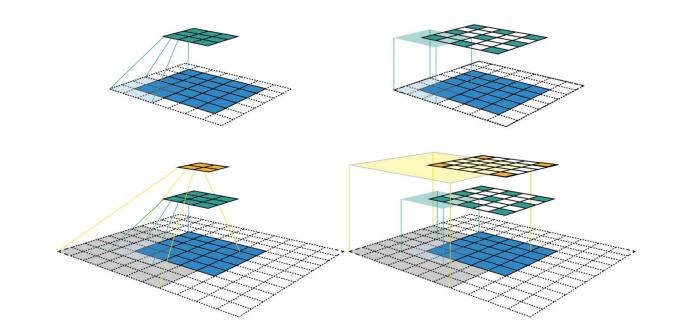
University of Ljubljana, Faculty of Computer and Information Science

## Neural networks





Prof Dr Marko Robnik-Šikonja Intelligent Systems, November 2021

#### Topics overview

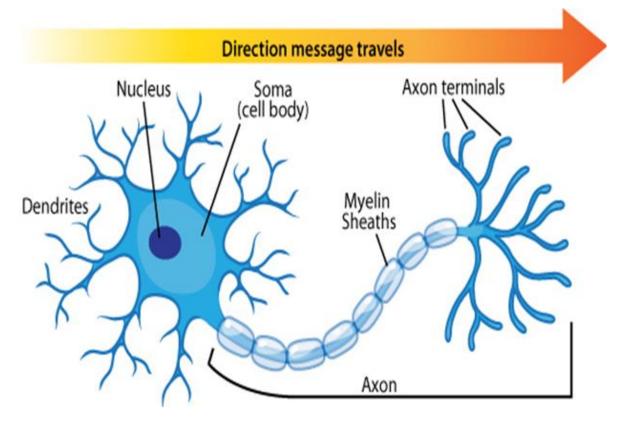
- basics of artificial neural networks
- backpropagation
- deep learning
- convolutional neural networks
- autoencoders
- generative adversarial networks
- robustness

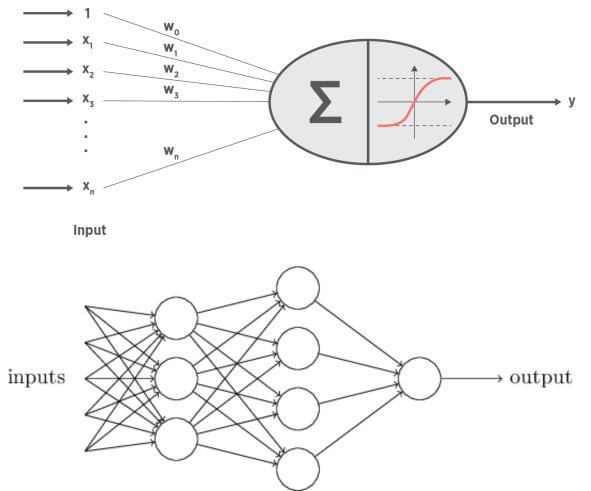
We will mention transformer networks in the natural language processing topic.

#### Artificial neural networks

- many approaches, we shall cover the basic ideas
- currently revival of interest, see deep neural networks
- <u>http://www.deeplearningbook.org</u>

# Artificial neural networks: brain analogy -

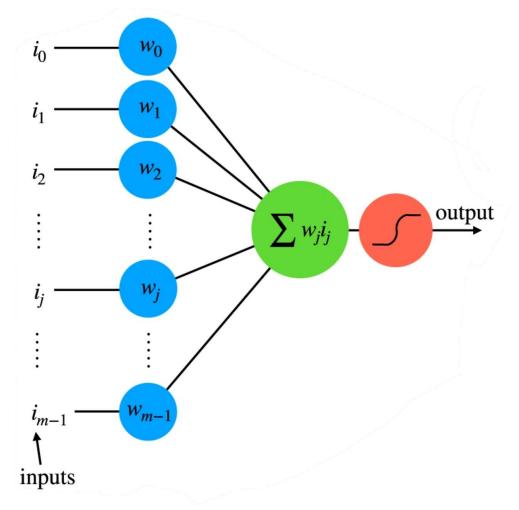




learning: error backpropagation

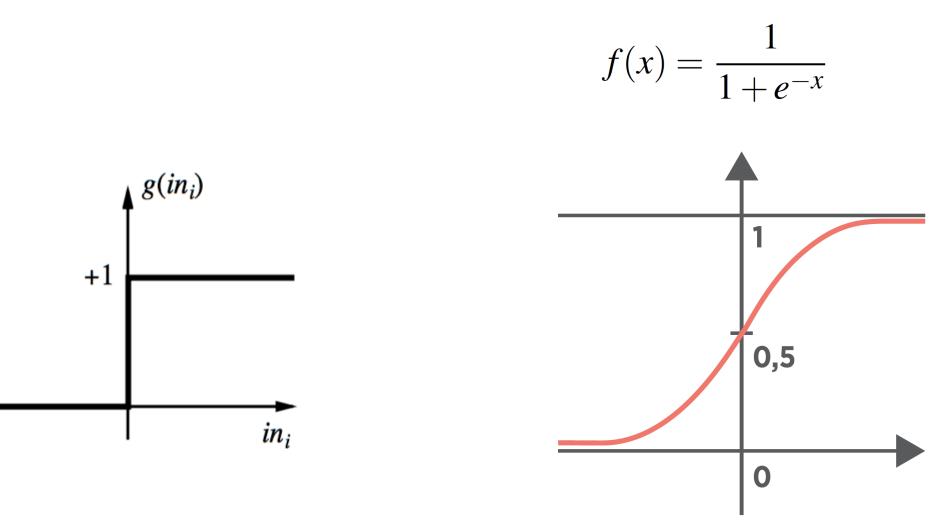
#### Neuron

• Computational units, passing messages (information) in the network, typically organized into layers



#### Activation functions

• examples: step function, sigmoid (logistic)



#### Activation functions

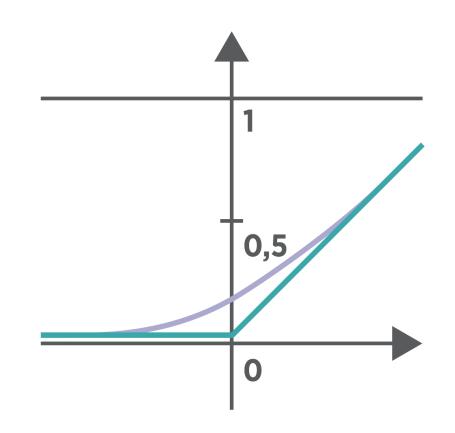
• ReLU (rectified linear unit)

f(x) = max(0, x)

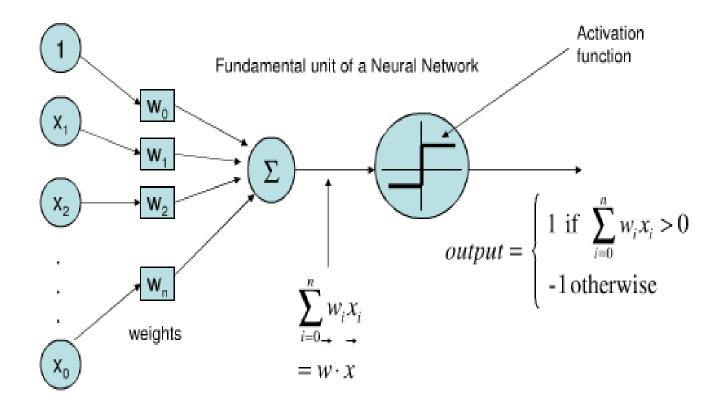
- softplus / approximation of ReLU with continuous derivation f(x) = ln(1+e<sup>x</sup>)
- ELU (Exponential Linear Unit)

$$ELU(x) = \begin{cases} c \cdot (e^x - 1), & \text{for } x < 0\\ x & \text{for } x \ge 0 \end{cases}$$

• many others

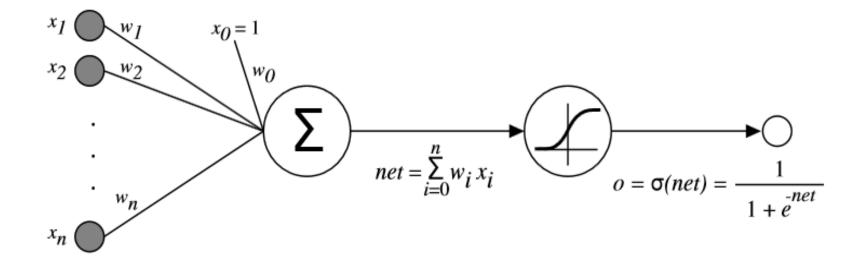


#### Historically: Perceptron



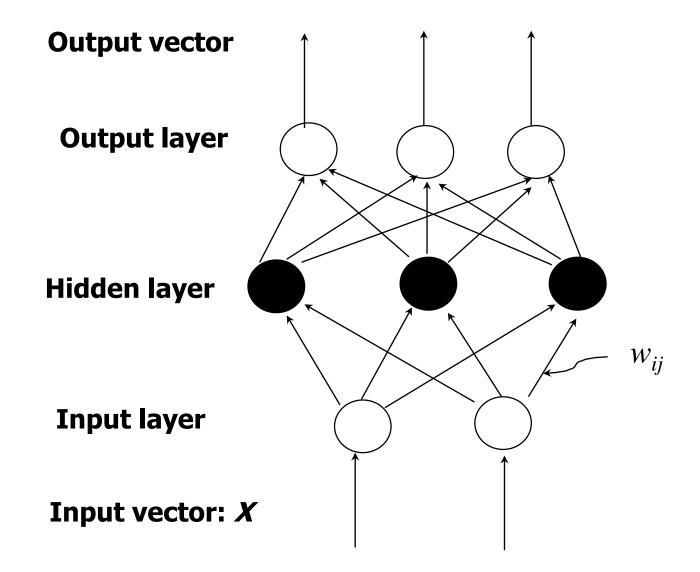
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#### Why nonlinear?



What is a derivative of a sigmoid?

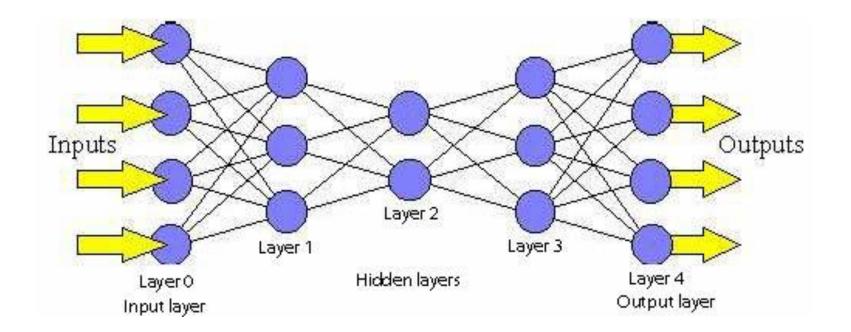
A multi-layer feed-forward NN



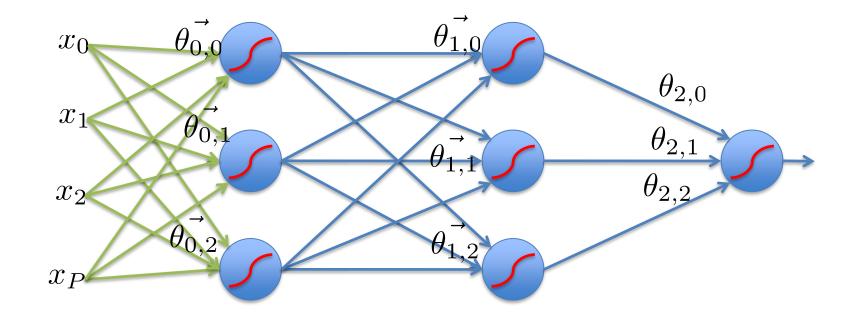
#### How a multi-layer NN works?

