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INF 5860 Machine learning for image classification
Lecture 6 : Introduction to neural nets
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## Reading material

- Reading material:
- http://cs231n.github.io/neural-networks-1/
- http://cs231n.github.io/neural-networks-2/
- http://cs231n.github.io/optimization-2/ Youtube: CS 231n: Lectures 4-6 covers the next 3 lectures
- Deep learning Chapter 6.1-6.5


## Today

- The concept of feed-forward neural nets
- Capacity of traditional feed-forward nets
- Forward propagation from input to output class labels
- Cost functions for neural net classification
- Net architecture
- Introduction to learning using backpropagation (as far as time permits)
- Backpropagation in detail next week.


## Feed-forward neural nets

- The focus today is a feed-forward neural net with few hidden layers.
- Input will be the image pixel values
- Or features like SIFT, orientation histograms etc.
- The net will play the role of a classifier that maps the input data through some hidden layers to a score for each class.
For a network with 2 layers, the score would be $s=f\left(W 2^{*} f(W 1 * x)\right)$
- f is a non-linear function called activation function
- Later, we will see recurrent networks that feeds the output back to itself.


## Non-linear data example



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## Two-layer net



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## Two-layer net for image classification



- This architecture with some hidden layers and fully forward connected layers is also called a multilayer perceptron.
- Fully connected: each node in layer i-1 is connected to each node in layer i .
- $x_{i}$ is still a 1D vector of pixel values (e.g. $3072 \times 1$ for CIFAR-10)
- This network does not use any information about which pixel is a neighbor of which pixel, or any spatial features relating neighboring pixel values.
- A Convolutional neural net will include this information and perform much better for image classification purposes.
- We can add as many hidden layers as we want, and the number of nodes in a hidden layer is a parameter we set.


## Modelling one neuron

- One node in the network is inspired by a neuron in the brain.
- It received inputs from its dendrites and produce outputs along a single axon.
- We have about 86 billion neurons of different types.
- Neurons are connected by synaptic junctions or synapses.
- A cell will fire (send a pulse) if its potential reach a certain level. The frequency of firing carries information.
- In mathematics this is modelled using activation function f .
- The weights that connect neurons are learnable.


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## McColloch-Pitt's mathematical neuron model



Simple illustration


McColloch and Pitts (1943) modelled this as a binary threshold unit

## Pseudo-code for forward progatating a single neuron

```
class Neuron(object):
    #
    def forward(inputs):
        #assume inputs and weights are 1D arrays
        cell_sum = np.sum(input*self.weights)+self.bias
        firing_rate = 1(1.0+math.exp(-cell_sum)) # Sigmoid activation
        return
                                    Other activation functions can
                                    be better, like RELU
```

Note: not an accurate actual model for a human neuron, see
http://www.sciencedirect.com/science/article/pii/S0959438814000130

# Topic for a later lecture: which activation function to choose 

## Activation Functions

Sigmoid

$$
\sigma(x)=1 /\left(1+e^{-x}\right)
$$


$\tanh \tanh (x)$

ReLU $\max (0, x)$


Leaky ReLU $\max (0.1 x, x)$


Maxout $\max \left(w_{1}^{T} x+b_{1}, w_{2}^{T} x+l\right.$ ELU


## Architecture for a feed-forward net



4-layered net

- input layer not counted


## One neuron as a binary logistic classifier


$\sigma(z)=1 /\left(1+e^{-x}\right)$ is the sigmoid function
$\sigma\left(\sum_{i} w_{i} x_{i}+b\right)$ can be interpreted as a probability of class1 $\mathrm{P}\left(\mathrm{y}_{\mathrm{i}}=1 \mid \mathrm{x}_{\mathrm{i}}, \mathrm{w}\right)$, and
$\mathrm{P}\left(\mathrm{y}_{\mathrm{i}}=0 \mid \mathrm{x}_{\mathrm{i}}, \mathrm{w}\right)=1-\mathrm{P}\left(\mathrm{y}_{\mathrm{i}}=1 \mid \mathrm{x}_{\mathrm{i}}, \mathrm{w}\right)$

