# Lecture 4: Backpropagation and Neural Networks (part 1) 

Tuesday January 31, 2017

## Announcements!

- If you are adversely affected by immigration ban, please talk to me about accommodations
- Send in paper choices by tonight
- Should be able to run Jupyter server on Tufts was and network machines now
- (deep-venv)> pip install --upgrade jupyter
- hw1 deadline in two days - Thurs Feb 2: Don't forget to read the course notes.
- Redo calculation of dL/dW for hinge loss


## Python/Numpy of the Day

- y_pred = scores.argmax(axis=1)
- inds $=$ np.random.choice(X.shape[0],batch_size)
- randomly select $N$ numbers in a range,
- useful for subsampling
- [: , np.newaxis]
- reshapes matrices of size ( $N$, ) to size ( $N, 1$ )


## Where we are...

$$
\begin{array}{lc}
s=f(x ; W)=W x & \text { scores function } \\
L_{i}=\sum_{j \neq y_{i}} \max \left(0, s_{j}-s_{y_{i}}+1\right) & \text { SVM loss } \\
L=\frac{1}{N} \sum_{i=1}^{N} L_{i}+\sum_{k} W_{k}^{2} & \text { data loss + regularization } \\
\text { want } \nabla_{W} L &
\end{array}
$$

## Optimization


(image credits to Alec Radford)

## Gradient Descent

$$
\frac{d f(x)}{d x}=\lim _{h \rightarrow 0} \frac{f(x+h)-f(x)}{h}
$$

Numerical gradient: slow :(, approximate :(, easy to write :) Analytic gradient: fast :), exact :), error-prone :(

In practice: Derive analytic gradient, check your implementation with numerical gradient

## Hinge Loss Gradient wrt Weights W

$$
L_{i}=\sum_{j \neq y_{i}}\left[\max \left(0, w_{j}^{T} x_{i}-w_{y_{i}}^{T} x_{i}+\Delta\right)\right]
$$

- We want the Jacobian Matrix of all gradients
- partial derivatives of all output dimensions by all input dimensions

$$
\nabla w L=\left[\begin{array}{cccc}
\nabla w_{1} L_{1} & \ldots & \ldots & \nabla w_{1} L_{N} \\
\vdots & \nabla w_{j} L_{i} & \ddots & \vdots \\
\nabla w_{k} L_{1} & \ldots & \ldots & \nabla w_{k} L_{N}
\end{array}\right]
$$

For all rows of $d W$ where the row corresponds to the
GT value for that training instance, i.e. $\mathrm{j}=\mathrm{y}_{\mathrm{i}}$

$$
\nabla_{w_{r_{i}}} L_{i}=-\left(\sum_{j \neq y_{i}} \mathbb{1}\left(w_{j}^{T} x_{i}-w_{y_{i}}^{T} x_{i}+\Delta>0\right)\right) x_{i}
$$

For all rows of $d W$ where $j \neq y_{i}$

$$
\nabla_{w_{j}} L_{i}=1\left(w_{j}^{T} x_{i}-w_{y_{i}}^{T} x_{i}+\Delta>0\right) x_{i}
$$

## Softmax Loss Gradient wrt Score S

* note change of subscripts from last slide

$$
\begin{aligned}
& a_{j}=w_{j}^{T} x_{j} \\
& S_{j}=\frac{e^{a_{j}}}{\sum_{k=1}^{N} e^{a_{k}}} \quad \forall j \in 1 \ldots N \\
& \frac{\partial S_{i}}{\partial a_{j}}=\frac{\partial \frac{e^{a_{i}}}{\sum_{k=1}^{e} e^{a_{k}}}}{\partial a_{j}} \\
& \nabla a_{j} S_{i}, \text { when } i=j \\
& \frac{\partial \frac{e^{a_{i}}}{\sum_{k=1}^{e^{a_{k}}}}}{\partial a_{j}}=\frac{e^{a_{i}} \Sigma-e^{a_{j}} e^{a_{i}}}{\Sigma^{2}} \\
& =\frac{e^{a_{i}}}{\Sigma} \frac{\Sigma-e^{a_{j}}}{\Sigma} \\
& =S_{i}\left(1-S_{j}\right) \\
& \nabla a_{j} S_{i} \text {, when } i \neq j
\end{aligned}
$$

$$
\begin{aligned}
& =-\frac{e^{a_{j}}}{\Sigma} \frac{e^{a_{i}}}{\Sigma} \\
& =-S_{j} S_{i}
\end{aligned}
$$ please see original notes.

