Lecture 7:
Training Neural Networks, Part I

Next: Training Neural Networks

Overview

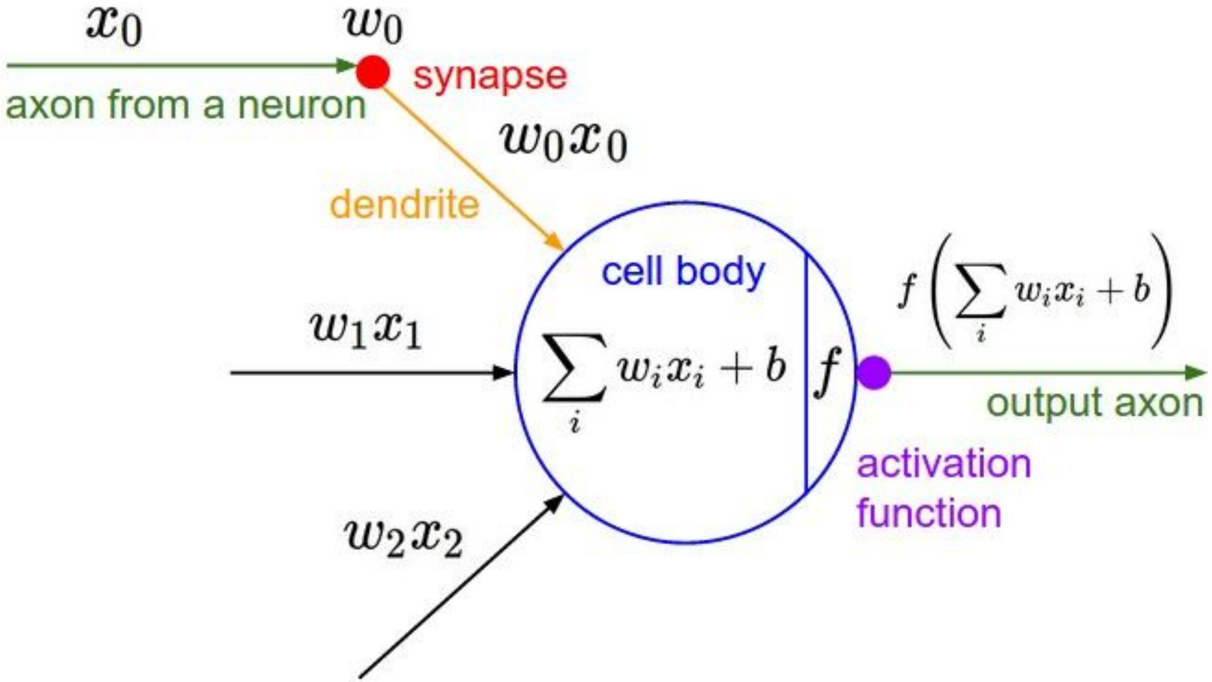
1. **One time setup**
   activation functions, preprocessing, weight initialization, regularization, gradient checking
2. **Training dynamics**
   babysitting the learning process, parameter updates, hyperparameter optimization
3. **Evaluation**
   model ensembles, test-time augmentation

Part 1

- Activation Functions
- Data Preprocessing
- Weight Initialization
- Batch Normalization
- Babysitting the Learning Process
- Hyperparameter Optimization

