# Deep Learning I Supervised Learning 

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## Mining for Structure

Massive increase in both computational power and the amount of data available from web, video cameras, laboratory measurements.


- Develop statistical models that can discover underlying structure, cause, or statistical correlation from data in unsupervised or semi-supervised way.
- Multiple application domains.


## Mining for Structure

Massive increase in both computational power and the amount of data available from web, video cameras, laboratory measurements.


- Develop statistical models that can discover underlying structure, cause, or statistical correlation from data in unsupervised or semi-supervised way.
- Multiple application domains.


## Impact of Deep Learning

- Speech Recognition

- Computer Vision
- Recommender Systems
- Language Understanding
- Drug Discovery and Medical Image Analysis


## Deep Generative Model

Model P(document)

(Hinton \& Salakhutdinov, Science 2006)

## Example: Understanding Images



TAGS:
strangers, coworkers, conventioneers, attendants, patrons

Nearest Neighbor Sentence: people taking pictures of a crazy person

Model Samples

- a group of people in a crowded area .
- a group of people are walking and talking .
- a group of people, standing around and talking .


## Caption Generation


a car is parked in the middle of nowhere .
a ferry boat on a marina with a group of people.

a wooden table and chairs arranged in a room .


there is a cat sitting on a shelf .

a little boy with a bunch of friends on the street .

## Talk Roadmap

Part 1: Supervised Learning: Deep Networks

- Definition of Neural Networks
- Training Neural Networks
- Recent Optimization / Regularization Techniques

Part 2: Unsupervised Learning: Learning Deep
Generative Models

Part 3: Open Research Questions

## Learning Feature Representations



## Learning Feature Representations



## Traditional Approaches



## Learning algorithm



## Computer Vision Features



## Audio Features



## Audio Features



## Neural Networks Online Course

- Disclaimer: Some of the material and slides for this lecture were borrowed from Hugo Larochelle's class on Neural Networks: https://sites.google.com/site/deeplearningsummerschool2016/
- Hugo's class covers many other topics: convolutional networks, neural language model, Boltzmann machines, autoencoders, sparse coding, etc.
- We will use his material for some of the other lectures.


## http://info.usherbrooke.ca/hlarochelle/neural_networks



Topics: RBM, visible layer, hidden layer, energy function


$$
\text { Energy function: } \begin{aligned}
E(\mathbf{x}, \mathbf{h}) & =-\mathbf{h}^{\top} \mathbf{W} \mathbf{x}-\mathbf{c}^{\top} \mathbf{x}-\mathbf{b}^{\top} \mathbf{h} \\
& =-\sum_{j} \sum_{k} W_{j, k} h_{j} x_{k}-\sum_{k} c_{k} x_{k}-\sum_{j} b_{j} h_{j}
\end{aligned}
$$

Distribution: $p(\mathbf{x}, \mathbf{h})=\exp (-E(\mathbf{x}, \mathbf{h})) / Z_{\mathbf{k}}$


## Feedforward Neural Networks

- Definition of Neural Networks
- Forward propagation
- Types of units
- Capacity of neural networks
- How to train neural nets:
- Loss function
- Backpropagation with gradient descent
- More recent techniques:
- Dropout
- Batch normalization
- Unsupervised Pre-training



## Artificial Neuron

- Neuron pre-activation (or input activation):

$$
a(\mathbf{x})=b+\sum_{i} w_{i} x_{i}=b+\mathbf{w}^{\top} \mathbf{x}
$$

- Neuron output activation:

$$
h(\mathbf{x})=g(a(\mathbf{x}))=g\left(b+\sum_{i} w_{i} x_{i}\right)
$$

where
$\mathbf{W}$ are the weights (parameters)
$b$ is the bias term
$g(\cdot)$ is called the activation function


