

# **10701: Introduction to Machine Learning**

#### Neural Networks and Deep Learning (1)

01010001 Ω

- Basics in artificial neural networks

Eric Xing Lecture 10, October 7, 2020

Reading: see class homepage



# ML vs DL





# Outline

An overview of DL components

- Historical remarks: early days of neural networks
  - Perception
  - ANN
  - Reverse-mode automatic differentiation (aka backpropagation)
  - Pretrain
  - CNN
- Modern building blocks: units, layers, activations functions, loss functions, etc. (next lecture)



# Learning highly non-linear functions

#### $f\colon X \boldsymbol{\rightarrow} Y$

- f might be non-linear function
- X (vector of) continuous and/or discrete vars
- Y (vector of) continuous and/or discrete vars



**Speech recognition** 



## **Perceptron and Neural Nets**

• From biological neuron to artificial neuron (perceptron)



From biological neuron network to artificial neuron networks





# **Connectionist Models**

- Consider humans:
  - Neuron switching time
    - ~ 0.001 second
  - Number of neurons
    - ~ 10<sup>10</sup>
  - Connections per neuron
     ~ 10<sup>4-5</sup>
  - Scene recognition time
    - $\sim 0.1$  second
  - 100 inference steps doesn't seem like enough
     → much parallel computation
- Properties of artificial neural nets (ANN)
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed processes





# **Jargon Pseudo-Correspondence**

- Independent variable = input variable
- Dependent variable = output variable
- Coefficients = "weights"
- Estimates = "targets"

#### Logistic Regression Model (the sigmoid unit)





# The perceptron learning algorithm



- Recall the nice property of sigmoid function
- Consider regression problem f: X  $\rightarrow$  Y, for scalar Y:  $\frac{d\sigma}{dt} = \sigma(1 \sigma)$ We used to maximize the conditional data likelihood  $y = f(x) + \epsilon$

$$\vec{w} = \arg \max_{\vec{w}} \ln \prod_{i} P(y_i | x_i; \vec{w})$$
$$\vec{w} = \arg \min_{\vec{w}} \sum_{i} \frac{1}{2} (y_i - \hat{f}(x_i; \vec{w}))^2$$

Here ... 

#### The perceptron learning algorithm

$$\frac{\partial E_D[\vec{w}])}{\partial w_j} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_l (t_d - o_d)^2$$

$$= \frac{1}{2} \sum_d 2(t_d - o_d) \frac{\partial}{\partial w_i} (t_d - o_d)$$

$$= \sum_d (t_d - o_d) \left( -\frac{\partial o_d}{\partial w_i} \right)$$

$$= -\sum_d (t_d - o_d) \frac{\partial o_d}{\partial net_i} \frac{\partial net_d}{\partial w_i}$$

$$= -\sum_d (t_d - o_d) o_d (1 - o_d) x_d^i$$
Batch mode:

Do until converge: 1. compute gradient  $\nabla E_D[w]$ 2.  $\vec{w} = \vec{w} - \eta \nabla E_D[\vec{w}]$  x<sub>d</sub> = input t<sub>d</sub> = target output

 $o_d$  = observed output

Incremental mode: Do until converge: • For each training example *d* in *D* 1. compute gradient  $\nabla E_d[w]$ 2. $\vec{w} = \vec{w} - \eta \nabla E_d[\vec{w}]$ where  $\nabla E_d[\vec{w}] = -(t_d - o_d)o_d(1 - o_d)\vec{x}_d$ 



#### What decision surface does a perceptron define?



some possible values for  $w_1$  and  $w_2$ 





#### What decision surface does a perceptron define?



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#### What decision surface does a perceptron define?

1





a possible set of values for  $(W_1, W_2, W_3, W_4, W_5, W_6)$ : (0.6, -0.6, -0.7, 0.8, 1, 1)



## **Non Linear Separation**





#### **Neural Network Model**





# "Combined logistic models"





# "Combined logistic models"





# "Combined logistic models"





# **Neural Network Training**



- Back-Propagation (BP)
  - A routine to compute gradient
  - Use chain rule of derivative



# **Backpropagation: Reverse-mode differentiation**

 Artificial neural networks are nothing more than complex functional compositions that can be represented by computation graphs:





# **Backpropagation: Reverse-mode differentiation**

 Artificial neural networks are nothing more than complex functional compositions that can be represented by computation graphs:

$$x$$
  $1$   $3$   $f(x)$   $\frac{\partial f_n}{\partial x} =$ 

By applying the chain rule and using reverse accumulation, we get

$$\frac{\partial f_n}{\partial x} = \sum_{i_1 \in \pi(n)} \frac{\partial f_n}{\partial f_{i_1}} \frac{\partial f_{i_1}}{\partial x} = \sum_{i_1 \in \pi(n)} \frac{\partial f_n}{\partial f_{i_1}} \sum_{i_2 \in \pi(i_1)} \frac{\partial f_{i_1}}{\partial f_{i_2}} \frac{\partial f_{i_1}}{\partial x} = \dots$$

