# Lecture 7:

# Neural Networks Part 2

## Neural networks: the original linear classifier

(**Before**) Linear score function: 
$$f = Wx$$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

## Neural networks: 2 layers

(**Before**) Linear score function: 
$$f = Wx$$
(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$ 

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

(In practice we will usually add a learnable bias at each layer as well)

## Neural networks: also called fully connected network

(**Before**) Linear score function: 
$$f = Wx$$
  
(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$ 

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

"Neural Network" is a very broad term; these are more accurately called "fully-connected networks" or sometimes "multi-layer perceptrons" (MLP)

(In practice we will usually add a learnable bias at each layer as well)

## Neural networks: 3 layers

(**Before**) Linear score function: 
$$f = Wx$$
(**Now**) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$  or 3-layer Neural Network

$$f=W_3\max(0,W_2\max(0,W_1x))$$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H_1 \times D}, W_2 \in \mathbb{R}^{H_2 \times H_1}, W_3 \in \mathbb{R}^{C \times H_2}$$

(In practice we will usually add a learnable bias at each layer as well)

# Training Neural Networks

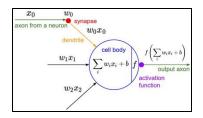
A bit of history...

The **Mark I Perceptron** machine was the first implementation of the perceptron algorithm.

The machine was connected to a camera that used 20×20 cadmium sulfide photocells to produce a 400-pixel image.

recognized letters of the alphabet

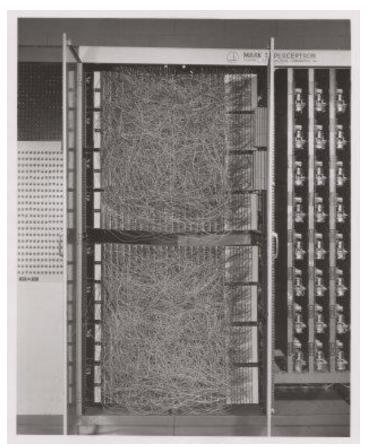
 $f(x) = \begin{cases} 1 & \text{if } w \cdot x + b > 0 \\ 0 & \text{otherwise} \end{cases}$ 

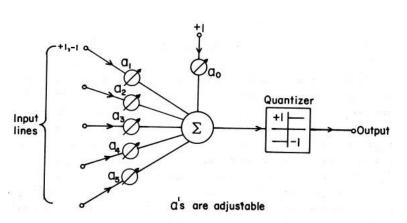


#### update rule:

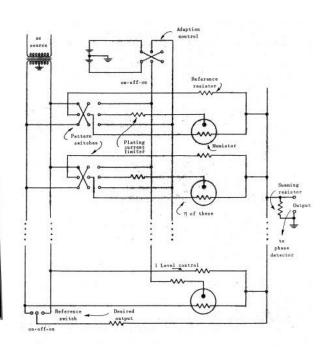
$$w_i(t+1) = w_i(t) + \alpha(d_j - y_j(t))x_{j,i}$$

Frank Rosenblatt, ~1957: Perceptron

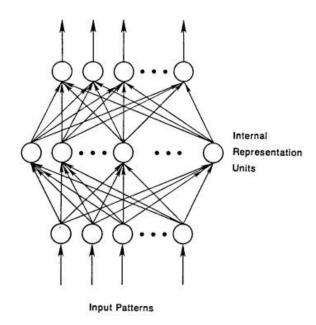








Widrow and Hoff, ~1960: Adaline/Madaline



To be more specific, then, let

$$E_{p} = \frac{1}{2} \sum_{i} (t_{pj} - o_{pj})^{2}$$
 (2)

be our measure of the error on input/output pattern p and let  $E = \sum E_p$  be our overall measure of the error. We wish to show that the delta rule implements a gradient descent in E when the units are linear. We will proceed by simply showing that

$$-\frac{\partial E_p}{\partial w_{ji}} = \delta_{pj} i_{pi},$$

which is proportional to  $\Delta_p w_{ji}$  as prescribed by the delta rule. When there are no hidden units it is straightforward to compute the relevant derivative. For this purpose we use the chain rule to write the derivative as the product of two parts: the derivative of the error with respect to the output of the unit times the derivative of the weight.

$$\frac{\partial E_p}{\partial w_{ji}} = \frac{\partial E_p}{\partial o_{pj}} \frac{\partial o_{pj}}{\partial w_{ji}}.$$
(3)

The first part tells how the error changes with the output of the jth unit and the second part tells how much changing  $w_{jj}$  changes that output. Now, the derivatives are easy to compute. First, from Equation 2

$$\frac{\partial E_p}{\partial o_{pj}} = -(t_{pj} - o_{pj}) = -\delta_{pj}. \tag{4}$$

