# CS60020: Foundations of Algorithm Design and Machine Learning

Sourangshu Bhattacharya

## **Neural Network Basics**

 Given several inputs: and several weights: and a bias value:



• A neuron produces a single output:  $o_1 = s(\sum_i w_i x_i + b)$ 

 $\sum_{i} w_i x_i + b$ 

- This sum is called the **activation** of the neuron
- The function *s* is called the **activation function** for the neuron
- The weights and bias values are typically initialized randomly and learned during training

## McCulloch-Pitts "unit"

Output is a "squashed" linear function of the inputs:

 $a_i \leftarrow g(in_i) = g\left(\sum_j W_{j,i}a_j\right)$ 



A gross oversimplification of real neurons, but its purpose is to develop understanding of what networks of simple units can do

## Activation functions



(a)is a step function or threshold function

(b) is a sigmoid function  $1/(1 + e^{-x})$ 

Changing the bias weight  $W_{0,i}$  moves the threshold location

### **Feed forward example**



Feed-forward network = a parameterized family of nonlinear functions:

$$a_5 = g(W_{3,5} \cdot a_3 + W_{4,5} \cdot a_4) = g(W_{3,5} \cdot g(W_{1,3} \cdot a_1 + W_{2,3} \cdot a_2) + W_{4,5} \cdot g(W_{1,4} \cdot a_1 + W_{2,4} \cdot a_2))$$

Adjusting weights changes the function: do learning this way!

### **Expressiveness of perceptrons**

Consider a perceptron with g = step function (Rosenblatt, 1957, 1960) Can represent AND, OR, NOT, majority, etc., but not XOR Represents a linear separator in input space:



Minsky & Papert (1969) pricked the neural network balloon

## **Feed Forward Neural Networks**

Layers are usually fully connected; numbers of hidden units typically chosen by hand



## Hidden-Layer

- The hidden layer (L<sub>2</sub>, L<sub>3</sub>) represent learned non-linear combination of input data
- For solving the XOR problem, we need a hidden layer
  - some neurons in the hidden layer will activate only for some combination of input features
  - the output layer can represent combination of the activations of the hidden neurons
- Neural network with one hidden layer is a universal approximator
  - Every function can be modeled as a shallow feed forward network
  - Not all functions can be represented *efficiently* with a single hidden layer  $\Rightarrow$  we still need deep neural networks

## **Going from Shallow to Deep Neural Networks**

- Neural Networks can have several hidden layers
- Initializing the weights randomly and training all layers at once does hardly work
- Instead we train layerwise on unannotated data Img-Source: http://neuralnetworksanddeeplearning.com
  (a.k.a. pre-training):
  - Train the first hidden layer
  - Fix the parameters for the first layer and train the second layer.
  - Fix the parameters for the first & second layer, train the third layer



- After the pre-training, train all layers using your annotated data
- The pre-training on your unannotated data creates a high-level abstractions of the input data
- The final training with annotated data fine tunes all parameters in the network

## How to learn the weights

- Initialise the weights i.e.  $W_{k,j}W_{j,i}$  with random values
- With input entries we calculate the predicted output
- We compare the prediction with the true output
- The error is calculated
- The error needs to be sent as feedback for updating the weights



#### Example: Classify 'Paris' in the context of this sentence with window length 2:

... museums in Paris are amazing ....  $X_{window} = [x_{museums} \quad x_{in} \quad x_{Paris} \quad x_{are} \quad x_{amazing}]^T$ Resulting vector  $x_{window} \in R^{5d}$  is a column vector.

$$s = U^T f(Wx + b) \qquad x \in \mathbb{R}^{20 \times 1}, W \in \mathbb{R}^{8 \times 20}, U \in \mathbb{R}^{8 \times 1}$$



#### Idea

Ensure that the score computed for "true" labeled data points is higher than the score computed for "false" labeled data points.