## Artificial Neuron

- Output activation of the neuron:

$$
h(\mathbf{x})=g(a(\mathbf{x}))=g\left(b+\sum_{i} w_{i} x_{i}\right)
$$

Range is determined by $g(\cdot)$


Bias only changes the position of the riff

## Activation Function

- Sigmoid activation function:
> Squashes the neuron's output between 0 and 1
> Always positive
> Bounded
> Strictly Increasing

$$
g(a)=\operatorname{sigm}(a)=\frac{1}{1+\exp (-a)}
$$



## Activation Function

- Rectified linear (ReLU) activation function:
> Bounded below by 0 (always non-negative)
> Tends to produce units with sparse activities
> Not upper bounded
> Strictly increasing

$$
g(a)=\operatorname{reclin}(a)=\max (0, a)
$$

## Single Hidden Layer Neural Net

- Hidden layer pre-activation:

$$
\begin{aligned}
& \mathbf{a}(\mathbf{x})=\mathbf{b}^{(1)}+\mathbf{W}^{(1)} \mathbf{x} \\
& \quad\left(a(\mathbf{x})_{i}=b_{i}^{(1)}+\sum_{j} W_{i, j}^{(1)} x_{j}\right)
\end{aligned}
$$

- Hidden layer activation:

$$
\mathbf{h}(\mathbf{x})=\mathbf{g}(\mathbf{a}(\mathbf{x}))
$$

- Output layer activation:


$$
f(\mathbf{x})=o \underbrace{\left(b^{(2)}+\mathbf{w}^{(2)^{\top}} \mathbf{h}^{(1)} \mathbf{x}\right)}_{\substack{\text { Output activation } \\ \text { function }}}
$$

## Multilayer Neural Net

- Consider a network with L hidden layers.
- layer pre-activation for $\mathrm{k}>0$

$$
\mathbf{a}^{(k)}(\mathbf{x})=\mathbf{b}^{(k)}+\mathbf{W}^{(k)} \mathbf{h}^{(k-1)}(\mathbf{x})
$$

- hidden layer activation from 1 to L :

$$
\mathbf{h}^{(k)}(\mathbf{x})=\mathbf{g}\left(\mathbf{a}^{(k)}(\mathbf{x})\right)
$$

- output layer activation ( $k=L+1$ ):

$$
\left(\mathbf{h}^{(0)}(\mathbf{x})=\mathbf{x}\right)
$$

$$
\mathbf{h}^{(L+1)}(\mathbf{x})=\mathbf{o}\left(\mathbf{a}^{(L+1)}(\mathbf{x})\right)=\mathbf{f}(\mathbf{x})
$$

## Capacity of Neural Nets

- Consider a single layer neural network

(from Pascal Vincent's slides)


## Capacity of Neural Nets

- Consider a single layer neural network



## Universal Approximation

- Universal Approximation Theorem (Hornik, 1991):
- "a single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units"
- This applies for sigmoid, tanh and many other activation functions.
- However, this does not mean that there is learning algorithm that can find the necessary parameter values.


## Feedforward Neural Networks

- How neural networks predict $f(x)$ given an input $x$ :
- Forward propagation
- Types of units
- Capacity of neural networks
- How to train neural nets:
- Loss function
- Backpropagation with gradient descent
- More recent techniques:
- Dropout
- Batch normalization
- Unsupervised Pre-training



## Training

- Empirical Risk Minimization:

$$
\underset{\boldsymbol{\theta}}{\arg \min } \frac{1}{T} \sum_{t} \underbrace{l\left(f\left(\mathbf{x}^{(t)} ; \boldsymbol{\theta}\right), y^{(t)}\right)}_{\text {Loss function }}+\underbrace{\lambda \Omega(\boldsymbol{\theta})}_{\text {Regularizer }}
$$

- Learning is cast as optimization.
> For classification problems, we would like to minimize classification error.
> Loss function can sometimes be viewed as a surrogate for what we want to optimize (e.g. upper bound)