Not surprisingly, the contribution of unit  $u_j$  to the error is simply proportional to  $\delta_{pj}$ . Moreover, since we have linear units,

$$o_{pj} = \sum_{i} w_{ji} l_{pi}, \qquad (5)$$

from which we conclude that

$$\frac{\partial o_{pj}}{\partial w_{ii}} = i_{pi}$$

Thus, substituting back into Equation 3, we see that

$$-\frac{\partial E_p}{\partial w_{ij}} = \delta_{pj} i_i \tag{6}$$

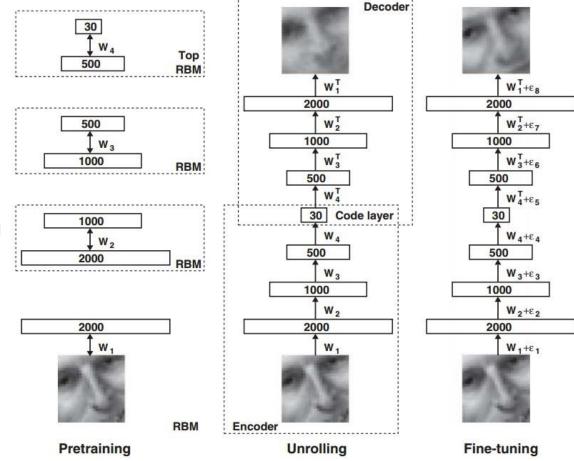
recognizable maths

Rumelhart et al. 1986: First time back-propagation became popular

[Hinton and Salakhutdinov 2006]

Reinvigorated research in Deep Learning

NOT NEURAL NETWORKS!



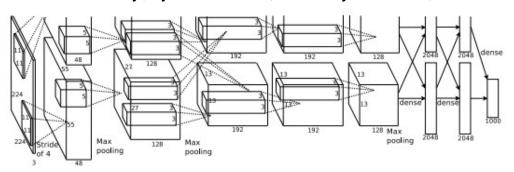
#### First strong results in neural nets

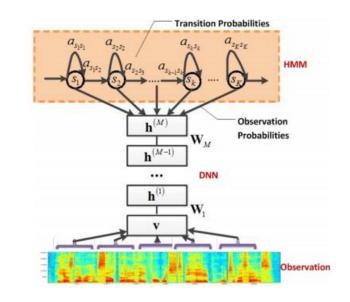
Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition

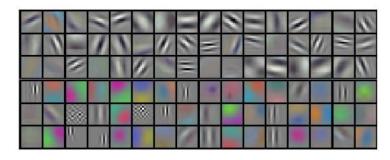
George Dahl, Dong Yu, Li Deng, Alex Acero, 2010

## Imagenet classification with deep convolutional neural networks

Alex Krizhevsky, Ilya Sutskever, Geoffrey E Hinton, 2012





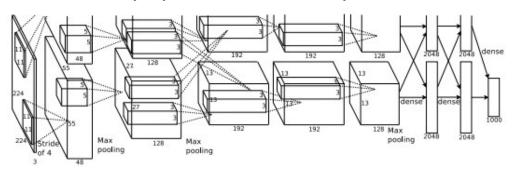


#### First strong results

Dropout training and ReLU's...

## Imagenet classification with deep convolutional neural networks

Alex Krizhevsky, Ilya Sutskever, Geoffrey E Hinton, 2012





# Overview

#### 1. One time setup

activation functions, preprocessing, weight initialization, regularization, gradient checking

## 1. Training dynamics

babysitting the learning process, parameter updates, hyperparameter optimization

#### 1. Evaluation

model ensembles

#### Activation Function: Non-linearities

(**Before**) Linear score function: f = Wx

(Now) 2-layer Neural Network  $f = W_2 \max(0, W_1 x)$ 

The function  $\max(0, z)$  is called the **activation function**.

Q: What if we try to build a neural network without one?

$$f = W_2 W_1 x$$

### Activation Function: Non-linearities

(**Before**) Linear score function: 
$$f = Wx$$

(**Now**) 2-layer Neural Network 
$$f = W_2 \max(0, W_1 x)$$

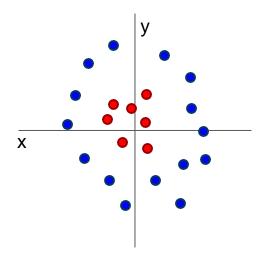
The function  $\max(0, z)$  is called the **activation function**.

**Q:** What if we try to build a neural network without one?

$$f = W_2 W_1 x$$
  $W_3 = W_2 W_1 \in \mathbb{R}^{C \times H}, f = W_3 x$ 

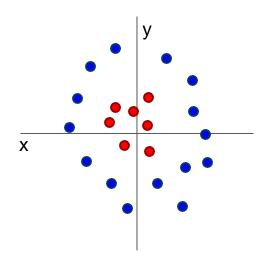
A: We end up with a linear classifier again!