- *s* = score(museums in Paris are amazing)
- s<sub>c</sub> = score(Not all museums in Paris)

#### Objective

Maximize  $(s - s_c)$  or to minimize  $(s_c - s)$ . One possible objective function: minimize  $J = max(s_c - s, 0)$ 

#### What is the problem with this?

- Does not attempt to create a margin of safety. We would want the "true" labeled data point to score higher than the "false" labeled data point by some positive margin Δ.
- We would want error to be calculated if (s s<sub>c</sub> < Δ) and not just when (s s<sub>c</sub> < 0). The modified objective: minimize J = max(Δ + s<sub>c</sub> s, 0)

- Objective for a single window:  $J = max(1 + s_c s, 0)$
- Each window with a location at its center should have a score +1 higher than any window without a named entity at its center.

• 
$$s = U^T f(Wx + b), s_c = U^T f(Wx_c + b)$$

 Assuming cost J is > 0, compute the derivatives of s and s<sub>c</sub> with respect to the involved variables: U, W, b, x

### Training with backpropagation

#### Derivative of weight W<sub>ij</sub>:





#### Derivative continued ...



where  $f^{\prime}(z)=f(z)(1-f(z))$  for logistic f

### *From single weight* W<sub>ij</sub> *to full* W:

$$\frac{\partial s}{\partial W_{ij}} = \delta_i x_j$$

- We want all combinations of i = 1, 2, ... and j = 1, 2, 3, ...
- Solution: Outer product

$$\frac{\partial J}{\partial W} = \delta x^T$$

## **Computation Graphs**



## BACKPROPAGATION

Slides from Intel

## How to Train a Neural Net?



- Put in Training inputs, get the output
- Compare output to correct answers: Look at loss function J
- Adjust and repeat!
- Backpropagation tells us how to make a single adjustment using calculus.

How have we trained before?

- Gradient Descent!
- 1. Make prediction
- 2. Calculate Loss
- 3. Calculate gradient of the loss function w.r.t. parameters
- 4. Update parameters by taking a step in the opposite direction
- 5. Iterate

How have we trained before?

- Gradient Descent!
- 1. Make prediction
- 2. Calculate Loss
- 3. Calculate gradient of the loss function w.r.t. parameters
- 4. Update parameters by taking a step in the opposite direction
- 5. Iterate

## Feedforward Neural Network



## Forward Propagation









How have we trained before?

- Gradient Descent!
- 1. Make prediction
- 2. Calculate Loss
- 3. Calculate gradient of the loss function w.r.t. parameters
- 4. Update parameters by taking a step in the opposite direction
- 5. Iterate

## How to Train a Neural Net?

- How could we change the weights to make our Loss Function lower?
- Think of neural net as a function F: X -> Y
- F is a complex computation involving many weights W\_k
- Given the structure, the weights "define" the function F (and therefore define our model)
- Loss Function is J(y,F(x))

## How to Train a Neural Net?

- Get  $\frac{\partial J}{\partial W_k}$  for every weight in the network.
- This tells us what direction to adjust each  $W_k$  if we want to lower our loss function.
- Make an adjustment and repeat!

## Feedforward Neural Network



## Calculus to the Rescue

- Use calculus, chain rule, etc. etc.
- Functions are chosen to have "nice" derivatives
- Numerical issues to be considered

### Punchline

$$\frac{\partial J}{\partial W^{(3)}} = (\hat{y} - y) \cdot a^{(3)}$$
$$\frac{\partial J}{\partial W^{(2)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'(z^{(3)}) \cdot a^{(2)}$$
$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'(z^{(3)}) \cdot W^{(2)} \cdot \sigma'(z^{(2)}) \cdot X$$

- Recall that:  $\sigma'(z) = \sigma(z)(1 \sigma(z))$
- Though they appear complex, above are easy to compute!








How have we trained before?

- Gradient Descent!
- 1. Make prediction
- 2. Calculate Loss
- 3. Calculate gradient of the loss function w.r.t. parameters
- 4. Update parameters by taking a step in the opposite direction
- 5. Iterate

## Vanishing Gradients

Recall that:

$$\frac{\partial J}{\partial W^{(1)}} = (\hat{y} - y) \cdot W^{(3)} \cdot \sigma'(z^{(3)}) \cdot W^{(2)} \cdot \sigma'(z^{(2)}) \cdot X$$

- Remember:  $\sigma'(z) = \sigma(z)(1 \sigma(z)) \le .25$
- As we have more layers, the gradient gets very small at the early layers.
- This is known as the "vanishing gradient" problem.
- For this reason, other activations (such as ReLU) have become more common.

