## Lecture 4: <br> Backpropagation and Neural Networks

## Administrative

## Assignment 1 due Thursday April 20, 11:59pm on Canvas

## Administrative

## Project: TA specialities and some project ideas are posted on Piazza

## Administrative

## Google Cloud: All registered students will receive an email this week with instructions on how to redeem $\$ 100$ in credits

## Where we are...

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

want $\nabla_{W} L$

## Optimization



```
# Vanilla Gradient Descent
while True:
    weights_grad = evaluate_gradient(loss_fun, data, weights)
    weights += - step_size * weights_grad # perform parameter update
```


## 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

## Computational graphs



## Convolutional network (AlexNet)



## Neural Turing Machine

input image


Figure reproduced with permission from a Twitter post by Andrej Karpathy.

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April 13, 2017

## Neural Turing Machine



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Backpropagation: a simple example

$$
\begin{aligned}
& f(x, y, z)=(x+y) z \\
& \text { e.g. } x=-2, y=5, z=-4
\end{aligned}
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q=x+y \quad \frac{\partial q}{\partial x}=1, \frac{\partial q}{\partial y}=1
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$$
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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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$


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

Backpropagation: a simple example

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

Chain rule:

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









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


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

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[local gradient] x [upstream gradient]

$$
x 0:[2] \times[0.2]=0.4
$$

$$
\text { w0: }[-1] \times[0.2]=-0.2
$$

$$
\text { w2 } \frac{-3.00}{0.20}
$$

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

$$
\sigma(x)=\frac{1}{1+e^{-x}}
$$

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



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$$

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## Patterns in backward flow

add gate: gradient distributor


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add gate: gradient distributor
Q : What is a max gate?


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## Patterns in backward flow

add gate: gradient distributor
max gate: gradient router


## Patterns in backward flow

add gate: gradient distributor
max gate: gradient router
Q: What is a mul gate?


## Patterns in backward flow

add gate: gradient distributor max gate: gradient router mul gate: gradient switcher


## Gradients add at branches

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## Gradients for vectorized code ( $x, y, z$ are <br> 

## Vectorized operations



## Vectorized operations

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

Jacobian matrix

4096-d
input vector
Q: what is the size of the Jacobian matrix?


## Vectorized operations

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\frac{\partial L}{\partial x}=\frac{\partial f}{\partial x} \frac{\partial L}{\partial f}
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Jacobian matrix

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input vector
Q: what is the size of the Jacobian matrix? [4096 x 4096!]

## Vectorized operations



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Jacobian matrix

4096-d
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$$
\in \mathbb{R}^{n} \in \mathbb{R}^{n \times n}
$$

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A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$
$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right] \mathbf{W}$


$$
\begin{aligned}
& q=W \cdot x=\left(\begin{array}{c}
W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\
\vdots \\
W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}
\end{array}\right) \\
& f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2}
\end{aligned}
$$

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q=W \cdot x=\left(\begin{array}{cc}
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\vdots \\
W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}
\end{array}\right) \quad \frac{\partial f}{\partial q_{i}}=2 q_{i}, \quad \nabla_{q} f=2 q
$$

$$
f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2}
$$

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$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right] \mathbf{W}$


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W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}
\end{array}\right) \\
f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2} & =\begin{aligned}
\frac{\partial f}{\partial W_{i, j}} & =\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial W_{i, j}} \\
& \left.=\sum_{k}\right)\left(\mathbf{1}_{k=i} x_{j}\right) \\
& =2 q_{i} x_{j}
\end{aligned} \text { ( } r l
\end{array}
$$

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$$
\begin{aligned}
& \text { A vectorized example: } f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2} \\
& q=W \cdot x=\left(\begin{array}{c}
W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\
\vdots \\
W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}
\end{array}\right) \\
& \frac{\partial f}{\partial W_{i, j}}=\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial W_{i, j}} \\
& =\sum_{k}\left(2 q_{k}\right)\left(\mathbf{1}_{k=i} x_{j}\right) \\
& f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2} \\
& =2 \stackrel{k}{q}{ }_{i} x_{j}
\end{aligned}
$$