## Why do we want non-linearity?

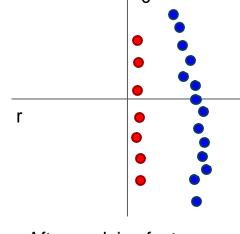


Cannot separate red and blue points with linear classifier

## Why do we want non-linearity?



$$f(x, y) = (r(x, y), \theta(x, y))$$



Cannot separate red and blue points with linear classifier

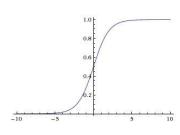
After applying feature transform, points can be separated by linear classifier

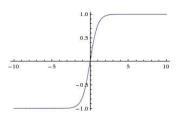
## **Sigmoid**

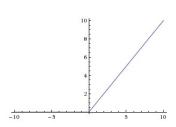
$$\sigma(x) = 1/(1 + e^{-x})$$

tanh tanh(x)

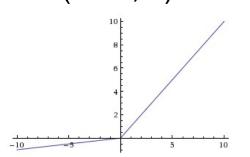
**ReLU** max(0,x)







# Leaky ReLU max(0.1x, x)

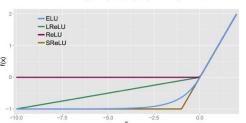


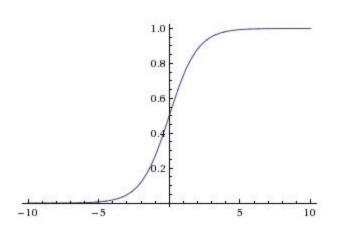
#### **Maxout**

ELU

$$\max(w_1^Tx+b_1,w_2^Tx+b_2)$$

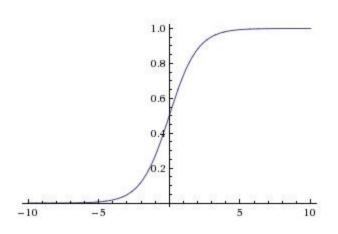
$$f(x) = \begin{cases} x & \text{if } x > 0\\ \alpha (\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$





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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron



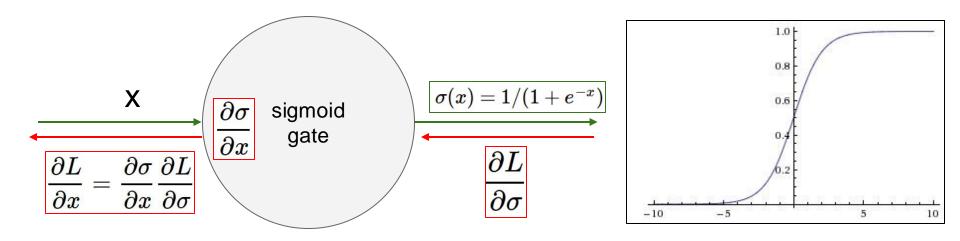
**Sigmoid** 

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

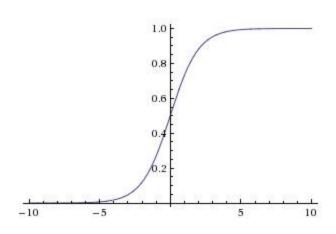
- Squashes numbers to range [0,1]
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#### 3 problems:

1. Saturated neurons "kill" the gradients



What happens when x = -10? What happens when x = 0? What happens when x = 10?



**Sigmoid** 

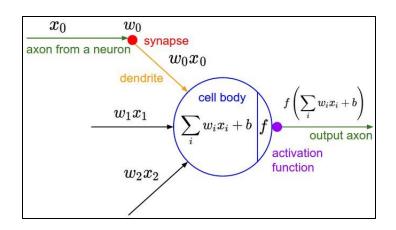
$$\sigma(x) = 1/(1 + e^{-x})$$

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

#### 3 problems:

- Saturated neurons "kill" the gradients
- 2. Sigmoid outputs are not zerocentered

Consider what happens when the input to a neuron (x) is always positive:



$$f\left(\sum_{\pmb{i}} w_{\pmb{i}} x_{\pmb{i}} + b
ight)$$

What can we say about gradients with respect to **w**?

$$f\left(\sum_i w_i x_i + b
ight)$$

$$\frac{\partial f}{\partial w}$$

$$y = \sum_{i} w_{i} x_{i}.$$
$$\frac{\partial f}{\partial w} = \frac{\partial f}{\partial y} \frac{\partial y}{\partial w}.$$

$$\frac{\partial y}{\partial w} = x.$$

$$\frac{\partial f}{\partial w} = \frac{\partial f}{\partial y} \frac{\partial y}{\partial w} = \frac{\partial f}{\partial y} x$$

