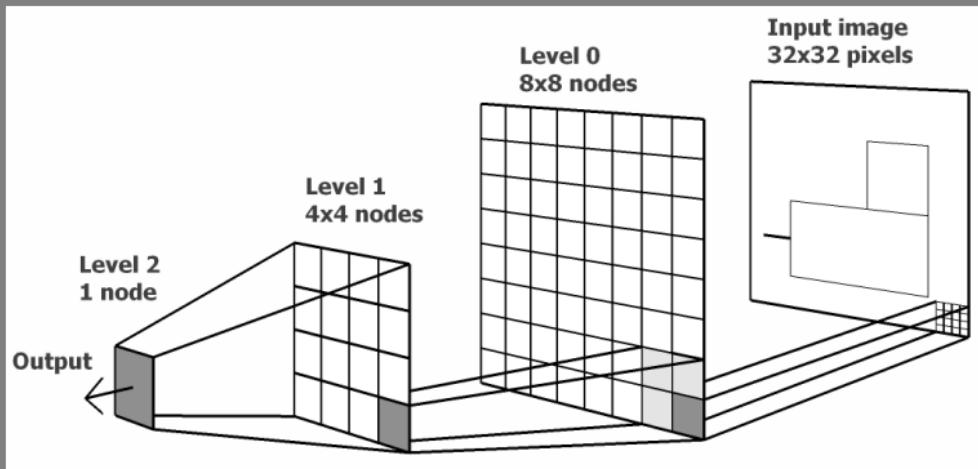
A Experimental setup



Source: Purves, Brains: How They Seem to Work

Source: youtube

- Instead of representing neurons stacked in columns, for image recognition it is easier to imagine them organized in matrices
- No difference in terms of mathematics



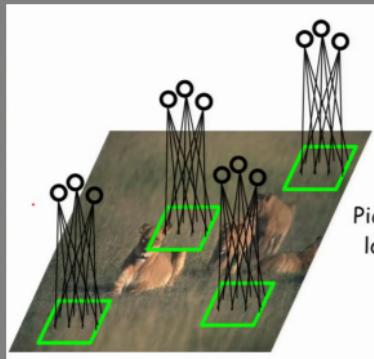
Source: Saulius Garalevicius 2010

Main idea

- In “classic” NN, we let it learn “wild” by
 - drawing all weights
 - let the weights take any value
- Can we learn from the cat?
 - Add structure to the architecture of the NN
 - Add constraints to the values of the weights
 - Do this by taking inspiration from the way vision works in living beings

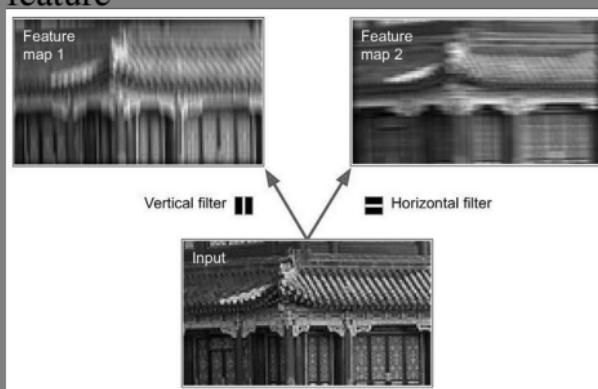
1st Hidden Layer: Feature Maps

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Source: Nando de Freitas, Lectures Machine Learning, University of British Columbia

- Each neuron in the 1st layer is only connected to a *patch* (e.g., 5px X 5px) of pixels.
- Several neurons (3 in the example) are attached to the same patch, each looking for a different *feature*. Output ~ 0 or ~ 1 .
- *Feature map*: Set of neurons looking for the same feature

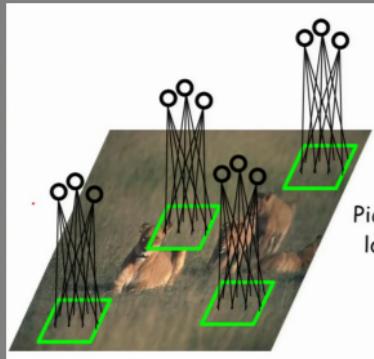


From [Ger19]

- A neuron “implements” a vertical filter when its weights are 1 in the center line and 0 elsewhere.