#### Neural Networks – What we learnt

- Neural networks for supervised learning
- Multiple Hidden layers as universal approximators
- Fully connected feed-forward networks for calssification
- Backpropagation for learning network parameters (Weights at layers)

#### **Up Next:**

- Paradigms for Deep Learning Models
  - CNNs
  - RNNs

## CONVOLUTIONAL NEURAL NETWORKS

#### Motivation – Image Data

- So far, the structure of our neural network treats all inputs interchangeably.
- No relationships between the individual inputs
- Just an ordered set of variables
- We want to incorporate domain knowledge into the architecture of a Neural Network.

#### Motivation

- Image data has important structures, such as;
- "Topology" of pixels
- Translation invariance
- Issues of lighting and contrast
- Knowledge of human visual system
- Nearby pixels tend to have similar values
- Edges and shapes
- Scale Invariance objects may appear at different sizes in the image.

#### Motivation – Image Data

- Fully connected would require a vast number of parameters
- MNIST images are small (32 x 32 pixels) and in grayscale
- Color images are more typically at least (200 x 200) pixels x
  3 color channels (RGB) = 120,000 values.
- A single fully connected layer would require (200x200x3)<sup>2</sup> = 14,400,000,000 weights!
- Variance (in terms of bias-variance) would be too high
- So we introduce "bias" by structuring the network to look for certain kinds of patterns

#### Motivation

- Features need to be "built up"
- Edges -> shapes -> relations between shapes
- Textures
- Cat = two eyes in certain relation to one another + cat fur texture.
- Eyes = dark circle (pupil) inside another circle.
- Circle = particular combination of edge detectors.
- Fur = edges in certain pattern.

#### Kernels

- A *kernel* is a grid of weights "overlaid" on image, centered on one pixel
- Each weight multiplied with pixel underneath it
- Output over the centered pixel is  $\sum_{p=1}^{P} W_p \cdot pixel_p$
- Used for traditional image processing techniques:
  - o Blur
  - o Sharpen
  - Edge detection
  - o Emboss

#### Kernel: 3x3 Example







## Kernel: 3x3 Example





#### Kernel: 3x3 Example



	Kernel				
-1	0	1			
-2	0	2			
-1	0	1			



 $= (3 \cdot -1) + (2 \cdot 0) + (1 \cdot 1)$  $+ (1 \cdot -2) + (2 \cdot 0) + (3 \cdot 2)$  $+ (1 \cdot -1) + (1 \cdot 0) + (1 \cdot 1)$ 

= -3 + 1 - 2 + 6 - 1 + 1 = 2

#### Kernels as Feature Detectors

Can think of kernels as a "local feature detectors"

-1	1	-1
-1	1	-1
-1	1	-1

Vertical Line Detector Horizontal Line Detector Corner Detector

-1	-1	-1
1	1	1
-1	-1	-1



## Convolutional Neural Nets

Primary Ideas behind Convolutional Neural Networks:

- Let the Neural Network learn which kernels are most useful
- Use same set of kernels across entire image (translation invariance)
- Reduces number of parameters and "variance" (from biasvariance point of view)

#### Convolutions





## Convolution Settings – Grid Size

#### Grid Size (Height and Width):

- The number of pixels a kernel "sees" at once
- Typically use odd numbers so that there is a "center" pixel
- Kernel does not need to be square



Height: 1, Width: 3







## **Convolution Settings - Padding**

#### Padding

- Using Kernels directly, there will be an "edge effect"
- Pixels near the edge will not be used as "center pixels" since there are not enough surrounding pixels
- Padding adds extra pixels around the frame
- So every pixel of the original image will be a center pixel as the kernel moves across the image
- Added pixels are typically of value zero (zero-padding)

#### Without Padding

1	2	0	3	1
1	0	0	2	2
2	1	2	1	1
0	0	1	0	0
1	2	1	1	1

-1	1	2		
1	1	0		
-1	-2	0		
kernel				



input

## With Padding

0	0	0	0	0	0	0
0	1	2	0	3	1	0
0	1	0	0	2	2	0
0	2	1	2	1	1	0
0	0	0	1	0	0	0
0	1	2	1	1	1	0
0	0	0	0	0	0	0