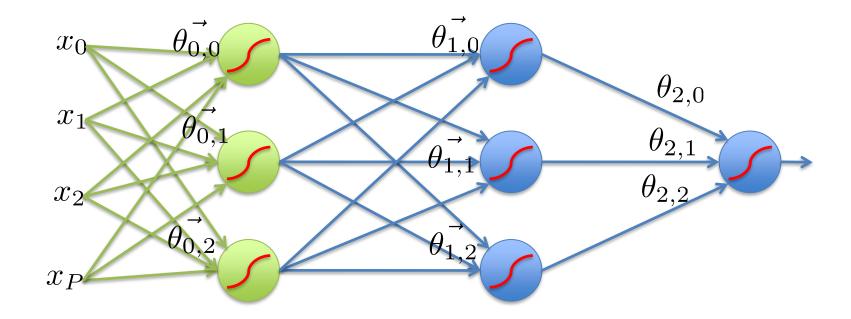
- The **inputs** to the network correspond to the attributes measured for each training tuple
- Inputs are fed simultaneously into the units making up the **input layer**
- They are then weighted and fed simultaneously to a hidden layer
- The number of hidden layers is arbitrary; if more than 1 hidden layer is used, the network is called deep neural network
- The weighted outputs of the last hidden layer are input to units making up the **output layer**, which emits the network's prediction
- The network is **feed-forward**: None of the weights cycles back to an input unit or to an output unit of a previous layer
- If we have backwards connections the network is called recurrent neural network
- From a statistical point of view, networks perform **nonlinear regression**: Given enough hidden units and enough training samples, they can closely approximate any function

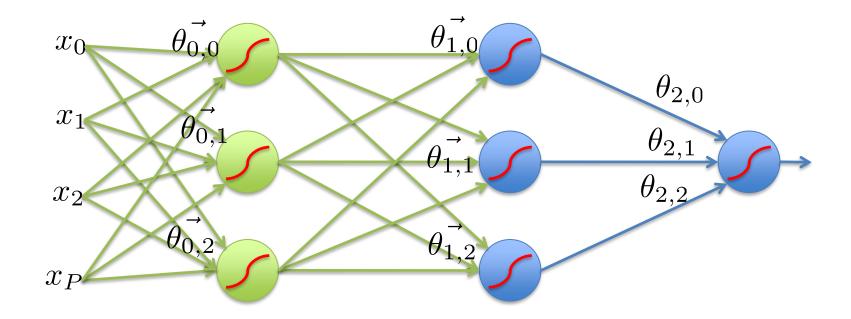
 neurons are activated progressively throug layers from input to output

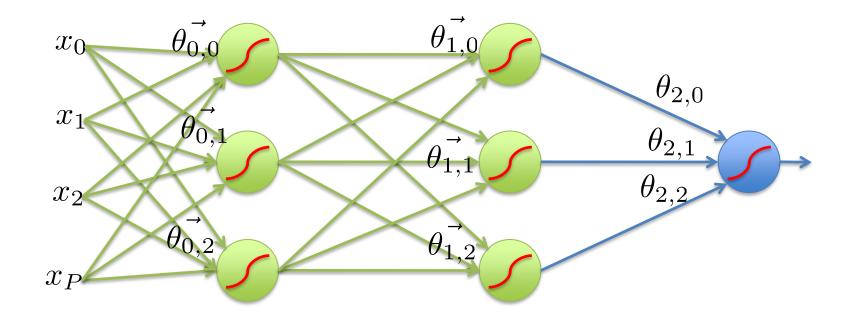


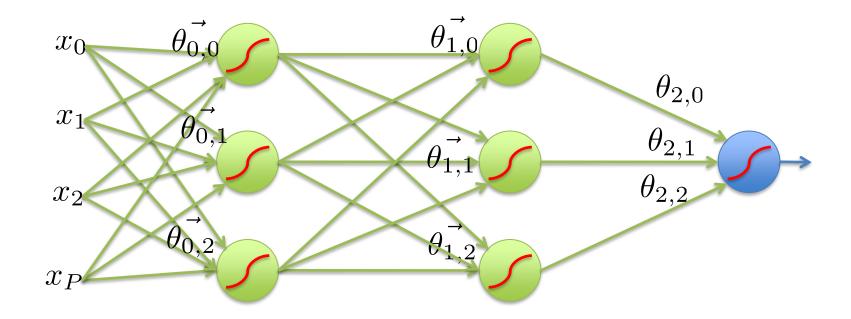
• Values are propagated through the network to the output, which returns the prediction

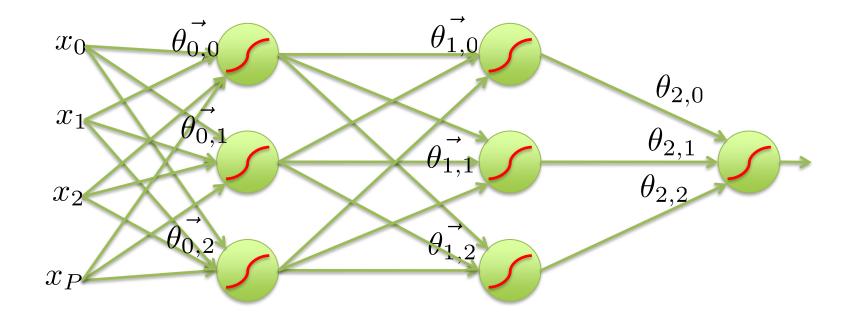










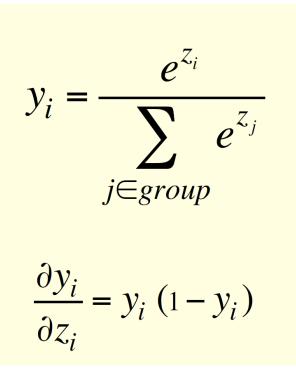


### Backpropagation learning algorithm for NN

- Backpropagation: a neural network learning algorithm
- Started by psychologists and neurobiologists to develop and test computational analogues of neurons
- A neural network: a set of connected input/output units where each connection has a weight associated with it
- During the learning phase, the network learns by adjusting the weights so as to be able to predict the correct class label of the input tuples
- Also referred to as connectionist learning due to the connections between units

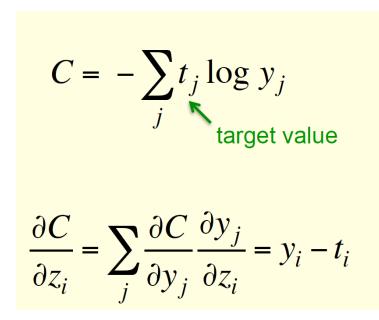
#### Softmax

 normalizes the output scores to be a probability distribution (values between 0 and 1, the sum is 1)



#### Criterion function

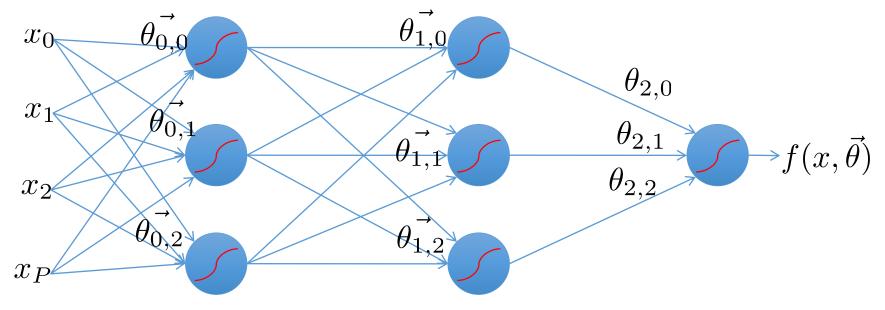
 together with softmax we frequently use cross entropy as cost function C



#### Backpropagation algorithm

- Iteratively process a set of training tuples & compare the network's prediction with the actual known target value
- For each training tuple, the weights are modified to **minimize the mean squared error** between the network's prediction and the actual target value
- Modifications are made in the "backwards" direction: from the output layer, through each hidden layer down to the first hidden layer, hence "backpropagation"
- Steps
  - Initialize weights to small random numbers, associated with biases
  - Propagate the inputs forward (by applying activation function)
  - Backpropagate the error (by updating weights and biases)
  - Terminating condition (when error is very small, etc.)

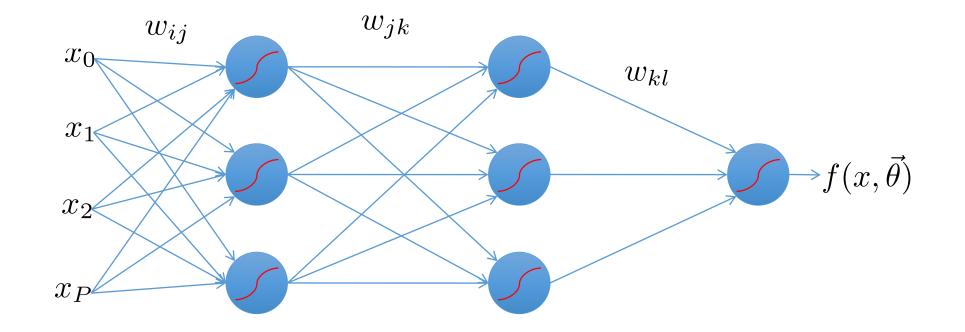
- We will do gradient descent on the whole network.
- Training will proceed from the last layer to the first.



