Lecture 7:

Training Neural Networks Part II

Projects as a mini-conference

1. You will write a paper with your team.
   a. A suggested format will make sure you cover the right kinds of topics.
2. Everyone will participate in “paper reviewing”.
   a. These will be highly structured so you know what to comment on.
3. Subhransu and I will grade all the final write-ups at the same time as the reviews. We will not use the review scores directly

Project Ideas

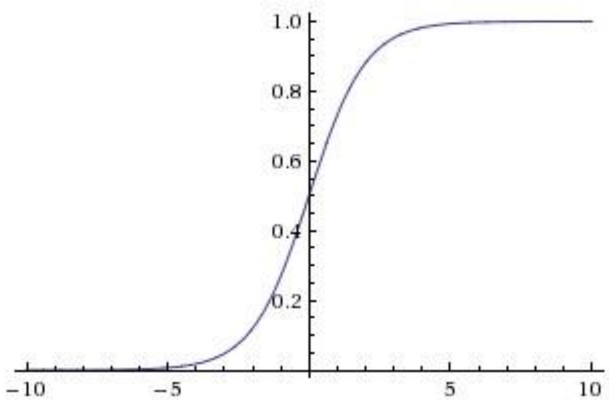
TA will give presentations
on Oct. 1 (Next Tuesday)!!

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 Functions

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



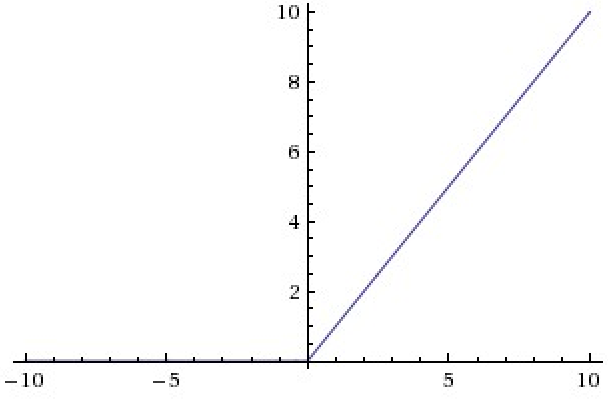
Sigmoid

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

2 problems:

1. Saturated neurons “kill” the gradients
2. exp() is a bit compute expensive

Activation Functions

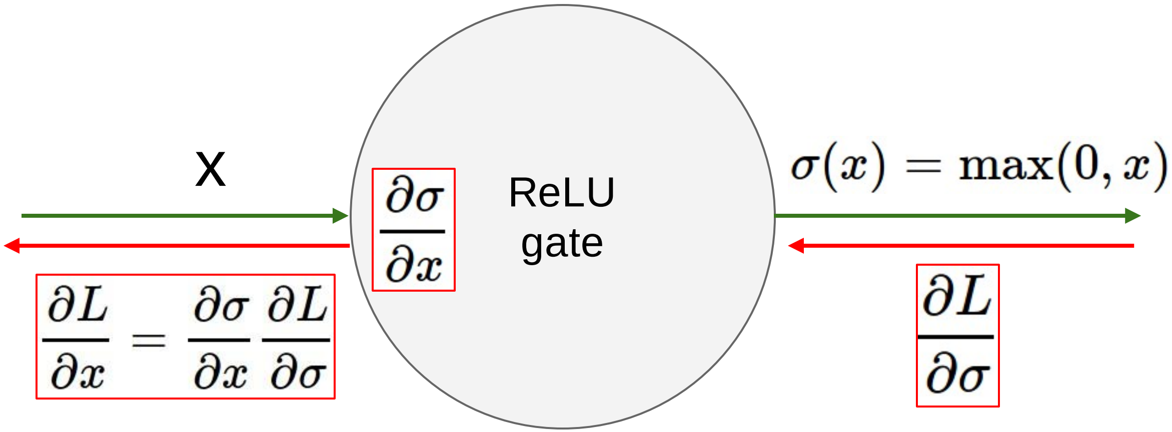


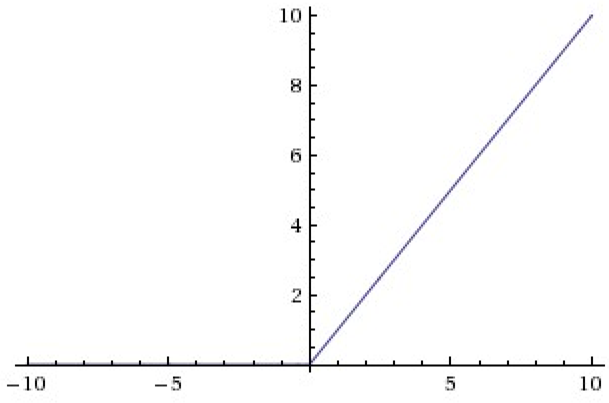
ReLU
(Rectified Linear Unit)