- The algorithm is commonly known as backpropagation
- What if some of the functions are stochastic?
- Then use stochastic backpropagation! (to be covered in the next part)
- Modern packages can do this *automatically* (more later)

# **Backpropagation (continue)**





a

# **Backpropagation (continue)**

• Say, 
$$E = (t - o)^2$$
,  $F_n = \sigma$ 

- Initialize all weights to small random numbers Until convergence, Do
  - Input the training example to the network 1. and compute the network outputs
  - For each output unit k1.

$$\delta_k \leftarrow o_k^2 (1 - o_k^2) (t - o_k^2)$$

2. For each hidden unit h

$$\delta_h \leftarrow o_h^1 (1 - o_h^1) \sum_{k \in outputs} w_{h,k} \delta_k$$

Undate each network weight  $w_{i,i}$ 3.

$$w_{i,j} \leftarrow w_{i,j} + \Delta w_{i,j}$$
 where  $\Delta w_{i,j} = \eta \delta_j x^j$ 

 $x_d = input$  $t_d$  = target output  $o_d$  = observed output  $w_i$  = weight i





# More on Backpropatation

It is doing gradient descent over entire network weight vector

- Easily generalized to arbitrary directed graphs
- Will find a local, not necessarily global error minimum
  - In practice, often works well (can run multiple times)
- Often include weight *momentum*  $\alpha$

 $\Delta w_{i,j}(t) = \eta \delta_j x_{i,j} + \alpha \Delta w_{i,j}(t-1)$ 

- Minimizes error over *training* examples
  - Will it generalize well to subsequent testing examples?
- Training can take thousands of iterations,  $\rightarrow$  very slow!
- Using network after training is very fast



## **Minimizing the Error**





# **Overfitting in Neural Nets**





## **Alternative Error Functions**

Penalize large weights:

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{k,d} - o_{k,d})^2 + \gamma \sum_{i,j} w_{j,i}^2$$

Training on target slopes as well as values

$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{k,d} - o_{k,d})^2 + \mu \sum_{j \in inputs} \left( \frac{\partial t_{k,d}}{\partial x_d^j} - \frac{\partial o_{k,d}}{\partial x_d^j} \right)$$

Tie together weights



# Pretraining

A better initialization strategy of weight parameters

- Based on Restricted Boltzmann Machine
- An auto-encoder model
- Unsupervised
- □ Layer-wise, greedy
- Useful when training data is limited
- Not necessary when training data is rich



## **Restricted Boltzmann Machines**

- RBM is a Markov random field represented with a bi-partite graph
- All nodes in one layer/part of the graph are connected to all in the other; no inter-layer connections



• Joint distribution:

$$P(v,h) = \frac{1}{Z} \exp\left\{\sum_{i,j} w_{ij} v_i h_i + \sum_i b_i v_i + \sum_j c_j h_j\right\}$$
































### Layer-wise Unsupervised Pre-training





### **Learning Hidden Layer Representation**

A network:

A target function:

Can	this	be	learned?

Input		Output
10000000	$\rightarrow$	10000000
01000000	$\rightarrow$	01000000
00100000	$\rightarrow$	00100000
00010000	$\rightarrow$	00010000
00001000	$\rightarrow$	00001000
00000100	$\rightarrow$	00000100
00000010	$\rightarrow$	0000010
0000001	$\rightarrow$	00000001





### **Learning Hidden Layer Representation**

A network:



• Learned hidden layer representation:

Input		Hidden				Output			
Values									
10000000	$\rightarrow$	.89	.04	.08	$\rightarrow$	10000000			
01000000	$\rightarrow$	.01	.11	.88	$\rightarrow$	01000000			
00100000	$\rightarrow$	.01	.97	.27	$\rightarrow$	00100000			
00010000	$\rightarrow$	.99	.97	.71	$\rightarrow$	00010000			
00001000	$\rightarrow$	.03	.05	.02	$\rightarrow$	00001000			
00000100	$\rightarrow$	.22	.99	.99	$\rightarrow$	00000100			
00000010	$\rightarrow$	.80	.01	.98	$\rightarrow$	00000010			
00000001	$\rightarrow$	.60	.94	.01	$\rightarrow$	00000001			



## Training





## Training





### Non-linear LR vs. ANN



$$Y = a(X_1) + b(X_2) + c(X_3) + d(X_1X_2) + ...$$



### **Expressive Capabilities of ANNs**

- Boolean functions:
  - Every Boolean function can be represented by network with single hidden layer
  - But might require exponential (in number of inputs) hidden units
- Continuous functions:
  - Every bounded continuous function can be approximated with arbitrary small error, by network with one hidden layer [Cybenko 1989; Hornik et al 1989]
  - Any function can be approximated to arbitrary accuracy by a network with two hidden layers [Cybenko 1988].