## Stochastic Gradient Descend

- Perform updates after seeing each example:
- Initialize: $\boldsymbol{\theta} \equiv\left\{\mathbf{W}^{(1)}, \mathbf{b}^{(1)}, \ldots, \mathbf{W}^{(L+1)}, \mathbf{b}^{(L+1)}\right\}$
- For $\mathrm{t}=1: \mathrm{T}$
- for each training example $\left(\mathbf{x}^{(t)}, y^{(t)}\right)$

$$
\begin{aligned}
& \Delta=-\nabla_{\boldsymbol{\theta}} l\left(f\left(\mathbf{x}^{(t)} ; \boldsymbol{\theta}\right), y^{(t)}\right)-\lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta}) \\
& \boldsymbol{\theta} \leftarrow \boldsymbol{\theta}+\alpha \Delta
\end{aligned}
$$

Training epoch
$=$

Iteration of all examples

- To train a neural net, we need:
> Loss function: $l\left(\mathbf{f}\left(\mathbf{x}^{(t)} ; \boldsymbol{\theta}\right), y^{(t)}\right)$
$>$ A procedure to compute gradients: $\nabla_{\boldsymbol{\theta}} l\left(\mathbf{f}\left(\mathbf{x}^{(t)} ; \boldsymbol{\theta}\right), y^{(t)}\right)$
$>$ Regularizer and its gradient: $\Omega(\boldsymbol{\theta}), \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$


## Computational Flow Graph

- Forward propagation can be represented as an acyclic flow graph
- Forward propagation can be implemented in a modular way:
> Each box can be an object with an fprop method, that computes the value of the box given its children
> Calling the fprop method of each box in the right order yields forward propagation



## Computational Flow Graph

- Each object also has a bprop method
- it computes the gradient of the loss with respect to each child box.
- By calling bprop in the reverse order, we obtain backpropagation



## Model Selection

- Training Protocol:
- Train your model on the Training Set $\mathcal{D}^{\text {train }}$
- For model selection, use Validation Set $\mathcal{D}^{\text {valid }}$
> Hyper-parameter search: hidden layer size, learning rate, number of iterations/epochs, etc.
- Estimate generalization performance using the Test Set $\mathcal{D}^{\text {test }}$
- Generalization is the behavior of the model on unseen examples.


## Early Stopping

- To select the number of epochs, stop training when validation set error increases (with some look ahead).



## Mini-batch, Momentum

- Make updates based on a mini-batch of examples (instead of a single example):
> the gradient is the average regularized loss for that mini-batch
> can give a more accurate estimate of the gradient
> can leverage matrix/matrix operations, which are more efficient
- Momentum: Can use an exponential average of previous gradients:

$$
\bar{\nabla}_{\boldsymbol{\theta}}^{(t)}=\nabla_{\boldsymbol{\theta}} l\left(\mathbf{f}\left(\mathbf{x}^{(t)}\right), y^{(t)}\right)+\beta \bar{\nabla}_{\boldsymbol{\theta}}^{(t-1)}
$$

> can get pass plateaus more quickly, by "gaining momentum"

## Feedforward Neural Networks

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## Learning Distributed Representations

- Deep learning is research on learning models with multilayer representations
> multilayer (feed-forward) neural networks
> multilayer graphical model (deep belief network, deep Boltzmann machine)
- Each layer learns "distributed representation"
> Units in a layer are not mutually exclusive
- each unit is a separate feature of the input
- two units can be "active" at the same time
> Units do not correspond to a partitioning (clustering) of the inputs
- in clustering, an input can only belong to a single cluster


## Local vs. Distributed Representations

- Clustering, Nearest Neighbors, RBF SVM, local density estimators
- Parameters for each region.
- \# of regions is linear with \# of parameters.

- RBMs, Factor models, PCA, Sparse Coding, Deep models



## Local vs. Distributed Representations

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## Local vs. Distributed Representations

- Clustering, Nearest Neighbors, RBF SVM, local density estimators
- Parameters for each region.
- \# of regions is linear with \# of parameters.

- RBMs, Factor models, PCA, Sparse Coding, Deep models $\quad$ C1=1
- Each parameter affects many regions, not just local.
- \# of regions grows (roughly) exponentially in \# of parameters.



