## Statistical Natural Language Processing Artificial Neural networks & deep learning

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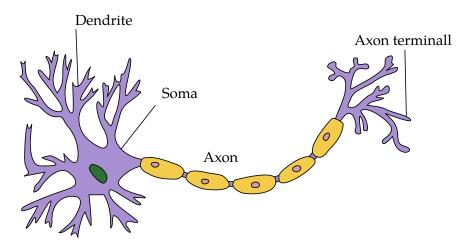
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#### Artificial neural networks

- Artificial neural networks (ANNs) are machine learning models inspired by biological neural networks
- ANNs are powerful non-linear models
- Power comes with a price: there are no guarantees of finding a global minimum of the error function
- ANNs have been used in ML, AI, Cognitive science since 1950's with some ups and downs
- Currently they are the driving force behind the popular *'deep learning'* methods

# The biological neuron

(showing a picture of a real neuron is mandatory in every ANN lecture)



# Artificial and biological neural networks

- ANNs are *inspired* by biological neural networks
- Similar to biological networks, ANNs are made of many simple processing units
- Despite the similarities, there are many differences: ANNs do not mimic biological networks
- ANNs are a practical statistical machine learning methods

## Recap: the perceptron

$$y = f\left(\sum_{j}^{m} w_{j} x_{j}\right)$$

where

$$f(x) = \begin{cases} +1 & \text{if } wx > 0\\ -1 & \text{otherwise} \end{cases}$$

In ANN-speak  $f(\cdot)$  is called an *activation function*.

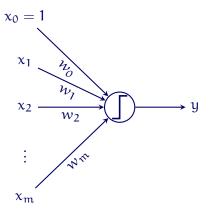
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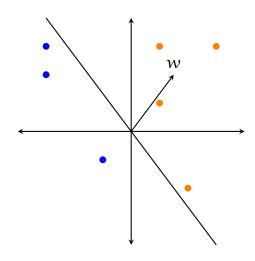
where

$$f(x) = \begin{cases} +1 & \text{if } wx > 0 \\ -1 & \text{otherwise} \end{cases}$$

In ANN-speak  $f(\cdot)$  is called an *activation function*.



# Recap: perceptron algorithm



 Perceptron algorithm minimizes the function

$$J(w) = \sum_{i} max(0, -wx_{i}y_{i})$$

• The online version picks an misclassified example, and sets

$$w \leftarrow w + x_i y_i$$

• Algorithm is guaranteed to converge if classes are linearly separable

#### Recap: logistic regression

$$P(y) = f\left(\sum_{j}^{m} w_{j} x_{j}\right)$$

where

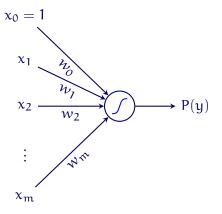
$$f(x) = \frac{1}{1 + e^{-wx}}$$

#### Recap: logistic regression

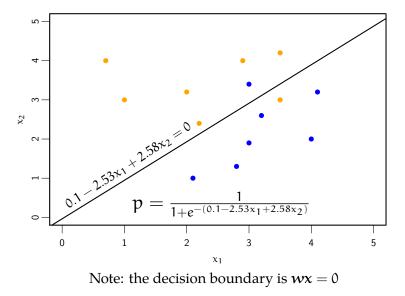
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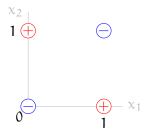


Logistic regression is also a linear classifier



### Linear separability

- A classification problem is said to be *linearly separable* if one can find a linear discriminator
- A well-known counter example is the logical XOR problem



There is no line that can separate positive and negative classes.

#### Can a linear classifier learn the XOR problem?

#### Can a linear classifier learn the XOR problem?

• We can use non-linear basis functions

$$w_0 + w_1 x_1 + w_2 x_2 + w_3 \phi(x_1, x_2)$$

is still linear in *w* for any choice of  $\phi(\cdot)$ 

• For example, adding the product  $x_1x_2$  as an additional feature would allow a solution like:  $x_1 + x_2 - 2x_1x_2$ 

x1	x <sub>2</sub>	$x_1 + x_2 - 2x_1x_2$
0	0	0
0	1	1
1	0	1
1	1	0

• Choosing proper basis functions like x<sub>1</sub>x<sub>2</sub> is called *feature engineering* 

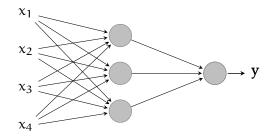
# Multi-layer perceptron

- The simplest modern ANN architecture is called multi-layer perceptron (MLP)
- (MLP) is a *fully connected, feed-forward* network consisting of perceptron-like units
- Unlike perceptron, the units in an MLP use a continuous activation function
- The MLP can be trained using gradient-based methods
- The MLP can represent many interesting machine learning problems
  - It can be used for both regression and classification

# Multi-layer perceptron

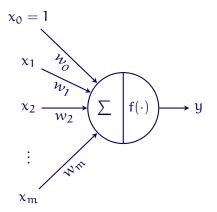
the picture





Each unit takes a weighted sum of their input, and applies a (non-linear) *activation function*.