## 2-layer net, 3 pixels, with notation



## Notation

$a_{i}^{(j)}$ - activation of unit $i$ and layer $j$
$\Theta^{(j)}$ - matrix of weights controlling function mapping from layer j to $\mathrm{j}+1$
$\Theta^{(j)}$ has dimension (nodes in layer $\left.(\mathrm{j})\right) \times($ nodes in layer $(\mathrm{j}-1)+1)$
$\mathrm{s}_{\mathrm{j}-1}$ nodes in layer $\mathrm{j}-1, \mathrm{~s}_{\mathrm{j}}$ nodes in layer j : $\Theta^{(j)}$ has size $\mathrm{s}_{\mathrm{j}} \times\left(\mathrm{s}_{\mathrm{j}-1}+1\right)$
$\mathrm{a}_{1}^{(1)}=g\left(\Theta_{10}^{(1)} \mathrm{x}_{0}+\Theta_{11}^{(1)} \mathrm{x}_{1}+\Theta_{12}^{(1)} \mathrm{x}_{2}+\Theta_{13}^{(1)} \mathrm{x}_{3}\right)$
$\mathrm{a}_{2}^{(1)}=g\left(\Theta_{20}^{(1)} \mathrm{x}_{0}+\Theta_{21}^{(1)} \mathrm{x}_{1}+\Theta_{22}^{(1)} \mathrm{x}_{2}+\Theta_{23}^{(1)} \mathrm{x}_{3}\right)$
$\mathrm{a}_{3}^{(1)}=g\left(\Theta_{30}^{(1)} \mathrm{x}_{0}+\Theta_{31}^{(1)} \mathrm{x}_{1}+\Theta_{32}^{(1)} \mathrm{x}_{2}+\Theta_{33}^{(1)} \mathrm{x}_{3}\right)$
$h_{\Theta}(x)=\mathrm{a}_{1}^{(2)}=g\left(\Theta_{10}^{(2)} \mathrm{a}_{0}{ }^{(2)}+\Theta_{11}^{(2)} \mathrm{a}_{1}{ }^{(2)}+\Theta_{12}^{(2)} \mathrm{a}_{2}{ }^{(2)}+\Theta_{13}^{(2)} \mathrm{a}_{3}{ }^{(2)}\right)$

## 2-layer net - what do the layers do?



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HIDDEN LAYER:
Each $\mathrm{a}_{1}{ }^{(1)}$ is a weighted linear combination of all input pixels $x_{1}, \ldots x_{3}$


## Example net: MNIST-classification

- Input $20 \times 20$ images=400 input nodes +1 bias
- 25 nodes in hidden layer: $\Theta^{(1)}$ is $25 \times 401$ (add bias term $\mathrm{x}_{0}$ )
- 10 classes: digits ' 0 ' $-{ }^{\prime} 9^{\prime}: \Theta^{(2)}$ is $10 \times 26$ (add bias term $\mathrm{a}_{0}{ }^{(2)}$
- One vs. all loss function


## Example of trained network MNIST data

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 7 | 1 | 1 | 1 | 1 | 1 | 7 | 1 | 1 |
| 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 |
| 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 |
| 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 | 5 |
| 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 | 6 |
| 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 | 7 |
| 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 | 8 |
| 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 | 9 |

$20 \times 20$ images
of handwritten digits,
10 classes

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## Weights for the output layer 25 hidden nodes, 10 classes



## Weights for the output classes



## 

20
High value for feature/node 13 and 1


Maybe this responds to objects with a center in the right half (13) and seeing a diagonal edge????

## What if the object is rotated or translated?



Maybe this responds to objects with a center in the right half (13) and seeing a diagonal edge????

Would this be the case for the rotated object?


## Some remarks

- With the output layer, it is possible to use a net with or without the activation function.
- The size of network is measured by the number of neurons.


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## Example feed-forward computation



- Input x: $3 \times 1$ vector
$\Theta^{(1)}: 4 \times 4$ (nof. hidden nodes in layer $1 \times$ nof.inputs +1 )
$\Theta^{(2)}: 2 \times 5$ (nof.classes $\times$ nof. hidden nodes in layer $1+1$ )
If we have N training samples we can predict
all $\mathrm{n}=1 \ldots \mathrm{~N}$ at one time :

z1 = Theta1.dot(X)
a1 = sigmoid(z1)
\#Append 1 to a1 before computing z2
Continue with layer 2..........


## Back to the non-linearly separable case



## A similiar, simple example: XNOR



## Coding the AND-functions

(

## Which logical function is this?



## Creating the XNOR-function



## Representation power of the net

- Fully-connected nets define a family of functions that are parameterized by the weights of the network.
- It turns out that nets with at least one hidden layer are universal approximators
- Given any continuous function $f(x)$ and some $e>0$, there is a net $g(x)$ (with a non-linear activation) that can represent the function such that
- $|f(x)-g(x)|<e$
- But why do we need more than one hidden layer?
- `In practise, 3-layers feed-forward nets often works better then 2-layers, but going deeper rarely helps.
- This is NOT the case for Convolutional nets where depth helps, more on this later.


