

# CSCE 633: Machine Learning

Lecture 8



# Overview

- Deep neural networks
  - Motivation & Challenges
  - Unsupervised pretraining: Deep belief networks & autoencoders
  - (Supervised) fine-tuning
  - Alternative optimization methods
  - Convolutional neural networks
  - Recurrent neural networks
  - Long short term memory neural networks

[Contents of the following slides have been summarized from the NIPS 2010 & CVPR 2012 Deep Learning

Tutorials, and the Stanford CS231 class by Drs. Li, Johnson, & Yeung]



# Overview

- Deep neural networks
  - Motivation & Challenges
  - •
  - •
  - •
  - •
  - •
  - •







# Deep Learning

Specialized components, domain knowledge required



- End-to-end learning
- Richer solution space







- Deep Representations might allow for a hierarchy or representation
  - Non-local generalization
  - Comprehensibility
- Multiple levels of latent variables allow combinatorial sharing of statistical strength
- Deep architectures work well (vision, audio, NLP, etc.)!



- Learn features from data
- Use differentiable functions that produce features efficiently
- End-to-end learning: no distinction between feature extractor and classifier
- "Deep" architectures: cascade of simpler non-linear modules



- Natural progression from low level to high level structure as seen in natural complexity
- Easier to monitor what is being learnt and to guide the machine to better subspaces
- A good lower level representation can be used for many distinct tasks

#### Feature representation



3rd layer "Objects"



2nd layer "Object parts"



1st layer "Edges"



Pixels



- Multi-task learning
- Unsupervised training





# Deep neural networks: Challenges

- Memory is used to store input data, weight parameters and activations as an input propagates through the network
- Activations from a forward pass must be retained until they can be used to calculate the error gradients in the backwards pass
- Example: 50-layer neural network
  - 26 million weight parameters, 16 million activations in the forward pass
  - 168MB memory (assuming 32-bit float)

Parallelize computations with GPU (graphics processing units)



# Deep neural networks: Challenges

- Deep networks trained with backpropagation (without unsupervised pretraining) perform worse than shallow networks
- Gradient is progressively getting more dilute
  - Weight correction is minimal after moving back a couple of layers
- High risk of getting "stuck" to local minima
- In practice, a small portion of data is labelled

# Perform pretraining to mitigate this issue

Example error rates with and without pretraining

	train.	valid.	test
DBN, unsupervised pre-training	0%	1.2%	1.2%
Deep net, auto-associator pre-training	0% 0	1.4%	1.4%
Deep net, supervised pre-training	0	1.7%	-2.0%
Deep net, no pre-training	.004%	-2.1%	-2.4%
Shallow net, no pre-training	.004%	1.8%	1.9%

(Bengio et al., NIPS 2007)



# Overview

- Deep neural networks
  - •
  - Unsupervised pretraining: Deep belief networks & autoencoders
  - ٠
    - •
  - •
  - •
  - •



- This idea came into play when research studies found that a DNN trained on a particular task (e.g. object recognition) can be applied on another domain (e.g. object subcategorization) giving state-of-the-art results
- 1st part: Greedy layer-wise unsupervised pre-training
  - Each layer is pre-trained with an unsupervised learning algorithm
  - Learning a nonlinear transformation that captures the main variations in its input (the output of the previous layer)
- 2nd part: Supervised fine-tuning
  - The deep architecture is fine-tuned with respect to a supervised training criterion with gradient-based optimization
- We will examine the deep belief networks and stacked autoencoders

Unusual form of regularization: minimizing variance and introducing bias towards configurations of the parameter space that are useful for unsupervised learning





[Source: Erhan et al., 2010]