## An artificial neuron



• The unit calculates a weighted sum of the inputs

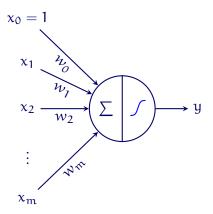
$$\sum_{j}^{m} w_{j} x_{j} = w x$$

- Result is a linear transformation
- Then the unit applies a non-linear activation function f(·)
- Output of the unit is

y = f(wx)

#### Artificial neuron

an example



• A common activation function is *logistic sigmoid* function

$$f(x) = \frac{1}{1 + e^{-x}}$$

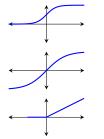
• The output of the network becomes

$$y = \frac{1}{1 + e^{-wx}}$$

# Activation functions in ANNs

hidden units

- The activation functions in MLP are typically continuous (differentiable) functions
- For hidden units common choices are



Sigmoid (logistic) 
$$\frac{1}{1+e^x}$$

Hyperbolic tangent (tanh) 
$$\frac{e^{2x}-1}{e^{2x}+1}$$

Rectified linear unit (relu) max(0, x)

## Activation functions in ANNs

output units

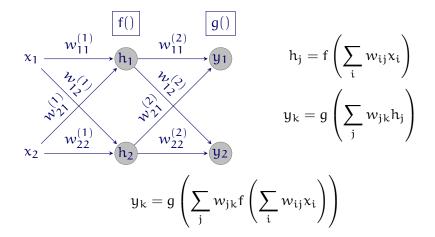
- The activation functions of the output units depends on the task
  - For regression, identity function
  - For binary classification, logistic sigmoid

$$P(y = 1 \mid x) = \frac{1}{1 + e^{-wx}} = \frac{e^{wx}}{1 + e^{-wx}}$$

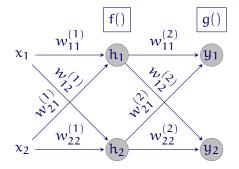
- For multi-class classification, softmax

$$\mathsf{P}(\mathsf{y}=\mathsf{k}\,|\,\mathsf{x}) = \frac{e^{w_{\mathsf{k}}\mathsf{x}}}{\sum_{\mathsf{j}}e^{w_{\mathsf{j}}\mathsf{x}}}$$

# MLP: a simple example



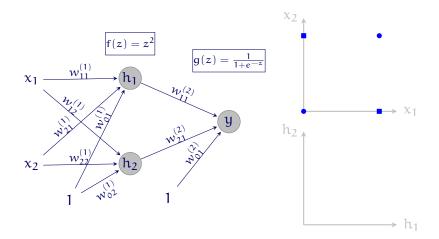
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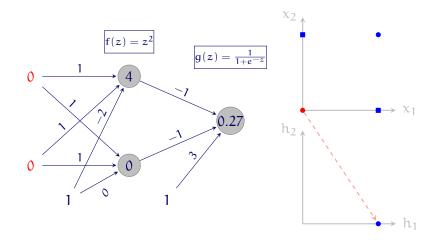


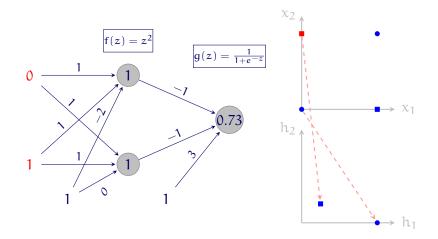
• Alternatively, we can write the computations in matrix form

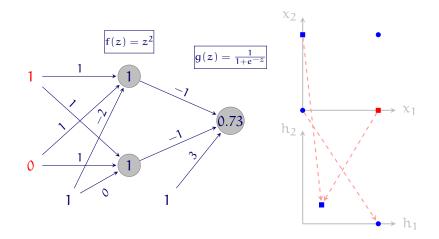
$$\mathbf{h} = f(W^{(1)}\mathbf{x})$$
$$\mathbf{y} = g(W^{(2)}\mathbf{h})$$
$$= g\left(W^{(2)}f(W^{(1)}\mathbf{x})\right)$$