Next 18 slides by Andrew Rosenberg

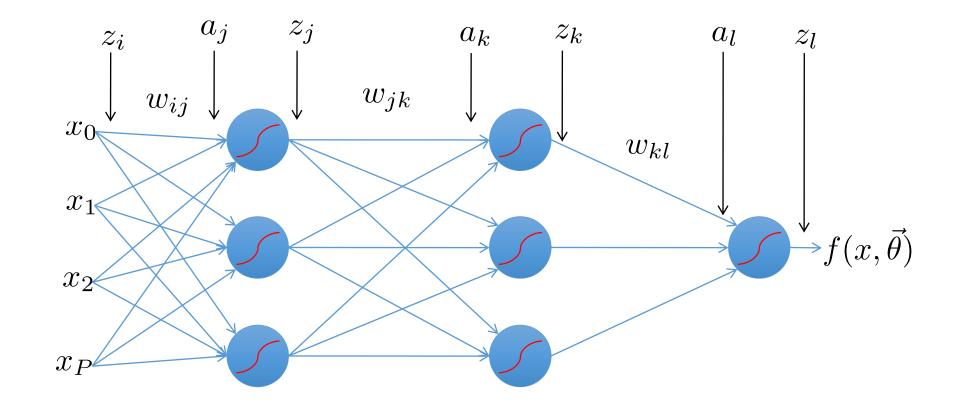
• Introduce variables over the neural network

 $\vec{\theta} = \{w_{ij}, w_{jk}, w_{kl}\}$ 



$$\vec{\theta} = \{w_{ij}, w_{jk}, w_{kl}\}$$

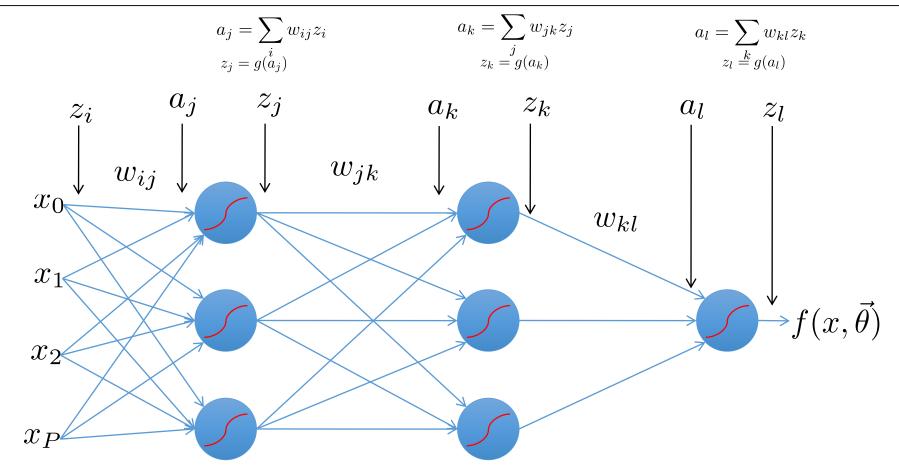
- Introduce variables over the neural network
  - Distinguish the input and output of each node

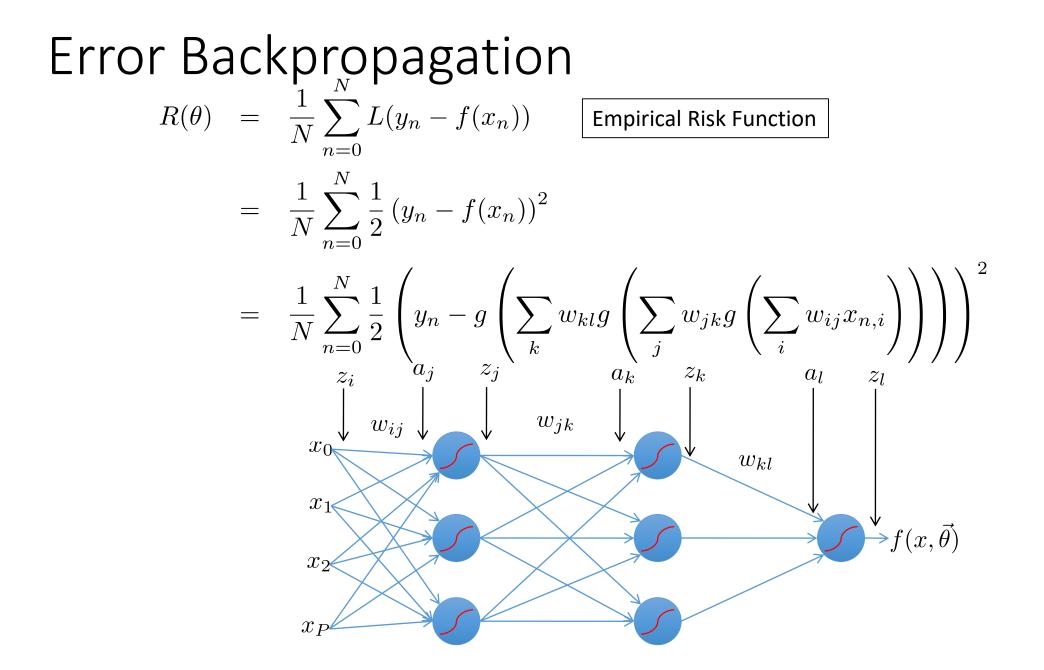


#### **Error Backpropagation** $\vec{\theta} = \{w_{ij}, w_{jk}, w_{kl}\}$ $a_j = \sum_i w_{ij} z_i \qquad a_k = \sum_j w_{jk} z_j \qquad a_l = \sum_k w_{kl} z_k$ $z_j = g(a_j) \qquad \qquad z_k = g(a_k) \qquad \qquad z_l = g(a_l)$ $a_k$ $z_k$ $a_l$ $z_i$ $z_l$ $x_0$ $w_{kl}$ $x_1$ $\rightarrow f(x, \vec{\theta})$ $x_2$ $\mathcal{X}_{P}$

$$\vec{\theta} = \{w_{ij}, w_{jk}, w_{kl}\}$$

Training: Take the gradient of the last component and iterate backwards

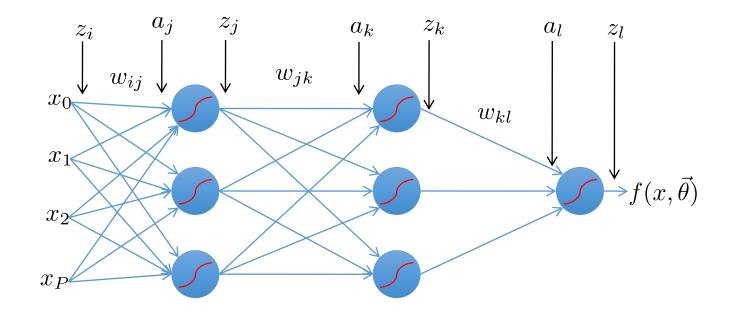




Optimize last layer weights w<sub>kl</sub>

$$L_n = \frac{1}{2} \left( y_n - f(x_n) \right)^2$$

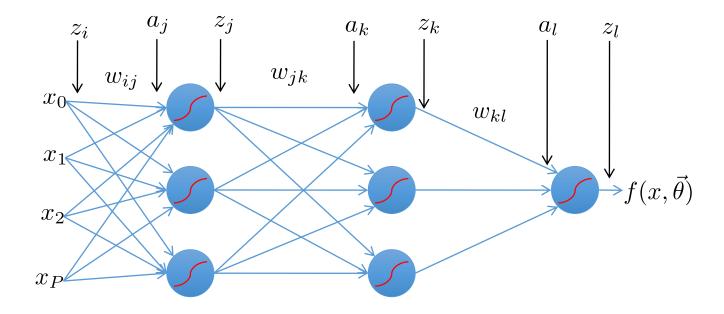
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial L_n}{\partial a_{l,n}} \right] \left[ \frac{\partial a_{l,n}}{\partial w_{kl}} \right]$$
 Calculus chain rule

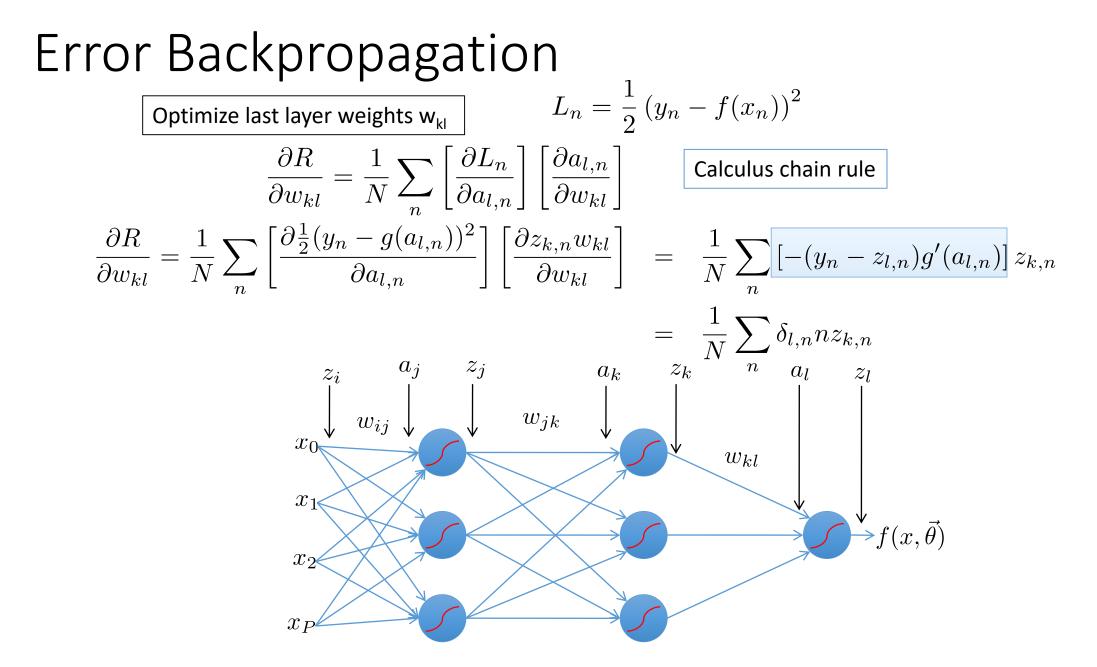


#### Error Backpropagation Optimize last layer weights $w_{kl}$ $L_n = \frac{1}{2} \left( y_n - f(x_n) \right)^2$ $\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum \left[ \frac{\partial L_n}{\partial a_{l,n}} \right] \left[ \frac{\partial a_{l,n}}{\partial w_{kl}} \right]$ Calculus chain rule $\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum \left[ \frac{\partial \frac{1}{2} (y_n - g(a_{l,n}))^2}{\partial a_{l,n}} \right] \left[ \frac{\partial a_{l,n}}{\partial w_{kl}} \right]$ $x_0$ $w_{kl}$ $x_1$ $f(x, \vec{\theta})$ $x_2 \leqslant$ $x_I$

#### **Error Backpropagation** Optimize last layer weights $w_{kl}$ $L_n = \frac{1}{2} \left( y_n - f(x_n) \right)^2$ $\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum \left[ \frac{\partial L_n}{\partial a_{l,n}} \right] \left[ \frac{\partial a_{l,n}}{\partial w_{kl}} \right]$ Calculus chain rule $\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial \frac{1}{2} (y_n - g(a_{l,n}))^2}{\partial a_{l,n}} \right] \left[ \frac{\partial z_{k,n} w_{kl}}{\partial w_{kl}} \right]$ $x_0$ $w_{kl}$ $x_1$ $f(x, \vec{\theta})$ $x_2 \leqslant$ XF

$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial \frac{1}{2} (y_n - g(a_{l,n}))^2}{\partial a_{l,n}} \right] \left[ \frac{\partial z_{k,n} w_{kl}}{\partial w_{kl}} \right] = \frac{1}{N} \sum_{n} \left[ -(y_n - z_{l,n})g'(a_{l,n}) \right] z_{k,n}$$

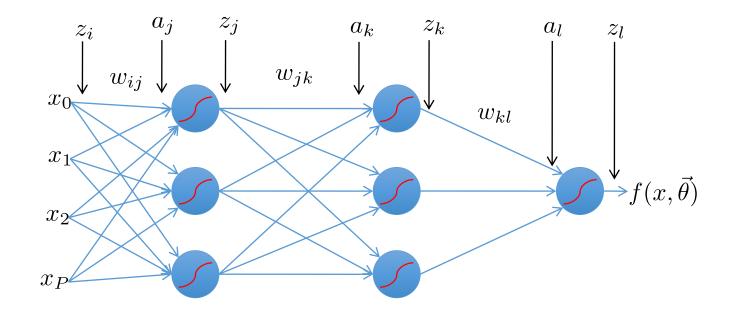


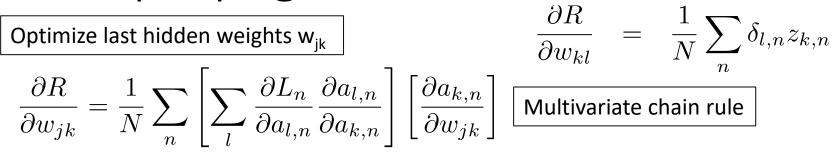


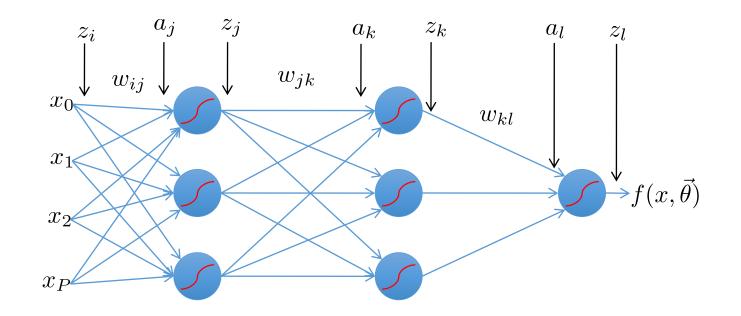
Optimize last hidden weights w<sub>ik</sub>