## Inspiration from Visual Cortex



## Why Training is Hard

- First hypothesis: Hard optimization problem (underfitting)
> vanishing gradient problem
> saturated units block gradient propagation
- This is a well known problem in recurrent neural networks



## Why Training is Hard

- Second hypothesis: Overfitting
> we are exploring a space of complex functions
> deep nets usually have lots of parameters
- Might be in a high variance / low bias situation



## Why Training is Hard

- First hypothesis (underfitting): better optimize
> Use better optimization tools (e.g. batch-normalization, second order methods, such as KFAC)
> Use GPUs, distributed computing.
- Second hypothesis (overfitting): use better regularization
> Unsupervised pre-training
Stochastic drop-out training
- For many large-scale practical problems, you will need to use both: better optimization and better regularization!


## Unsupervised Pre-training

- Initialize hidden layers using unsupervised learning
> Force network to represent latent structure of input distribution

character image

random image
> Encourage hidden layers to encode that structure


## Unsupervised Pre-training

- Initialize hidden layers using unsupervised learning
> This is a harder task than supervised learning (classification)

character image

random image
> Hence we expect less overfitting


## Autoencoders: Preview

- Feed-forward neural network trained to reproduce its input at the output layer


## Decoder



$$
\begin{aligned}
\widehat{\mathbf{x}} & =o(\widehat{\mathbf{a}}(\mathbf{x})) \\
& =\underbrace{\operatorname{sigm}\left(\mathbf{c}+\mathbf{W}^{*} \mathbf{h}(\mathbf{x})\right)}_{\text {For binary units }}
\end{aligned}
$$

Encoder

$$
\begin{aligned}
\mathbf{h}(\mathbf{x}) & =g(\mathbf{a}(\mathbf{x})) \\
& =\operatorname{sigm}(\mathbf{b}+\mathbf{W} \mathbf{x})
\end{aligned}
$$

## Autoencoders: Preview

- Loss function for binary inputs

$$
\begin{aligned}
& l(f(\mathbf{x}))=-\sum_{k}\left(x_{k} \log \left(\widehat{x}_{k}\right)+\left(1-x_{k}\right) \log \left(1-\widehat{x}_{k}\right)\right) \\
& >\quad \text { Cross-entropy error function } \quad f(\mathbf{x}) \equiv \widehat{\mathbf{x}}
\end{aligned}
$$

- Loss function for real-valued inputs

$$
l(f(\mathbf{x}))=\frac{1}{2} \sum_{k}\left(\widehat{x}_{k}-x_{k}\right)^{2}
$$

> sum of squared differences
> we use a linear activation function at the output

## Pre-training

- We will use a greedy, layer-wise procedure
> Train one layer at a time with unsupervised criterion
> Fix the parameters of previous hidden layers
> Previous layers can be viewed as feature extraction



## Fine-tuning

- Once all layers are pre-trained
> add output layer
> train the whole network using supervised learning
- We call this last phase fine-tuning
> all parameters are "tuned" for the supervised task at hand
> representation is adjusted to be more discriminative



## Why Training is Hard

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## Dropout

- Key idea: Cripple neural network by removing hidden units stochastically
> each hidden unit is set to 0 with probability 0.5
> hidden units cannot co-adapt to other units
> hidden units must be more generally useful
- Could use a different dropout probability, but 0.5 usually works well



## Dropout

- Use random binary masks $\mathrm{m}^{(k)}$
> layer pre-activation for $\mathrm{k}>0$

$$
\mathbf{a}^{(k)}(\mathbf{x})=\mathbf{b}^{(k)}+\mathbf{W}^{(k)} \mathbf{h}^{(k-1)}(\mathbf{x})
$$

> hidden layer activation ( $\mathrm{k}=1$ to L ):

$$
\mathbf{h}^{(k)}(\mathbf{x})=\mathbf{g}\left(\mathbf{a}^{(k)}(\mathbf{x})\right) \odot \mathrm{m}^{(k)}
$$

> Output activation ( $\mathrm{k}=\mathrm{L}+1$ )

$$
\mathbf{h}^{(L+1)}(\mathbf{x})=\mathbf{o}\left(\mathbf{a}^{(L+1)}(\mathbf{x})\right)=\mathbf{f}(\mathbf{x}) \quad \mathbf{W}^{(1)}
$$



## Dropout at Test Time

- At test time, we replace the masks by their expectation
> This is simply the constant vector 0.5 if dropout probability is 0.5
> For single hidden layer: equivalent to taking the geometric average of all neural networks, with all possible binary masks
- Can be combined with unsupervised pre-training
- Beats regular backpropagation on many datasets
- Ensemble: Can be viewed as a geometric average of exponential number of networks.