-1	1	2			
1	1	0			
-1	-2	0			
kernel					

-1		

output

input

## **Convolution Settings**

#### Stride

- The "step size" as the kernel moves across the image
- Can be different for vertical and horizontal steps (but usually is the same value)
- When stride is greater than 1, it scales down the output dimension

## Stride 2 Example – No Padding



-1	1	2		
1	1	0		
-1	-2	0		
kernel				



output

input

## Stride 2 Example – With Padding

			•				
	0	0	0	0	0	0	0
	0	1	2	0	3	1	0
4	0	1	0	0	2	2	0
	0	2	1	2	1	1	0
	0	0	0	1	0	0	0
	0	1	2	1	1	1	0
	0	0	0	0	0	0	0

-1	1	2
1	1	0
-1	-2	0

kernel





input

## Convolutional Settings - Depth

- In images, we often have multiple numbers associated with each pixel location.
- These numbers are referred to as "channels"
  - RGB image 3 channels
  - CMYK 4 channels
- The number of channels is referred to as the "depth"
- So the kernel itself will have a "depth" the same size as the number of input channels
- Example: a 5x5 kernel on an RGB image
  - There will be 5x5x3 = 75 weights

#### Convolutional Settings - Depth

- The output from the layer will also have a depth
- The networks typically train many different kernels
- Each kernel outputs a single number at each pixel location
- So if there are 10 kernels in a layer, the output of that layer will have depth 10.

## Pooling

- Idea: Reduce the image size by mapping a patch of pixels to a single value.
- Shrinks the dimensions of the image.
- Does not have parameters, though there are different types of pooling operations.

Pooling: Max-pool

- For each distinct patch, represent it by the maximum
- 2x2 maxpool shown below



Pooling: Average-pool

- For each distinct patch, represent it by the average
- 2x2 avgpool shown below.



# ConvNet: CONV, RELU, POOL and FC Layers



# **Convolution** Layer

#### 32x32x3 image



Filters always extend the full depth of the input volume

5x5x3 filter

**Convolve** the filter with the image i.e. "slide over the image spatially, computing dot products"

# **Convolution Layer**

consider a second, greenfilter



# Convolution Layer

For example, if we had 6 5x5 filters, we'll get 6 separate activation maps:



We stack these up to get a "new image" of size 28x28x6!

# ReLU (Rectified Linear Units) Layer

- This is a layer of neurons that applies the activation function f(x)=max(0,x).
- It increases the nonlinear properties of the decision function and of the overall network without affecting the receptive fields of the convolution layer.
- Other functions are also used to increase nonlinearity, for example the hyperbolic tangent f(x)=tanh(x), and the sigmoid function.
- This is also known as a ramp function.



# A Basic ConvNet

**Preview:** ConvNet is a sequence of Convolutional Layers, interspersed with activation functions



# What is convolution of an image with a filter



Image

Convolved Feature
# Details about the convolution layer



7x7 input (spatially) assume 3x3 filter applied **with stride 3?** 

doesn't fit! cannot apply 3x3 filter on 7x7 input with stride 3.

# Details about the convolutionlayer

Ν

F F

Ν

Output size: (N - F) / stride + 1

e.g. N = 7, F = 3:  
stride 1 => 
$$(7 - 3)/1 + 1 = 5$$
  
stride 2 =>  $(7 - 3)/2 + 1 = 3$   
stride 3 =>  $(7 - 3)/3 + 1 = 2.33$ 

## Details about the convolutionlayer In practice: Common to zero pad the border

0	0	0	0	0	0		
0							
0							
0							
0							

e.g. input 7x7
3x3 filter, applied with stride 1
pad with 1 pixel border => what is the output?