- Computes **f(x) = max(0,x)**

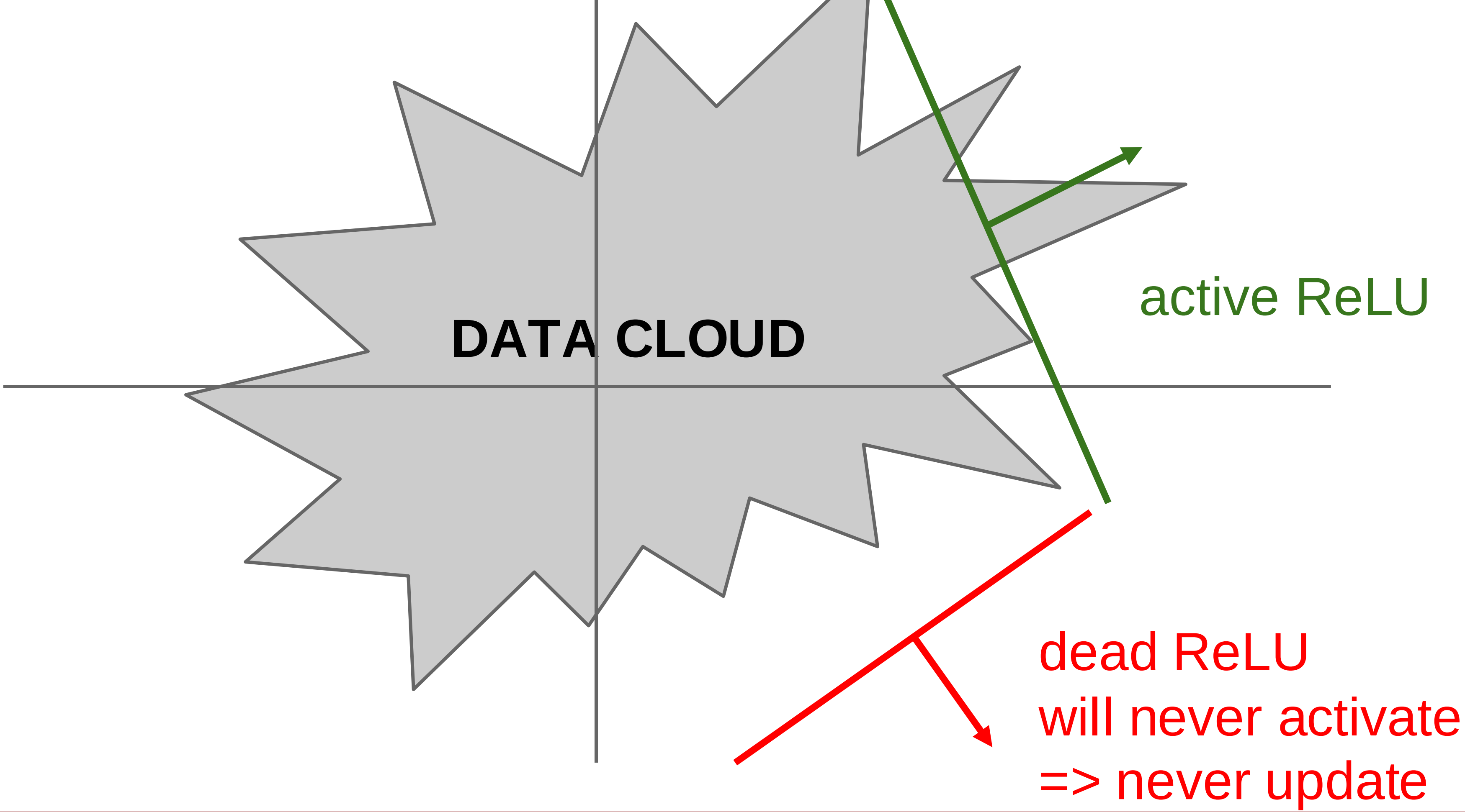
- Does not saturate (in +region)
- Very little computation
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

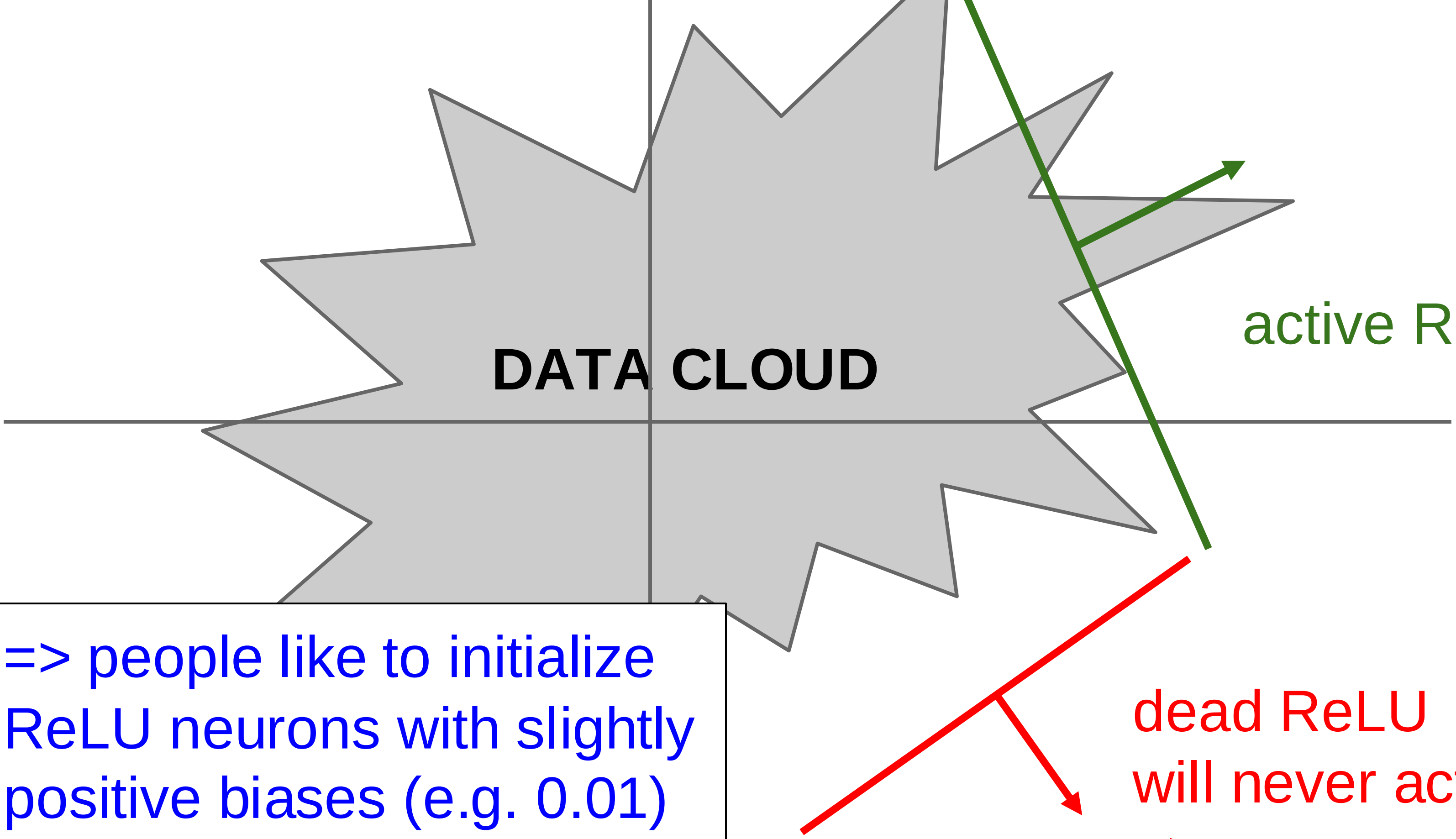
[Krizhevsky et al., 2012]