### **Feature learning**

 Successful learning of intermediate representations [Lee et al ICML 2009, Lee et al NIPS 2009]





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### **Computer vision features**



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## **Unsupervised learning of object-parts**



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Courtesy: Lee and Ng

## **Using ANN to learn hierarchical representation**



#### Good Representations are hierarchical

- In Language: hierarchy in syntax and semantics
  - Words->Parts of Speech->Sentences->Text
  - Objects, Actions, Attributes...-> Phrases -> Statements -> Stories
- In Vision: part-whole hierarchy
  - Pixels->Edges->Textons->Parts->Objects->Scenes



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# "Deep" learning: learning hierarchical representations



- Deep Learning: learning a hierarchy of internal representations
- From low-level features to mid-level invariant representations, to object identities
- Representations are increasingly invariant as we go up the layers
- Using multiple stages gets around the specificity/invariance dilemma



### Filtering+NonLinearity+Pooling = 1 stage of a Convolutional Net

- [Hubel & Wiesel 1962]:
  - simple cells detect local features
  - complex cells "pool" the outputs of simple cells within a retinotopic neighborhood.



### **Convolutional Network: Multi-Stage Trainable Architecture**



#### Hierarchical Architecture

Representations are more global, more invariant, and more abstract as we go up the layers

#### Alternated Layers of Filtering and Spatial Pooling

- Filtering detects conjunctions of features
- Pooling computes local disjunctions of features

#### Fully Trainable

All the layers are trainable



# **Convolutional Net Architecture for Hand-writing recognition**



Convolutional net for handwriting recognition (400,000 synapses)

- Convolutional layers (simple cells): all units in a feature plane share the same weights
- Pooling/subsampling layers (complex cells): for invariance to small distortions.
- Supervised gradient-descent learning using back-propagation
- The entire network is trained end-to-end. All the layers are trained simultaneously.
- □ [LeCun et al. Proc IEEE, 1998]



### **Training CNN: depth matters!**



- 21 Layers!
- Gradient vanishes when the network is too deep: Lazy to learn!
  - Add intermediate loss layers to produce error signals!
  - Do contrast normalization after each conv layer!
  - Use ReLU to avoid saturation!



### Training CNN: huge model, more data!





- Only 7 layers, 60M parameters!
- Need more labeled data to train!
- Data augmentation: crop, translate, rotate, add noise!



### Training CNN: highly nonconvex objective

Demand more advanced optimization techniques

Add momentum as we have done for NN

### • Learning rate policy

- decrease learning rate regularly!
- different layers use different learning rate!
- observe the trend of objective curve more often!
- Initialization really cares!
  - Supervised pretraining
  - Unsupervised pretraining



## **Training CNN: avoid overfitting**

More data are always the best way to avoid overfitting
 data augmentation

Add regualizations: recall what we have done for linear regression

Dropout





# Summary: artificial neural networks – what you should know

- Highly expressive non-linear functions
- Highly parallel network of logistic function units
- Minimizing sum of squared training errors
  - Gives MLE estimates of network weights if we assume zero mean Gaussian noise on output values
- Minimizing sum of sq errors plus weight squared (regularization)
  - MAP estimates assuming weight priors are zero mean Gaussian
- Gradient descent as training procedure
  - How to derive your own gradient descent procedure
- Discover useful representations at hidden units
- Local minima is greatest problem
- Overfitting, regularization, early stopping



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## Limitations

- Supervised Training
  - Need huge amount of labeled data, but label is scarce!
  - □ Pre-training, self-supervised training ...
- Slow Training
  - Train an AlexNet on a single machine need one week!
- Optimization
  - Highly nonconvex objective
- Parameter tuning is hard
  - The parameter space is so large...





#### Detailed Tutorial on Convolutional Neural Network

Some contents are borrowed from Rob Fergus, Yan Lecun and Stanford's course



Ordinary Neural Network





Figure courtesy, Fei-Fei, Andrej Karpathy



All Neural Net activations arranged in 3 dimensions



## For example, a CIFAR-10 image is a 32\*32\*3 volume: 32 width, 32 height, 3 depth (RGB)





## Local connectivity



image: 32 \* 32 \* 3 volume

before: full connectivity: 32 \* 32 \* 3 weights for each neuron

now: one unit will connect to, e.g. 5\*5\*3 chunk and only have 5\*5\*3 weights

Note the connectivity is:

- local in space
- full in depth



## Convolution

- One local region only gives one output
- Convolution: Replicate the column of hidden units across space, with some stride







- 7 \* 7 Input
- Assume 3\*3 connectivity, stride = 1

- Produce a map
- What's the size of the map?
  5 \* 5



## Convolution

- One local region only gives one output
- Convolution: Replicate the column of hidden units across space, with some stride



- 7 \* 7 Input
- Assume 3\*3 connectivity, stride = 1

• What if stride = 2?