- Pretraining is implemented by stacking several layers of Restricted Boltzmann Machines (RBM) in a greedy manner
- Assuming joint distribution between hidden  $h_i$  and observed variables  $x_j$  with parameters  $\mathbf{W}, \mathbf{b}, \mathbf{c}$  $P(\mathbf{x}, \mathbf{h}) \propto \exp(\mathbf{h}^T \mathbf{W} \mathbf{x} + \mathbf{b}^T \mathbf{x} + \mathbf{c}^T \mathbf{h})$  $P(\mathbf{x}|\mathbf{h}) = \prod_j P(x_j|\mathbf{h}), P(x_j = 1|\mathbf{h}) = \operatorname{sigmoid}(b_j + \sum_i W_{ij}h_i)$  $P(\mathbf{h}|\mathbf{x}) = \prod_i P(h_i|\mathbf{x}), P(h_i = 1|\mathbf{x}) = \operatorname{sigmoid}(c_i + \sum_j W_{ij}x_j)$
- RBM trained by approximate stochastic gradient descent
- This representation is extended to all hidden layers
- The RBM parameters correspond to the parameters of the feed-forward multi-layer neural network



- Step 1: Construct an RBM with an input and hidden layer and train to find  $\boldsymbol{W}^{(1)}$
- Step 2: Stack another hidden layer on top of the RBM to form a new RBM
  - Fix  $W^1$ . Assume  $h^{(1)}$  as input. Train to find  $W^{(2)}$ .
- Step 3: Continue to stack layers and find weights  $\mathbf{W}^{(3)}$ , etc.





- Unsupervised algorithm that tries to learn an approximation of the identity function  $h_{\mathbf{W},\mathbf{b}}(x)\approx\mathbf{x}$
- Trivial problem unless we place constraints on the network, such as by limiting the number of hidden units, we can discover interesting structure about the data

e.g. if some of the input features are correlated, then this algorithm will be able to discover some of those correlations



• 
$$\alpha_j^{(i)} = f(W_{i1}^{(1)}x_1 + W_{i2}^{(1)}x_2 + \ldots + b_i^{(1)})$$

- Trained using back-propagation and additional sparsity constraints
- Can be also used for feature transformation

[http://ufldl.stanford.edu/wiki/index.php/Autoencoders\_ and\_Sparsity]







- Capture a "hierarchical grouping" of the input
- First layer learns a good representation of input features (e.g. edges)
- Second layer learns a good representation of the patterns in the first layer (e.g. corners), etc.

http://ufldl.stanford.edu/wiki/index.php/Stacked\_Autoencoders



# Overview

- Deep neural networks
  - •
  - •
  - (Supervised) fine-tuning
  - •
  - •
  - •
  - •



# Deep neural networks: Fine-tuning

- Taking advantage of labelled data from large (publicly available) datasets, e.g., VGG16
- Tweak the parameters of an already trained network so that it adapts to the new task at hand
- Initial layers  $\rightarrow$  learn general features
- Last layers  $\rightarrow$  learn features more specific to the task of interest
- Fine-tuning freezes the first layers, and relearns weights from the last





# Overview

- Deep neural networks
  - •
  - •
  - •
  - Alternative optimization methods
  - •
  - •
  - •



- $\bullet\,$  Gradient becomes zero as we increase the # layers
- Local optima and saddle points become more common in high dimensions







- Movement through the parameter space is averaged over multiple time steps
- Momentum speeds up movement along directions of strong improvement (loss decrease) and also helps the network avoid local minima

# SGDSGD+Momentum $x_{t+1} = x_t - \alpha \nabla f(x_t)$ $v_{t+1} = \rho v_t + \nabla f(x_t)$ $x_{t+1} = x_t - \alpha v_{t+1}$

```
while True:
dx = compute_gradient(x)
x += learning_rate * dx
```

```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x += learning rate * vx
```

- Build up "velocity" as a running mean of gradients
- Rho gives "friction"; typically rho=0.9 or 0.99



# Issue with noisy trajectories that diverge from optima \$G\$ radient Noise\$





- Gradient term is not computed from current parameter position x<sub>t</sub>
- Gradient term is computed using the current position and momentum x<sub>t</sub> + ρv<sub>t</sub>
- While the gradient term always points in the right direction, the momentum term may not
- If the momentum term points in the wrong direction or overshoots, the gradient can still "go back" and correct it in the same update step.