## Multiple classes: One-vs-all

- Train one output node for each class, e.g. CAR (yes/no), CAT(yes/n0)


$$
\begin{aligned}
& \text { Want }: \mathrm{h}_{\Theta}\left(x_{i}\right) \approx y_{i}=\left[\begin{array}{l}
1 \\
0 \\
0 \\
0
\end{array}\right] \quad \mathrm{h}_{\Theta}\left(x_{i}\right) \approx y_{i}=\left[\begin{array}{l}
0 \\
1 \\
0 \\
0
\end{array}\right] \quad \mathrm{h}_{\Theta}\left(x_{i}\right) \approx y_{i}=\left[\begin{array}{l}
0 \\
0 \\
1 \\
0
\end{array}\right] \quad \mathrm{h}_{\Theta}\left(x_{i}\right) \approx y_{i}=\left[\begin{array}{l}
0 \\
0 \\
0 \\
1
\end{array}\right] \\
& \text { if CAR }
\end{aligned}
$$

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## Neural network classification



Binary classification:

$$
y=1 \text { or } 0
$$

1 output unit

$$
y \in R_{k} \text {, e.g. }\left[\begin{array}{l}
1 \\
0 \\
0 \\
0
\end{array}\right] \cdot\left[\begin{array}{l}
0 \\
1 \\
0 \\
0
\end{array}\right] \cdot\left[\begin{array}{l}
0 \\
0 \\
1 \\
0
\end{array}\right],\left[\begin{array}{l}
0 \\
0 \\
0 \\
1
\end{array}\right]
$$

## Cost function for neural networks

- For logistic regression it was:

$$
J(\theta)=-\frac{1}{m}\left[\sum _ { i = 1 } ^ { m } y ( i ) \operatorname { l o g } h _ { \theta } \left(X(i,:)+(1-y(i)) \log \left(1-h_{\theta}(X(i,:))\right]+\frac{\lambda}{2 m} \sum_{j=1}^{n} \theta_{j}^{2}\right.\right.
$$

- For neural nets it is:

Output: $h_{\Theta}(x) \in R^{K}$
$J(\Theta)=-\frac{1}{m}\left[\sum_{i=1}^{m} \sum_{k=1}^{K} y_{k}(i) \log h_{\theta k}(X(i,:))+\left(1-y_{k}(i)\right) \log \left(1-h_{\theta k}(X(i,:))\right)\right]+\frac{\lambda}{2 m} \sum_{l=1}^{L-1} \sum_{i=1}^{s_{l}} \sum_{j=1}^{s_{j}+1}\left(\Theta_{j i}^{(l)}\right)^{2}$
L: number of layers
$s_{1}$ : Number of units (without bias) in layer 1

## Implementing the cost function

- Create an indicator matrix $Y$ with one row per sample, where each row encodes the class as:

$$
\text { IF } y=\left[\begin{array}{c}
2 \\
2 \\
1 \\
4 \\
\vdots \\
3
\end{array}\right], \quad \operatorname{let} Y=\left[\begin{array}{cccc}
0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & 1 & 0
\end{array}\right]
$$

- Compute the cost without regularization, then add the regularization term.
- Use a loop over the training samples if you want.


## Introduction to backpropagation and computational graphs

- We now have a network architecture and a cost function.
- A learning algorithm for the net should give us a way to change the weights in such a manner that the output is closer to the correct class labels.
- The activation function should assure that a small change in weights results in
small change in any weight (ior bias)
 a small change in ouputs.
- Backpropagation use partial derivatives to compute the derivative of the cost function $J$ with respect to all the weights.


## Neural net optimization problem

- Given a cost function $L$ (or $J$ ), a set of training data ( $\mathrm{x}_{\mathrm{i}}, \mathrm{y}_{\mathrm{i}}$ ), and the weights W .
- Normally we use backpropagation to compute the gradient of the cost function with respect to W
- We can also compute it with respect to input $x_{i}$ (useful for visualization)


## Gradients and partial derivatives

$$
\begin{aligned}
& f(x, y)=x y \rightarrow \frac{\partial f}{\partial x}=y \frac{\partial f}{\partial y}=x \\
& f(x, y)=x+y \rightarrow \frac{\partial f}{\partial x}=1 \frac{\partial f}{\partial y}=1 \\
& f(x, y)=\max (x, y) \rightarrow \frac{\partial f}{\partial x}=1(x \geq y) \frac{\partial f}{\partial y}=1(y \geq x)
\end{aligned}
$$