#### 7x7 output!

in general, common to see CONV layers with stride 1, filters of size FxF, and zero-padding with (F-1)/2. (will preserve size spatially) e.g. F = 3 => zero pad with 1 F = 5 => zero pad with 2 F = 7 => zero pad with 3

## Convolution layer examples

Input volume: **32x32x3** 10 5x5 filters with stride 1, pad 2

Output volume size: ?

```
(32+2*2-5)/1+1 = 32 spatially, so 32x32x10
```

## **Pooling Layer**

makes the representations smaller and more manageable X operates over each activation map independently:



- Invariance to image transformation and increases compactness to representation.
- Pooling types: Max, Average, L2 etc.

#### Single depth slice



y

max pool with 2x2 filters and stride 2

6	8
3	4

#### **Convolutional Neural Networks**



 $z_j = f(V_{1:n}^u * K_j + b_j)$  Where ReLu is used as f.

#### **Convolutional Neural Networks**



#### **Applications**

## Localization and Detection













Results from Faster R-CNN, Ren et al 2015

#### **Applications**

#### **Computer Vision Tasks**

 Classification
 Object Detection
 Instance Segmentation

 Image: Classification + Localization
 Object Detection
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification
 Image: Classification
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification
 Image: Classification
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification
 Image: Classification
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification
 Image: Classification
 Image: Classification

 Image: Classification + Localization
 Image: Classification
 Image: Classification

#### Is deep learning all about CNNs?

- Consider a language modelling task
- Given a vocabulary, the task is to predict the next word in a sentence
- Sequence information of words are important
- Typically in cases where sequential data is involved, recurrent neural networks (RNNs) are widely used

#### Recurrent neural networks

#### **Recurrent neural networks**

- Lots of information is sequential and requires a memory for successful processing
- Sequences as input, sequences as output



- Recurrent neural networks(RNNs) are called recurrent because they perform same task for every element of sequence, with output dependent on previous computations
- RNNs have memory that captures information about what has been computed so far
- RNNs can make use of information in arbitrarily long sequences – in practice they limited to looking back only few steps

#### **Topologies of Recurrent Neural Network**



1) Common Neural Network (e.g. feed forward network)

- 2) Prediction of future states base on single observation
- 3) Sentiment classification
- 4) Machine translation
- 5) Simultaneous interpretation

#### Language Model

• Compute the probability of a sentence

- Useful in machine translation
  - Word ordering: p(the cat is small) > p(small the cat is)
  - Word choice: p(walking home after school) > p(walking house after school)







- Recurrent Neural Network have an internal state
- State is passed from input  $x_t$  to  $x_{t+1}$

#### Language Models with RNN

- Let  $x_0, x_1, x_2...$  denote words (input)
- Let o<sub>0</sub>, o<sub>1</sub>, o<sub>2</sub>... denote the probability of the sentence(output)
- Memory requirement scales nicely (linear with the number of word embeddings / number of character)





#### **Recurrent neural networks**

- RNN being unrolled (or unfolded) into full network
- Unrolling: write out network for complete sequence



• Image credits: Nature

#### **RNN (Problem Revisited)**



#### No Magic Involved (in Theory)

- You unroll your data in time
- You compute the gradients
- You use back propagation to train your network
- Karpathy presents a Python implementation for Char-RNN with 112 lines
- Training RNNs is hard:
  - Inputs from many time steps ago can modify output
  - Vanishing / Exploding Gradient Problem
- Vanishing gradients can be solved by Gated-RNNs like Long-Short-Term-Memory (LSTM) Models
  - LSTM became popular in NLP in 2015

#### Vanishing and exploding gradients

- For training RNNs, calculate gradients for U, V, W – ok for V but for W and U ...
- ► Gradients for *W*:

$$\frac{\partial \mathcal{L}_3}{\partial W} = \frac{\partial \mathcal{L}_3}{\partial o_3} \frac{\partial o_3}{\partial s_3} \frac{\partial s_3}{\partial W} = \sum_{k=0}^3 \frac{\partial \mathcal{L}_3}{\partial o_3} \frac{\partial o_3}{\partial s_3} \frac{\partial s_3}{\partial s_k} \frac{\partial s_k}{\partial W}$$

