# Statistical Machine Learning (BE4M33SSU) <br> Lecture 8: Deep Neural Networks 

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## Overview

Topics covered in the lecture:

- Deep Architectures
- Convolutional Neural Networks (CNNs)
- Transfer learning
- Weight initialization
- Autoencoders and unsupervised pre-training


## Why Deep Architectures?

- Is it better to use deep architectures rather than the shallow ones for complex nonlinear mappings?
- We know that deep architectures evolved in Nature (e.g., cortex)
- Universal approximation theorem: one layer is enough so why to bother with more layers?
- Poggio et al: Why and When Can Deep - but Not Shallow - Networks Avoid the Curse of Dimensionality, 2016:
- deep networks can be exponentially better (have less units) than shallow networks for learning compositional functions
- Handcrafted features vs. automatic extraction
- Gradually increasing complexity, intermediate representations: each successive layer brings higher abstraction


## Processing Images

- Topographical mapping in the visual cortex - nearby cells represent nearby regions in the visual field
- Input: grayscale image $32 \times 32$ pixels
- Output: layer of $32 \times 32$ features
- How many parameters do we need when input and output is fully connected?



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$$
\underset{\text { outputs }}{32^{2}} \times\left(\underset{\text { inputs }}{32^{2}}+\underset{\text { biases }}{1}\right) \approx 1 \mathrm{M}
$$



## Locally Connected Layer

- Each neuron has a receptive field of $3 \times 3$ pixels
- It is fully connected only to the corresponding set of 9 inputs
- How many parameters do we need now?



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$\underset{\text { outputs }}{30^{2}} \times\left(\underset{\text { inputs }}{3^{2}}+\underset{\text { bias }}{1}\right)=9 \mathrm{k}$



## Multiple Input Channels

- We can have more input channels, e.g., colors
- Now the input is defined by width, height and depth: $32 \times 32 \times 3$

The number of parameters is $30^{2} 3 \times(\underset{\text { chatputs }}{3} \times \underset{\text { inputs }}{3}+\underset{\text { bias }}{1}) \approx 25 \mathrm{k}$


## Sharing Parameters

- We can further reduce the number of parameters by sharing weights
- Use the same set of weights and bias for all outputs, define a filter
- The number of parameters drops to $\underset{\text { inputs }}{ } \times 3^{2}+\underset{\text { bias }}{1}=28$
- Translation equivariance



## Multiple Output Channels

- Extract multiple different of features
- Use multiple filters to get more feature maps
- For 4 filters we have $\underset{\text { filters }}{4} \times\left(\underset{\text { inputs }}{ } \times 3^{2}+\underset{\text { bias }}{1}\right)=112$ parameters

This is the convolutional layer

- Processes volume into volume


1D convolution with no bias, single input channel and filter size $F$ :

$$
\begin{array}{ll}
z_{i^{\prime}} & =\sum_{i=1}^{F} w_{i} x_{i^{\prime}+(i-1)} \\
\text { correlations (similarity) } \\
z_{i^{\prime}} & =\sum_{i=1}^{F} \bar{w}_{i} x_{i^{\prime}-(i-F)} \\
\text { convolution }
\end{array}
$$

where $\overline{\boldsymbol{w}}$ is a reverse of $\boldsymbol{w}\left(\bar{w}_{i}=w_{F-i+1}\right)$ and $i \in\{1, \ldots, N-F+1\}$ for the input size $N$


## Convolution in 2D: Example

- Input volume $5 \times 5 \times 3$, single $3 \times 3$ filter, $3 \times 3^{2}+1=28$ parameters



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## Convolution in 2D: Example

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## Convolution in 2D: Forward Message



$$
z_{k l d}=f_{k l d}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{b})=b_{d}+\sum_{i=1}^{F} \sum_{j=1}^{F} \sum_{c=1}^{C} x_{k+i-1, l+j-1, c} w_{i j c d}
$$

## Convolution in 2D: Parameter Gradient


$z_{k l d}=f_{k l d}(\boldsymbol{x}, \boldsymbol{w}, \boldsymbol{b})=b_{d}+\sum_{i=1}^{F} \sum_{j=1}^{F} \sum_{c=1}^{C} x_{k+i-1, l+j-1, c} w_{i j c d}$

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial w_{i j c d}} & =\sum_{k^{\prime}, l^{\prime}, d^{\prime}} \frac{\partial \mathcal{L}}{\partial f_{k^{\prime}, l^{\prime}, d^{\prime}}} \frac{\partial f_{k^{\prime}, l^{\prime}, d^{\prime}}}{\partial w_{i j c d}}=\sum_{k^{\prime}, l^{\prime}, d^{\prime}} \delta_{k^{\prime}, l^{\prime}, d^{\prime}}^{l+1} \frac{\partial f_{k^{\prime}, l^{\prime}, d^{\prime}}}{\partial w_{i j c d}}= \\
& =\sum_{k^{\prime}, l^{\prime}} \delta_{k^{\prime}, l^{\prime}, d}^{l+1} x_{k^{\prime}+i-1, l^{\prime}+j-1, c}
\end{aligned}
$$