• This corresponds to a series of transformations followed by element-wise (non-linear) function applications

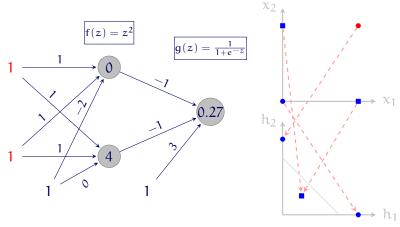








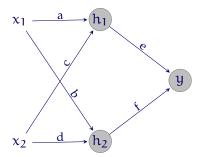
# Solving non-linear problems with ANNs a solution to XOR problem



Is this different from non-linear basis functions?

#### Non-linear activation functions are necessary

Without non-linear activation functions, an ANN with any number of layers is equivalent to a linear model.



 $h_1 = ax_1 + cx_2$   $h_2 = bx_1 + dx_2$   $y = eh_1 + fh_2$  $= (ea + fb)x_1 + (ec + fd)x_2$ 

y is still a linear function of  $x_i$ 

#### Where do non-linearities come from?

non-linearities are abundant in nature, it is not only the XOR problem

In a linear model,  $y = w_0 + w_1 x_1 + \ldots + w_k x_k$ 

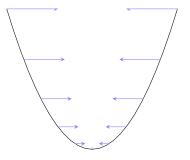
- The outcome is *linearly-related* to the predictors
- The effects of the inputs are *additive*

This is not always the case:

- Some predictors affect the outcome in a non-linear way
  - The effect may be strong or positive only in a certain range of the variable (e.g., reaction time change by age)
  - Some effects are periodic (e.g., many measures of time)
- Some predictors interact 'not bad' is not 'not' + 'bad' (e.g., for sentiment analysis)

# Finding the minimum of a loss function

- Derivative of a function points to the largest direction of change
- Derivative is 0 at minima/maxima
- To find the minimum (or maximum) of error function f(x), we solve f'(x) = 0, for x
- If no analytic solution exist, we search for the minimum iteratively
- -f'(x) for any x points towards the minimum



#### Gradient descent: a refresher

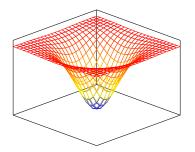
• The general idea is to approach a minimum of the error function in small steps

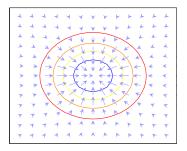
$$\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla J(\boldsymbol{w})$$

- $\nabla J$  is the gradient of the loss function, it points to the direction of the maximum increase
- $-\eta$  is the learning rate
- The updates can be performed
- batch for the complete training set
- on-line after every training instance

- this is known as *stochastic gradient descent* (SGD) mini-batch after small fixed-sized batches

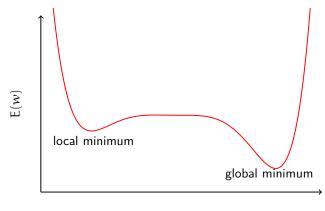
# Gradient descent: the picture





$$\nabla f(x_1, \dots, x_n) = \left(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n}\right)$$





w

#### A function is *convex* if there is only one (global) minimum.

## Error functions in ANN training

depend on the task

• If we assume Gaussian noise, a natural choice is the minimizing the sum of squared error

$$E(w) = \sum_i (y_i - \hat{y}_i)^2$$

• For binary classification, we use *cross entropy* 

$$E(w) = -\sum_{i} y_i \log \hat{y}_i + (1 - y_i) \log(1 - \hat{y}_i)$$

• Similarly, for multi-class classification, also cross entropy

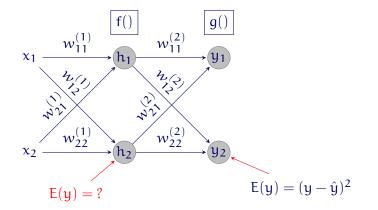
$$\mathsf{E}(w) = -\sum_{i}\sum_{k}y_{i,k}\log\hat{y}_{k}$$

In practice, the ANN loss functions will not be convex.