$$
\nabla a_{j} S_{i}=S_{i}\left(\mathbb{1}(i=j)-S_{j}\right)
$$

## Softmax Loss Gradient wrt Score S

$$
a_{j}=w_{j}^{T} x_{j}
$$

$S_{j}=\frac{e^{a_{j}}}{\sum_{k=1}^{N} e^{a_{k}}} \quad \forall j \in 1 . . N$

$$
\nabla a_{j} S_{i}=S_{i}\left(\mathbb{1}(i=j)-S_{j}\right)
$$

$$
\nabla S_{i} L=\frac{\partial}{\partial S_{i}}-\log \left(S_{i}\right)=S_{j}-\mathbb{1}(i=j)
$$

$$
\nabla W_{j} L=\frac{\partial L}{\partial S_{i}} * \frac{\partial S_{i}}{\partial W_{j}}=\left(S_{j}-\mathbb{1}(i=j)\right) x_{i}
$$

Skipping some steps for space, please see original notes.

## Computational Graph



## Convolutional Network (AlexNet)



$$
\begin{aligned}
& f(x, y, z)=(x+y) z \\
& \text { e.g. } x=-2, y=5, z=-4
\end{aligned}
$$



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$$
q=x+y \quad \frac{\partial q}{\partial x}=1, \frac{\partial q}{\partial y}=1
$$



$$
f=q z \quad \frac{\partial f}{\partial q}=z, \frac{\partial f}{\partial z}=q
$$

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

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Chain rule:

$$
\frac{\partial f}{\partial y}=\frac{\partial f}{\partial q} \frac{\partial q}{\partial y}
$$



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



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$\begin{array}{lllll}f(x)=e^{x} & \rightarrow & \frac{d f}{d x}=e^{x} & f(x)=\frac{1}{x} & \rightarrow\end{array}$

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| $f(x)=e^{x}$ |  | $\rightarrow$ | $\frac{d f}{d x}=e^{x}$ | $f(x)=\frac{1}{x}$ | $\rightarrow$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $f_{a}(x)=a x$ | $\rightarrow$ | $\frac{d f}{d x}=a$ | $f_{c}(x)=c+x$ | $\frac{d f}{d x}=-1 / x^{2}$ |  |
|  |  | $\rightarrow$ | $\frac{d f}{d x}=1$ |  |  |

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\end{array}
$$

sigmoid function

$$
\begin{aligned}
& f(w, x)=\frac{1}{1+e^{-\left(w_{0} x_{0}+w_{1} x_{1}+w_{2}\right)}} \\
& \sigma(x)=\frac{1}{1+e^{-x}} \\
& \frac{d \sigma(x)}{d x}=\frac{e^{-x}}{\left(1+e^{-x}\right)^{2}}=\left(\frac{1+e^{-x}-1}{1+e^{-x}}\right)\left(\frac{1}{1+e^{-x}}\right)=(1-\sigma(x)) \sigma(x)
\end{aligned}
$$

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$$
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\end{aligned}
$$

## Patterns in backward flow



## Gradients add at branches

## Implementation: forward/backward API



Graph (or Net) object. (Rough psuedo code)

```
class ComputationalGraph(object):
    #..
    def forward(inputs):
        # 1. [pass inputs to input gates...]
        # 2. forward the computational graph:
        for gate in self.graph.nodes_topologically_sorted():
        gate.forward()
        return loss # the final gate in the graph outputs the loss
    def backward():
        for gate in reversed(self.graph.nodes_topologically_sorted()):
        gate.backward() # little piece of backprop (chain rule applied)
        return inputs_gradients
```


## Implementation: forward/backward API


class MultiplyGate(object):
def forward $(x, y)$ :
$z=x^{*} y$
return $z$
def backward(dz):
\# $\mathrm{dx}=\ldots$ \#todo
\# dy = . . . \#todo
return [dx, dy]


$$
\frac{\partial L}{\partial x}
$$

## Implementation: forward/backward API



```
class MultiplyGate(object):
    def forward(x,y):
        z = x*y
        self.x = x # must keep these around!
        self.y = y
        return z
def backward(dz):
    dx = self.y * dz # [dz/dx * dL/dz]
    dy = self.x * dz # [dz/dy * dL/dz]
    return [dx, dy]
```


