#### Statistical Natural Language Processing Neural networks

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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

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

where  $\mathbf{x} = (x_1, \dots, x_m)$ ,  $\mathbf{w} = (w_1, \dots, w_m)$ 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

- Logistic regression estimates  $\mathsf{P}(\boldsymbol{y} \,|\, \boldsymbol{x})$ 

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

The function

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

is called the logistic sigmoid function

• To find the solution, we minimize the minus log likelihood

$$-\log \mathcal{L}(\boldsymbol{w}) = \sum_i y_i \log p + (1-y_i) \log(1-p)$$

• The above objective function is simply cross entropy

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

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

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 classical 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



### MLP: a simple example



• 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, the ANN 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 functions

- 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





$$abla f(x_1,\ldots,x_n) = \left(\frac{\partial f}{\partial x_1},\ldots,\frac{\partial f}{\partial x_n}\right)$$

### Global and local minima



w

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

### Error functions in ANN training

depends on the task

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

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

• 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 any practical ANN, the loss function 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> are easy: we can use gradient descent directly

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# Backpropagation: visualization



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- 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 adapt the learning rate during learning
    - A common trick is adding a momentum: if we move in the same direction a long time accelarate

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

• 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) become popular: lots of excitement in AI, cognitive science
  - 1970s Not much interest
    - criticims 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 popularity and 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 trined with backpropaation 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 netowrks 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
    - optimiaztion 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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# 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., 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

Preliminaries ANNs

# 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

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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



### Strided convolution



- It is common to use *strided* convolution in some applications
- This is equivalent to convolution + down sampling

# 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 NNs tend to be complex (with some repetition)

- Many layers
- 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

 $| \setminus / -$ 

 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) ngrams 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 NN 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

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#### Recurrent neural networks



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- 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



### Processing sequences with RNNs

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



not

- RNNs process sequences one unit at a time
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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 reding:

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)

# Summary

- ANNs are powerfull non-linear learners
  - based on some inspiration from bioloical 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

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Next:

Fri exercises (continued)

Mon parsing