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

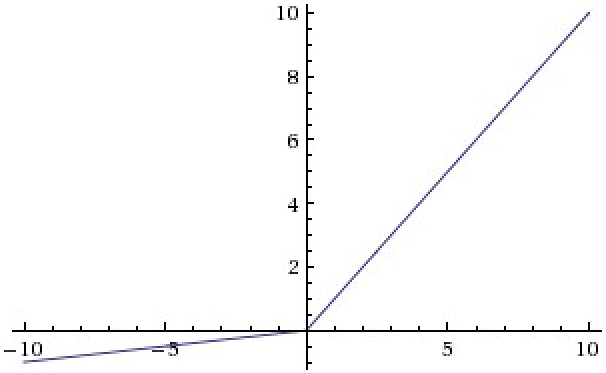

DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update



=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

Activation Functions

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



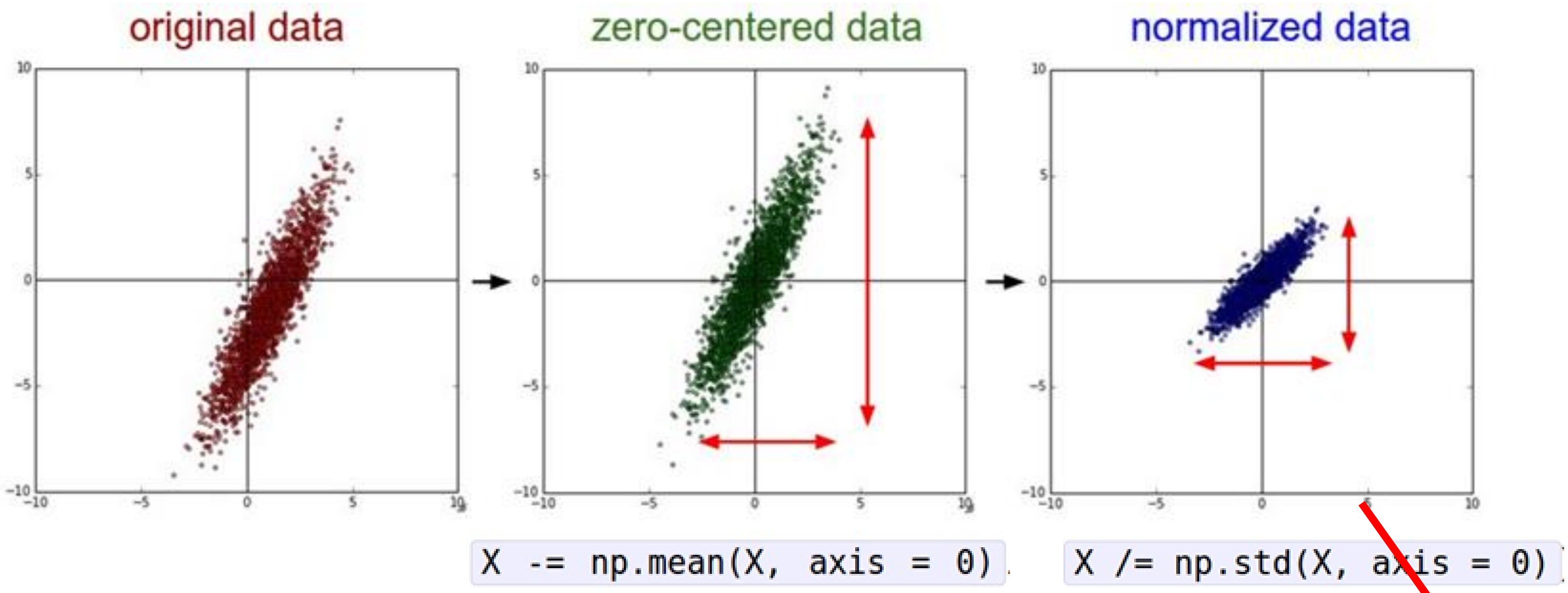
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