# Learning in ANNs

- ANNs implement complex functions: we need to use optimization methods (e.g., gradient descent) to train them
- Typically error functions for ANNs are not convex, gradient descent will find a local minimum
- Optimization requires updating multiple layers of weights
- Assigning credit (or blame) to each weight during learning is not trivial
- An effective solution to the last problem is the *backpropagation* algorithm

### Learning in multi-layer networks: the problem



We want a way to update non-final weights based on final error.

# Backpropagation

- The final output of the network is computed by calculating the output of each layer and passing it to the next (*forward propagation*)
- Weight updates on the final layer is easy: we need the relevant component of the gradient:

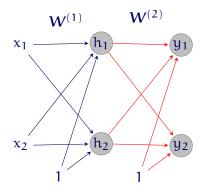
$$\Delta w_{ij} = \eta \frac{\partial E}{\partial w_{ij}}$$

• For the non-final weights we make use of chain rule of derivatives

if 
$$F(w) = f(g(w))$$
,  $F'(x) = f'(g(w))g'(w)$ 

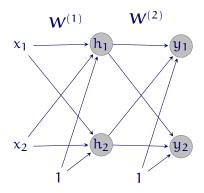
• Backpropagation propagates the error from output units to the input weights using the chain rule of derivatives

## Backpropagation: visualization



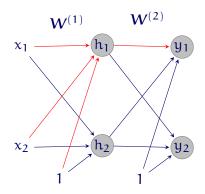
• Updating weights **W**<sup>(2)</sup> is easy: we can use gradient descent directly

## Backpropagation: visualization



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- We update weights **W**<sup>(1)</sup> using the chain rule

## Backpropagation: visualization



- Updating weights **W**<sup>(2)</sup> is easy: we can use gradient descent directly
- We update weights **W**<sup>(1)</sup> using the chain rule
- Backpropagation algorithm uses dynamic programming to do this efficiently

Regularization in neural networks

• As in linear models, we can use L1 and L2 regularization by adding a regularization term to the error function (known as *weight decay*). For example,

 $J(w) = E(w) + \|W\|$ 

- There are other ways to fight overfitting
  - With *early stopping*, one stops the training before it reaches to the smallest training error
  - With *dropout*, random units (with all of their connections) are dropped during training
  - Injecting noise at the output, as a way to (implicitly) model the noise in the target classes/values

# Adapting learning rate

- The choice of learning rate  $\boldsymbol{\eta}$  is important
- too small slow convergence
  - too big overshooting may fluctuate around the minimum, or even jump away
    - The idea is to adapt the learning rate during learning
    - A common trick is adding a momentum: if we move in the same direction a long time accelerate

$$\Delta w_{ij}(t) = \eta \frac{\partial E}{\partial w_{ij}} + \alpha \Delta w_{ij}(t-1)$$

• There are many adaptive optimization algorithms: Adagrad, Adadelta, RMSprop, Adam, ...

## How many layers, units

- A network with single hidden layer is said to be *a universal approximator*: it can approximate any continuous function with arbitrary precision
- However, in practice multiple interconnected layers are useful and commonly used in modern ANN models
- The choice of layers, in general the architecture of the system, depends on the application

## A bit of history

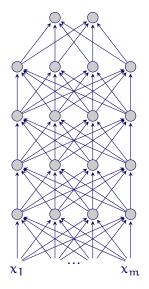
- 1950-60 ANNs (perceptron) became popular: lots of excitement in AI, cognitive science
  - 1970s Not much interest
    - criticism on perceptron: linear separability
  - 1980s ANNs became popular again
    - backpropagation algorithm
    - multi-layer networks
  - 1990s ANNs had again fallen 'out of fashion'
    - Engineering: other algorithms (such as SVMs) performed generally better
    - From the cognitive science perspective: ANNs are difficult to interpret

present ANNs (again) enjoy a renewed popularity with the name 'deep learning'

Summary, so far...

- ANNs are non-linear machine learning methods
- they can be used for both regression and classification
- they are trained with backpropagation algorithm
- ANN loss functions are not convex, what we find is a local minimum

# Deep feed-forward networks



- Deep neural networks (>2 hidden layers) have recently been successful in many tasks
- They are particularly useful in problems where layers/hierarchies of features are useful
- They often use sparse connectivity and shared weights
- We will review two important architectures: CNNs and RNNs

# Training deep networks

difficulties

- Training deep networks is more difficult
- A common practical problem is unstable gradients: the gradients may vanish, or explode
- Often we have lots of hyper parameters:
  - the number of layers
  - For each layer:
    - what architecture to use (dense, CNN, RNN, ...)
    - activation function(s)
    - regularization method / parameters
    - optimization algorithm
    - initialization
    - ...