## Convolution

- One local region only gives one output
- Convolution: Replicate the column of hidden units across space, with some stride







- 7 \* 7 Input
- Assume 3\*3 connectivity, stride = 1

• What if stride = 3?



## **Convolution: In Practice**

- Zero Padding
  - Input size: 7 \* 7
  - □ Filter Size: 3\*3, stride 1
  - Pad with 1 pixel border
  - Output size?
    - $\square$  7 \* 7 => preserved size!

0	0	0	0	0	0		
0							
0							
0							
0							



## **Convolution: Summary**

#### Zero Padding

- Input volume of size [W1 \* H1 \* D1]
- □ Using K units with receptive fields F x F and applying them at strides of S gives

Output volume: [W2, H2, D2]

- W2 = (W1 F)/S + 1
- H2 = (H1 F) / S + 1
- D2 =k



## **Convolution: Problem**

- □ Assume input [32 \* 32 \* 3]
- Gounits with receptive field 5 \* 5, applied at stride 1/pad 1
  - => Output volume: [30 \* 30 \* 30]
- At each position of the output volume, we need 5 \* 5 \* 3 weights => Number of weights in such layer: 27000 \* 75 = 2 million  $\otimes$

Idea: Weight sharing!

Learn one unit, let the unit convolve across all local receptive fields!



## **Convolution: Problem**

- □ Assume input [32 \* 32 \* 3]
- Gounits with receptive field 5 \* 5, applied at stride 1/pad 1
  - => Output volume: [30 \* 30 \* 30] = 27000 units

Weight sharing

- => Before: Number of weights in such layer: 27000 \* 75 = 2 million  $\otimes$
- => After: weight sharing: 30 \* 75 = 2250 ©

But also note that sometimes it's not a good idea to do weight sharing! When?

## **Convolutional Layers**

- Connect units only to local receptive fields
- Use the same unit weight parameters for units in each "depth slice" (i.e. across spatial positions)



computed with one set of weights

Can call the units "filters"

We call the layer convolutional because it is related to convolution of two signals

$$f[x,y] * g[x,y] = \sum_{n_1 = -\infty}^{\infty} \sum_{n_2 = -\infty}^{\infty} f[n_1,n_2] \cdot g[x-n_1,y-n_2]$$

Sometimes we also add a bias term b, y = Wx + b, like what we have done for ordinary NN

Short question: Will convolution layers introduce nonlinearity?



### **Stacking Convolutional Layers**



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

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## **Pooling Layers**

- In ConvNet architectures, Conv layers are often followed by Pool layers
  - makes the representations smaller and more manageable without losing too much information. Computes MAX operation (most common)





## **Pooling Layers**

In ConvNet architectures, Conv layers are often followed by Pool layers

 makes the representations smaller and more manageable without losing too much information. Computes MAX operation (most common)

□ Input volume of size [W1 x H1 x D1]

- Pooling unit receptive fields F x F and applying them at strides of S gives
- Output volume: [W2, H2, D1]: depth unchanged!

W2 = (W1-F)/S+1,H2 = (H1-F)/S+1

Short question: Will pooling layer introduce nonlinearity?


# Nonlinerity

□ Similar to NN, we need to introduce nonlinearity in CNN

- Sigmoid
- Tanh
- RELU: Rectified Linear Units -> preferred
  - Simplifies backpropagation
  - Makes learning faster
  - Avoids saturation issues





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### **Convolutional Networks: 1989**



 LeNet: a layered model composed of convolution and subsampling operations followed by a holistic representation and ultimately a classifier for handwritten digits. [LeNet ]

## **Convolutional Nets: 2012**





- + gpu
- + non-saturating nonlinearity
- + regularization

- AlexNet: a layered model composed of convolution, subsampling, and further operations followed by a holistic representation and all-in-all a landmark classifier on
- □ ILSVRC12. [AlexNet]



## **Convolutional Nets: 2014**



- □ ILSVRC14 Winners: ~6.6% Top-5 error

  - VGG: 16 layers of 3x3 convolution interleaved with max pooling + 3 fully-connected layers

### Training CNN: Use GPU

- Convolutional layers
  - Reduce parameters BUT Increase computations





#### **Visualize and Understand CNN**



A CNN transforms the image to 4096 numbers that are then linearly classified.



#### Visualize and Understand CNN

lemon

bell pepper

• Find images that maximize some class score:

husky



goose

limousine

ostrich