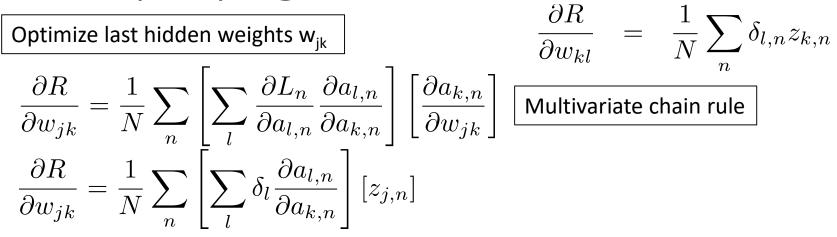
$$\frac{\partial R}{\partial w_{jk}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial L_n}{\partial a_{k,n}} \right] \left[ \frac{\partial a_{k,n}}{\partial w_{jk}} \right]$$

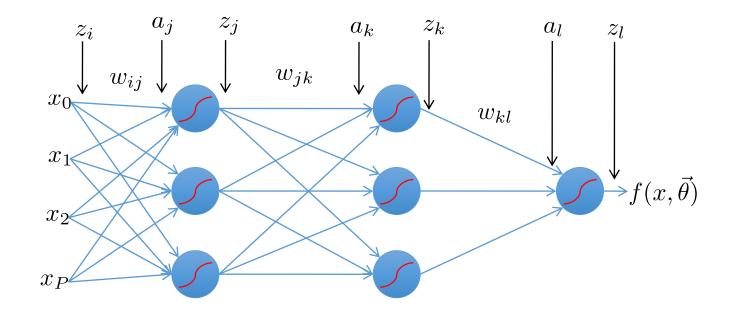
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum_{n} \delta_{l,n} z_{k,n}$$

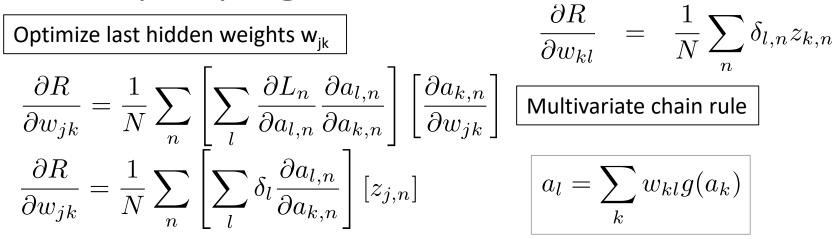


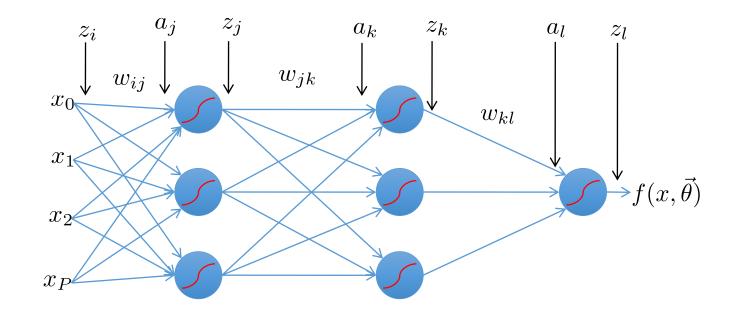




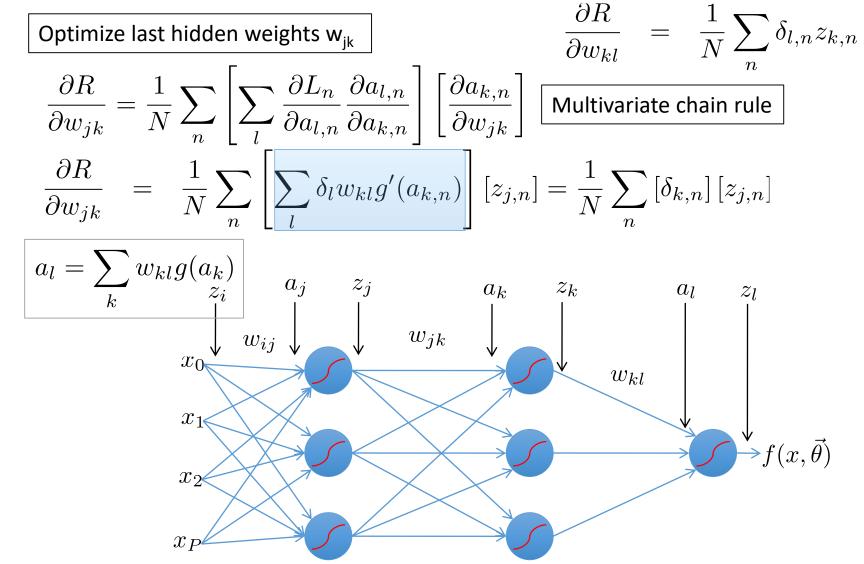








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Repeat for all previous layers

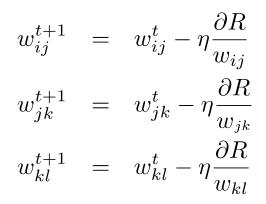
$$\frac{\partial R}{\partial w_{kl}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial L_{n}}{\partial a_{l,n}} \right] \left[ \frac{\partial a_{l,n}}{\partial w_{kl}} \right] = \frac{1}{N} \sum_{n} \left[ -(y_{n} - z_{l,n})g'(a_{l,n}) \right] z_{k,n} = \frac{1}{N} \sum_{n} \delta_{l,n} z_{k,n}$$

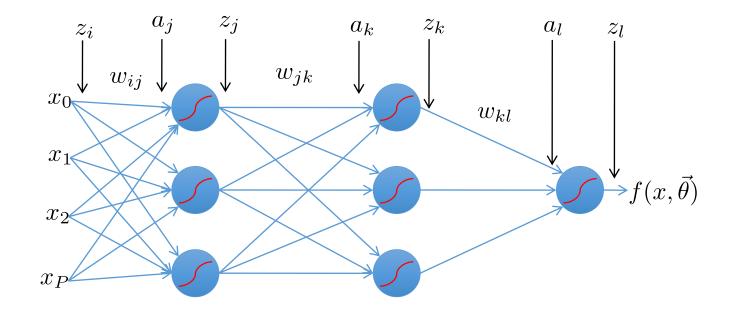
$$\frac{\partial R}{\partial w_{jk}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial L_{n}}{\partial a_{k,n}} \right] \left[ \frac{\partial a_{k,n}}{\partial w_{jk}} \right] = \frac{1}{N} \sum_{n} \left[ \sum_{l} \delta_{l,n} w_{kl} g'(a_{k,n}) \right] z_{j,n} = \frac{1}{N} \sum_{n} \delta_{k,n} z_{j,n}$$

$$\frac{\partial R}{\partial w_{ij}} = \frac{1}{N} \sum_{n} \left[ \frac{\partial L_{n}}{\partial a_{j,n}} \right] \left[ \frac{\partial a_{j,n}}{\partial w_{ij}} \right] = \frac{1}{N} \sum_{n} \left[ \sum_{k} \delta_{k,n} w_{jk} g'(a_{j,n}) \right] z_{i,n} = \frac{1}{N} \sum_{n} \delta_{j,n} z_{i,n}$$

$$\frac{z_{i}}{w_{ij}} \int w_{jk} \int w_{jk} \int w_{jk} \int w_{kl} \int w_{kl} \int w_{kl} \int f(x,\vec{\theta})$$

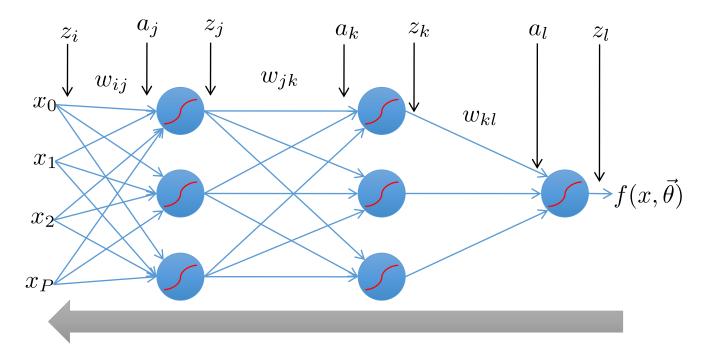
Now that we have well defined gradients for each parameter, update using Gradient Descent





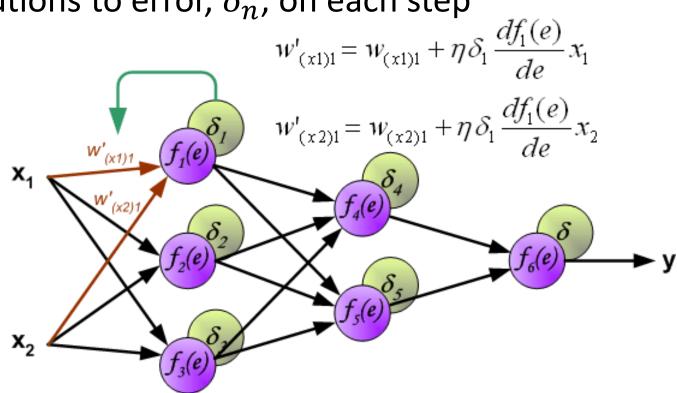
40

- Error backpropagation unravels the multivariate chain rule and solves the gradient for each partial component separately.
- The target values for each layer come from the next layer.
- This feeds the errors back along the network.