Activation Functions

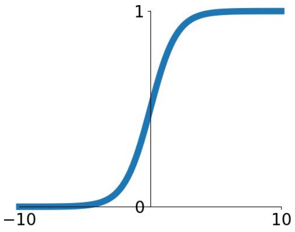
Activation Functions



Activation Functions

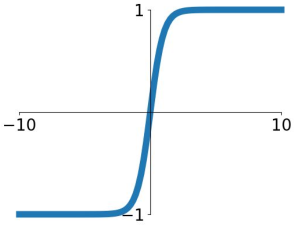
Sigmoid

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



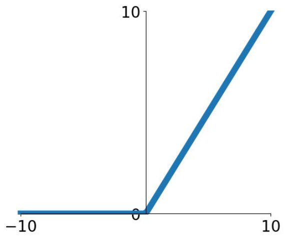
tanh

$$\tanh(x)$$



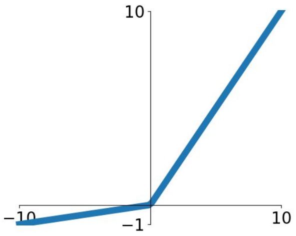
ReLU

$$\max(0, x)$$



Leaky ReLU

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

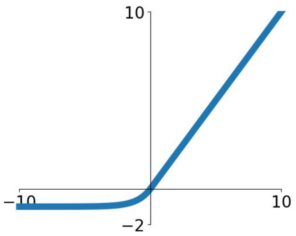


Maxout

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

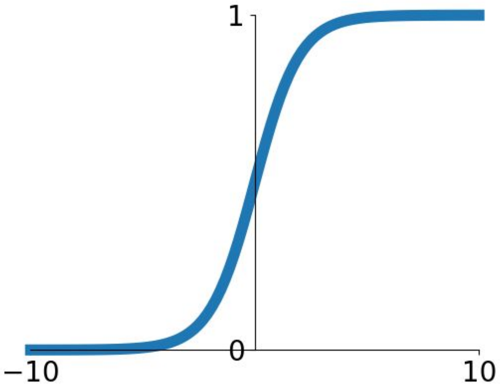
ELU

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



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

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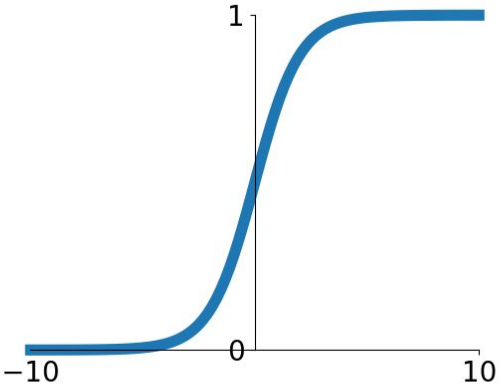

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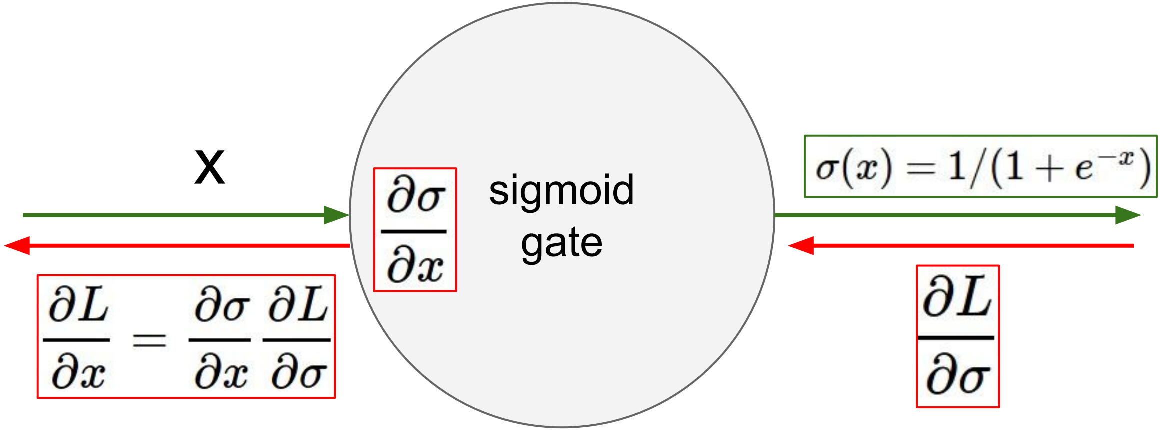
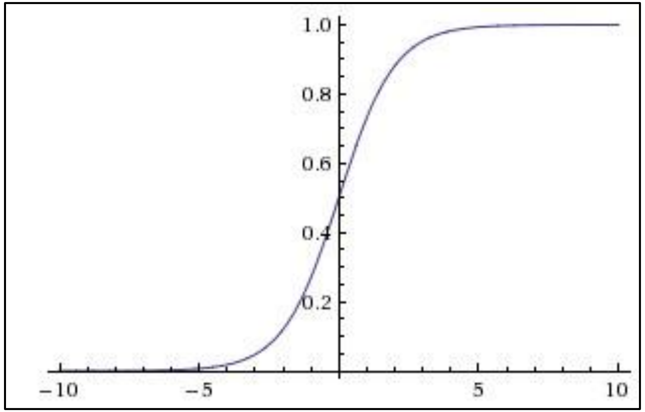
3 problems:

1. Saturated neurons “kill” the gradients





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

Activation Functions

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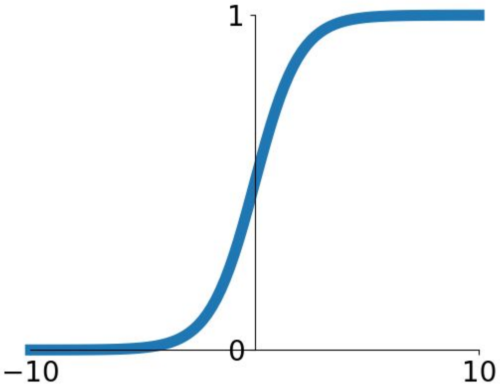

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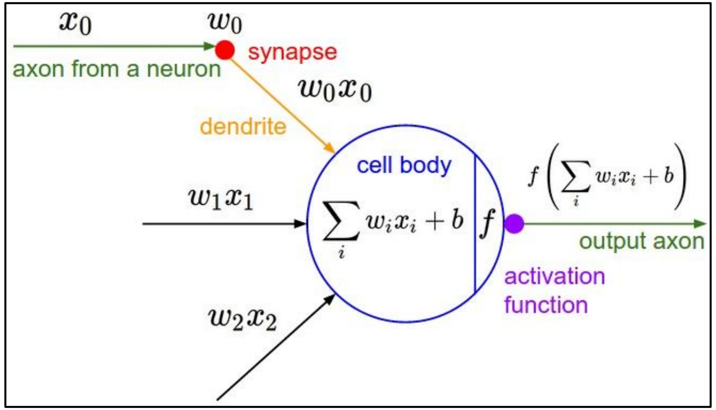
3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered

Consider what happens when the input to a neuron is always positive...

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



What can we say about the gradients on **w**?

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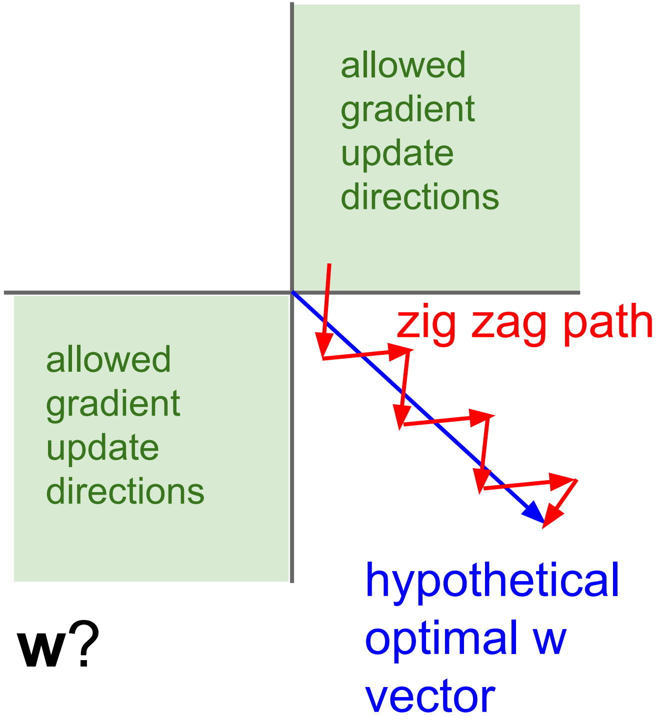