 $\label{eq:constraints} \fboxlabel{eq:constraints} \fboxlabel{eq:constraints} \fboxlabel{eq:constraints} \fboxlabel{eq:constraints} \vspace{-1.5} \vspac$ 







# Added element-wise scaling of the gradient based on the historical sum of squares in each dimension









# Combination of RMSProp and Momentum

first moment =	
second moment =	
while ";	
dx = compute gradient(x)	
first moment = beta1 ' first moment → ( - beta1) ' dx	
second moment = beta2 ' second moment + (i - beta2) ' dx ' dx	
<pre>x ++&gt; learning rate * first moment / (np.sqrt(second moment) + * * ))</pre>	AdaGrad / RIVISProp







- Gradient term is not computed from current parameter position x<sub>t</sub>
- Gradient term is computed using the current position and momentum x<sub>t</sub> + ρv<sub>t</sub>
- While the gradient term always points in the right direction, the momentum term may not
- If the momentum term points in the wrong direction or overshoots, the gradient can still "go back" and correct it in the same update step.

 $\begin{bmatrix} v_{t+1} = \rho v_t - \alpha \nabla f(\overline{x_t + \rho v_t}) \\ x_{t+1} = x_t + v_{t+1} \end{bmatrix} \qquad \begin{array}{l} \text{Annoying, usually we want} \\ \text{update in terms of } x_t, \nabla f(x_t) \\ \text{Change of variables } \tilde{x}_t = x_t + \rho v_t \text{ and} \\ \hline v_{t+1} = \rho v_t - \alpha \nabla f(\tilde{x}_t) \\ \tilde{x}_{t+1} = \tilde{x}_t - \rho v_t + (1 + \rho) v_{t+1} \\ = \tilde{x}_t + v_{t+1} + \rho (v_{t+1} - v_t) \\ \end{array} \\ \begin{array}{l} \text{dx = compute gradient(x)} \\ \text{old } v = v \\ v = \text{rho } v - \text{ilearning rate } \text{dx} \\ v = v \text{ old } v + (1 + rho) \text{ vy} \\ v = \text{rho } v - \text{ilearning rate } \text{dx} \\ \end{array}$ 



- Adam is a good default choice
- A more informed selection of the optimization method can be done through hyper-parameter tuning



# Overview

- Deep neural networks
  - •
  - •
  - •
  - •
  - Convolutional neural networks
  - •



# **Convolutional neural networks**

- Similar to regular neural networks
  - made up of neurons, each with an input and an activation function
  - have weights and biases to be learned
  - have a loss function on the last (fully-connected) layer
- Explicit assumption that the inputs are images
  - vastly reduce the amount of parameters in the network




- Grayscale image (1-channel)
  - 2d-matrix
  - each pixel ranges from 0 to 255 0: black, 255: white
- Color image (3-channel, RGB)
  - three 2d-matrices stacked over each other
  - each with pixel values ranging between 0 and 255









- 1000  $\times$  1000 image, 1M hidden units  $\rightarrow$  10^{12} parameters
- Since spatial correlation is local, we can significantly simplify this





- 1000  $\times$  1000 image, 1M hidden units, 10  $\times$  10 filter size  $\rightarrow$  10  $^8$  parameters
- Since spatial correlation is local, we can significantly simplify this



- Stationarity: Statistics are similar at different locations
- Share the same parameters across different locations







- Let us assume filter is an "eye" detector
- How can we make the detection robust to the exact location of the eye?
- By pooling (e.g., max or average) filter responses at different locations we gain robustness to the exact spatial location of features