1st Hidden Layer: Feature Maps

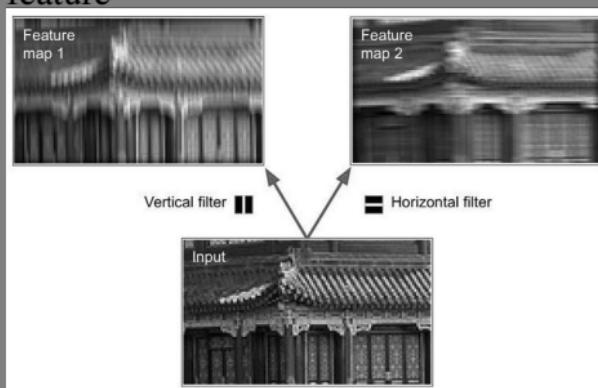
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Source: Nando de Freitas, Lectures Machine Learning, University of British Columbia

Who decides the filters?

- Each neuron in the 1st layer is only connected to a *patch* (e.g., 5px X 5px) of pixels.
- Several neurons (3 in the example) are attached to the same patch, each looking for a different *feature*. Output ~ 0 or ~ 1 .
- *Feature map*: Set of neurons looking for the same feature

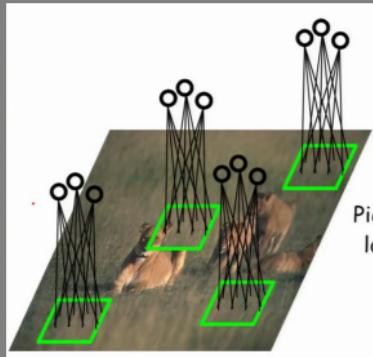


From [Ger19]

- A neuron “implements” a vertical filter when its weights are 1 in the center line and 0 elsewhere.

1st Hidden Layer: Feature Maps

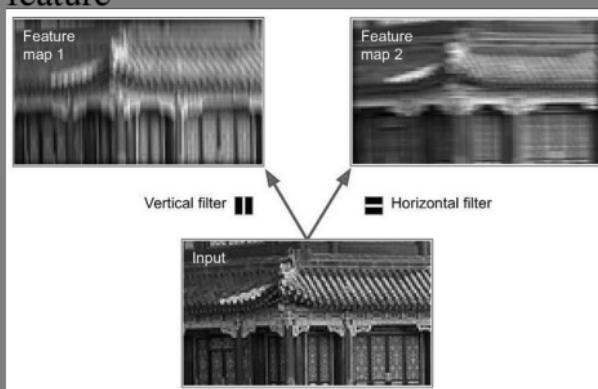
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Source: Nando de Freitas, Lectures Machine Learning, University of British Columbia

Who decides the filters?
Gradient descent

- Each neuron in the 1st layer is only connected to a *patch* (e.g., 5px X 5px) of pixels.
- Several neurons (3 in the example) are attached to the same patch, each looking for a different *feature*. Output ~ 0 or ~ 1 .
- *Feature map*: Set of neurons looking for the same feature

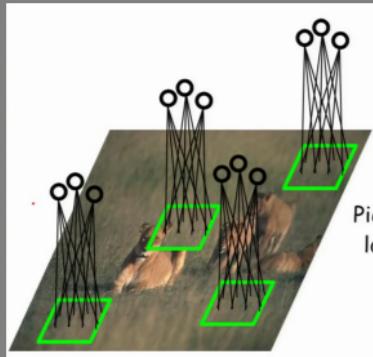


From [Ger19]

- A neuron “implements” a vertical filter when its weights are 1 in the center line and 0 elsewhere.

1st Hidden Layer: Feature Maps

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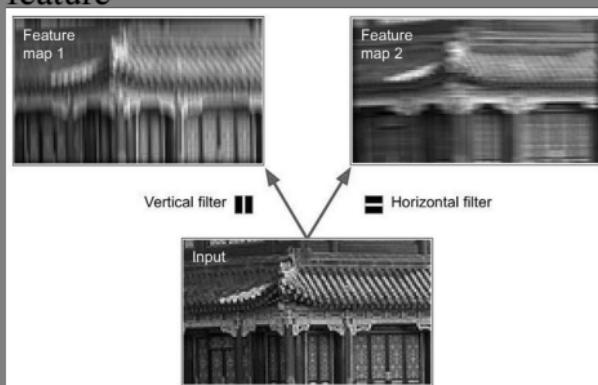


Source: Nando de Freitas, Lectures Machine Learning, University of British Columbia

Who decides the filters?
Gradient descent

How to force the neurons of a feat.map to look for the same feature?

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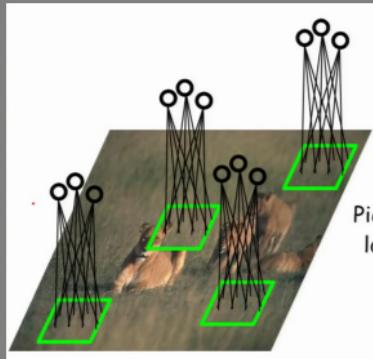


From [Ger19]

- A neuron “implements” a vertical filter when its weights are 1 in the center line and 0 elsewhere.