## (x,y,z are scalars)

## Example: Torch Layers



* Original slides borrowed from Andrej Karpathy and Li Fei-Fei, Stanford cs231n

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## Example: Torch Layers


self, inplase - ip or false
If (ip and type(1p) $\sim$ 'boolean') then
error('in-place flag must be boolean')
end
function Mulconstant aplateoutput(input)
function MulConst ant supolateoutput (iqput)
If self, inplace thes
isput:sul(self.constant_walar)
salf_output = input
*1se
salf_outpot:resizaAs(inpot)
self_output :copy(input)
self_outpot:copy(input)
self_output imul(self.constant_scalar)
end
retarn self.output
function MulConstant :upolatebraalnput(1aput, graobutput)
If self.grasInput then
if self. Inplace then
gradoutput: :mil(self_constant_scalar)
self-gradInput = gradoutput
restore previows ingut valos
Anput:alv(selr.conatant_acalar)
else
self.gradInput : resizedas(grasoutput)
self.gradInput icopy(grasoutput)
self_gradinput: inul(self.constant_scalar)
and
return self.gradloput
(nd

## Example：Caffe Layers

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## Caffe Sigmoid Layer


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vold Shufflecotype* botton_datd, Dtype* top dota, const ist itellusize,
conat bool forward, const int* shiffle orster, const int count) i
I/ data shape is expected to be the shope (count, M) of the blob
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for (int $1=0 ; 1 \times$ count; $+*$ i) $i$
for (int $j=0 ; j<i$ ten_size; + +1) $\{$ if (formard) ?
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$/ /$ Oneck there is only one botton laydr
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If Make a vector of ordered Ind
for (int ief; ispottom(e)-shhope(1); iv*) shuffle_order.push_bock(1);
// Mirsenne twistar initialized with inpot seed
std::mt19917 pen(shuffle_seed.)
std::Shuffle(shuffle_order,beginO. ihuffle_order, end). gen):
// copy rondomized shuffle order to leyer nerber variable shuffie_order.

for (int $1=0 ; 1 \times$ shiffle_order,size (); $1++$ ) ? Shuffle_order_.wioble_qpu_doteC)[shuffle_order_-offset(i)] = shuffle_order[I]:
template stypenane Otyper
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const vectorellobotyper*st too) ?
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const int* shiffle_onder = shiffle_order_.cpu_data()

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victorcints orle_shope $=$ botton (el)-3shope ):
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top (0)->Reshape (new shape)

Otype* top_dato $=$ top $[$ ( )-xmutobte_cpu_doto .
const int* ithifla_order = shuffle_order_-cpu_datac):
bool formard = false;
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coult),

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shus_CPU(Shufflalayer'):
fendif
TNSTANTtate_Cuss (5huffletoyer):
itcisterlattrclass(Shuffle);
// namespace caffe

Gradients for vectorized code ( $x, y, z$ are now vectors)

This is now the Jacobian matrix (derivative of each element of $z$ w.r.t. each element of $x$ )

## $\frac{\partial L}{\partial z}$ <br> gradients

## Vectorized operations



## Vectorized operations

$$
\frac{\partial L}{\partial x}=\frac{\partial f}{\partial x} \frac{\partial L}{\partial f}
$$

Jacobian matrix
input vector


## Q: what is the size of the Jacobian matrix?

4096-d

output vector

## Vectorized operations

$$
\frac{\partial L}{\partial x}=\frac{\partial f}{\partial x} \frac{\partial L}{\partial f}
$$



## Vectorized operations

in practice we process an entire minibatch (e.g. 100) of examples at one time:
$1004096-d$
input vectors


## Assignment: Writing SVM/Softmax Stage your forward/backward computation!



```
loss = data_loss + reg_loss
# backward pass (we have 5 lines)
dmargins = # ... (optionally, we go direct to dscores)
dscores = #...
dW = #...
```


## Summary so far

- neural nets will be very large: no hope of writing down gradient formula by hand for all parameters
- backpropagation = recursive application of the chain rule along a computational graph to compute the gradients of all inputs/parameters/ intermediates
- implementations maintain a graph structure, where the nodes implement the forward() / backward().
- forward: compute result of an operation and save any intermediates needed for gradient computation in memory
- backward: apply the chain rule to compute the gradient of the loss function with respect to the inputs.