#### Learning with error backpropagation

- Backpropagation
- randomly initialize parameters (weights)
- compute error on the output
- compute contributions to error,  $\delta_n$ , on each step backwards  $w'_{(x1)1} = w_{(x1)1} + \eta \delta_1 \frac{df_1}{df_1}$
- gradient
- step
- iteratively
- batch
- minibatch



#### Defining a network topology

- Decide the network topology: Specify # of units in the *input layer*, # of *hidden layers* (if > 1), # of units in *each hidden layer*, and # of units in the *output layer*
- Normalize the input values for each attribute measured in the training tuples to [0.0—1.0]
- One input unit per domain value, each initialized to 0
- Output, if for classification and more than two classes, one output unit per class is used
- Once a network has been trained and its accuracy is unacceptable, repeat the training process with a *different network topology* or a *different set of initial* weights

## Neural network as a classifier

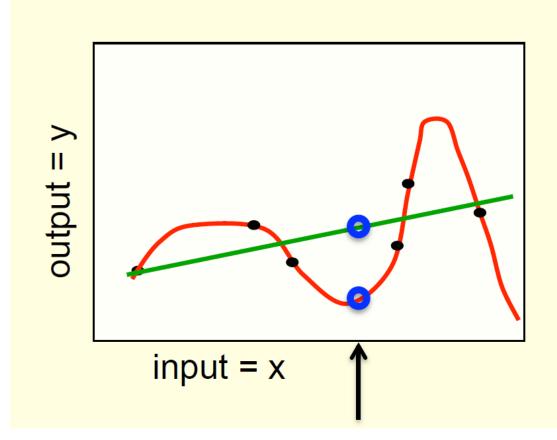
- Weakness
  - Long training time
  - Require a number of parameters typically best determined empirically, e.g., the network topology or "structure."
  - Poor interpretability: difficult to interpret the symbolic meaning behind the learned weights and of "hidden units" in the network
- Strength
  - High tolerance to noisy data
  - Ability to classify untrained patterns
  - Well-suited for continuous-valued inputs and outputs
  - Successful on an array of real-world data, e.g., hand-written letters
  - Algorithms are inherently parallel
  - Builds more advanced representation
  - Techniques exist for the extraction of explanations from trained neural networks

#### Efficiency and interpretability

- Efficiency of backpropagation: Each epoch (one iteration through the training set) takes O(|D| \* w), with |D| tuples and w weights, but # of epochs can be exponential to n, the number of inputs, in worst case
- For easier comprehension: Rule extraction by network pruning
  - Simplify the network structure by removing weighted links that have the least effect on the trained network
  - Then perform link, unit, or activation value clustering
  - The set of input and activation values are studied to derive rules describing the relationship between the input and hidden unit layers
- Sensitivity analysis: assess the impact that a given input variable has on a network output. The knowledge gained from this analysis can be represented in rules
- Recent attempts tend to learn interpreation along learning

# Overfitting and model complexity

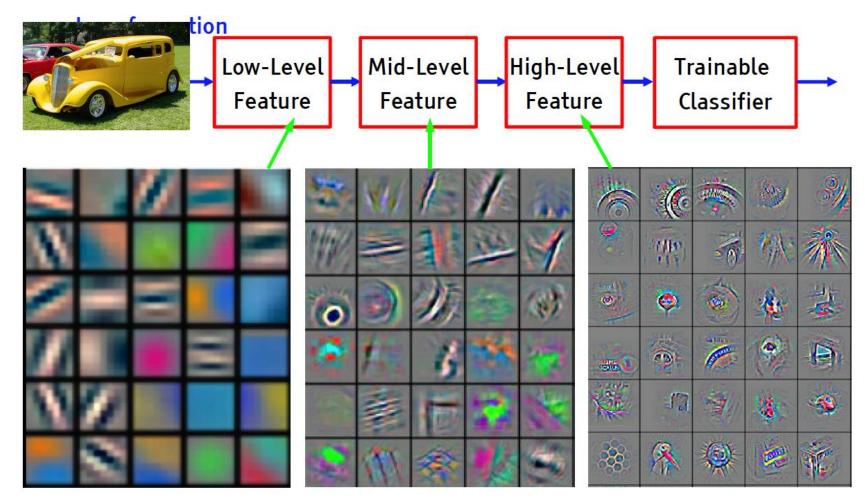
- which curve is more plausible given the data?
- overfitting
- neural nets are especially prone to overfitting
- why?



# Prevention of overfitting

- Weight-decay
- Weight-sharing
- Early stopping
- Model averaging
- Bayesian fitting of neural nets
- Dropout
- Generative pre-training
- etc.

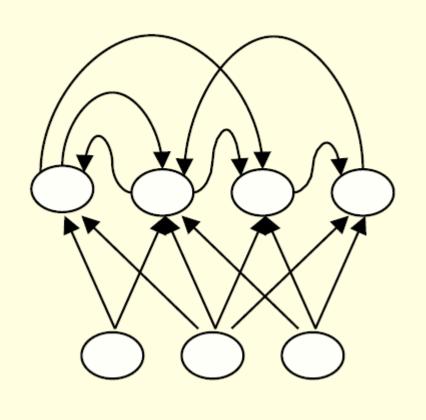
#### Deep learning = learning of hierarchical represenation

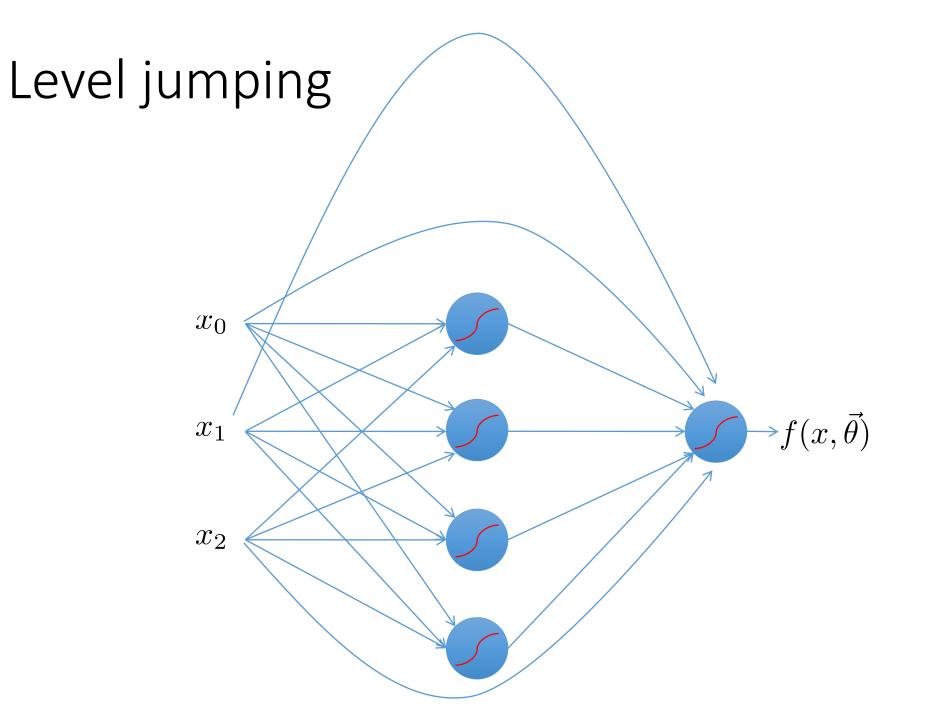


Feature visualization of convolutional net trained on ImageNet from [Zeiler & Fergus 2013]

#### Recurrent networks

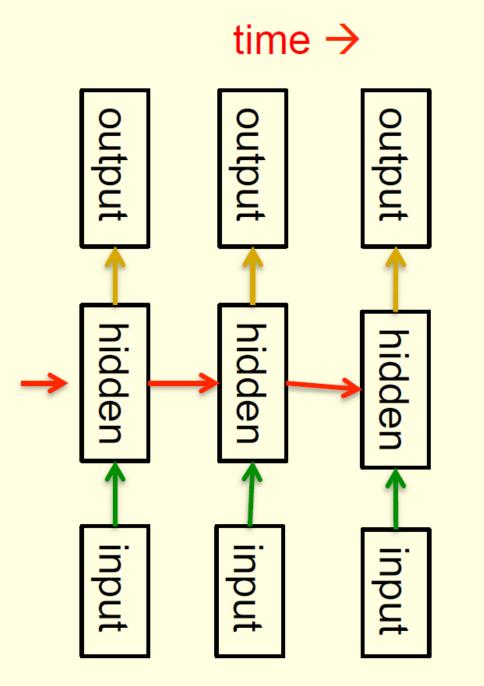
- back connections
- biologically more realistic
- store information from the past
- more difficult to learn



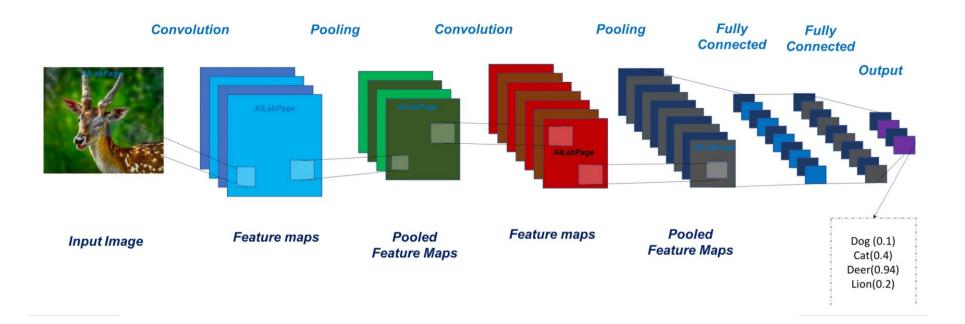


Recurrent networks for sequence learning

- unrolled network
- equivalent to deep networks with one hidden level per time slot
- but: hidden layers share weight (less parameters)



#### Convolutional neural networks (CNN)



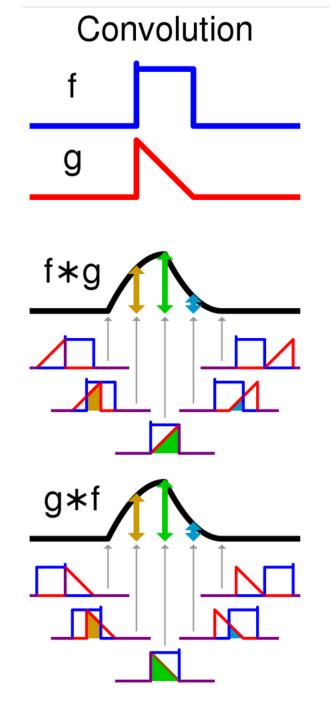
# Convolution

 an operation on two functions (f and g) that produces a third function expressing how the shape of one is modified by the other.

$$(f*g)(t) riangleq \int_{-\infty}^\infty f( au)g(t- au)\,d au.$$

• for discrete functions

$$(fst g)[n] = \sum_{m=-\infty}^\infty f[m]g[n-m].$$

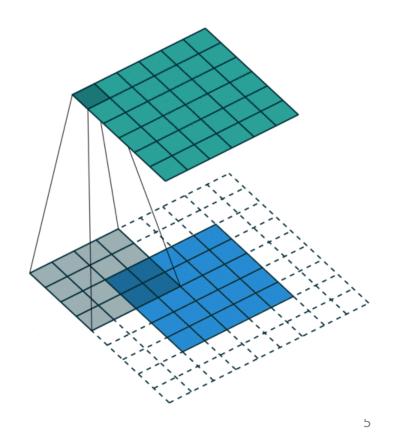


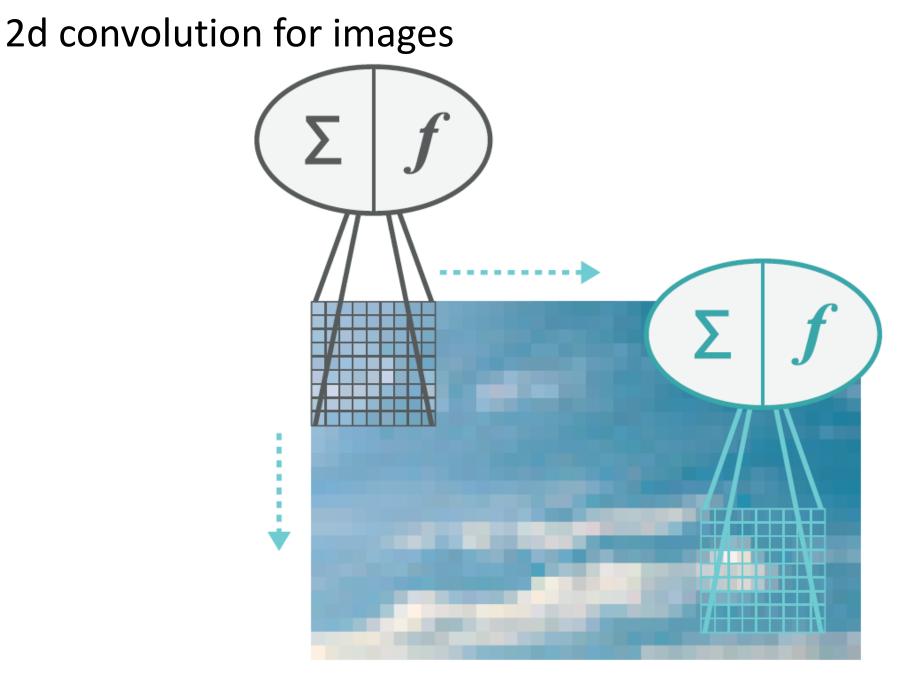
# Convolutional Neural Network (CNN)

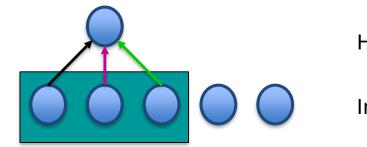
- Convolutional Neural Networks are inspired by mammalian visual cortex.
  - The visual cortex contains a complex arrangement of cells, which are sensitive to small sub-regions of the visual field, called a receptive field. These cells act as local filters over the input space and are well-suited to exploit the strong spatially local correlation present in natural images.
  - Two basic cell types:
    - Simple cells respond maximally to specific edge-like patterns within their receptive field.
    - Complex cells have larger receptive fields and are locally invariant to the exact position of the pattern.