1st Hidden Layer: Feature Maps

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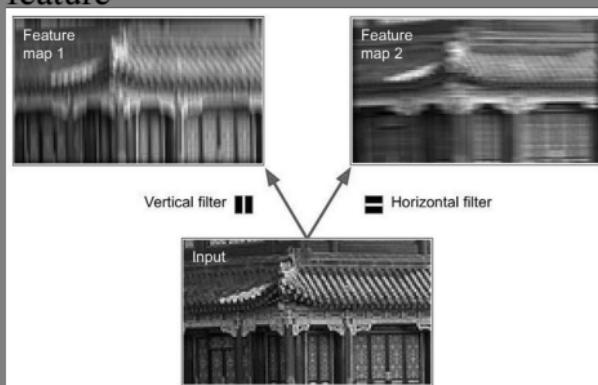


Source: Nando de Freitas, Lectures Machine Learning, University of British Columbia

Who decides the filters?
Gradient descent

How to force the neurons of a feat.map to look for the same feature?
Shared weights

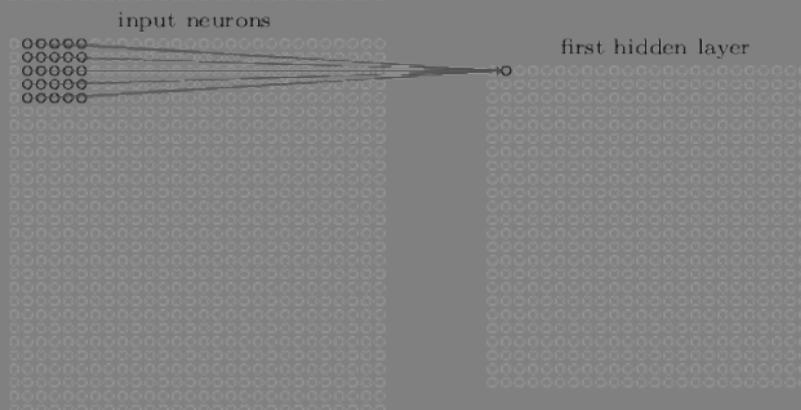
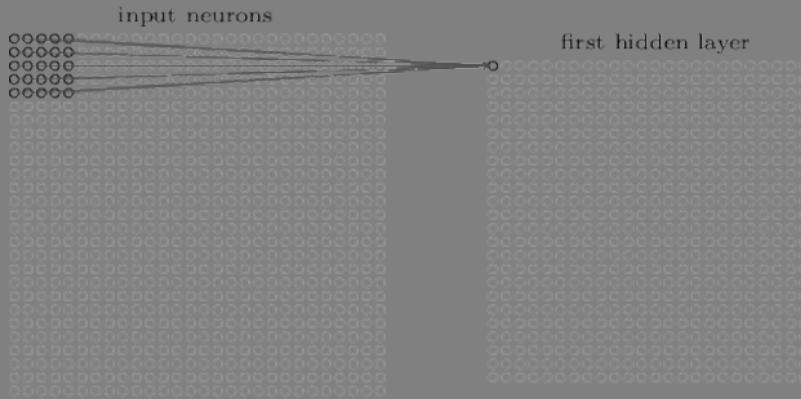
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1st Hidden Layer: Feature Map