Leaky ReLU

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

Data Preprocessing

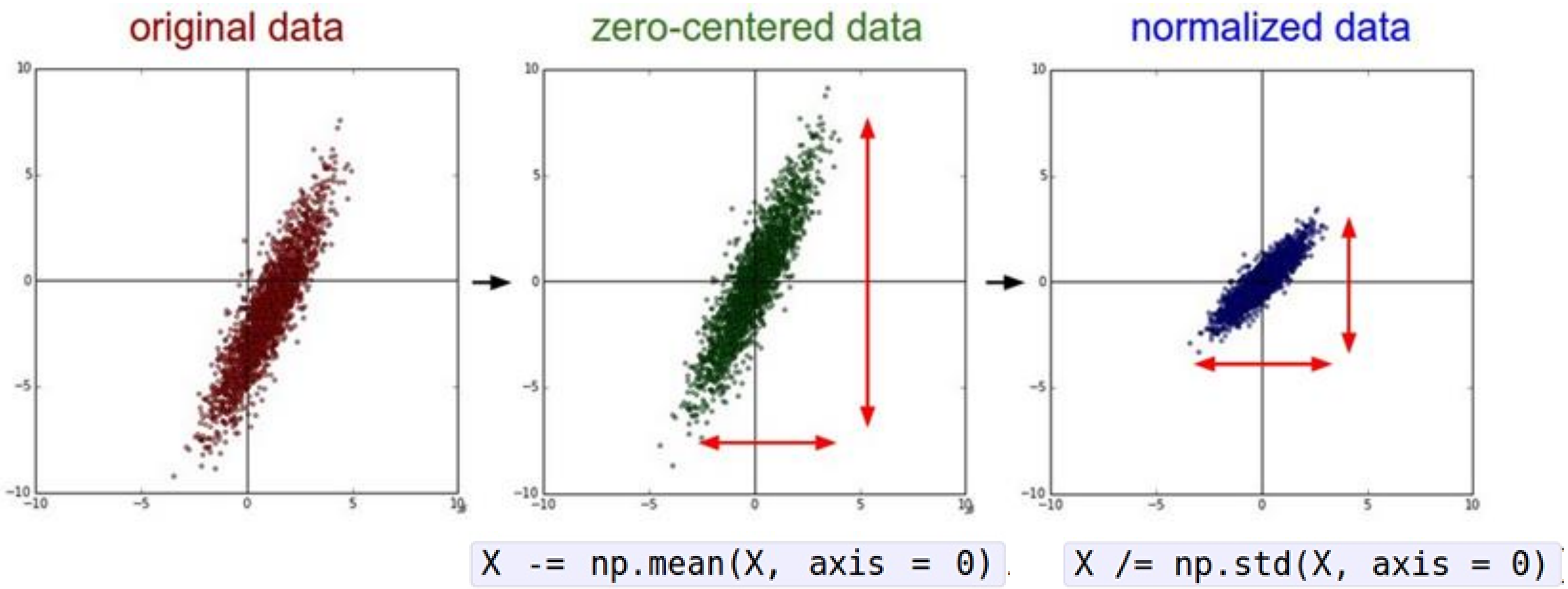
Step 1: Preprocess the data



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

Invariance of units

Step 1: Preprocess the data



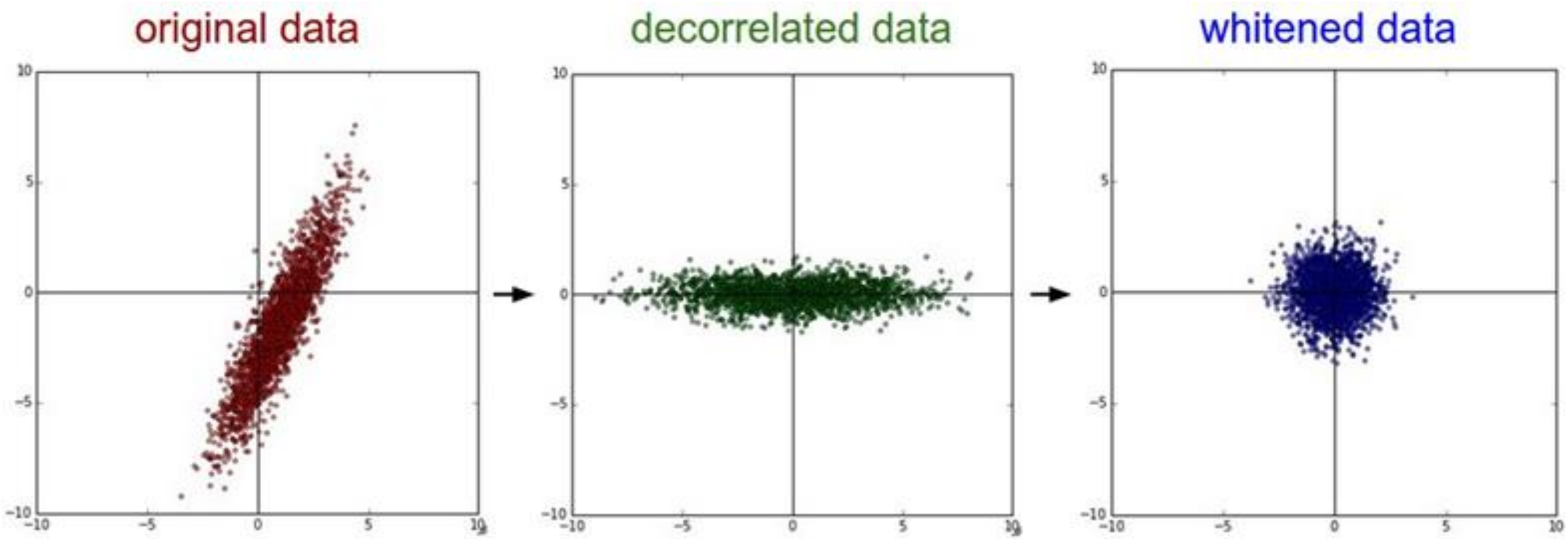
(Assume X [NxD] is data matrix,
each example in a row)

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



(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

In practice for Images: center only

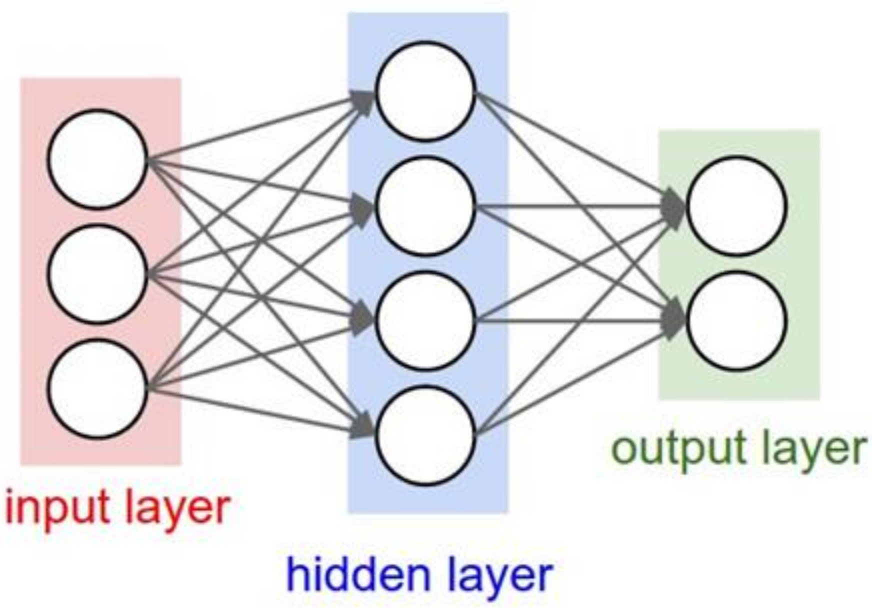
e.g. consider CIFAR-10 example with [32,32,3] images

- 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)
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```