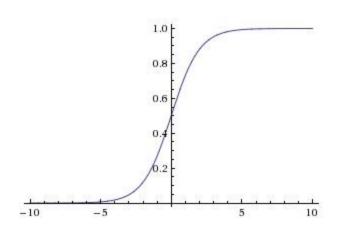
Consider what happens when the input to a neuron is

always positive...

$$f\left(\sum_{\pmb{i}} w_{\pmb{i}} x_{\pmb{i}} + b
ight)$$

What can we say about the gradients on **w**? Always all positive or all negative:(
(this is also why you want zero-mean data!)

allowed gradient update directions zig zag path allowed gradient update directions hypothetical optimal w vector



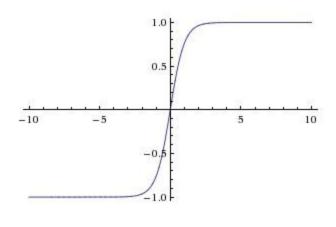
**Sigmoid** 

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

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

#### 3 problems:

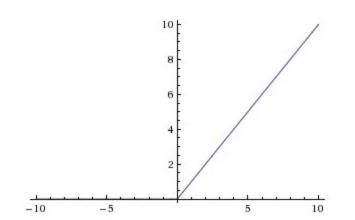
- 1. Saturated neurons "kill" the gradients
- 2. Sigmoid outputs are not zerocentered
- 3. exp() is a bit compute expensive



tanh(x)

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

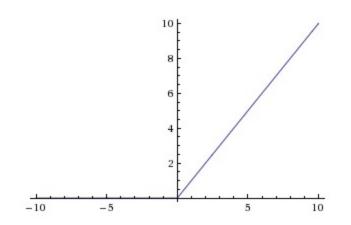
[LeCun et al., 1991]



**ReLU** (Rectified Linear Unit)

- Computes f(x) = max(0,x)
- Does not saturate (in +region)
- Very little computation
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

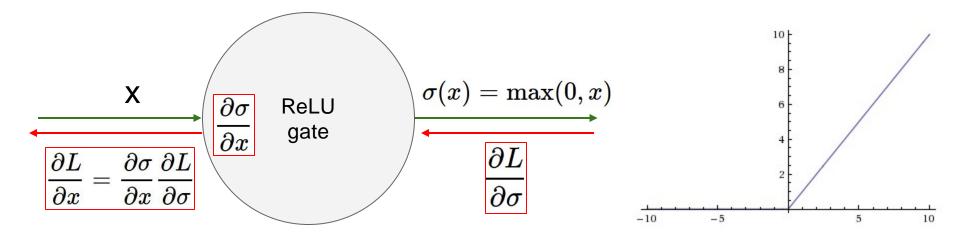
[Krizhevsky et al., 2012]



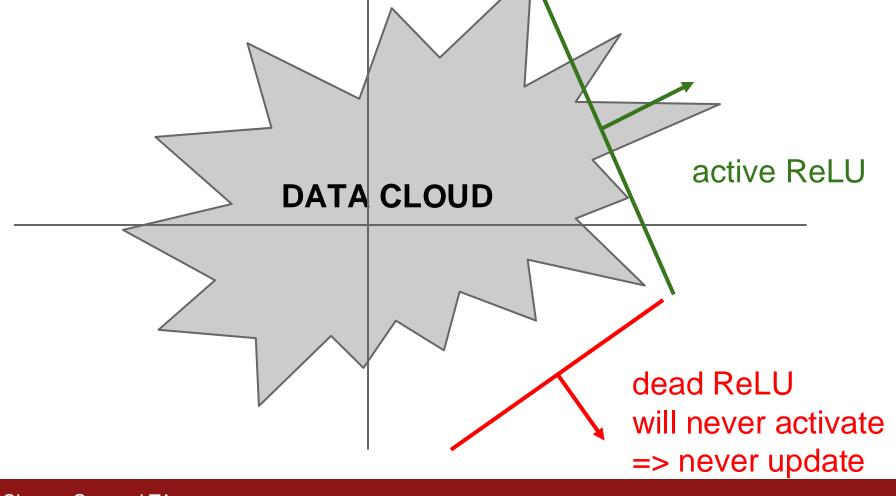
**ReLU** (Rectified Linear Unit)