## Convolutional neural networks (CNN)

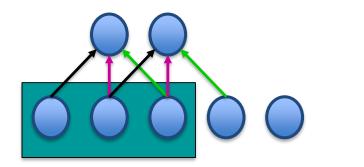
- currently, the most successful approach in image analysis, successful in language
- idea: many copies of small detectors used all over the image, recursively combined,
- detectors are learned, combination are learned



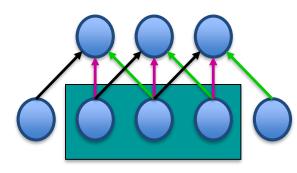




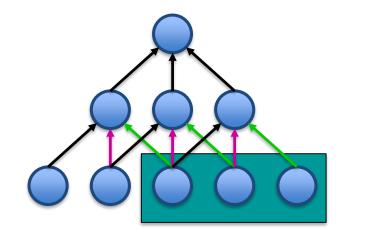
Hidden layer



Hidden layer



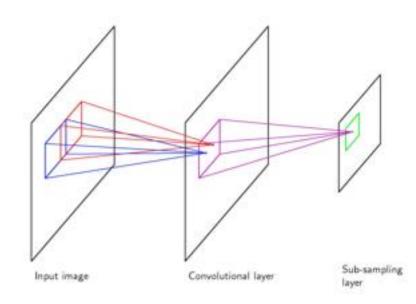
Hidden layer



Hidden layer

## **Convolutional Network**

- The network is not fully connected.
- Different nodes are responsible for different regions of the image.
- This allows for robustness to transformations.
- Convolution is combined with subsampling.

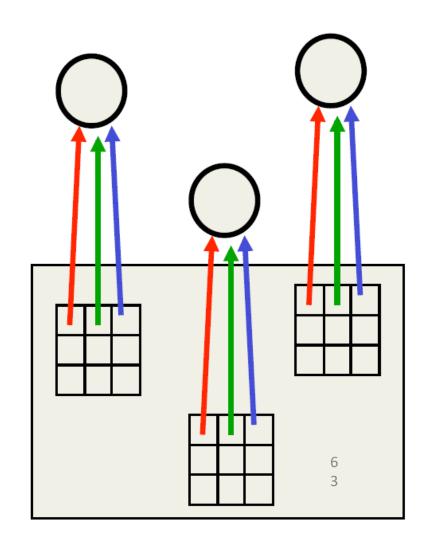


# **CNN Architecture: Convolutional Layer**

- The core layer of CNNs
- The convolutional layer consists of a set of filters.
  - Each filter covers a spatially small portion of the input data.
- Each filter is convolved across the dimensions of the input data, producing a multidimensional feature map.
  - As we convolve the filter, we are computing the dot product between the parameters of the filter and the input.
- Intuition: the network will learn filters that activate when they see some specific type of feature at some spatial position in the input.
- The key architectural characteristics of the convolutional layer is local connectivity and shared weights.

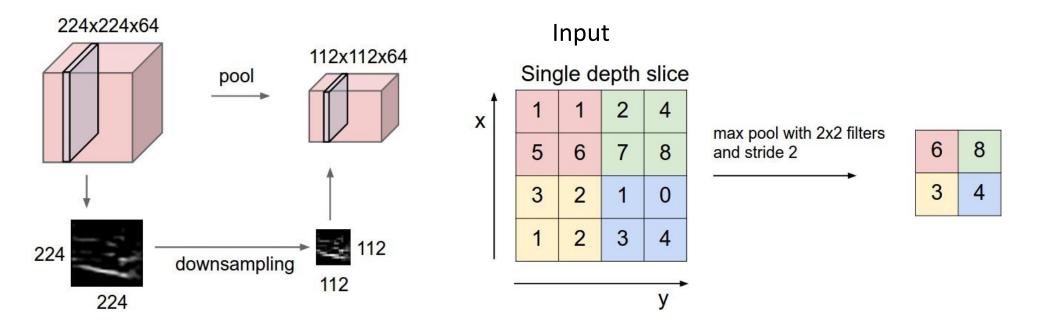
## Neural implementation of convolution

- weights of the same colors have equal weights
- adapted backpropagation
- images: 2d convolution
- languages: 1d convolution



## **CNN Architecture: Pooling Layer**

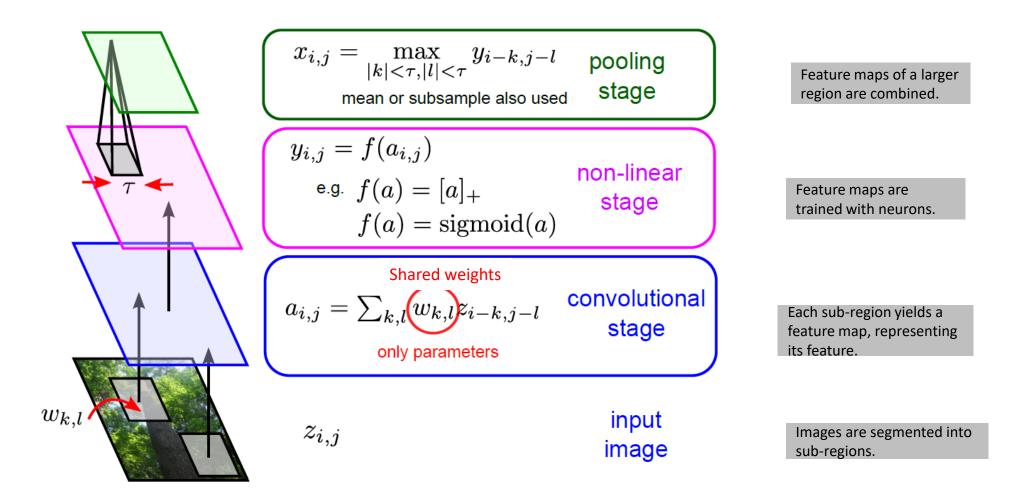
- Intuition: to progressively reduce the spatial size of the representation, to reduce the amount of parameters and computation in the network, and hence to also control overfitting
- Pooling partitions the input image into a set of non-overlapping rectangles and, for each such sub-region, outputs the maximum value of the features in that region.



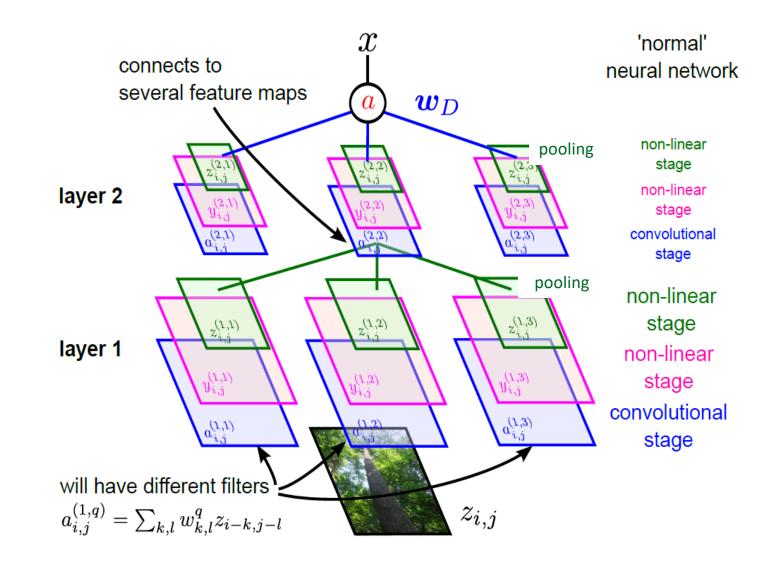
# CNN: pooling

- reduces the number of connections to the next layer (prevents the excessive number of parameters, speeds-up learning, reduces overfitting)
- max-pooling, min-pooling, average-pooling
- the problem: after several layers of pooling we lose the information about the exact location of the recognized pattern and about spatial relations between different patterns and features, e.g., a nose on a forehead

## Building-blocks for CNN's

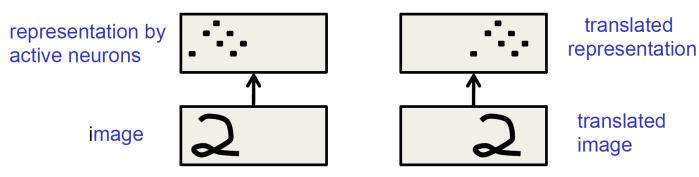


# Full CNN



# Convolutional networks: illustration on image recognition

- a useful feature is learned and used on several positions
- prevents dimension hopping
- max-pooling

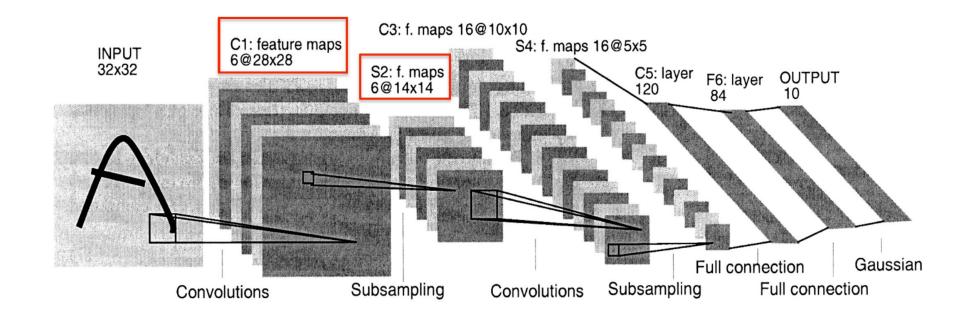


## CNN success: LeNet

- handwritten digit recognition by Yann LeCun,
- several hidden layers
- several convolutional filters
- pooling
- several other tricks