## Why Training is Hard

- First hypothesis (underfitting): better optimize
> Use better optimization tools (e.g. batch-normalization, second order methods, such as KFAC)
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## Batch Normalization

- Normalizing the inputs will speed up training (Lecun et al. 1998)
> could normalization be useful at the level of the hidden layers?
- Batch normalization is an attempt to do that (loffe and Szegedy, 2014)
> each unit's pre-activation is normalized (mean subtraction, stddev division)
> during training, mean and stddev is computed for each minibatch
> backpropagation takes into account the normalization
> at test time, the global mean / stddev is used


## Batch Normalization

Input: Values of $x$ over a mini-batch: $\mathcal{B}=\left\{x_{1 \ldots m}\right\}$; Parameters to be learned: $\gamma, \beta$
Output: $\left\{y_{i}=\mathrm{BN}_{\gamma, \beta}\left(x_{i}\right)\right\}$

$$
\begin{aligned}
& \mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_{i} \\
& \sigma_{\mathcal{B}}^{2} \leftarrow \frac{1}{m} \sum_{i=1}^{m}\left(x_{i}-\mu_{\mathcal{B}}\right)^{2} \quad \text { // mini-batch variance } \\
& \widehat{x}_{i} \leftarrow \frac{x_{i}-\mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^{2}+\epsilon}} \\
& y_{i} \leftarrow \gamma \widehat{x}_{i}+\beta \equiv \mathrm{BN}_{\gamma, \beta}\left(x_{i}\right) \\
& \text { // normalize } \\
&
\end{aligned}
$$

Learned linear transformation to adapt to non-linear activation function ( $\gamma$ and $\beta$ are trained)

## Batch Normalization

-Why normalize the pre-activation?
> can help keep the pre-activation in a non-saturating regime (though the linear transform $y_{i} \leftarrow \gamma \widehat{x}_{i}+\beta$ could cancel this effect)

- Use the global mean and stddev at test time.
> removes the stochasticity of the mean and stddev
> requires a final phase where, from the first to the last hidden layer - propagate all training data to that layer
- compute and store the global mean and stddev of each unit
> for early stopping, could use a running average


## Optimization Tricks

- SGD with momentum, batch-normalization, and dropout usually works very well
- Pick learning rate by running on a subset of the data
> Start with large learning rate \& divide by 2 until loss does not diverge
$>$ Decay learning rate by a factor of $\sim 100$ or more by the end of training
- Use ReLU nonlinearity
- Initialize parameters so that each feature across layers has similar variance. Avoid units in saturation.


## Visualization

- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance

- Good training: hidden units are sparse across samples
hidden unit


## Visualization

- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance
- Visualize parameters: learned features should exhibit structure and should be uncorrelated and are uncorrelated


too noisy

too correlated

BAD

lack structure

## Visualization

- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance

- Bad training: many hidden units ignore the input and/or exhibit strong correlations


## hidden unit

## Computer Vision

- Design algorithms that can process visual data to accomplish a given task:
> For example, object recognition: Given an input image, identify which object it contains



## Deep Convolutional Nets

Very deep network
Prediction


- Convolution
- Pooling

High-level feature space

- Normalization
- Densely connected


## Deep Convolutional Nets



## ConvNets: Examples

- Optical Character Recognition, House Number and Traffic Sign classification


Ciresan et al. "MCDNN for image classification" CVPR 2012
Wan et al. "Regularization of neural networks using dropconnect" ICML 2013
Goodfellow et al. "Multi-digit nuber recognition from StreetView..." ICLR 2014
Jaderberg et al. "Synthetic data and ANN for natural scene text recognition" arXiv 2014