## Convolution in 2D: Backward Message



Substitute $m=k+i-1$ and $n=l+j-1$

$$
\begin{aligned}
\delta_{m n c}^{l} & =\frac{\partial \mathcal{L}}{\partial x_{m n c}}=\sum_{k^{\prime}, l^{\prime}, d^{\prime}} \delta_{k^{\prime}, l^{\prime}, d^{\prime}}^{l+1} \frac{\partial f_{k^{\prime}, l^{\prime}, d^{\prime}}}{\partial x_{m n c}} \\
& =\sum_{k^{\prime}, l^{\prime}, d^{\prime}} \delta_{k^{\prime}, l^{\prime}, d^{\prime}}^{l+1} w_{m-k^{\prime}+1, n-l^{\prime}+1, c, d^{\prime}}
\end{aligned}
$$

## Stride

- Stride hyper parameter, typically $S \in\{1,2\}$
- Higher stride produces smaller output volumes spatially

$S=2$



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- Higher stride produces smaller output volumes spatially

$S=2$



## Zero Padding

- Convolutional layer reduces the spatial size of the output w.r.t. the input
- For many layers this might be a problem

This is often fixed by zero padding the input
The size of the zero padding is denote $P$

| $P=1, S=1$ |  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 0 | 0 | 0 | 0 | 0 |
| 0 |  |  |  |  | 0 |
| 0 |  |  |  |  | 0 |
| 0 |  |  |  |  | 0 |
| 0 |  |  |  |  | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 |


|  |  |  |  |  |
| :--- | :--- | :--- | :--- | :--- |

## Convolutional Layer Summary

- Input volume: $W_{\text {input }} \times H_{\text {input }} \times C$
- Output volume: $W_{\text {output }} \times H_{\text {output }} \times D$
- Having $D$ filters:
- receptive field of $F \times F$ units,
- stride $S$
- zero padding $P$

$$
\begin{aligned}
W_{\text {output }} & =\left(W_{\text {input }}-F+2 P\right) / S+1 \\
H_{\text {output }} & =\left(H_{\text {input }}-F+2 P\right) / S+1
\end{aligned}
$$

- Needs $F^{2} C D$ weights and $D$ biases
- The number of activations and $\delta$ s to store: $W_{\text {output }} \times H_{\text {output }} \times D$


## Convolution Applied to an Image

mp
18/46


Filters of the first layer


Krizhevsky, Sutskever, Hinton: ImageNet Classification with Deep Convolutional Neural Networks, 2012

http://cs231n.github.io/convolutional-networks/

## Convolutional Layer: Nonlinearities

- In most cases a nonlinearity (sigmoid, tanh, ReLU) is applied to the outputs of the convolutional layer

Example: ReLU units


## Max Pooling

- Reduces spatial resolution $\rightarrow$ less parameters $\rightarrow$ helps with overfitting
- Introduces translation invariance
- Depth is not affected
$F=2, S=2$

| 2 | 2 | 0 | 4 | 3 | 4 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 0 | 5 | 0 | 4 | 1 |
| 4 | 5 | 2 | 5 | 1 | 4 |
| 5 | 2 | 1 | 0 | 2 | 1 |
| 2 | 3 | 3 | 3 | 5 | 3 |
| 0 | 3 | 0 | 4 | 0 | 1 |


| 2 | 5 | 4 |
| :--- | :--- | :--- |
| 5 | 5 | 4 |
| 3 | 4 | 5 |

- No changes to the depth
- Forward message: $z_{k l}=f_{k l}(\boldsymbol{x})=\max _{(i, j) \in \Omega(k, l)} x_{i j}$
- Backward message:

$$
\delta_{i j}^{l}=\sum_{k^{\prime}, l^{\prime}} \delta_{k^{\prime} l^{\prime}}^{l+1} \frac{\partial f_{k^{\prime} l^{\prime}}}{\partial x_{i j}}=\sum_{k^{\prime}, l^{\prime}} \delta_{k^{\prime} l^{\prime}}^{l+1} \mathbb{I}\left\{(i, j)=\underset{\left(i^{\prime}, j^{\prime}\right) \in \Omega\left(k^{\prime}, l^{\prime}\right)}{\operatorname{argmax}} x_{i^{\prime} j^{\prime}}\right\}
$$

- Backward message propagates only for the selected max unit



## Convolutional vs. Fully-Connected Layers

- Convolutional layer can be simply transformed to a Fully-connected layer $\rightarrow$ sparse weight matrix