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Always all positive or all negative :(

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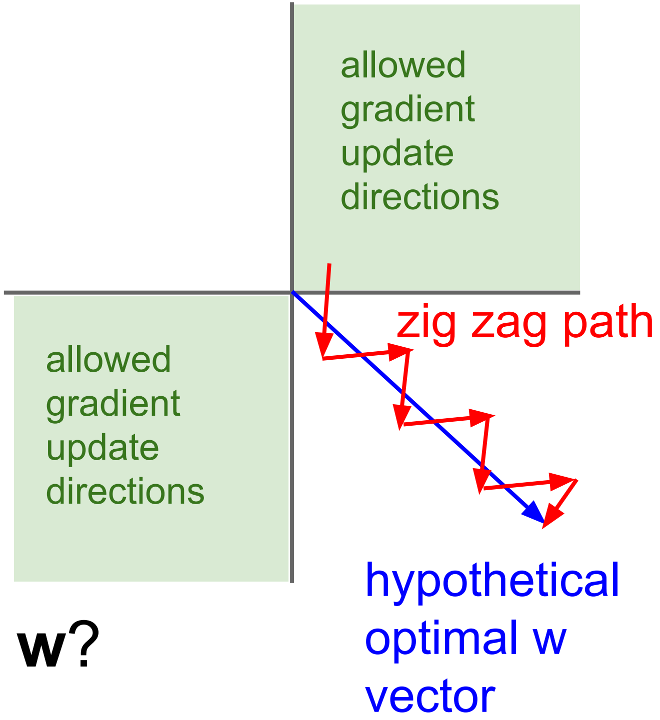

What can we say about the gradients on **w**?

Always all positive or all negative :(

(For a single element! Minibatches help)

Activation Functions

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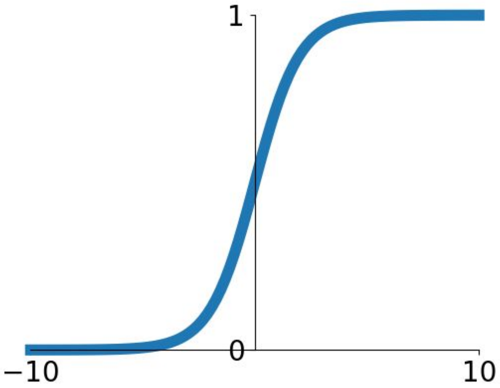

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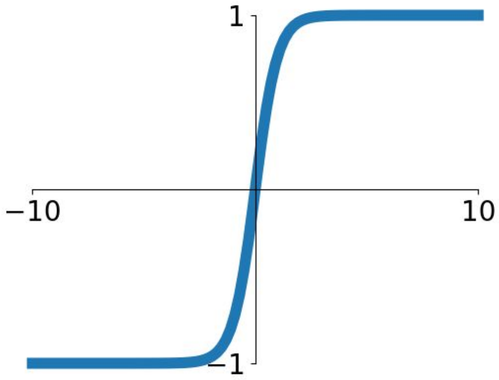
3 problems:

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

Activation Functions



tanh(x)

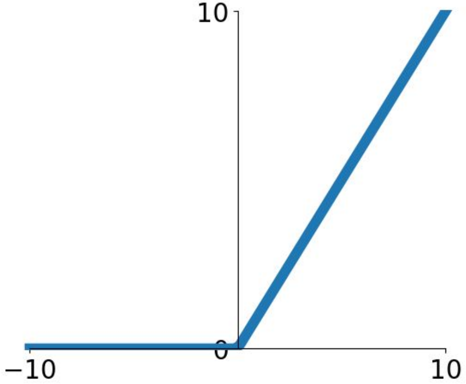
- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