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

```
# 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

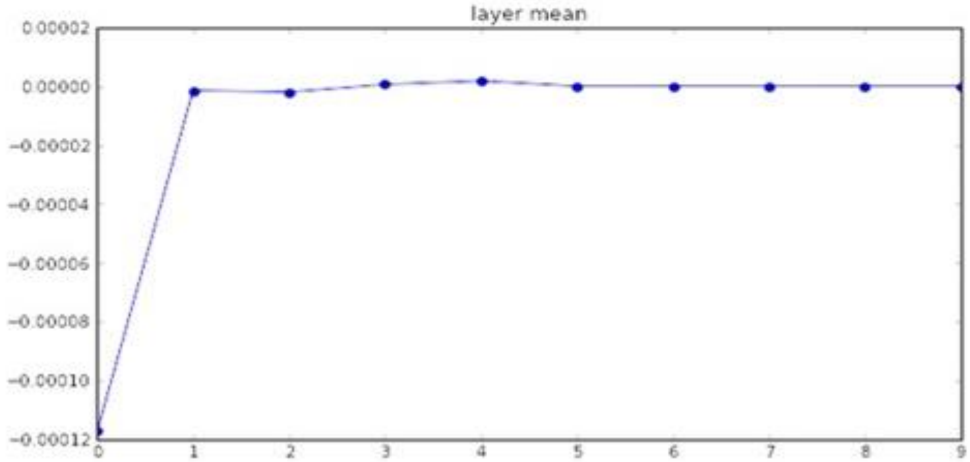
# look at distributions at each layer
print 'input layer had mean %f and std %f' % (np.mean(D), np.std(D))
layer_means = [np.mean(H) for i,H in Hs.iteritems()]
layer_stds = [np.std(H) for i,H in Hs.iteritems()]
for i,H in Hs.iteritems():
    print 'hidden layer %d had mean %f and std %f' % (i+1, layer_means[i], layer_stds[i])

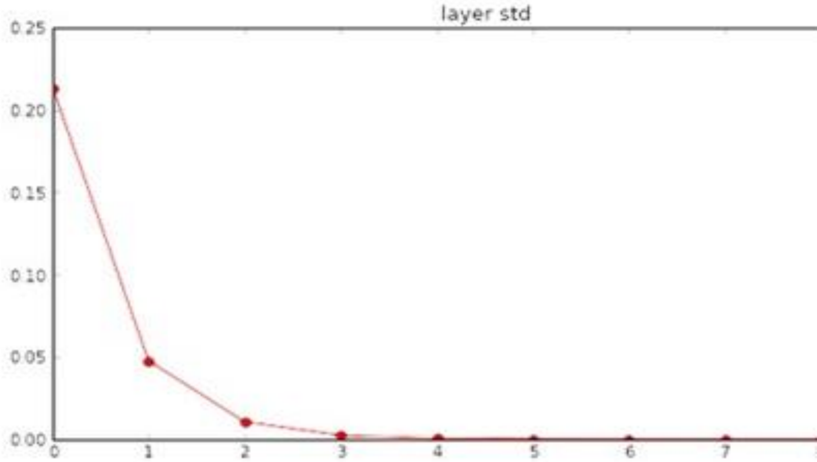
# plot the means and standard deviations
plt.figure()
plt.subplot(121)
plt.plot(Hs.keys(), layer_means, 'ob-')
plt.title('layer mean')
plt.subplot(122)
plt.plot(Hs.keys(), layer_stds, 'or-')
plt.title('layer std')

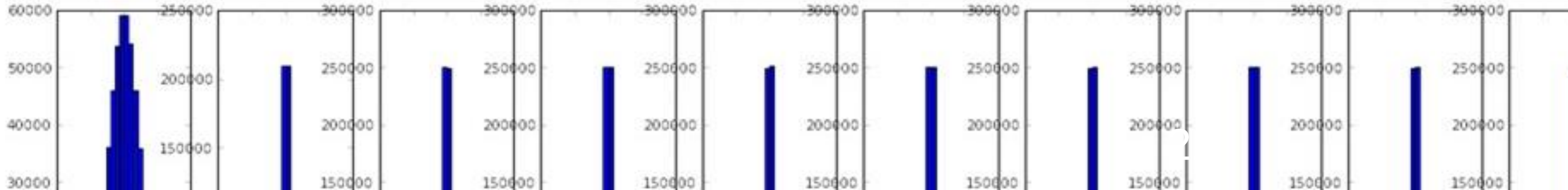
# plot the raw distributions
plt.figure()
for i,H in Hs.iteritems():
    plt.subplot(1,len(Hs),i+1)
    plt.hist(H.ravel(), 30, range=(-1,1))
```

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

```
input layer had mean 0.000927 and std 0.998388
hidden layer 1 had mean -0.000117 and std 0.213081
hidden layer 2 had mean -0.000001 and std 0.047551
hidden layer 3 had mean -0.000002 and std 0.010630
hidden layer 4 had mean 0.000001 and std 0.002378
hidden layer 5 had mean 0.000002 and std 0.000532
hidden layer 6 had mean -0.000000 and std 0.000119
hidden layer 7 had mean 0.000000 and std 0.000026
hidden layer 8 had mean -0.000000 and std 0.000006
hidden layer 9 had mean 0.000000 and std 0.000001
hidden layer 10 had mean -0.000000 and std 0.000000
```







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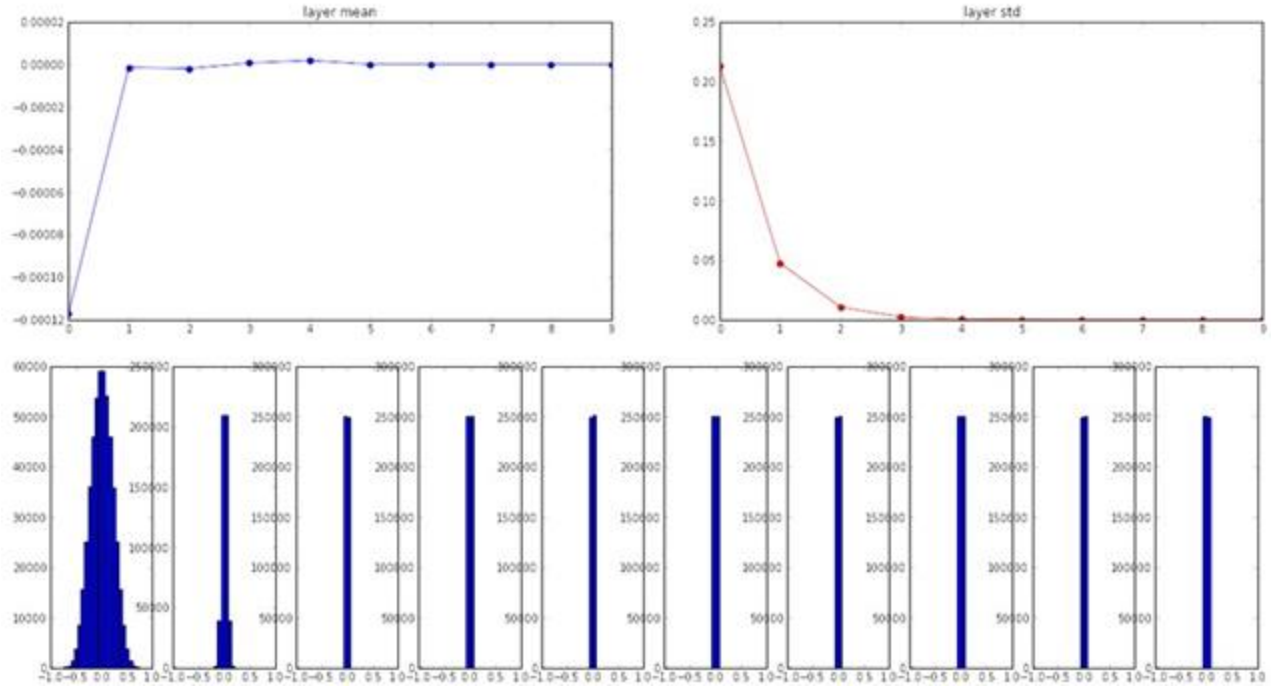
```



All activations become zero!

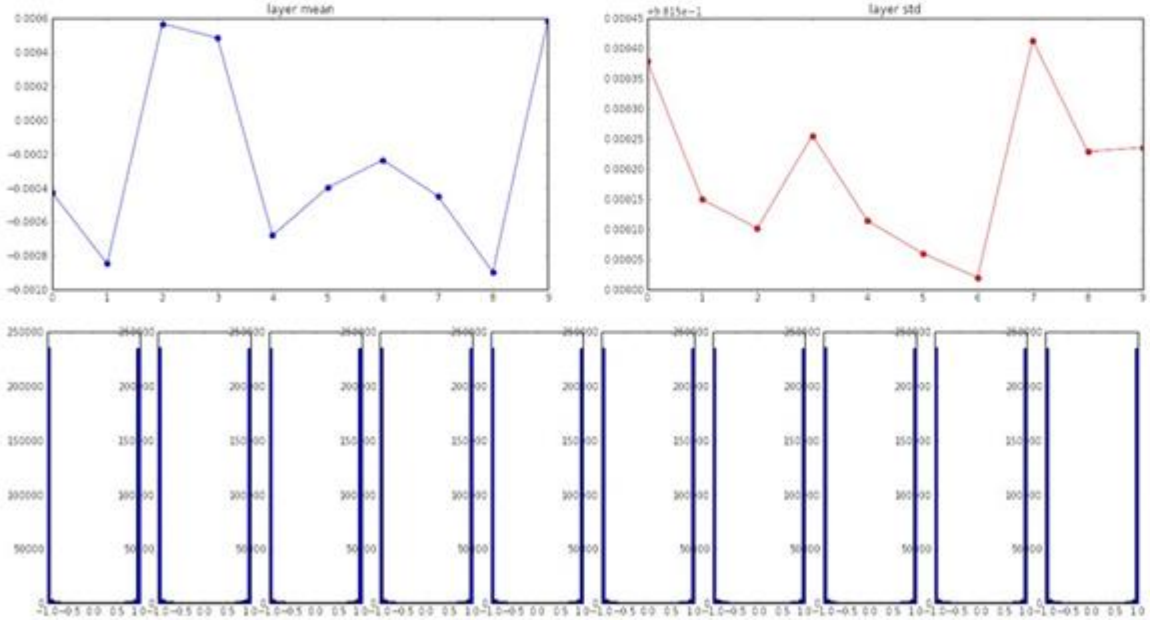
Q: think about the backward pass. What do the gradients look like?

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