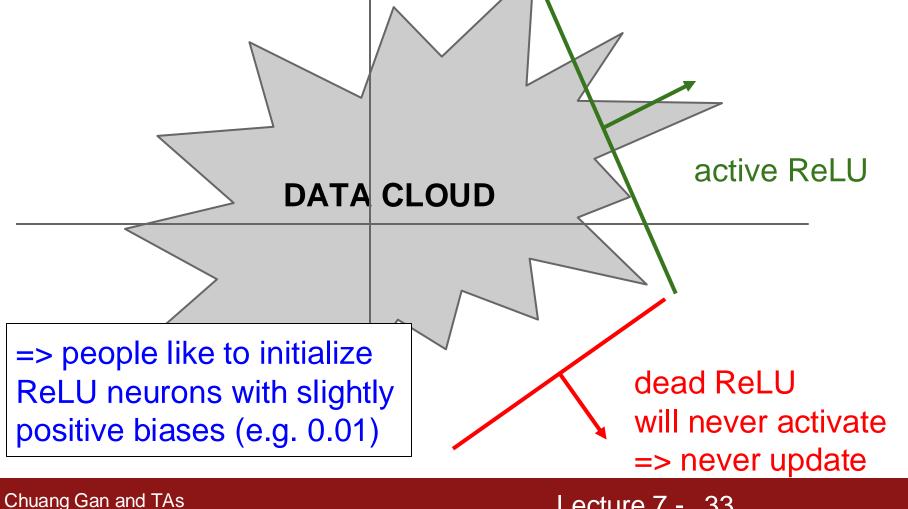
- Computes f(x) = max(0,x)
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?

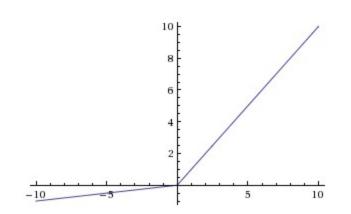


What happens when x = -10? What happens when x = 0? What happens when x = 10?





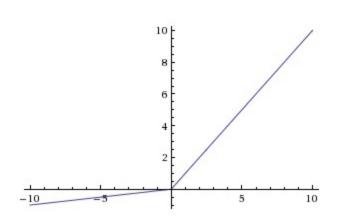
[Mass et al., 2013] [He et al., 2015]



- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- will not "die".

## Leaky ReLU

$$f(x) = \max(0.01x, x)$$

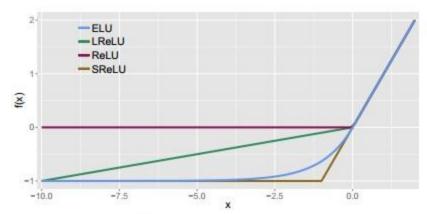


## **Leaky ReLU**

$$f(x) = \max(0.01x, x)$$

- Make up your own parametric rectifier! (Project idea!!!)
  - How about shifting the hinge?
  - How about shifting the slope?
  - How about changing the shape of the right side?
  - How about a diversity of ReLU's. What are pros and cons?

### **Exponential Linear Units (ELU)**



$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha (\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$

- Most benefits of ReLU
- Does not die
- Closer to zero mean outputs
- Computation requires exp()

#### Maxout "Neuron"

- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

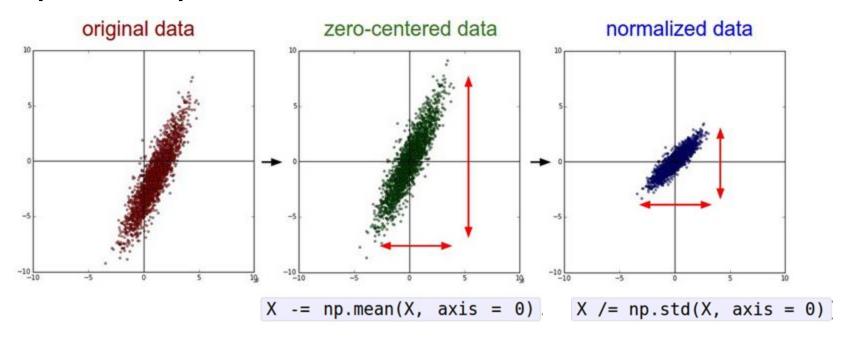
Problem: doubles the number of parameters/neuron:(

#### **TLDR:** In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU
- Try out tanh but don't expect much
- Don't use sigmoid

## Data Preprocessing

#### Step 1: Preprocess the data



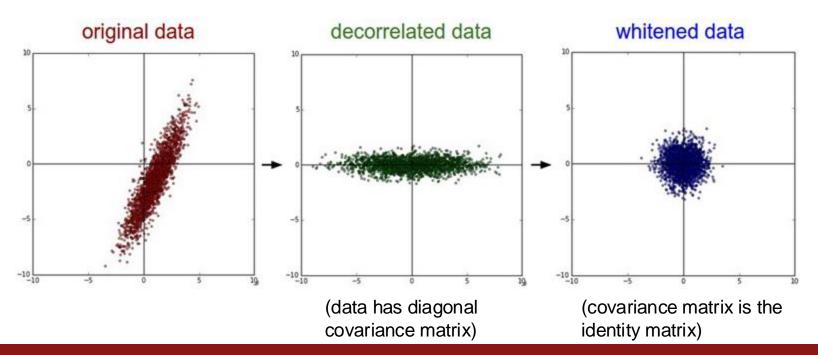
(Assume X [NxD] is data matrix, each example in a row)

#### Preprocessing: Why are we doing this?

- Subtracting off the mean
  - Avoid gradients that only point in two different orthants.
- Normalizing the magnitude
  - Kilometers vs. millimeters...
    - Invariance to the specific \*units\* of the inputs...