The other direction is also possible:
FC layer of $D$ units following a $F \times F \times C$ convolutional layer can be replaced by a $1 \times 1 \times D$ convolutional layer using $F \times F$ filters $(P=0$, $S=1$ )

## Fully-Connected Layer to Convolutional Example



## Fully-Connected Layer to Convolutional Example



## Fully-Connected Layer to Convolutional Example



CONV, MP layers

$12 \times 12 \times 512$


- Use zero padding to preserve the spatial resolution
- Reduce the resolution only by means of max pooling
- Prefer image size with factorization containing higher power of 2 for pooling with $F=2$ (e.g., $224=2^{5} \times 7$ for ImageNet networks)
- Set the number of filters to powers of 2 (optimization)
- Read Andrej Karpathy's blog and see his course on CNNs http://cs231n.stanford.edu/


## LeNet-5 (1998)

- Yann LeCun
- CNN for written character recognition dataset MNIST
- Training set 60,000 , testing set 10,000 examples


LeCun et al.: Gradient-based learning applied to document recognition, 1998

## Errors by LeNet-5

- 82 errors (current best 21)

Human error expected to be between 20 to 30


LeCun et al.: Gradient-based learning applied to document recognition, 1998

## ImageNet Dataset

- Dataset of high-resolution color images: 15M training examples, 22k classes
- ImageNet Large Scale Visual Recognition Challenge (ILSVRC) uses subset of the ImageNet: 1.3 M training, 50 k validation, 100 k testing samples, 1000 classes


(a) Siberian husky

(b) Eskimo dog


## AlexNet 2012

- Two separate streams for 2 GPUs, 60M parameters
- Data augmentation (increasing dataset size): $224 \times 224$ patches (+ mirrored) of $256 \times 256$ original images, altering RGB intensities
- Uses ReLU and dropout
- Top five error $18.2 \%$ for the basic net decreased to $15.4 \%$ for an ensemble of 7 CNNs, pre-CNN best was $25.6 \%$




Krizhevsky et al.: ImageNet Classification with Deep Convolutional Neural Networks, 2012

## ZFNet 2013

- Smaller filters for the first convolutional layer CONV1: $7 \times 7, S=2$ instead of $11 \times 11, S=4$
- CONV3-5: more depth
- Top five error $16.5 \%, 14.8 \%$ for an ensemble of 6 CNN



## VGGNet 2014

- Simonyan, Zisserman: Very Deep Convolutional Networks for Large-Scale Image Recognition, 2014
- Simplification: lowering filter spatial resolution $(F=3, S=1, P=1)$, increasing depth
- A sequence of $3 \times 3$ filters can emulate a single large one Top five error $7.3 \%, 6.8 \%$ for an ensemble of 2 CNNs



## GoogLeNet 2014

- Use of inception layers instead of pure convolutional ones
- Fully connected output layer preceded by the global average pooling: the last layer before average pooling has $7 \times 7 \times 1024$ it is spatially reduced to $1 \times 1 \times 1024$
- Only 5M parameters (60M AlexNet)
- Auxiliary classifiers: their losses are added with discount weight
- Top five error $6.7 \%$



## ResNet 2015

- He et al.: Deep Residual Learning for Image Recognition, 2015
- 152 layers (2-3 weeks on 8 GPUs)
- Using skip connections
- Batch normalization instead of dropout
- Top five error $3.6 \%$ (human performance $5.1 \%$ expected)


## CNNs for Natural Language Processing (NLP)



## Transfer Learning

- Idea: use an existing model as a base to solve a similar problem
- Often used when not enough data available to solve the target problem directly
- Example: reuse an ImageNet network for object localization



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- Often used when not enough data available to solve the target problem directly
- Example: reuse an ImageNet network for object localization
- You can:
- cut the original network at various layers,
- fix or not the weights of the original network or use different learning rates
- use different type of model for the head, e.g., linear SVM


## Parameter Initialization

- Is it a good idea to set all weights to zero?


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- Is it a good idea to set all weights to zero?
- No. All neurons would behave the same: the same $\delta$ s are backpropagated. We need to break the symmetry
- Use small numbers, e.g., sample from a Gaussian distribution with zero mean:
- works well for shallow networks,
- for deep networks it is not a good idea


## Gaussian Initialization

- MLP, ten tanh layers, 500 units each. Each input fed with $\mathcal{N}(0,1)$
- Weights initialized to $\mathcal{N}\left(0, \sigma^{2}\right)$