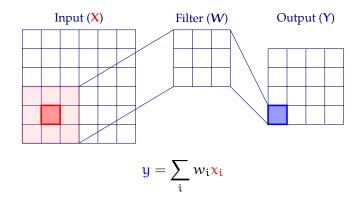
Why now?

- Increased computational power, especially advances in graphical processing unit (GPU) hardware
- Availability of large amounts of data
  - mainly unlabeled data (more on this later)
  - but also labeled data through 'crowd sourcing' and other sources
- Some new developments in theory and applications

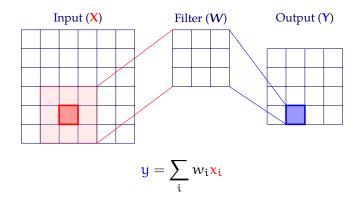
### Convolutional networks

- Convolutional networks are particularly popular in image processing applications
- They have also been used with success some NLP tasks
- Unlike feed-forward networks we have discussed so far,
  - CNNs are not fully connected
  - The hidden layer(s) receive input from only a set of neighboring units
  - Some weights are shared
- A CNN learns features that are location invariant
- CNNs are also computationally less expensive compared to fully connected networks

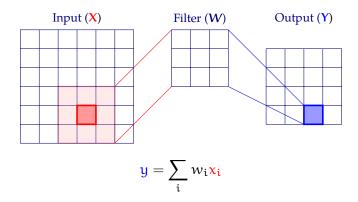
- Convolution is a common operation in image processing for effects like edge detection, blurring, sharpening, ...
- The idea is to transform each pixel with a function of the local neighborhood



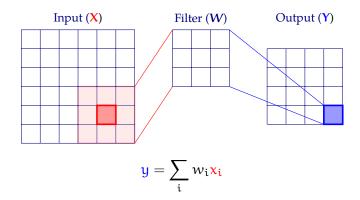
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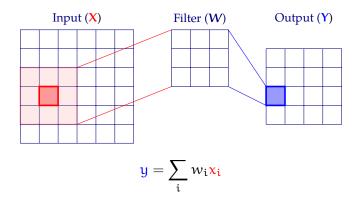
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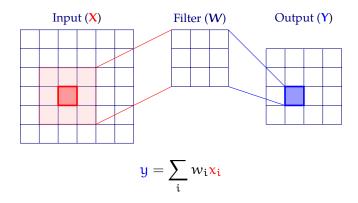
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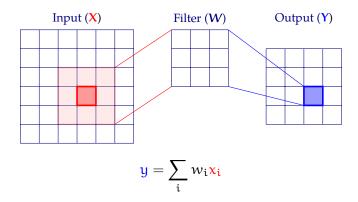
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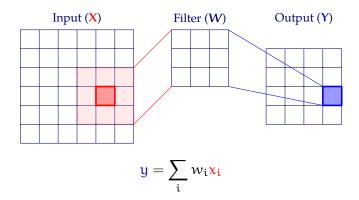
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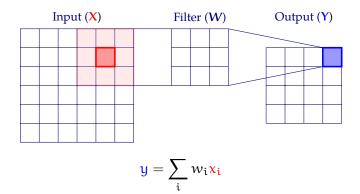
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## Example convolutions

• Blurring

$$\frac{1}{16} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1 \end{bmatrix}$$

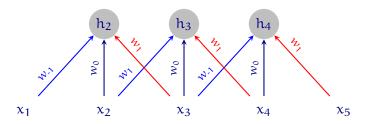
• Edge detection

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

## Learning convolutions

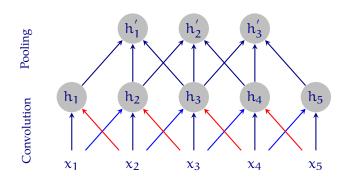
- Some filters produce features that are useful for classification (e.g., of images, or sentences)
- In machine learning we want to *learn* the convolutions
- Typically, we learn multiple convolutions, each resulting in a different feature map
- Repeated application of convolutions allow learning higher level features
- The last layer is typically a standard fully-connected classifier

#### Convolution in neural networks



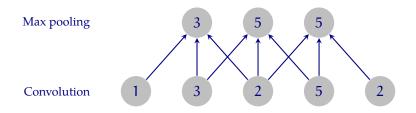
- Each hidden layer corresponds to a local window in the input
- Weights are shared: each convolution detects the same type of features