- Convolution is the mathematical operation that implements filtering
- Given an input image x[m, n] and an impulse response h[m, n] (filter or kernel), the convolution output can be written as

$$y[m, n] = x[m, n] * h[m, n] = \sum_{j=-\infty}^{\infty} \sum_{i=-\infty}^{\infty} x[i, j]h[m-i, n-j]$$



http://www.songho.ca/dsp/convolution/convolution2d\_example.html





$$\begin{split} & [0,0] = x[-1,-1] \cdot h[1,1] + x[0,-1] \cdot h[0,1] + x[1,-1] \cdot h[-1,1] \\ & + x[-1,0] \cdot h[1,0] + x[0,0] \cdot h[0,0] + x[1,0] \cdot h[-1,0] \\ & + x[-1,1] \cdot h[1,-1] + x[0,1] \cdot h[0,-1] + x[1,1] \cdot h[-1,-1] \\ & = 0 \cdot 1 + 0 \cdot 2 + 0 \cdot 1 + 0 \cdot 0 + 1 \cdot 0 + 2 \cdot 0 + 0 \cdot (-1) + 4 \cdot (-2) + 5 \cdot (-1) = -13 \end{split}$$

$$\begin{split} y_1(1,0] &= x_1^*(0,-1) \cdot b_1(1,1] + x_1(1,-1) \cdot b_1(0,1] + x_1^*(2,-1) \cdot b_1(-1,1] \\ &+ x_1^*(0,0) \cdot b_1(1,0] + x_1(1,0) \cdot b_1(0,0) + x_1^*(2,0) \cdot b_1(-1,0] \\ &+ x_1^*(0,1) \cdot b_1(1,-1) + x_1(1,1) \cdot b_1(0,-1) + x_1(2,1) \cdot b_1(-1,-1] \\ &= 0 \cdot 1 + 0 \cdot 2 + 0 \cdot 1 + 1 \cdot 0 + 2 \cdot 0 + 3 \cdot 0 + 4 \cdot (-1) + 5 \cdot (-2) + 6 \cdot (-1) = -20 \end{split}$$





https://cs231n.github.io/assets/conv-demo/index.html









H

0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
0	0	0	90	90	90	90	90	0	0
0	0	0	90	90	90	90	90	0	0
0	0	0	90	90	90	90	90	0	0
0	0	0	90	0	90	90	90	0	0
0	0	0	90	90	90	90	90	0	0
0	0	0	0	0	0	0	0	0	0
0	0	90	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0
$\overline{F}$									

0	10	20	30	30	30	20	10	
0	20	40	60	60	60	40	20	
0	30	60	90	90	90	60	30	
0	30	50	80	80	90	60	30	
0	30	50	80	80	90	60	30	
0	20	30	50	50	60	40	20	
10	20	30	30	30	30	20	10	
10	10	10	0	0	0	0	0	

G





Original

Identical image





Original

	0	0	0	
<	1	0	0	
	0	0	0	



Shifted left By 1 pixel





Blur (with a mean filter)





Original

Sharpening filter (accentuates edges)





before

after













https://www.nervanasys.com/convolutional-neural-networks/

Also check:

http://cs231n.github.io/assets/conv-demo/index.html

https://ujjwalkarn.me/2016/08/11/intuitive-explanation-convnets/ (figure 6)



- Depth: the number of filters we use for the convolution operation
- Stride: the number of pixels by which we slide our filter matrix over the input
- Zero-padding: padding the input matrix with zeros around the border, so that we can apply the filter to bordering elements of our input image matrix





MAX POOL2

Max POOL3

Assuming no zero-padding and weight sharing throughout the entire image



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images

First layer (CONV1): 96 11x11 filters applied at stride 4 =>

Q: what is the output volume size? Hint: (227-11)/4+1 = 55



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images

First layer (CONV1): 96 11x11 filters applied at stride 4 => Output volume [55x55x96]

Q: What is the total number of parameters in this layer?



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images

First layer (CONV1): 96 11x11 filters applied at stride 4 => Output volume [55x55x96] Parameters: (11\*11\*3)\*96 = 35K



#### Convolutional neural networks: Max-pooling

- Reduces the dimensionality of each feature map but retains the most important information
- Can be of different types: Max, Average, Sum etc.
- Makes the input representations (feature dimension) smaller and more manageable
- Promotes an almost scale invariant representation of the image



**Rectified Feature Map** 



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images After CONV1: 55x55x96

Second layer (POOL1): 3x3 filters applied at stride 2

Q: what is the output volume size? Hint: (55-3)/2+1 = 27



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images After CONV1: 55x55x96

Second layer (POOL1): 3x3 filters applied at stride 2 Output volume: 27x27x96

Q: what is the number of parameters in this layer?