```
W = np.random.randn(fan_in, fan_out) * 1.0 # layer initialization
```

*1.0 instead of *0.01

```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean -0.000430 and std 0.981879
hidden layer 2 had mean -0.000849 and std 0.981649
hidden layer 3 had mean 0.000566 and std 0.981601
hidden layer 4 had mean 0.000483 and std 0.981755
hidden layer 5 had mean -0.000682 and std 0.981614
hidden layer 6 had mean -0.000401 and std 0.981560
hidden layer 7 had mean -0.000237 and std 0.981520
hidden layer 8 had mean -0.000448 and std 0.981913
hidden layer 9 had mean -0.000899 and std 0.981728
hidden layer 10 had mean 0.000584 and std 0.981736
```

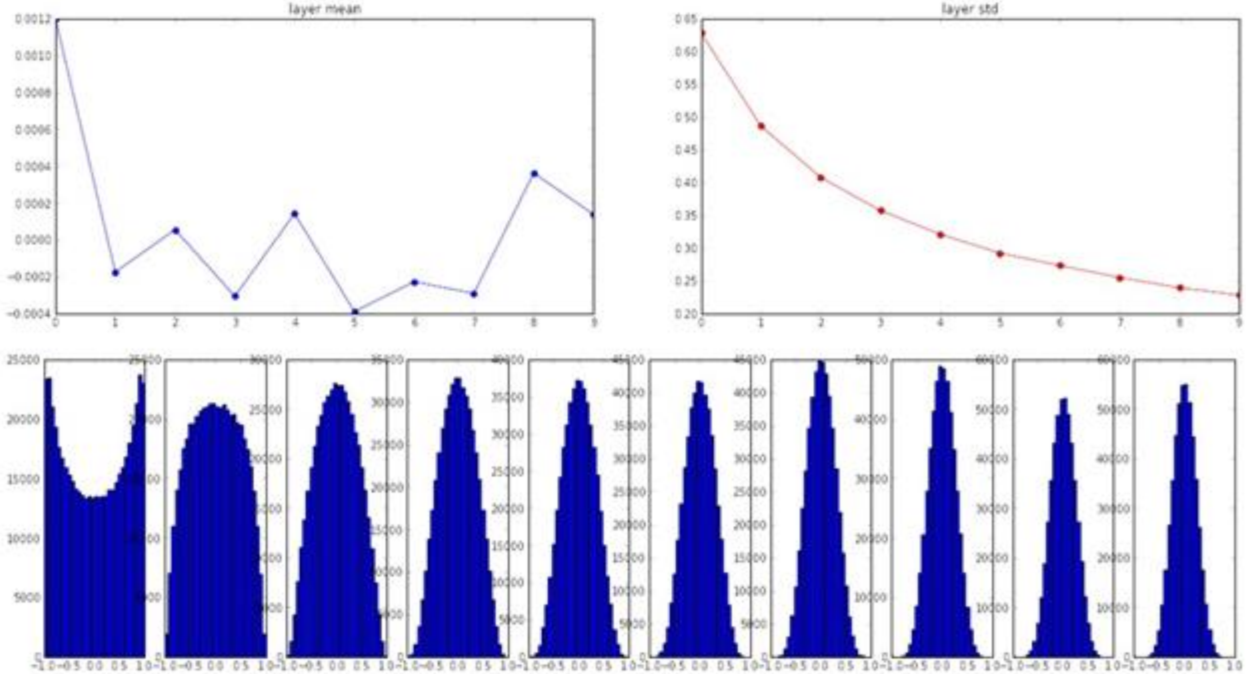


Almost all neurons completely saturated, either -1 and 1. Gradients will be all zero.

```
input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean 0.001198 and std 0.627953
hidden layer 2 had mean -0.000175 and std 0.486051
hidden layer 3 had mean 0.000055 and std 0.407723
hidden layer 4 had mean -0.000306 and std 0.357108
hidden layer 5 had mean 0.000142 and std 0.320917
hidden layer 6 had mean -0.000389 and std 0.292116
hidden layer 7 had mean -0.000228 and std 0.273387
hidden layer 8 had mean -0.000291 and std 0.254935
hidden layer 9 had mean 0.000361 and std 0.239266
hidden layer 10 had mean 0.000139 and std 0.228008
```

```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

“Xavier initialization”
[Glorot et al., 2010]



Reasonable initialization.
(Mathematical derivation assumes linear activations)