## ConvNets: Examples

- Pedestrian detection



## ConvNets: Examples

- Object Detection


Sermanet et al., OverFeat: Integrated recognition, localization, 2013
Girshick et al., Rich feature hierarchies for accurate object detection, 2013
Szegedy et al., DNN for object detection, NIPS 2013

## ImageNet Dataset

- 1.2 million images, 1000 classes

Examples of Hammer

(Deng et al., Imagenet: a large scale hierarchical image database, CVPR 2009)

## Important Breakthrough

## - Deep Convolutional Nets for Vision (Supervised)

Krizhevsky, A., Sutskever, I. and Hinton, G. E., ImageNet Classification with Deep Convolutional Neural Networks, NIPS, 2012.


IM AGENET
1.2 million training images 1000 classes


## Architecture

- How can we select the right architecture:
> Manual tuning of features is now replaced with the manual tuning of architechtures
- Depth
- Width
- Parameter count


## How to Choose Architecture

- Many hyper-parameters:
> Number of layers, number of feature maps
- Cross Validation
- Grid Search (need lots of GPUs)
- Smarter Strategies
> Random search
> Bayesian Optimization


## AlexNet

- 8 layers total
- Trained on Imagenet dataset [Deng et al. CVPR'09]
- $18.2 \%$ top-5 error



## AlexNet

- Remove top fully connected layer 7
- Drop ~16 million parameters
- Only $1.1 \%$ drop in performance!



## AlexNet

- Let us remove upper feature extractor layers and fully connected:
> Layers 3,4, 6 and 7
- Drop ~50 million parameters
- 33.5 drop in performance!
- Depth of the network is the key.



## GoogLeNet



- 24 layer model that uses so-called inception module.


## Convolution Pooling

Softmax
Other

## GoogLeNet

- GoogLeNet inception module:
> Multiple filter scales at each layer
D Dimensionality reduction to keep computational requirements down

(Szegedy et al., Going Deep with Convolutions, 2014)


## GoogLeNet



- Width of inception modules ranges from 256 filters (in early modules) to 1024 in top inception modules.
- Can remove fully connected layers on top completely
- Number of parameters is reduced to 5 million
- $6.7 \%$ top-5 validation error on Imagnet
(Szegedy et al., Going Deep with Convolutions, 2014)


## Residual Networks

Really, really deep convnets do not train well, E.g. CIFAR10:



Key idea: introduce "pass through" into each layer

Thus only residual now needs to be learned

| method | top-1 err. | top-5 err. |
| :--- | :---: | :---: |
| VGG [41] (ILSVRC'14) | - | $8.43^{\dagger}$ |
| GoogLeNet [44] (ILSVRC'14) | - | 7.89 |
| VGG [41] (v5) | 24.4 | 7.1 |
| PReLU-net [13] | 21.59 | 5.71 |
| BN-inception [16] | 21.99 | 5.81 |
| ResNet-34 B | 21.84 | 5.71 |
| ResNet-34 C | 21.53 | 5.60 |
| ResNet-50 | 20.74 | 5.25 |
| ResNet-101 | 19.87 | 4.60 |
| ResNet-152 | $\mathbf{1 9 . 3 8}$ | $\mathbf{4 . 4 9}$ |

Table 4. Error rates (\%) of single-model results on the ImageNet validation set (except ${ }^{\dagger}$ reported on the test set).

With ensembling, $3.57 \%$ top- 5 test error on ImageNet


(He, Zhang, Ren, Sun, CVPR 2016)



## Choosing the Architecture

- Task dependent
- Cross-validation
- [Convolution $\rightarrow$ pooling] ${ }^{*}+$ fully connected layer
- The more data: the more layers and the more kernels
> Look at the number of parameters at each layer
> Look at the number of flops at each layer
- Computational resources


## End of Part 1