Case Study: AlexNet

[Krizhevsky et al. 2012]



Input: 227x227x3 images After CONV1: 55x55x96

Second layer (POOL1): 3x3 filters applied at stride 2 Output volume: 27x27x96 Parameters: 0!



### Convolutional neural networks: Final fully connected layer

- Traditional multilayer perceptron
- Yields the classification/regression result





#### Convolutional neural networks: Putting it all together

- Step 1: Initialize weights
- Step 2: Take first image as input and go through the forward propagation step (convolution, ReLU and pooling operations along with forward propagation in the fully connected layer) and finds the output probabilities for each class
- Step 3: Calculate the total error at the output layer
- **Step 4**: Use backpropagation to update the weights, which are adjusted in proportion to their contribution to the total error
- Step 5: Repeat Steps 1-4 for all train images



Feature Extraction from Image

Classification











### Convolutional neural networks: Hyperparameter tuning

- Learning rate: how much to update the weight during optimization
- Number of epochs: number of times the entire training set pass through the neural network
- Batch size: the number of samples in the training set for weight update
- Activation function: the function that introduces non-linearity to the model (e.g. sigmoid, tanh, ReLU, etc.)
- Number of hidden layers and units
- Weight initialization: e.g., uniform distribution
- Dropout for regularization: probability of dropping a unit
- Optimization method: optimization method to learn the weights (e.g., Adam, RMSProp)

We can perform or search over all parameters



## Overview

- Deep neural networks
  - • • Recurrent neural networks

[The content for the following slides has been summarized from Li, Johnson, & Yeung, Stanford CSCE 231]



#### Recurrent neural networks: Motivation

- Networks with feedback loops (recurrent edges)
- Output at current time step depends on current input as well as previous state (via recurrent edges)



- one-to-one: e.g., image classification (image  $\rightarrow$  user ID)
- one-to-many: e.g., image captioning (image  $\rightarrow$  sequence of words)
- many-to-one: e.g., sentiment classification (sequence of words  $\rightarrow$  emotion)
- many-to-many: e.g., machine translation (e.g., sequence of words → sequence of words)



### Recurrent neural networks: Representation

We can process a sequence of vectors **x** by applying a **recurrence formula** at every time step:





The same function and the same set of parameters are used at every time step



### Recurrent neural networks: Representation

The state consists of a single "hidden" vector h:

1



$$egin{aligned} h_t &= f_W(h_{t-1}, x_t) \ &dots \ &dots\ \ &dots \ &dots \ &dots \ &dots \ &dots \ &d$$



#### Recurrent neural networks: Representation



The same function and the same set of parameters are used at every time step.


### Recurrent neural networks: Representation





#### Recurrent neural networks: Representation

## Character-level language model During training: learning sequence of characters





#### **Recurrent neural networks: Representation**

Character-level language model During testing: sample characters feed back to model one at a time









# Truncated Backpropagation through time



Run forward and backward through chunks of the sequence instead of whole sequence



# Truncated Backpropagation through time



Carry hidden states forward in time forever, but only backpropagate for some smaller number of steps



# Truncated Backpropagation through time





# Text generation THE SONNETS

#### by William Shakespeare

From Laters conducts we observe the control thereby boardy, one might never the, Bias as the riper should by time decrase. His scheck here might board has a server been board on the strength of the scheck and the scheck here and the scheck and the scheck and decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the decrases and the scheck and the scheck and the scheck and the decrases and the scheck and the scheck and the scheck and the decrases and scheck and the scheck and the scheck and the decrases and scheck and the scheck and the scheck and the decrases and scheck and the scheck and t

When forty winters shall heaving thy hms, And ing deep trents in the bearty's field. Thy youth's panal levery so gared on nose, Will be a latted weet of sound voorth hedre. Where all the transmer of thy histy days. The same that the transmer of the histy days. Where and all-outing dame, and thirtfless paids. It hous coulds answer "This fair child of mine Shall sum any communic entropy" has the child of mine Additional the transmer of the transfer entropy. It hous coulds answer "This fair child of mine Shall sum any communic entropy has the transfer in the seven in the new mark when those at thi. And we only block sums then those at the top of the transfer.