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> A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$ $\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$ 0.8 ]W
> $\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{\mathrm{W}}$

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A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$ $\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$ W

$$
\nabla_{W} f=2 q \cdot x^{T}
$$

$\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{\mathrm{W}}$
$\left.\left[\begin{array}{l}0.2 \\ 0.4\end{array}\right]_{\mathrm{X}}^{(2)} \xrightarrow[\frac{2 q_{k}}{0.44}]{0.52}\right] \rightarrow \mathbf{1}_{k=i} x_{j}$
Always check: The gradient with respect to a variable should have the same shape as the variable
$q=W \cdot x=\left(\begin{array}{c}W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\ \vdots \\ W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}\end{array}\right)$

$$
\begin{aligned}
\frac{\partial f}{\partial W_{i, j}} & =\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial W_{i, j}} \\
& =\sum_{k}\left(2 q_{k}\right)\left(\mathbf{1}_{k=i} x_{j}\right) \\
& =2 q_{i} x_{j}
\end{aligned}
$$

A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$
$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$
$\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{W}$

$q=W \cdot x=\left(\begin{array}{c}W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\ \vdots \\ W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}\end{array}\right)$
$\frac{\partial q_{k}}{\partial x_{i}}=W_{k, i}$
$f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2}$

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A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$
$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$
$\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{\mathrm{W}}$

$q=W \cdot x=\left(\begin{array}{c}W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\ \vdots \\ W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}\end{array}\right)$

$$
\begin{aligned}
\frac{\partial q_{k}}{\partial x_{i}} & =W_{k, i} \\
\frac{\partial f}{\partial x_{i}} & =\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial x_{i}} \\
& =\sum_{k} 2 q_{k} W_{k, i}
\end{aligned}
$$

Fei-Fei Li \& Justin Johnson \& Serena Yeung Lecture 4-72
A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$
$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$
$\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{W}$
$\left[\begin{array}{c}0.2 \\ 0.4\end{array}\right]$
$\left[\begin{array}{c}-0.112 \\ 0.636\end{array}\right] \mathrm{x}$
$q=W \cdot x=\left(\begin{array}{c}W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\ \vdots \\ W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}\end{array}\right)$
$f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2}$

$$
\begin{aligned}
\frac{\partial q_{k}}{\partial x_{i}} & =W_{k, i} \\
\frac{\partial f}{\partial x_{i}} & =\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial x_{i}} \\
& =\sum_{k} 2 q_{k} W_{k, i}
\end{aligned}
$$

Fei-Fei Li \& Justin Johnson \& Serena Yeung Lecture 4-73
A vectorized example: $f(x, W)=\|W \cdot x\|^{2}=\sum_{i=1}^{n}(W \cdot x)_{i}^{2}$
$\left[\begin{array}{cc}0.1 & 0.5 \\ -0.3 & 0.8\end{array}\right]$
$\left[\begin{array}{ll}0.088 & 0.176 \\ 0.104 & 0.208\end{array}\right]^{W}$
$\left[\begin{array}{c}0.2 \\ 0.4\end{array}\right]$
$\left[\begin{array}{c}-0.112 \\ 0.636\end{array}\right] \mathrm{x}$
$q=W \cdot x=\left(\begin{array}{c}W_{1,1} x_{1}+\cdots+W_{1, n} x_{n} \\ \vdots \\ W_{n, 1} x_{1}+\cdots+W_{n, n} x_{n}\end{array}\right)$
$f(q)=\|q\|^{2}=q_{1}^{2}+\cdots+q_{n}^{2}$

$$
\begin{aligned}
\frac{\partial q_{k}}{\partial x_{i}} & =W_{k, i} \\
\frac{\partial f}{\partial x_{i}} & =\sum_{k} \frac{\partial f}{\partial q_{k}} \frac{\partial q_{k}}{\partial x_{i}} \\
& =\sum_{k} 2 q_{k} W_{k, i}
\end{aligned}
$$