#### Step 1: Preprocess the data

In practice, you may also see PCA and Whitening of the data



#### In practice for Images: center only

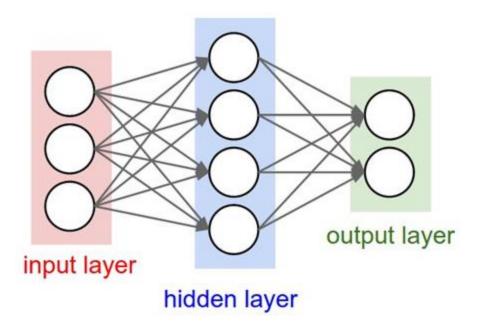
e.g. consider CIFAR-10 example with [32,32,3] images

- Subtract the mean image (e.g. AlexNet) (mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet)
   (mean along each channel = 3 numbers)

Not common to normalize variance, to do PCA or whitening

## Weight Initialization

Q: what happens when W=0 init is used?



- First idea: **Small random numbers** (Gaussian with zero mean and 1e-2 standard deviation)

W = 0.01\* np.random.randn(D,H)

- First idea: **Small random numbers** (Gaussian with zero mean and 1e-2 standard deviation)

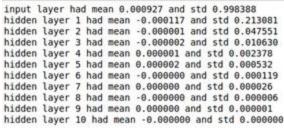
$$W = 0.01* np.random.randn(D,H)$$

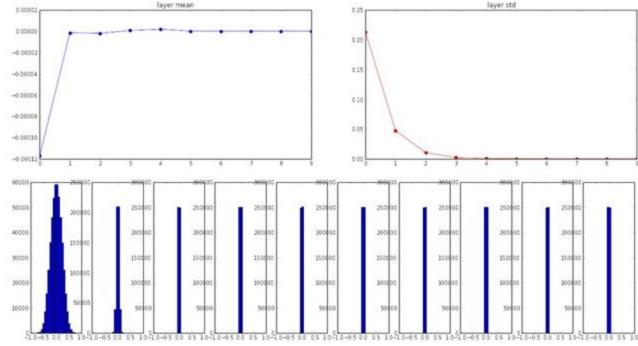
Works ~okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a network.

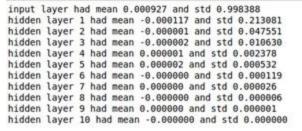
# Let's look at some activation statistics

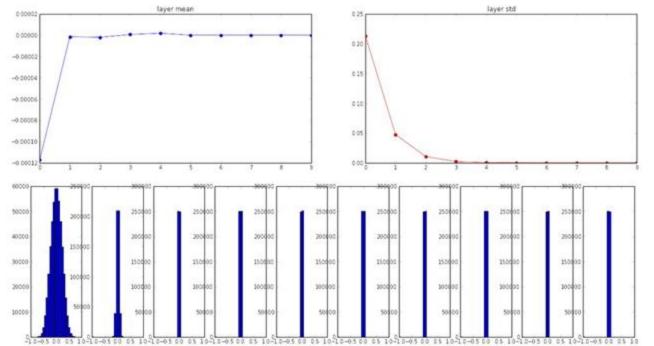
E.g. 10-layer net with 500 neurons on each layer, using tanh non-linearities, and initializing as described in last slide.

```
# assume some unit gaussian 10-D input data
D = np.random.randn(1000, 500)
hidden layer sizes = [500]*10
nonlinearities = ['tanh']*len(hidden layer sizes)
act = {'relu':lambda x:np.maximum(0,x), 'tanh':lambda x:np.tanh(x)}
Hs = \{\}
for i in xrange(len(hidden layer sizes)):
    X = D if i == 0 else Hs[i-1] # input at this layer
    fan in = X.shape[1]
    fan out = hidden layer sizes[i]
    W = np.random.randn(fan in, fan out) * 0.01 # layer initialization
    H = np.dot(X, W) # matrix multiply
   H = act[nonlinearities[i]](H) # nonlinearity
    Hs[i] = H # cache result on this layer
# look at distributions at each layer
print 'input layer had mean %f and std %f' % (np.mean(D), np.std(D))
layer means = [np.mean(H) for i,H in Hs.iteritems()]
layer stds = [np.std(H) for i,H in Hs.iteritems()]
for i,H in Hs.iteritems():
    print 'hidden layer %d had mean %f and std %f' % (i+1, layer means[i], layer stds[i])
# plot the means and standard deviations
plt.figure()
plt.subplot(121)
plt.plot(Hs.keys(), layer means, 'ob-')
plt.title('layer mean')
plt.subplot(122)
plt.plot(Hs.keys(), layer stds, 'or-')
plt.title('layer std')
# plot the raw distributions
plt.figure()
for i,H in Hs.iteritems():
    plt.subplot(1,len(Hs),i+1)
    plt.hist(H.ravel(), 30, range=(-1,1))
```