## Neural Network so far:

(Before) Linear score function:

$$
f=W x
$$

## Neural Network so far:

(Before) Linear score function:
(Now) 2-layer Neural Network

$$
f=W x
$$

$f=W_{2} \max \left(0, W_{1} x\right)$

## Neural Network so far:

(Before) Linear score function:
(Now) 2-layer Neural Network $\quad f=W_{2} \max \left(0, W_{1} x\right)$


## Neural Network so far:


(Before) Linear score function: $\quad f=W \boldsymbol{x}$
(Now) 2-layer Neural Network $\quad f=W_{2} \max \left(0, W_{1} x\right)$


## Neural Network so far:

(Before) Linear score function: $\quad f=W x$
(Now) 2-layer Neural Network $f=W_{2} \max \left(0, W_{1} x\right)$ or 3-layer Neural Network

$$
f=W_{3} \max \left(0, W_{2} \max \left(0, W_{1} x\right)\right)
$$

## Full implementation of training a 2-layer Neural Network needs ~11 lines:

1. 
2. 
3. 
4. 
5. 
6. 
7. 
8. 
9. 
10. 
11. 
```
X = np.array([ [0,0,1],[0,1,1],[1,0,1],[1,1,1] ])
y = np.array([[0,1,1,0]]).T
syn0 = 2*np.random.random((3,4)) - 1
syn1 = 2*np.random.random((4,1)) - 1
for j in xrange(60000):
    l1 = 1/(1+np.exp(-(np.dot(X,syn0))))
    12 = 1/(1+np.exp (-(np.dot (11,syn1))))
    l2_delta = (y - l2)* (12* (1-12))
    l1_delta = l2_delta.dot(syn1.T) * (11 * (1-11))
syn0 += X.T.dot(11_delta)

Backward
```

syn1 += l1.T.dot(12_delta)

```
```

syn1 += l1.T.dot(12_delta)

```
backprop of derivative
from @iamtrask, http://iamtrask.github.io/2015/07/12/basic-python-network/

\section*{Assignment: Writing 2layer Net Stage your forward/backward computation!}
```


# receive W1,W2,b1,b2 (weights/biases), X (data)

# forward pass:

h1 = \#... function of X,W1,b1
scores = \#... function of h1,W2,b2
loss = \#... (several lines of code to evaluate Softmax loss)

# backward pass:

dscores = \#...
dh1,dW2,db2 = \#...
dW1,db1 = \#...

```






Be very careful with your Brain analogies:

\section*{Biological Neurons:}
- Many different types
- Dendrites can perform complex nonlinear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate

\section*{Activation Functions}

\section*{Leaky ReLU} \(\max (0.1 x, x)\)

\section*{Sigmoid}
\[
\sigma(x)=1 /\left(1+e^{-x}\right)
\]

\(\boldsymbol{t a n h} \tanh (x)\)


Maxout \(\max \left(w_{1}^{T} x+b_{1}, w_{2}^{T} x+b_{2}\right)\) ELU \(\quad f(x)= \begin{cases}x \\ a(\exp (x)-1) & \text { if } i x>0 \\ i x \leq 0\end{cases}\)


\section*{Neural Networks: Architectures}


\section*{Example Feed-forward computation of a Neural Network}
```

class Neuron:
\#
def neuron_tick(inputs):
""" assume inputs and weights are 1-D numpy arrays and bias is a number """
cell_body_sum = np.sum(inputs * self.weights) + self.bias
firing_rate = 1.0 / (1.0 + math.exp(-cell body sum)) \# sigmoid activation function
return firing_rate

```

We can efficiently evaluate an entire layer of neurons.

\section*{Example Feed-forward computation of a Neural Network}

```


# forward-pass of a 3-layer neural network:

f = lambda x: 1.0/(1.0 + np.exp(-x)) \# activation function (use sigmoid)
x = np.random.randn(3, 1) \# random input vector of three numbers (3x1)
h1= f(np.dot(W1, x) + b1) \# calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) \# calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 \# output neuron (1\times1)

```

\section*{Setting the number of layers and their sizes}

more neurons \(=\) more capacity

Do not use size of neural network as a regularizer. Use stronger regularization instead:

(you can play with this demo over at ConvNetJS: http://cs.stanford.edu/people/ karpathy/convnetjs/demo/classify2d.html)

\section*{Summary}
- we arrange neurons into fully-connected layers
- the abstraction of a layer has the nice property that it allows us to use efficient vectorized code (e.g. matrix multiplies)
- neural networks are not really neural
- neural networks: bigger = better (but might have to regularize more strongly)

\section*{Next Lecture:}

\section*{More than you ever wanted to know about Neural Networks and how to train them.}```