## Xavier Initialization

- Glorot and Bengio: Understanding the difficulty of training deep feedforward neural networks, 2010
- For the linear neuron $s=\sum_{i} w_{i} x_{i}$, let $w_{i}$ and $x_{i}$ be independent random variables, $w_{i}$ and $x_{i}$ are i.i.d., $E\left(x_{i}\right)=E\left(w_{i}\right)=0$ :

$$
\begin{aligned}
\operatorname{Var}(s) & =\operatorname{Var}\left(\sum_{i} w_{i} x_{i}\right)=\sum_{i} \operatorname{Var}\left(w_{i} x_{i}\right)= \\
& =\sum_{i}\left[\mathbb{E}\left(w_{i}\right)\right]^{2} \operatorname{Var}\left(x_{i}\right)+\left[\mathbb{E}\left(x_{i}\right)\right]^{2} \operatorname{Var}\left(w_{i}\right)+\operatorname{Var}\left(x_{i}\right) \operatorname{Var}\left(w_{i}\right)= \\
& =\sum_{i} \operatorname{Var}\left(x_{i}\right) \operatorname{Var}\left(w_{i}\right)=n_{\text {in }} \operatorname{Var}(x) \operatorname{Var}(w)
\end{aligned}
$$

- We want $\operatorname{Var}(s)=\operatorname{Var}(x)$, so choose $\operatorname{Var}(w)=\frac{1}{n_{\text {in }}}$
- Similar analysis for the backpropagated signal: $\operatorname{Var}(w)=\frac{2}{n_{\text {in }}+n_{\text {out }}}$
- Standardized inputs
- Works well for tanh as it is linear near zero
- Xavier initialization does not work for ReLU


ReLU


## He Initialization

- He et al.: Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification, 2015
- Suggested ReLU initialization
- Uses $\operatorname{Var}(w)=\frac{2}{n_{\text {in }}}$



## Other Methods

- Recent data-driven techniques iteratively scaling weights in the network
- Batch normalization:
- specialized layer which sets unit variance,
- computes mean and variance estimates over batch,
- normalizes but allow linear transformation (parameters) of the distribution to better deal with nonlinearities


## Autoencoders

- Task: train the network for identity (same targets as inputs $\mathbf{Y}=\mathbf{X}$ )
- The number of hidden units is typically less than the number of inputs/outputs
- Compresses the input space
- May have tied weights $\left(\mathbf{W}^{\prime}=\mathbf{W}^{\mathbf{T}}\right)$
- Works as PCA for linear layers and squared loss: Bourlard and Kamp: Auto-Association by Multilayer Perceptrons and Singular Value Decomposition, 1988


Denoising Autoencoders

- Reconstruction from corrupted inputs



## Stacked Autoencoders

1. Train the first layer as a shallow autoencoder


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4. Fine-tune all parameters


- Use the encoder part of a stacked autoencoder for weight initialization of a different network
- Semi-supervised setup


POOL POOL POOL



32


32














$S=1$

$S=1$




## Sharpen

Box blur
(normalized)

$$
\frac{1}{9}\left[\begin{array}{lll}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1
\end{array}\right]
$$

$\frac{1}{16}\left[\begin{array}{lll}1 & 2 & 1 \\ 2 & 4 & 2 \\ 1 & 2 & 1\end{array}\right]$
Gaussian blur (approximation)

$$
\left[\begin{array}{rrr}
0 & -1 & 0 \\
-1 & 5 & -1 \\
0 & -1 & 0
\end{array}\right]
$$




POOL POOL POOL


## Input feature map



Output feature map

$F=2, S=2$

| 2 | 2 | 0 | 4 | 3 | 4 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 0 | 5 | 0 | 4 | 1 |
| 4 | 5 | 2 | 5 | 1 | 4 |
| 5 | 2 | 1 | 0 | 2 | 1 |
| 2 | 3 | 3 | 3 | 5 | 3 |
| 0 | 3 | 0 | 4 | 0 | 1 |


| 2 | 5 | 4 |
| :--- | :--- | :--- |
| 5 | 5 | 4 |
| 3 | 4 | 5 |



input
CONV, MP
layers
input



$$
\begin{aligned}
& \underset{4-99}{\substack{2 \rightarrow 8}}
\end{aligned}
$$



(a) Siberian husky

(b) Eskimo dog






input


input














## input


$\stackrel{\rightharpoonup}{2}$
$\stackrel{\rightharpoonup}{3}$
$\stackrel{3}{3}$

| 7 | 2 | 1 | 0 | 4 | 1 | 4 | 9 | 5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 6 | 9 | 0 | 1 | 5 | 9 | 7 | 3 |



| 7 | 2 | 1 | 0 | 4 | 1 | 4 | 9 | 5 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 6 | 9 | 0 | 1 | 5 | 9 | 7 | 3 |



| 72 | 0 | 4 | 7 | 4 | 9 | 8 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 6 | 9 | 0 | 1 | 5 | 4 |