#### LeNet5 architecture

handwritten digit recognition



#### Hand-written Digit Recognition

• Input: 00011(1112 

#### **Errors of LeNet5**

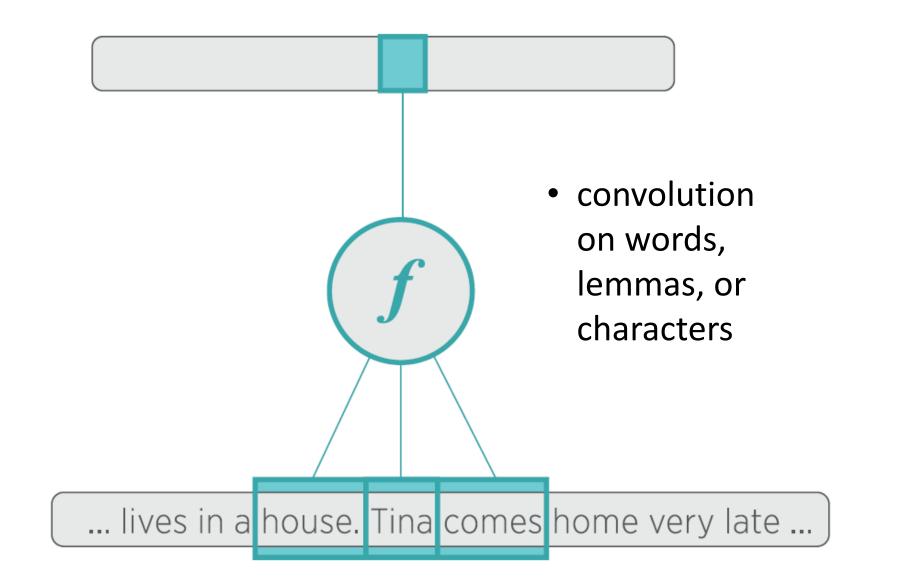
 $\int_{1->5} 9_{->8} \int_{6->3} 0_{->2} \int_{6->5} 9_{->5} \int_{0->7} 1_{->6} \int_{4->9} 2_{->1}$ 847769 1. 5 5 2->8 8->5 4->9 7->2 7->2 6->5 9->7 6->1 5->6 5->0

80 errors
 in
 10,000
 test
 cases

## Benefits of CNNs

- The number of weights can be much less than 1 million for a 1 mega pixel image.
- The small number of weights can use different parts of the image as training data. Thus we have several orders of magnitude more data to train the fewer number of weights.
- We get translation invariance for free.
- Fewer parameters take less memory and thus all the computations can be carried out in memory in a GPU or across multiple processors.

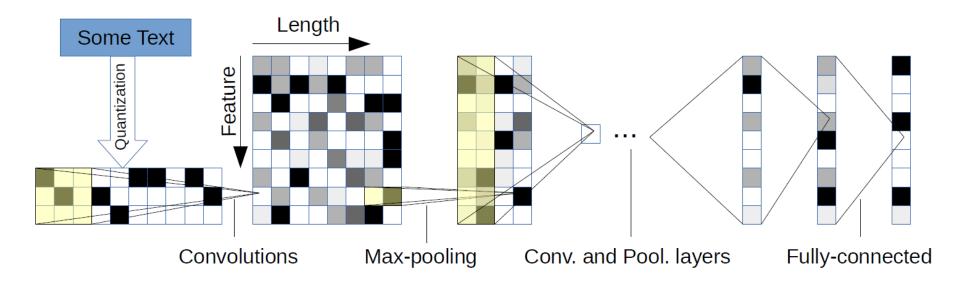
#### 1d convolution for text



# 2d convolution on characters

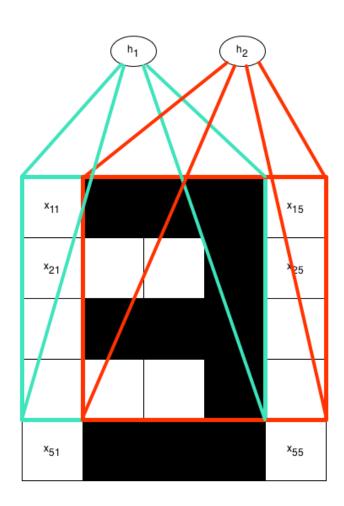
- text classification
- Zhang, Xiang, Junbo Zhao, and Yann LeCun. "Character-level convolutional networks for text classification." Advances in Neural Information Processing Systems. 2015.
- convolution, max-pooling
- ReLU activation h(x) = max(0, x)
- backpropagation with momentum 0.9
- minibatch =128, starting step 0.01 is halved every 3 epoch
- character quantization, alphabet of 70 characters abcdefghijklmnopqrstuvwxyz0123456789
   -,;.!?:'''/\|\_@#\$%^&\*~'+-=<>()[]{}
- one-hot encoding of characters

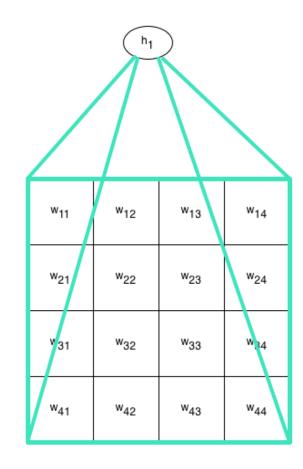
## Network architecture



- text blocks of 1014 characters (i.e. 1014 x 70)
- 6 convolutional layers with filter lengths 7, 7, 3, 3, 3, 3
- stride = 1
- between fully connected layers dropout, p=0.5
- good results on very large datasets >10<sup>6</sup>
- for smaller datasets bag of n-grams is very competitive

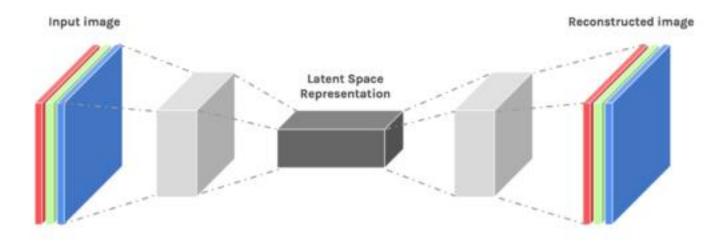
### Example: what the following CNN returns





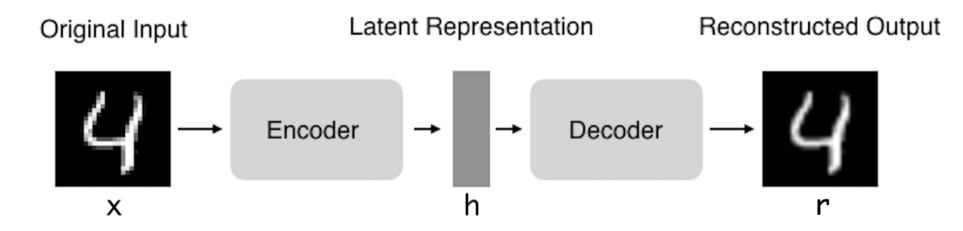
## Autoencoders

- Autoencoders are designed to reproduce their input, especially for images.
- The key point is to reproduce the input from a learned encoding.
- The loss function is the reproduction error



### Autoencoders: structure

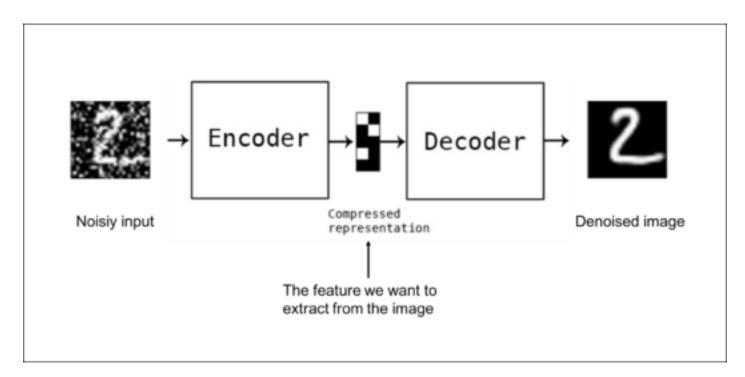
- Encoder: compress input into a latent-space of usually smaller dimension. h = f(x)
- Decoder: reconstruct input from the latent space. r = g(f(x)) with r as close to x as possible



https://towardsdatascience.com/deep-inside-autoencoders-7e41f319999f

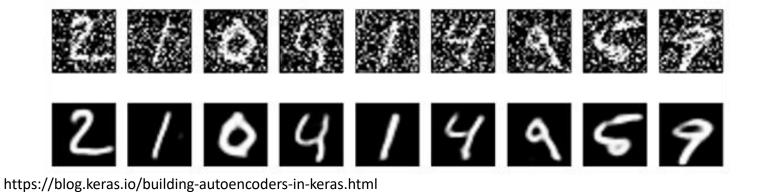
## Autoencoder applications: denoising

• Denoising: input clean image + noise and train to reproduce the clean image.



## Denoising autoencoders

- Basic autoencoder trains to minimize the loss between x and the reconstruction g(f(x)).
- Denoising autoencoders train to minimize the loss between x and g(f(x+w)), where w is random noise.
- Same possible architectures, different training data.



## Autoencoder applications: colorization

• Image colorization: input black and white and train to produce color images



## Autoencoder applications: watermark removal

• Watermark removal

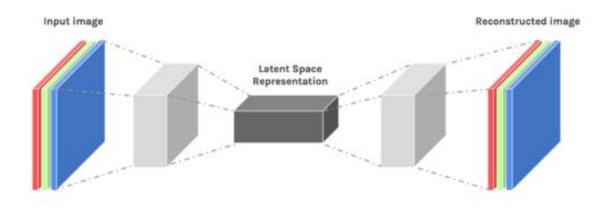


## Properties of autoencoders

- **Data-specific**: Autoencoders are only able to compress data similar to what they have been trained on.
- Lossy: The decompressed outputs will be degraded compared to the original inputs.
- Learned automatically from examples: It is easy to train specialized instances of the algorithm that will perform well on a specific type of input.

## Bottleneck layer (undercomplete)

- Suppose input images are n x n and the latent space is m < n x n.</li>
- Then the latent space is not sufficient to reproduce all images.
- Needs to learn an encoding that captures the important features in training data, sufficient for approximate reconstruction.



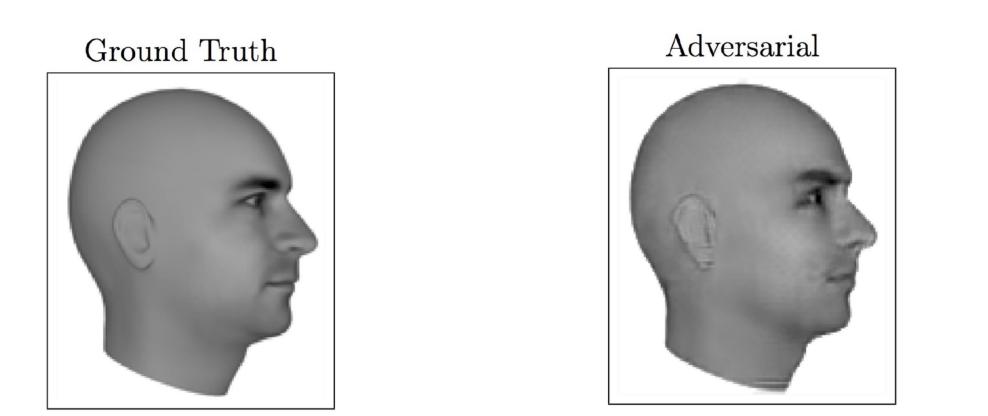
### GANs

- Generative
- Learn a generative model
- Adversarial
- Trained in an adversarial setting
- Networks
- Use Deep Neural Networks

### Why Generative Models?

- We've only seen discriminative models so far
- Given an image X, predict a label Y
- Estimates P(Y|X)
- Discriminative models have several key limitations
- Can't model P(X), i.e. the probability of seeing a certain image
- Thus, can't sample from P(X), i.e. can't generate new images
- Generative models (in general) cope with all of above
- Can model P(X)
- Can generate new images

### What GANs can do



Lotter, William, Gabriel Kreiman, and David Cox. "Unsupervised learning of visual structure using predictive generative networks." arXiv preprint arXiv:1511.06380 (2015).