• More generally: 
$$\frac{\partial \mathcal{L}}{\partial s_t} = \frac{\partial \mathcal{L}}{\partial s_m} \cdot \frac{\partial s_m}{\partial s_{m-1}} \cdot \frac{\partial s_{m-1}}{\partial s_{m-2}} \cdot \dots \cdot \frac{\partial s_{t+1}}{\partial s_t} \Rightarrow \ll 1$$
  
< 1 < 1 < 1

 Gradient contributions from far away steps become zero: state at those steps doesn't contribute to what you are learning

$$L_i$$
 – Loss, U, V, W – Parameters,  $S_i$  - states



#### Vanishing and exploding gradients



#### Vanishing and exploding gradients



Heatmap

#### Long Short Term Memory [Hochreiter and Schmidhuber, 1997]

LSTMs designed to combat vanishing gradients through gating mechanism

How LSTM calculates hidden state  $s_t$ 

$$i = \sigma(x_t U^i + s_{t-1} W^i)$$
  

$$f = \sigma(x_t U^f + s_{t-1} W^f)$$
  

$$o = \sigma(x_t U^o + s_{t-1} W^o)$$
  

$$g = \tanh(x_t U^g + s_{t-1} W^g)$$
  

$$c_t = c_{t-1} \circ f + g \circ i$$
  

$$s_t = \tanh(c_t) \circ o$$

#### Long-Short-Term Memory (LSTM)



- Long-term dependencies: *I grew up in France and lived there until I was 18. Therefore I speak fluent ???*
- Presented (vanilla) RNN is unable to learn long term dependencies
  - Issue: More recent input data has higher influence on the output
- Long-Short-Term Memory (LSTM) models solves this problem

#### **LSTM Model**



- The LSTM model implements a *forget-gate* and an *add-gate*
- The models learns when to forget something and when to update internal storage

Img Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

#### **LSTM Model**



- Core: Cell-state *C* (a vector of certain size)
- The model has the ability to remove or add information using Gates

Img Source: http://colah.github.io/posts/2015-08-Understanding-LSTMs/

### **Forget-Gate**



 $f_t = \sigma \left( W_f \cdot [h_{t-1}, x_t] + b_f \right)$ 

- Sigmoid function  $\sigma$  output a value between 0 and 1
- The output is point-wise multiplied with the cell state  $C_{t-1}$
- Interpretation:
  - 0: Let nothing through
  - 1: Let everything through
- Example: When we see a new subject, forget gender of old subject

#### Set-Gate



$$i_t = \sigma \left( W_i \cdot [h_{t-1}, x_t] + b_i \right)$$
$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C)$$

- Compute *i<sub>t</sub>* which cells we want to update and to which degree (σ: 0 ... 1)
- Compute the new cell value using the *tanh* function

## **Update Internal Cell State**



Update state cells

## Compute Output h<sub>t</sub>



- We use the updated cell state  $C_t$  to compute the output
- We might not need the complete cell state as output
  - Compute  $o_t$ , defining how relevant each cell is for the output
  - Pointwise multiply o<sub>t</sub> with tanh(C<sub>t</sub>)
- Cell state  $C_t$  and output  $h_t$  is passed to the next time step

### Conclusion

- Deep learning approaches Powerful mechanisms for introducing nonlinearity in learning
- Learning using backpropagation
- Embeddings for word representations
- Sequence Labelling using RNNs
- LSTMs, GRUs are special kind of RNNs
- CNNs for text and Image recognition.

## References

- Deep Learning for NLP <u>Nils Reimers</u>. <u>https://github.com/UKPLab/deeplearning4nlp-</u> <u>tutorial/tree/master/2017-07\_Seminar</u>
- <u>CS231n: Convolutional Neural Networks for Visual</u> <u>Recognition</u>. <u>Andrej Karpathy</u> <u>http://cs231n.github.io/convolutional-networks/</u>
- <a href="http://karpathy.github.io/2015/05/21/rnn-effectiveness/">http://karpathy.github.io/2015/05/21/rnn-effectiveness/</a>
- Neural Networks for Information Retrieval. SIGIR 2017 Tutorial <u>http://nn4ir.com/</u>
- CSE 446 Machine Learning Spring 2015, University of Washington. <u>Pedro Domingos</u>. <u>https://courses.cs.washington.edu/courses/cse446/15sp/</u>

# • Thanks