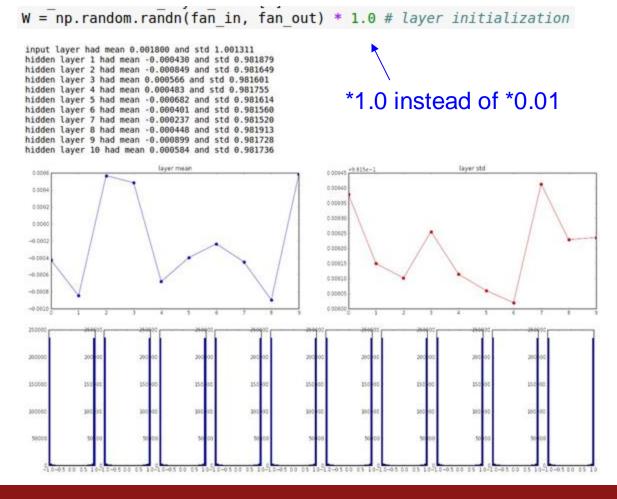




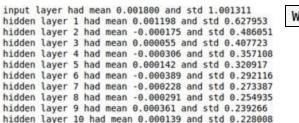
# All activations become zero!

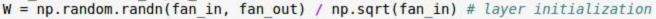
Q: think about the backward pass. What do the gradients look like?

Hint: think about backward pass for a W\*X gate.

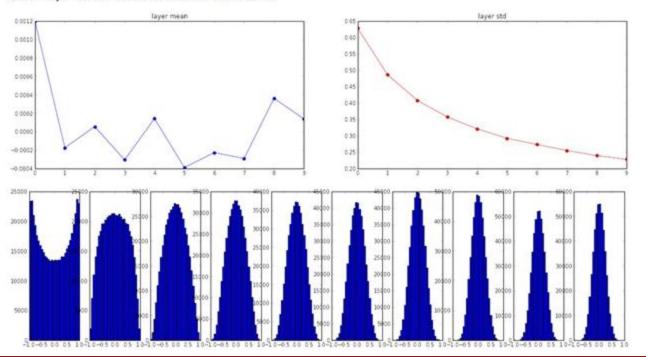


Almost all neurons completely saturated, either -1 and 1. Gradients will be all zero.

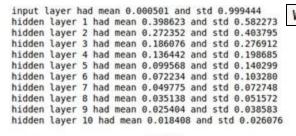




"Xavier initialization" [Glorot et al., 2010]

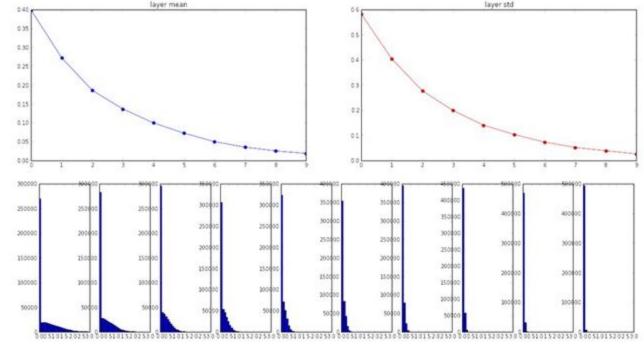


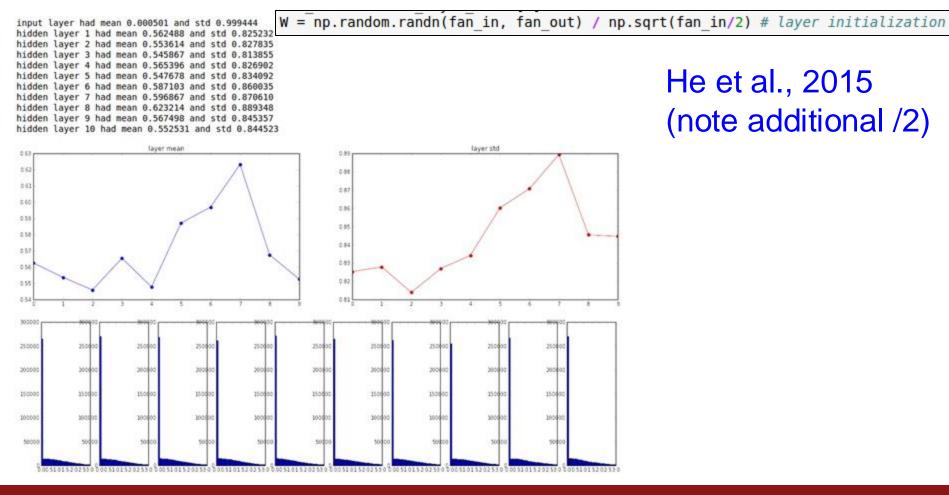
Reasonable initialization. (Mathematical derivation assumes linear activations)