## GANs in action

Which one is Computer generated?



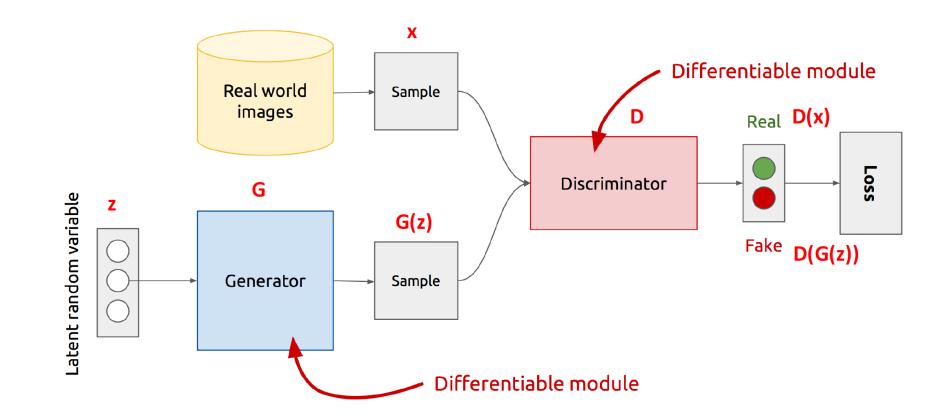


Ledig, Christian, et al. "Photo-realistic single image super-resolution using a generative adversarial network." arXiv preprint arXiv:1609.04802 (2016).

# Adversarial Training

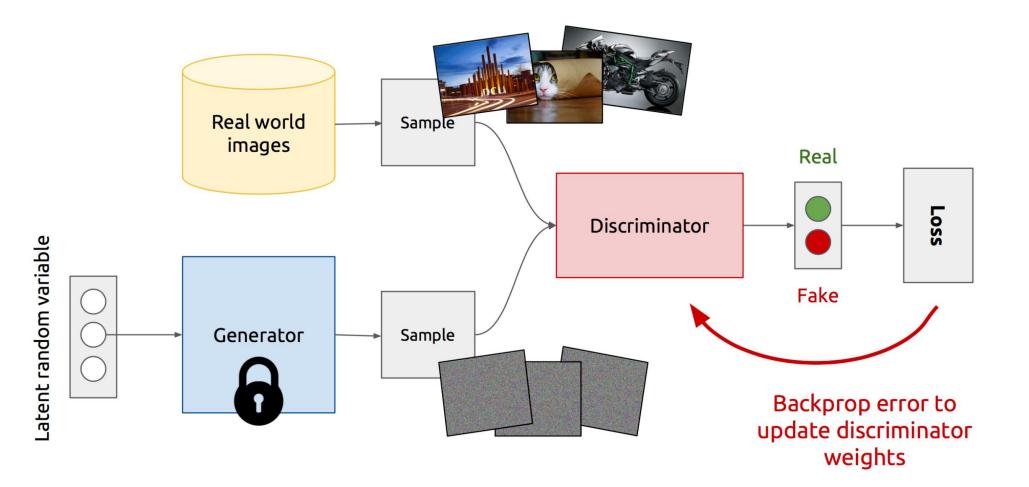
- Generator: generate fake samples, tries to fool the Discriminator
- Discriminator: tries to distinguish between real and fake samples
- Train them against each other
- Repeat this and we get better Generator and Discriminator

#### **GAN's Architecture**



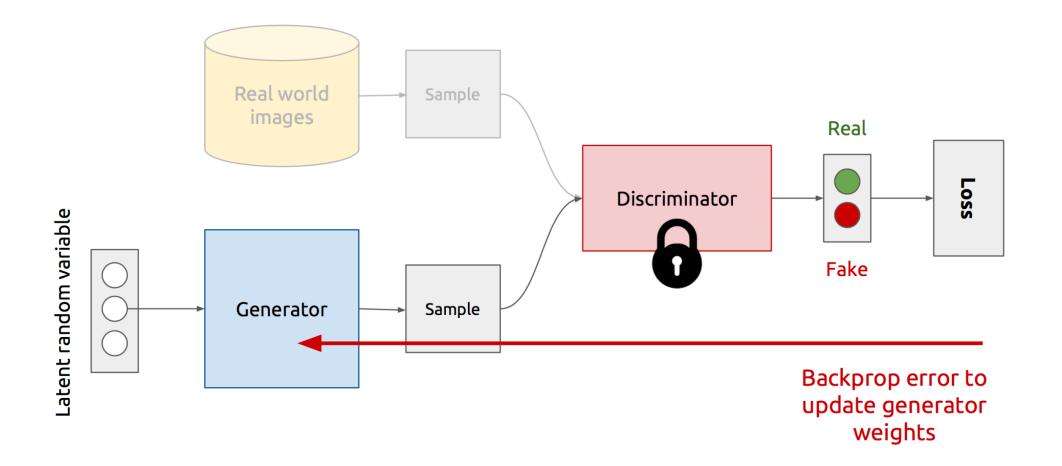
- **Z** is some random noise (Gaussian/Uniform).
- Z can be thought as the latent representation of the image.

### **Training Discriminator**



https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

### **Training Generator**



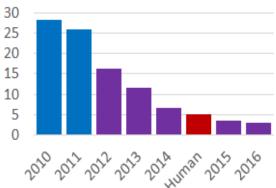
https://www.slideshare.net/xavigiro/deep-learning-for-computer-vision-generative-models-and-adversarial-training-upc-2016

### Sources

- Ian Goodfellow and Yoshua Bengio and Aaron Courville: *Deep Learning*. MIT Press, 2016, <u>http://www.deeplearningbook.org</u>
- Keras library in R or python
- HuggingFace library
- PyTorch
- TensorFlow

# Deep learnig sucesses

ILSVRC top-5 error rate on ImageNet

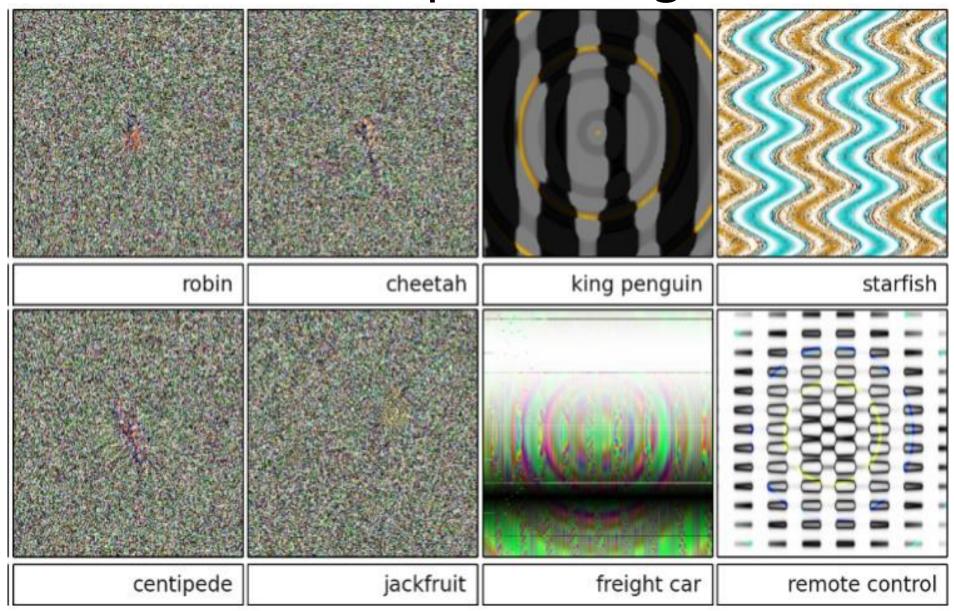


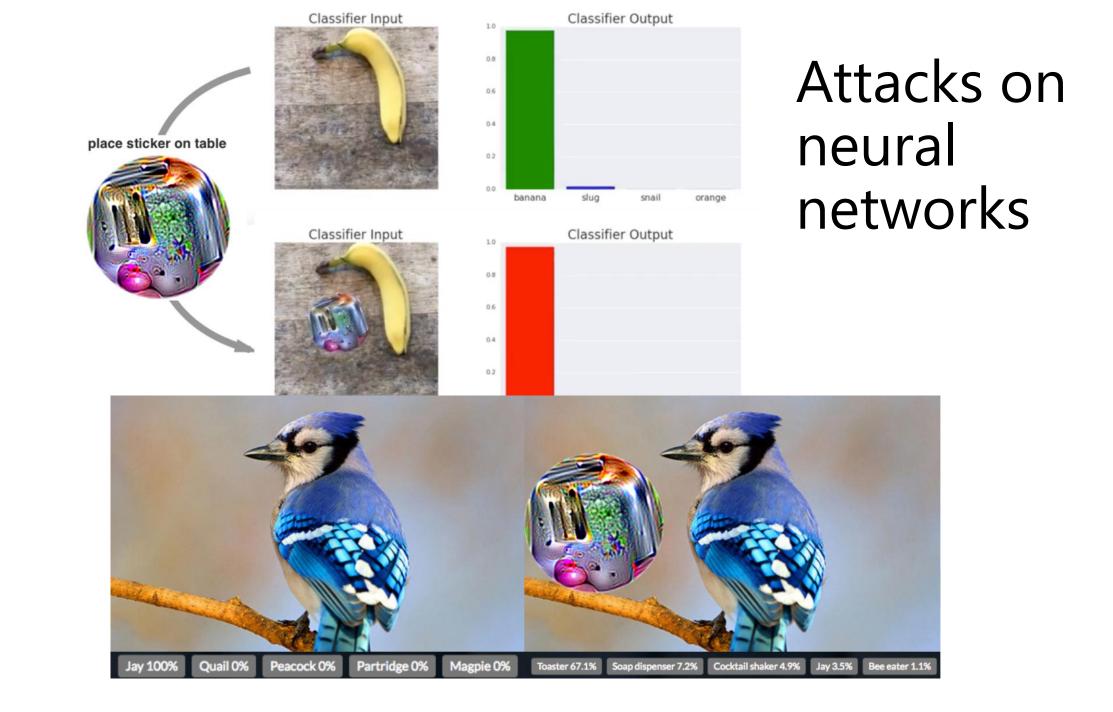


Microsoft claims new speech recognition record, achieving a super-human 5.1% error rate



# Weaknesses of deep learning





# Failures on outof-distribution examples

Michael A. Alcorn, Qi Li, Zhitao Gong, Chengfei Wang, Long Mai, Wei-Shinn Ku, Anh Nguyen (2018): Strike (with) a Pose: Neural Networks Are Easily Fooled by Strange Poses of Familiar Objects. arXiv:1811.11553



school bus 1.0 garbage truck 0.99 punching bag 1.0 snowplow 0.92



motor scooter 0.99 parachute 1.0

bobsled 1.0

parachute 0.54



school bus 0.98 fireboat 0.98 fire truck 0.99

bobsled 0.79