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

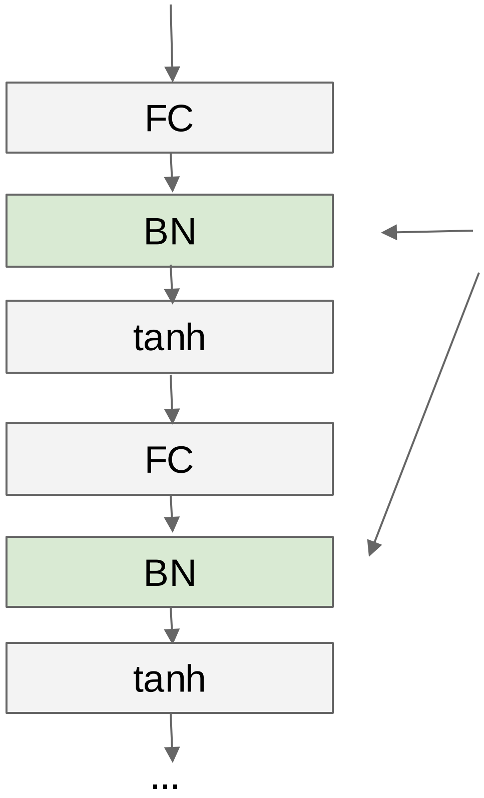
All you need is a good init, Mishkin and Matas, 2015

…

Batch Normalization

Batch Normalization

[Ioffe and Szegedy, 2015]



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

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

Batch Normalization

[Ioffe and Szegedy, 2015]

"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:

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

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

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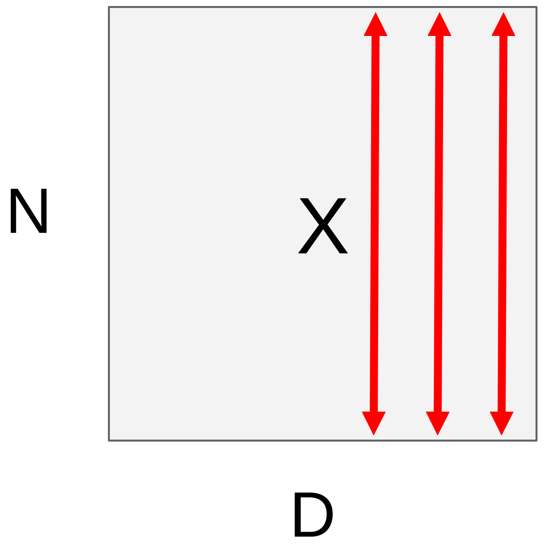


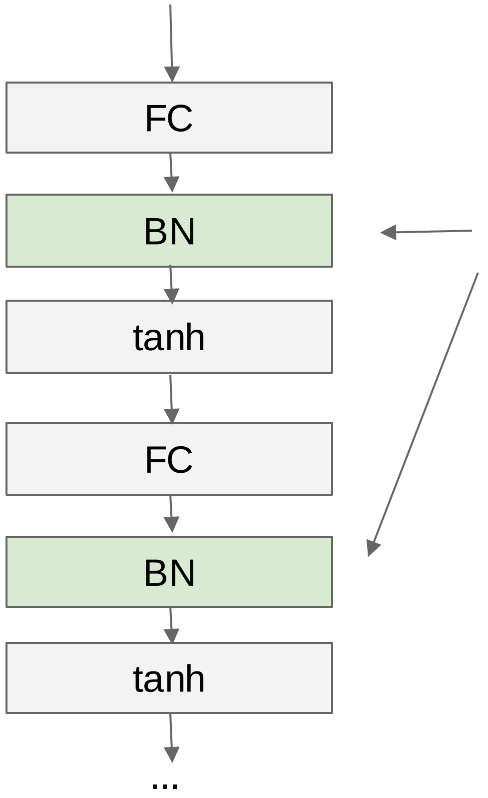
1. compute the empirical mean and variance independently for each dimension.

2. Normalize

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

Batch Normalization

[Ioffe and Szegedy, 2015]



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

Batch Normalization

[Ioffe and Szegedy, 2015]

Normalize:

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

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:

$$\gamma^{(k)} = \sqrt{\mathrm{Var}[x^{(k)}]}$$

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

to recover the identity mapping.

Batch Normalization

[Ioffe and Szegedy, 2015]

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

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization

Batch Normalization

[Ioffe and Szegedy, 2015]

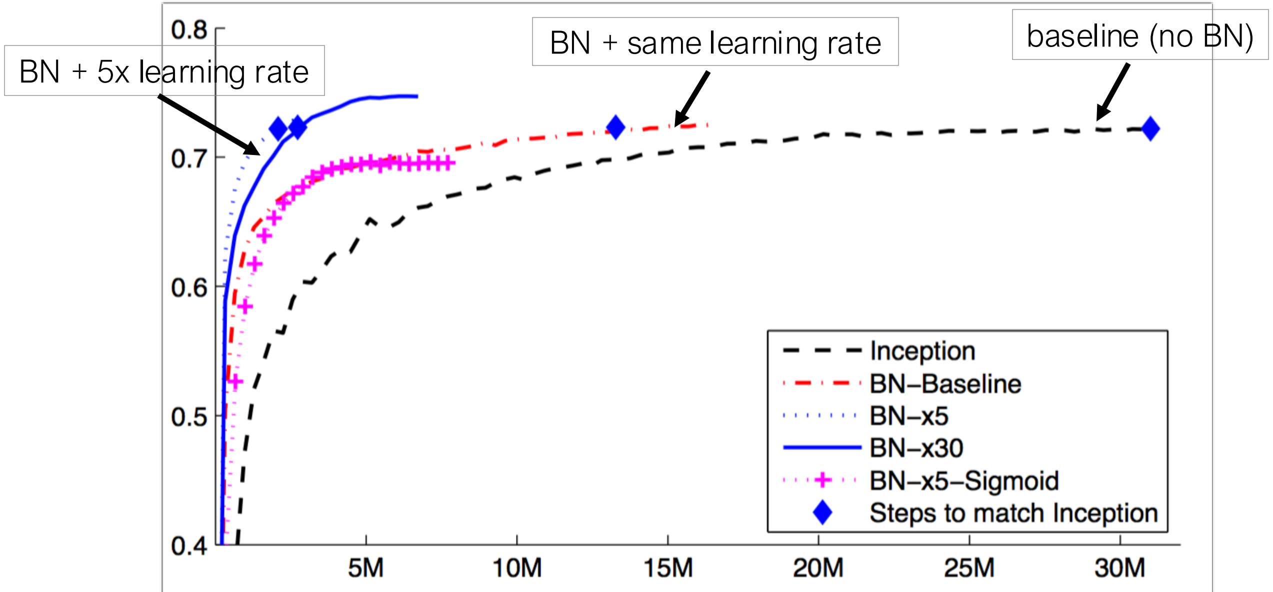

Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

Batch Normalization

[Ioffe and Szegedy, 2015]

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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)

Source of many bugs!