$f(x, y, z)=(x+y) z$ Let $\mathrm{q}=\mathrm{x}+\mathrm{y}$ and $f=q z$ and use the chain rule :
$\frac{\partial f}{\partial x}=\frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$

## Computational graph for $f=(x+y) z$



Z

$$
\text { Want: } \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}
$$

## Forward propagation of one sample



One sample, $x=-2, y=5, z=-4$

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

## Backwards propagation of gradients



Green numbers: forward propagation
Red numbers: backwards propagation

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Each gate: get input $x$ and $y$
Can compute output $x$ AND the local gradients of $z$


Green numbers: forward propagation
Red numbers: backwards propagation

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Green numbers: forward propagation
Red numbers: backwards propagation

## The sigmoid function

$$
f(w, x)=\frac{1}{1+e^{-\left(w_{0} x_{0}+w_{1} x_{1}+w_{2}\right)}}
$$

$$
\begin{array}{ccc}
f(x)=\frac{1}{x} & \rightarrow & \frac{d f}{d x}=-1 / x^{2} \\
f_{c}(x)=c+x & & \rightarrow \\
\frac{d f}{d x}=1 \\
f(x)=e^{x} & \rightarrow & \frac{d f}{d x}=e^{x} \\
f_{a}(x)=a x & & \frac{d f}{d x}=a
\end{array}
$$

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## The sigmoid gate

$$
\begin{gathered}
\sigma(x)=\frac{1}{1+e^{-x}} \\
\frac{d \sigma(x)}{d x}=\frac{e^{-x}}{\left(1+e^{-x}\right)^{2}}=\left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right)=(1-\sigma(x)) \sigma(x)
\end{gathered}
$$

Output: 0.73
Derivative of the sigmoid gate: $(1-0.73) 0.73=0.20$

## Forward and backward for a single neuron

```
w = [2,-3,-3] # assume some random weights and data
x = [-1, -2]
# forward pass
dot = w[0]*x[0] + w[1]*x[1] + w[2]
f = 1.0 / (1 + math.exp(-dot)) # sigmoid function
# backward pass through the neuron (backpropagation)
ddot = (1 - f) * f # gradient on dot variable, using the sigmoid gradient derivation
dx = [w[0] * ddot, w[1] * ddot] # backprop into x
dw = [x[0] * ddot, x[1] * ddot, 1.0 * ddot] # backprop into w
# we're done! we have the gradients on the inputs to the circuit
```


## A more tricky example

$$
f(x, y)=\frac{x+\sigma(y)}{\sigma(x)+(x+y)^{2}}
$$

- Stage the forward pass into simple operations that we now the derivative of:

```
x = 3# example values
```



## A more tricky example

$$
f(x, y)=\frac{x+\sigma(y)}{\sigma(x)+(x+y)^{2}}
$$

- In the backwards pass: compute the derivative of all these terms:

```
# backprop f = num * invden
dnum = invden # gradient on numerator # (8)
dinvden = num
# (8)
    # backprop invden = 1.0 / den
dden = (-1.0 / (den**2)) * dinvden
# backprop den = sigx + xpysqr
dsigx = (1) * dden #(6)
dxpysqr = (1) * dden #(6)
# backprop xpysqr = xpy**2 
# backprop xpy = x + y 
dy = (1) * dxpy # (4)
# backprop sigx = 1.0 / (1 + math.exp (-x))
dx += ((1 - sigx) * sigx) * dsigx # Notice += !! See notes below # (3)
# backprop num = x + sigy
dx += (1) * dnum
# (2)
dsigy = (1) * dnum #(2)
# backprop sigy = 1.0 / (1 + math.exp (-y))
dy += ((1 - sigy) * sigy) * dsigy
```

2

## Patterns in backward flow

add gate: gradient distributor max gate: gradient router mul gate: gradient.... «switcher»

Remark on multiplier gate: If a gate get one large and one small input, backprop will use the big input to cause a large change on the small input, and vice versa.
This is partly why feature scaling is important

## Gradients add at branches

## Next week:

- Next week: Backpropagation in detail
- Vectorized implementation of backpropagation
- Reading material:
- http://cs231n.github.io/optimization-2/
- Additional optional material:
- Lecture on backpropagation in Coursera Course on Machine Learning (Andrew Ng)
- http://yann.lecun.com/exdb/publis/pdf/lecun-98b.pdf
- http://colah.github.io/posts/2015-08-Backprop/
- http://neuralnetworksanddeeplearning.com/chap2.html