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## Modularized 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
```


## Modularized implementation: forward / backward API



## Modularized implementation: forward / backward API



## Example：Caffe layers

| Branch：master＊caffe／src／caffe／layers／ |  | Upload files | Find file | History | O ludnn＿｜cr＿ayer．cpp | dismantle layer headers | a year ago |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ．Shelhamer committed on Cithub Merge pull request \＃4630 from BlGenelload＿hdff＿fix－．．－Latest commit e687a71 21 days ago |  |  |  |  | R Cudnn＿lcn＿ayer．cu | dismantle layer headers | a year ago |
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| 目 argmax＿layer．cpp | dismantle layer headers | a year ago |  |  | 目 Cudnn＿relu＿layer．c．cp | Add cuDNN v5 support，drop cuDNn v3 support | 11 months ago |
| 目 base＿conv＿layer．cpp | enable dilated deconvolution |  |  |  | 目cudn＿＿relu＿layer．cu | Add cubNn v5 support，drop cuDNN v3 support | 11 montrs ago |
|  |  |  |  |  | 目cudnn＿sigmoid＿layer．cpp | Add cuDNN v5 support，drop cuDNN v3 support | 11 months ago |
| 目 base＿data＿layer．cpp | Using default from proto for prefetch | 3 months ago |  |  |  | Add cubNn v5 support，drop cuDNN v3 support | 11 months ago |
| 目 base＿data＿layer．cu | Switched multi－GPU to NCCL | 3 months ago |  |  | 目cudnn＿softmax＿layer．cpp | dismantil layer headers | a year ago |
| －${ }_{\text {B batch＿norm＿layer．cpp }}$ | Add missing spaces besides equal signs in batch＿norm＿layer．cpp | 4 months ago |  |  | 目cudnn＿softmax layer．cu | dismantle layer headers | a year ago |
| 目batch＿norm＿layer．cu | dismantle layer headers | a year ago |  |  | O Cudnn＿tanh＿layer．cpp | Add cuDNN V5 support，drop cuDNN v3 support | 11 months ago |
| －batch＿reindex＿layer．cpp | dismantle layer headers | a year ago |  |  | Oloudnn＿tanh＿layer．cu | Add cuDNN v5 support，drop cuDNN v3 support | ${ }^{11}$ months ago |
| 目 batch＿reindex＿layer．cu | dismantle layer headers | a year ago |  |  |  | Switched multi－GPU to NCCL | 3 months ago |
| 目 bias＿layer．cpp | Remove incorrect cast of gemm int arg to Dtype in BiasLayer | a year ago |  |  | 目deconv＿layer．cpp | enable dilated deconvolution | a year ago |
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| 目bonll＿ayer．cpp | dismantle layer headers | a year ago |  |  | 目dropout＿ayer．cpp | supporting $N$－D Blobs in Dropout layer Reshape | a year ago |
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| － Contrastive＿loss＿layer．cu | dismantle layer headers | a year ago |  |  | 目elu＿layer．cpp | ELU layer with basic tests | a year ago |
| 目conv＿layer．cpp | add support for 2 D dilated convolution | a year ago |  |  | 目embec＿layer．cpp | dismantil layer headers | a year ago |
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| 目crop＿layer．cpp | remove redundant operations in Crop layer（\＃5138） | 2 months ago |  |  | 目euclidean＿loss＿layer．cpp | dismantele layer headers | a year ago |
| 目crop＿layer．cu | remove redundant operations in Crop layer（\＃5138） | 2 months ago |  |  | 目eucilidean＿loss＿layer．cu | dismantle layer headers | a year ago |
| 目cudnn＿conv＿layer．cpp | dismante leyer headers | a year ago |  |  | 目exp＿layer．cpp | Solving issue with exp layer with base e | $a$ year ago |
| 目 cudnn＿conv＿layer．cu | Add cuDNN v5 support，drop cuDNN v3 support | 11 months ago |  |  | 目exp．ayer．cu | dismantle layer headers | a year ago |

[^0]
## Caffe Sigmoid Layer


\#ifdef CPU_ONLY
\#ifdef CPU_ONLY
STUB_GPU(SigmoidLayer);
\#endif
INSTANTIATE_CLASS(SigmoidLayer);

## In Assignment 1: Writing SVM / Softmax

## Stage your forward/backward computation!

## E.g. for the SVM:

loss $=$ data_loss + reg_loss

\# forward pass (we have lines)

scores = \#...
margins = \#. .
data_loss = \#. . .
reg_loss = \#...

## Summary so far...

- neural nets will be very large: impractical to write 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() API
- 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


## Next: Neural Networks

Neural networks: without the brain stuff
(Before) Linear score function: $\quad f=W x$

Neural networks: without the brain stuff
(Before) Linear score function: $\quad f=W x$
(Now) 2-layer Neural Network $\quad f=W_{2} \max \left(0, W_{1} x\right)$

Neural networks: without the brain stuff
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Neural networks: without the brain stuff
(Before) Linear score function: $\quad f=W x$
(Now) 2-layer Neural Network $\quad f=W_{2} \max \left(0, W_{1} x\right)$


Neural networks: without the brain stuff
(Before) Linear score function: $\quad f=W x$
(Now) 2-layer Neural Network $\quad f=W_{2} \max \left(0, W_{1} x\right)$ 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 ~20 lines:

```
import numpy as np
from numpy.random import randn
N, D_in, H, D_out = 64, 1000, 100, 10
x, y = randn(N, D_in), randn(N, D_out)
w1, w2 = randn(D_in, H), randn(H, D_out)
for t in range(2000):
    h = 1/ (1 + np.exp(-x.dot(w1)))
    y_pred = h.dot(w2)
    loss = np.square(y_pred - y).sum()
    print(t, loss)
    grad_y_pred = 2.0 * (y_pred - y)
    grad_w2 = h.T.dot(grad_y_pred)
    grad_h = grad_y_pred.dot(w2.T)
    grad_w1 = x.T.dot(grad_h * h * (1 - h))
    w1 -= 1e-4 * grad_w1
    w2 -= 1e-4 * grad_w2
```


## In Assignment 2: Writing a 2-layer net

```
# 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 = #. . .
```



Impulses carried toward cell body


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Impulses carried toward cell body


Fei-Fei Li \& Justin Johnson \& Serena Yeung Lecture 4 - 92
April 13, 2017

Impulses carried toward cell body


Impulses carried toward cell body


## Be very careful with your brain analogies!

## Biological Neurons:

- Many different types
- Dendrites can perform complex non-linear computations
- Synapses are not a single weight but a complex non-linear dynamical system
- Rate code may not be adequate
[Dendritic Computation. London and Hausser]


## Activation functions

Sigmoid
$\sigma(x)=\frac{1}{1+e^{-x}}$

tanh
$\tanh (x)$


ReLU
$\max (0, x)$

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



## Maxout

$\max \left(w_{1}^{T} x+b_{1}, w_{2}^{T} x+b_{2}\right)$

ELU
$\begin{cases}x & x \geq 0 \\ \alpha\left(e^{x}-1\right) & x<0\end{cases}$


## Neural networks: Architectures



## 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.

## Example feed-forward computation of a neural network


hidden layer 1 hidden layer 2

```
# 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 (3\times1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4xl)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)
```


## 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
- Next time: Convolutional Neural Networks


[^0]:    Fei－Fei Li \＆Justin Johnson \＆Serena Yeung
    Lecture 4－78
    April 13， 2017