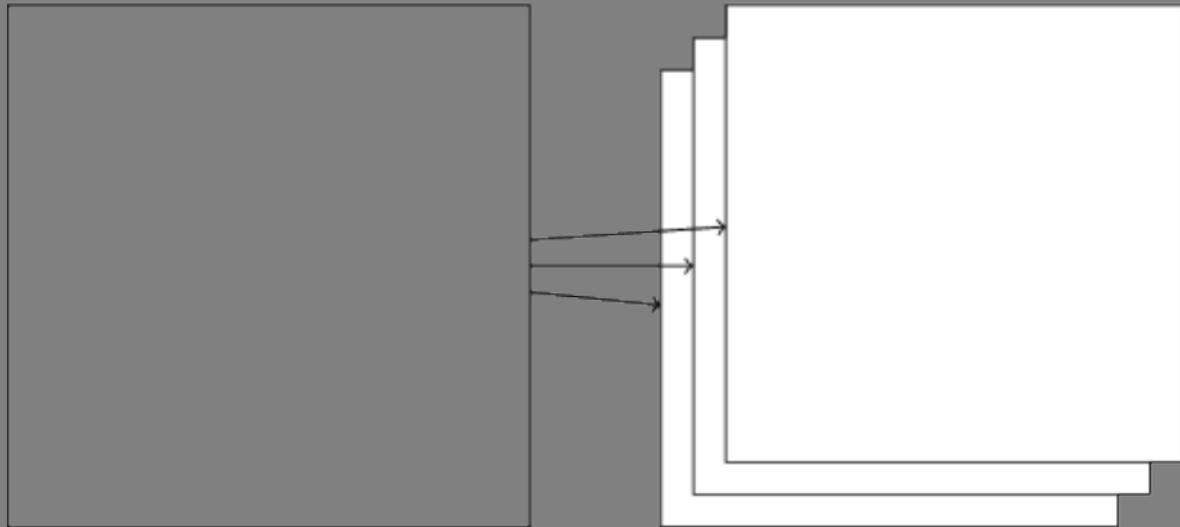


- Patches “seen” by neurons on the same feature map often overlaps
- Hyperparameter: *stride length* (by how much we slide the patch.)
- Sliding patch

Source: M. Nielsen - Neural Networks and Deep Learning

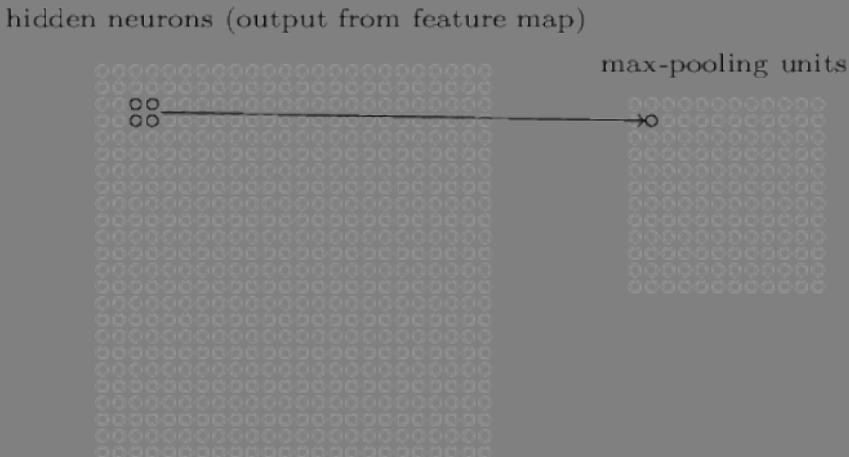
1st Hidden Layer: Feature Map

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- We can visually organize the 1st layer as a set of *feature maps*

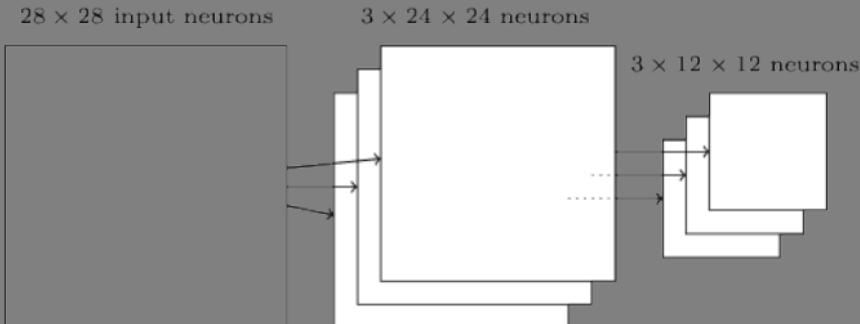
Source: M. Nielsen - Neural Networks and Deep Learning



- Max (or other function - hyperparameter!) of the output of a patch in a feature map
- Meaning: is the feature present in a region of the image?
- No weights to learn here