Pooling



- Convolution is combined with *pooling*
- Pooling 'layer' simply calculates a statistic (e.g., max) over the convolution layer
- Location invariance comes from pooling

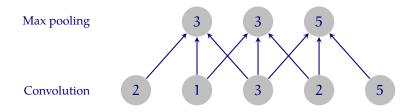
### Pooling and location invariance



• Note that the numbers at the pooling layer are stable in comparison to the convolution layer

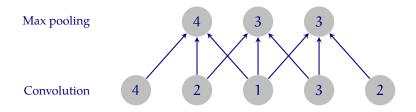
Ç. Çöltekin, SfS / University of Tübingen

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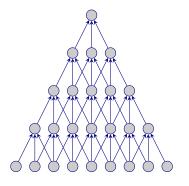


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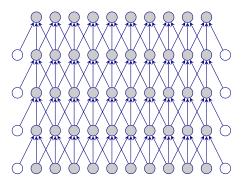
## Padding in CNNs

• With successive layers of convolution and pooling, the size of the later layers shrinks



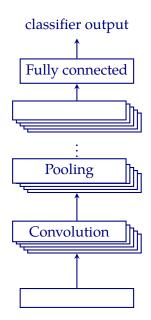
# Padding in CNNs

- With successive layers of convolution and pooling, the size of the later layers shrinks
- One way to avoid this is *padding* the input and hidden layers with enough number of zeros

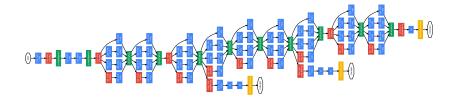


# CNNs: the bigger picture

- At each convolution/pooling step, we often want to learn multiple feature maps
- After a (long) chain of hierarchical features maps, the final layer is typically a fully-connected layer (e.g., softmax for classification)



## Real-world examples are complex



The real-world ANNs tend to be complex

- Many layers (sometimes with repetition)
- Large amount of branching

\* Diagram describes an image classification network, GoogLeNet (Szegedy et al. 2014).

# CNNs in natural language processing

- The use of CNNs in image applications is clear:
  - the first convolutional layer learns local features, e.g., edges

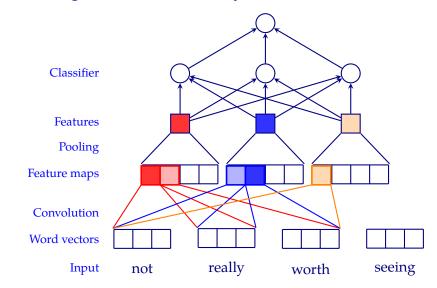


 successive layers learn more complex features that are combinations of these features



- In NLP, it is a bit less straight-forward
  - CNNs are typically used in combination with word vectors
  - The convolutions of different sizes correspond to (word) n-grams of different sizes
  - With pooling, CNNs produce summaries of documents or sentences similar to BoW approach

#### An example: sentiment analysis



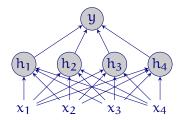
### Convolutional networks: summary

- Convolutional networks use sparse connectivity with weight sharing
- The resulting network is computationally more efficient (compared to fully-connected networks)
- They are suitable for inputs with local features with (some) location invariance
- CNNs are very popular in image classification / object detection
- They are also used in NLP, particularly for document/sentence classification

#### Recurrent neural networks

- Feed forward networks (also CNNs)
  - can only learn associations
  - they do not have memory of earlier inputs: they cannot handle sequences
- Recurrent neural networks are ANN solution for sequence learning
- This is achieved by recursive loops in the network

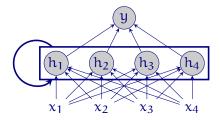
#### Recurrent neural networks



• Recurrent neural networks are similar to the standard feed-forward networks

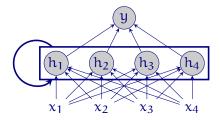
Ç. Çöltekin, SfS / University of Tübingen

#### Recurrent neural networks



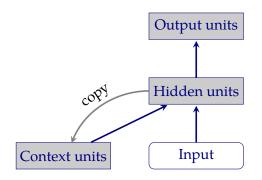
- Recurrent neural networks are similar to the standard feed-forward networks
- They include loops that use previous output (of the hidden layers) as well as the input