Gradient Checking

Gradient checks

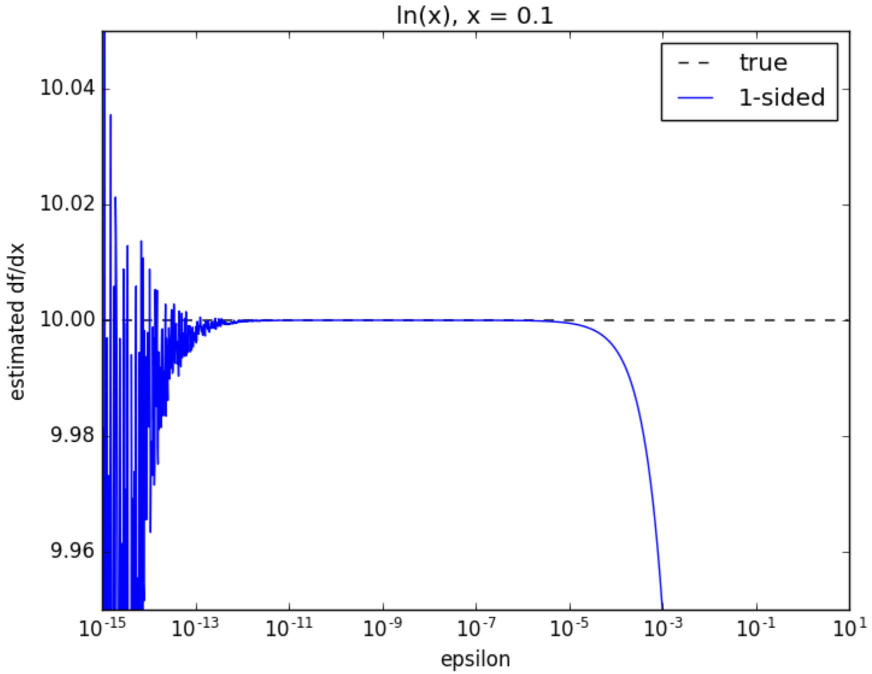
1-sided

$$\frac{df}{dx} \approx \frac{1}{h}(f(x+h) - f(x))$$

Compare gradient implementation with numerical gradients

Easy to implement, but slow

Numerical precision can be an issue (want *h* to be small but not too small)



Gradient checks

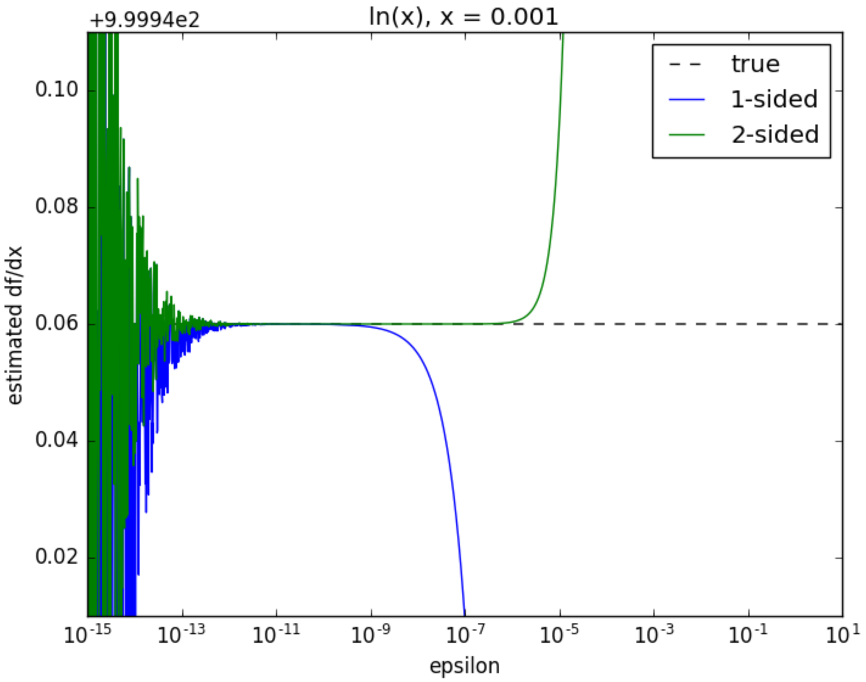
1-sided

$$\frac{df}{dx} \approx \frac{1}{h}(f(x+h) - f(x))$$

2-sided

$$\frac{df}{dx} \approx \frac{1}{2h}(f(x-h) - f(x+h))$$

2-sided gradients have better numerical stability!



Gradient checks

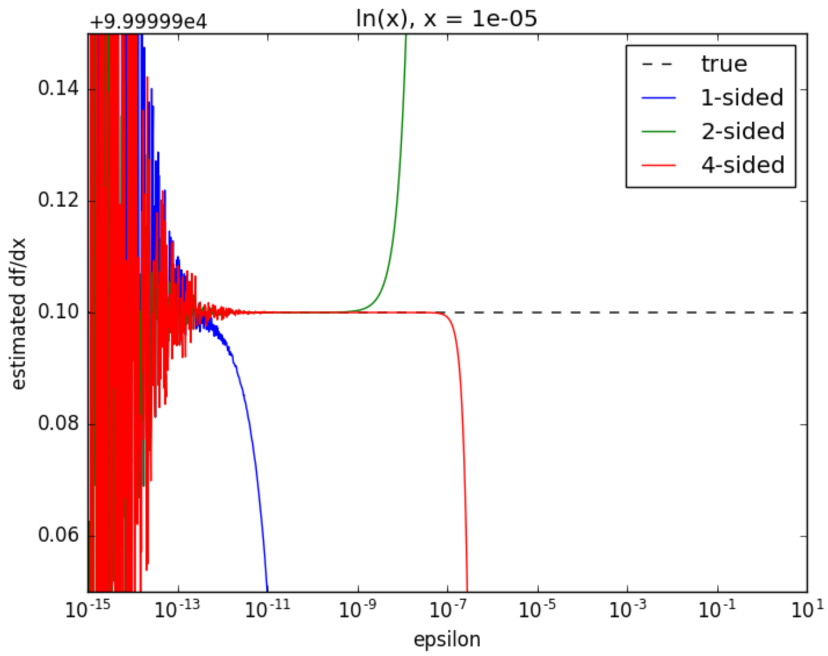
4-sided gradients are even better!

1-sided

$$\frac{df}{dx} \approx \frac{1}{h}(f(x+h) - f(x))$$

2-sided

$$\frac{df}{dx} \approx \frac{1}{2h}(f(x-h) - f(x+h))$$



4-sided

$$\frac{df}{dx} \approx \frac{1}{12h}(-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h))$$

How about 6 sided or 12 sided?

https://justindomke.wordpress.com/2017/04/22/you-deserve-better-than-two-sided-finite-differences/

Overview

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activation functions, preprocessing, weight initialization, regularization, *batch normalization, gradient checking*

2. Training dynamics

babysitting the learning process, hyperparameter optimization, parameter updates

3. Evaluation model ensembles