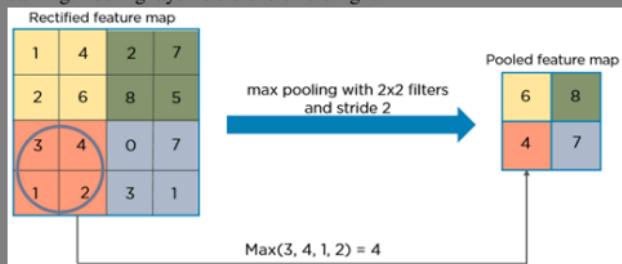
2nd Hidden Layer: Pooling

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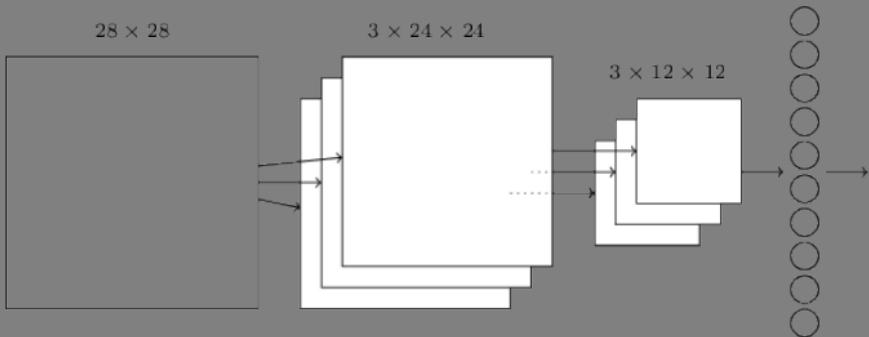


Source: M. Nielsen - Neural Networks and Deep Learning. Pooling layer is the one on the right.

- One pool per feature map
- Similar to convolutional layer, but no weights
 - Just take the average or the max of the patch
- Goal: summarizing features



From [video](#) on Simplilearn.

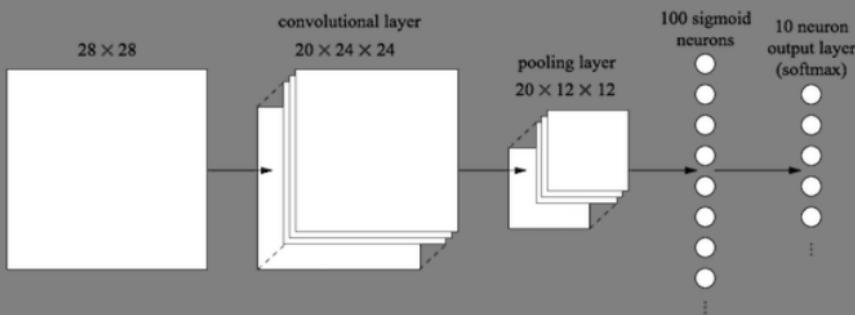


- One category per output neuron
- Ex: bus, car, truck, etc.

Source: M. Nielsen - Neural Networks and Deep Learning

Many possible architectures for convolutional NN

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- Ex: Add another hidden layer to summarize information further, before classification

Source: M. Nielsen - Neural Networks and Deep Learning

- In all the NN seen so far, all neurons take input that depends on the current sample forward-propagated
- In Recurrent NN, samples are submitted in sequences
- Some neurons is connected to previous samples
- What is this model aimed for?
- Language processing, Speach recognition
- Zaremba (NUY) and Sutskever (Google), “Learning to execute”
 - Their NN takes the words, one by one, of a (very simple) python scripts
 - It learns to predict the output!

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- Generative models
- Training: Find the weights submitting many images of cats
- Use: Give it a random input and get a synthetic cat image
- “Few” neurons in the hidden layer. Why?
- Serious use: drug discovery, music generation

In this lesson

- Structure of NNs
- Training (backpropagation)
- Design choices and hyper-parameters

In next lesson

- Random Forests

- [ADR18] Andrea Araldo, György Dán, and Dario Rossi, *Caching Encrypted Content via Stochastic Cache Partitioning*, IEEE/ACM Transactions on Networking **26** (2018), no. 1, 548–561.
- [Bis06] Christopher M. Bishop, *Pattern Recognition and Machine Learning*, 2006.
- [Ger19] Aurelien Geron, *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, O'Reilly, 2019.
- [SCYE17] Vivienne Sze, Yu Hsin Chen, Tien Ju Yang, and Joel S. Emer, *Efficient Processing of Deep Neural Networks: A Tutorial and Survey*, Proceedings of the IEEE **105** (2017), no. 12, 2295–2329.
- [Sen13] Andrew Senior, *An Empirical Study of the Learning Rates in Deep Neural Networks for Speech Recognition*, IEEE International Conference on Acoustics, Speech and Signal Processing, 2013.

- [Smi18] Leslie N. Smith, *A disciplined approach to neural network hyper-parameters: Part 1 – learning rate, batch size, momentum, and weight decay*, Tech. report, US Naval Research Laboratory, 2018.
- [Tai17] D. S. Taimanov, *Network disruption prediction based on neural networks*, 2017.

- Convolutional Neural Networks for Computer Vision (Ch.11 of [Ger19])
- Christopher M. Bishop. Pattern Recognition and Machine Learning, Springer - Sections 5.1, 5.2, 5.3
- <http://neuralnetworksanddeeplearning.com>