#### Recurrent neural networks



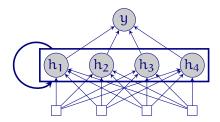
- Recurrent neural networks are similar to the standard feed-forward networks
- They include loops that use previous output (of the hidden layers) as well as the input
- Forward calculation is straightforward, learning becomes somewhat tricky

#### A simple version: SRNs Elman (1990)

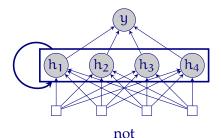


- The network keeps previous hidden states (context units)
- The rest is just like a feed-forward network
- Training is simple, but cannot learn long-distance dependencies

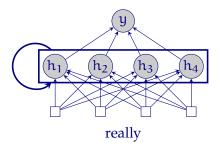
- RNNs process sequences one unit at a time
- The earlier input affects the output through the recurrent links



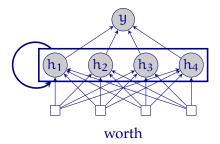
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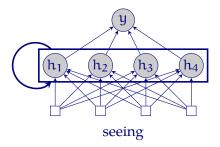
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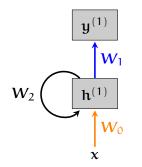
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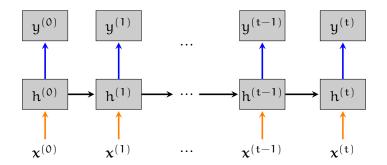
### Learning in recurrent networks



- We need to learn three sets of weights: W<sub>0</sub>, W<sub>1</sub> and W<sub>2</sub>
- Backpropagation in RNNs are at first not that obvious
- The main difficulty is in propagating the error through the recurrent connections

# Unrolling a recurrent network

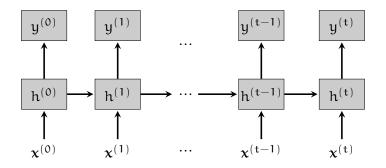
Back propagation through time (BPTT)



Note: the weights with the same color are shared.

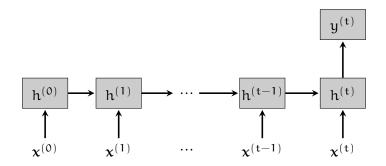
#### **RNN** architectures

Many-to-many (e.g., POS tagging)



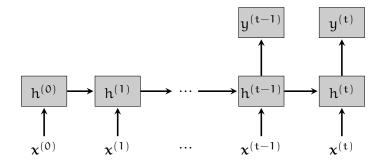
### **RNN** architectures

Many-to-one (e.g., document classification)

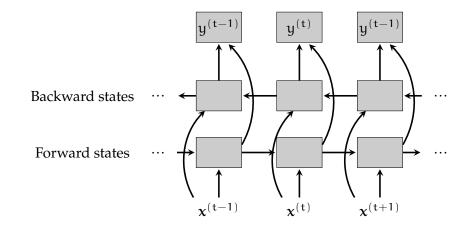


#### **RNN** architectures

Many-to-one with a delay (e.g., machine translation)



### **Bidirectional RNNs**



### RNNs as language models

- RNNs can function as language models
- We can train RNNs using unlabeled data for this purpose
- During training the task of RNN is to predict the next word
- Depending on the network configuration, an RNN can learn dependencies at a longer distance
- The resulting system can generate sequences

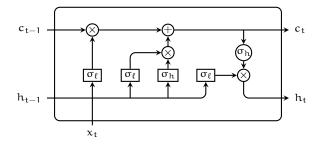
Recommended reading:

http://karpathy.github.io/2015/05/21/rnn-effectiveness/

### Unstable gradients revisited

- We noted earlier that the gradients may *vanish* or *explode* during backpropagation in deep networks
- This is especially problematic for RNNs since the effective dept of the network can be extremely large
- Although RNNs can theoretically learn long-distance dependencies, this is affected by unstable gradients problem
- The most popular solution is to use *gated* recurrent networks

#### Gated recurrent networks



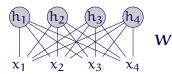
- Most modern RNN architectures are 'gated'
- The main idea is learning a mask that controls what to remember (or forget) from previous hidden layers
- Two popular architectures are
  - Long short term memory (LSTM) networks (above)
  - Gated recurrent units (GRU)

### Unsupervised learning in ANNs

- Restricted Boltzmann machines (RBM) similar to the latent variable models (e.g., Gaussian mixtures), consider the representation learned by hidden layers as hidden variables (h), and learn p(x, h) that maximize the probability of the (unlabeled)data
- Autoencoders

train a constrained feed-forward network to predict its output

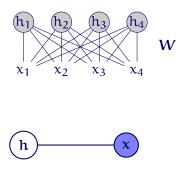
### Restricted Boltzmann machines (RBMs)



- RBMs are unsupervised latent variable models, they learn only from unlabeled data
- They are generative models of the joint probability p(h,x)
- They correspond to undirected graphical models
- No links within layers
- The aim is to learn useful features (h)

\*Biases are omitted in the diagrams and the formulas for simplicity.