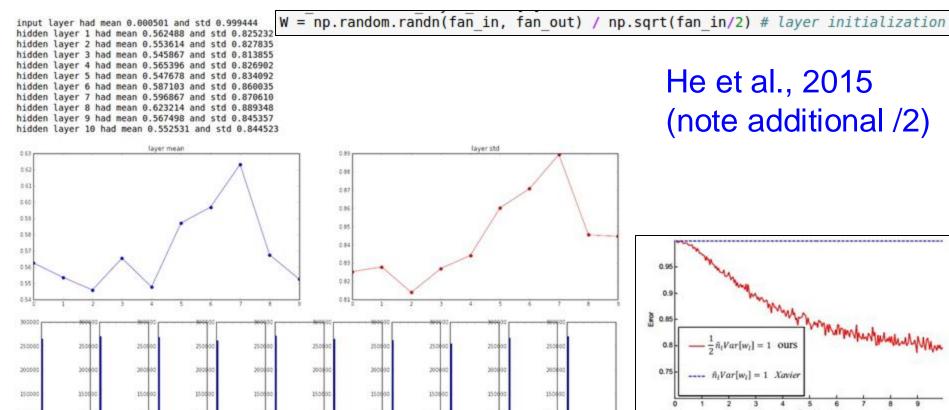
W = np.random.randn(fan\_in, fan\_out) / np.sqrt(fan\_in) # layer initialization

# but when using the ReLU nonlinearity it breaks.

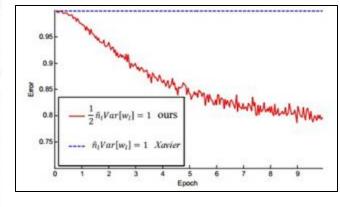




He et al., 2015 (note additional /2)



He et al., 2015 (note additional /2)



10000

100000

50000

30040

#### Proper initialization is an active area of research...

Understanding the difficulty of training deep feedforward neural networks by Glorot and Bengio, 2010

Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013

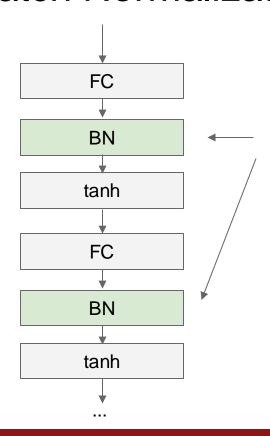
Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 2014

Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification by He et al., 2015

Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

All you need is a good init, Mishkin and Matas, 2015

• • •



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{Var[x^{(k)}]}}$$

"you want unit Gaussian activations? just make them so."
Not actually "Gaussian". Just zero mean, unit variance.

consider a batch of activations at some layer. To make each dimension unit normalized, apply:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

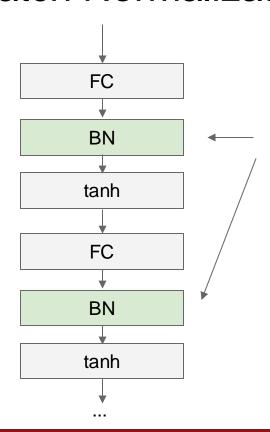
"you want unit Gaussian activations? just make them so." (you want NORMALIZED activations)

N X D

1. compute the empirical mean and variance independently for each dimension.

#### 2. Normalize

$$\widehat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$



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#### Normalize:

$$\widehat{x}^{(k)} = \frac{x^{(k)} - E[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)} \widehat{x}^{(k)} + \beta^{(k)}$$

Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\operatorname{Var}[x^{(k)}]}$$
$$\beta^{(k)} = \operatorname{E}[x^{(k)}]$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

to recover the identity mapping.

#### [loffe and Szegedy, 2015]

**Input:** Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma$ ,  $\beta$ 

Output: 
$$\{y_i = BN_{\gamma,\beta}(x_i)\}$$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$$
 // mini-batch mean

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$$
 // mini-batch variance

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$$
 // normalize

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)$$
 // scale and shift

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

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$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma,\beta}(x_i)$$
 // scale and shift

### Note: at test time BatchNorm layer functions differently:

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

(e.g. can be estimated during training with running averages)