#### Text generation

at first: tyntd-iafhatawiaoihrdemot lytdws e ,tfti, astai f ogoh eoase rrranbyne 'nhthnee e plia tklrgd t o idoe ns,smtt h ne etie h,hregtrs nigtike,aoaenns lng

train more

"Tmont thithey" fomesscerliund Keushey. Thom here sheulke, anmerenith ol sivh I lalterthend Bleipile shuwy fil on aseterlome coaniogennc Phe lism thond hon at. MeiDimorotion in ther thize."

#### train more

Aftair fall unsuch that the hall for Prince Velzonski's that me of her hearly, and behs to so arwage fiving were to it beloge, pavu say falling misfort how, and Gogition is so overelical and ofter.

#### train more

"Why do what that day," replied Natasha, and wishing to himself the fact the princess, Princess Mary was easier, fed in had oftened him. Pierre aking his soul came to the packs and drove up his father-in-law women.



#### Music generation



Music and Art Generation using Machine Learning | Curtis Hawthorne | TEDxMountainViewHighSchool

https://www.youtube.com/watch?v=Q-Qq8ipUHEI



Image captioning



Explain Images with Multimodal Recurrent Neural Networks, Mao et al.

Deep Visual-Semantic Alignments for Generating Image Descriptions, Karpathy and Fei-Fei Show and Tell: A Neural Image Caption Generator, Vinyals et al.

Long-term Recurrent Convolutional Networks for Visual Recognition and Description, Donahue et al. Learning a Recurrent Visual Representation for Image Caption Generation, Chen and Zitnick



Image captioning



# **Recurrent Neural Network**







## Image captioning

# Image Captioning: Example Results



A cat sitting on a suitcase on the floor



A cat is sitting on a tree branch



A dog is running in the grass with a frisbee



A white teddy bear sitting in the grass



Two people walking on the beach with surfboards



A tennis player in action on the court



Two giraffes standing in a grassy field



A man riding a dirt bike on a dirt track



Vanilla RNN Gradient Flow

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994 Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013





# Vanilla RNN Gradient Flow

Bengio et al, "Learning long-term dependencies with gradient descent is difficult", IEEE Transactions on Neural Networks, 1994 Pascanu et al, "On the difficulty of training recurrent neural networks", ICML 2013





# Overview

- Deep neural networks
  - •
  - Long short term memory neural networks

[The content for the following slides has been summarized from

https://colah.github.io/posts/2015-08-Understanding-LSTMs/]



A memory consists of an explicit memory and gating units which regulate the information flow into and out of the memory. RNN:



LSTM:





The cell state represents the memory of the network. The LSTM removes or adds information to the cell state, regulated by structures called gates.





Decides what information we will throw away from the previous cell state via a sigmoid function.



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



Decides what information from the current state we will store to the cell state. The sigmoid determined which input elements that will be updated. The *tanh* determines the new candidate values.



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



Update cell state based on the forget gate and input



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$



Provides an output based on the updated cell state and the current input.



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$



### What have we learnt so far

- DNNs allow hierarchical representations learned from raw data
- Challenges in terms of training  $\rightarrow$  pretraining
  - deep belief networks
  - autoencoders
- Convolutional neural networks  $\rightarrow$  image
  - convolution: local image properties
  - weight sharing: stationarity
  - max-pooling: robustness in the representation and reduced cost
- Additional links https://cs231n.github.io/convolutional-networks/