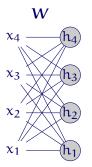
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### The distribution defined by RBMs



$$p(\mathbf{h}, \mathbf{x}) = \frac{e^{\mathbf{h}^{\mathsf{T}} \mathbf{W} \mathbf{x}}}{\mathsf{Z}}$$

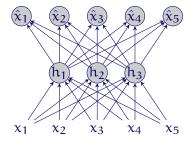
This calculation is intractable (Z is difficult to calculate). But conditional distributions are easy to calculate

$$p(\mathbf{h}|\mathbf{x}) = \prod_{j} p(\mathbf{h}_{j}|\mathbf{x}) = \frac{1}{1 + e^{\mathbf{W}_{j}\mathbf{x}}}$$
$$p(\mathbf{x}|\mathbf{h}) = \prod_{k} p(\mathbf{x}_{k}|\mathbf{h}) = \frac{1}{1 + e^{\mathbf{W}_{k}^{T}\mathbf{h}}}$$

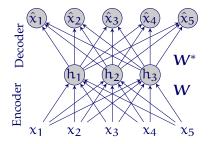
### Learning in RBMs

- We want to maximize the probability the model assigns to the input, p(x), or equivalently minimize  $-\log p(x)$
- In general, this is computationally expensive
- *Contrastive divergence algorithm* is a well known algorithm that efficiently finds an approximate solution

#### Autoencoders

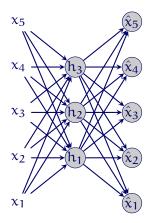


#### Autoencoders



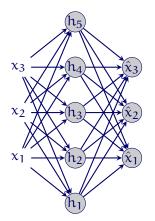
- Autoencoders are standard feed-forward networks
- The main difference is that they are trained to predict their input (they try to learn the identity function)
- The aim is to learn useful representations of input at the hidden layer
- Typically weights are tied (W\* = W<sup>T</sup>)

# Under-complete autoencoders



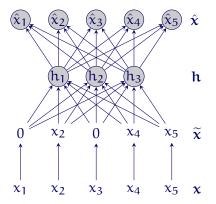
- An autoencoder is said to be *under-complete* if there are fewer hidden units than inputs
- The network is forced to learn a compact representation of the input (compress)
- An autoencoder with a single hidden layer approximates the PCA
- We need multiple layers for learning non-linear features

## Over-complete autoencoders



- An autoencoder is said to be *over-complete* if there are more hidden units than inputs
- The network can normally memorize the input perfectly
- This type of networks are useful if trained with a regularization term resulting in sparse hidden units (e.g., L1 regularization)

### Denoising autoencoders



- Instead of providing the exact input, we introduce noise by
  - randomly setting some inputs to 0 (dropout)
  - adding random (Gaussian) noise
- Network is still expected to reconstruct the original input (without noise)

### Unsupervised pre-training

- A common use case for RBMs and autoencoders are as pre-training methods for supervised networks
- Autoencoders or RBMs are trained using unlabeled data
- The weights learned during the unsupervised learning is used for initializing the weights of a supervised network
- This approach has been one of the reasons for success of deep networks

# Deep unsupervised learning

- Both autoencoders and RBMs can be 'stacked'
- Learn the weights of the first hidden layer from the data
- Freeze the weights, and using the hidden layer activations as input, train another hidden layer, ...
- This approach is called greedy layer-wise training
- In case of RBMs resulting networks are called *deep belief networks*
- Deep autoencoders are called *stacked autoencoders*

### Summary

- ANNs are powerful non-linear learners
  - based on some inspiration from biological NNs
  - using many simple processing units
  - built on linear models (logistic regression)
- For non-linear problems we need non-linear activation functions, and at least one hidden layer
- Deep networks use more than one hidden layer
- Common (deep) ANN architectures include:
- CNN location invariance
- RNN sequence learning

### Summary

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Next:

Wed work on assignments

Fri N-gram language models