[LeCun et al., 1991]

Activation Functions

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

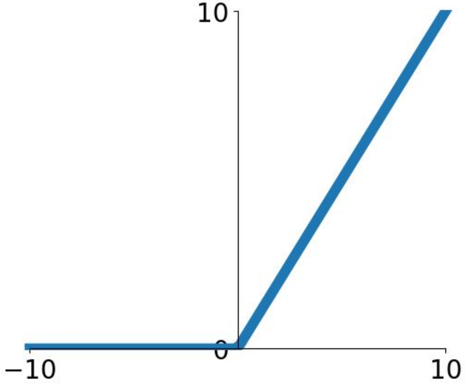
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)



ReLU
(Rectified Linear Unit)

[Krizhevsky et al., 2012]

Activation Functions



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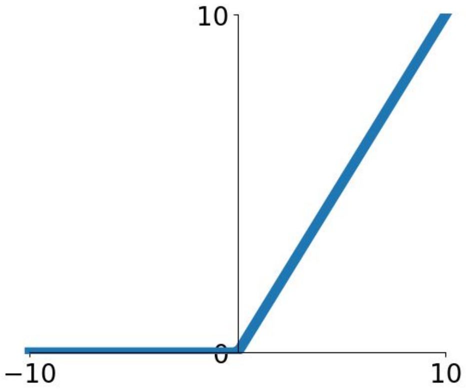

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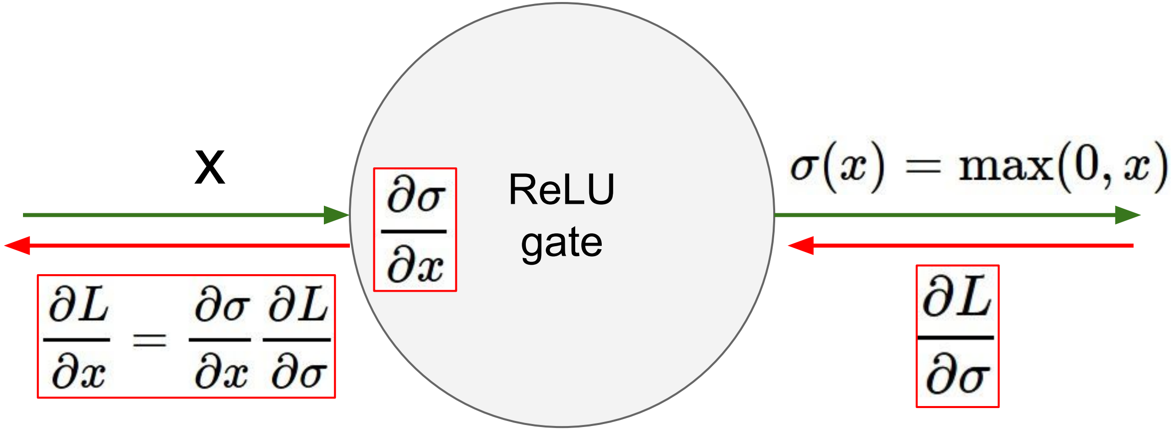
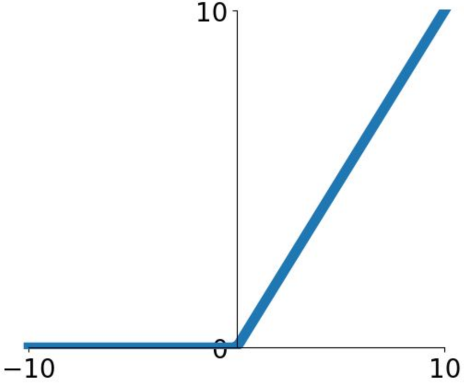
- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?





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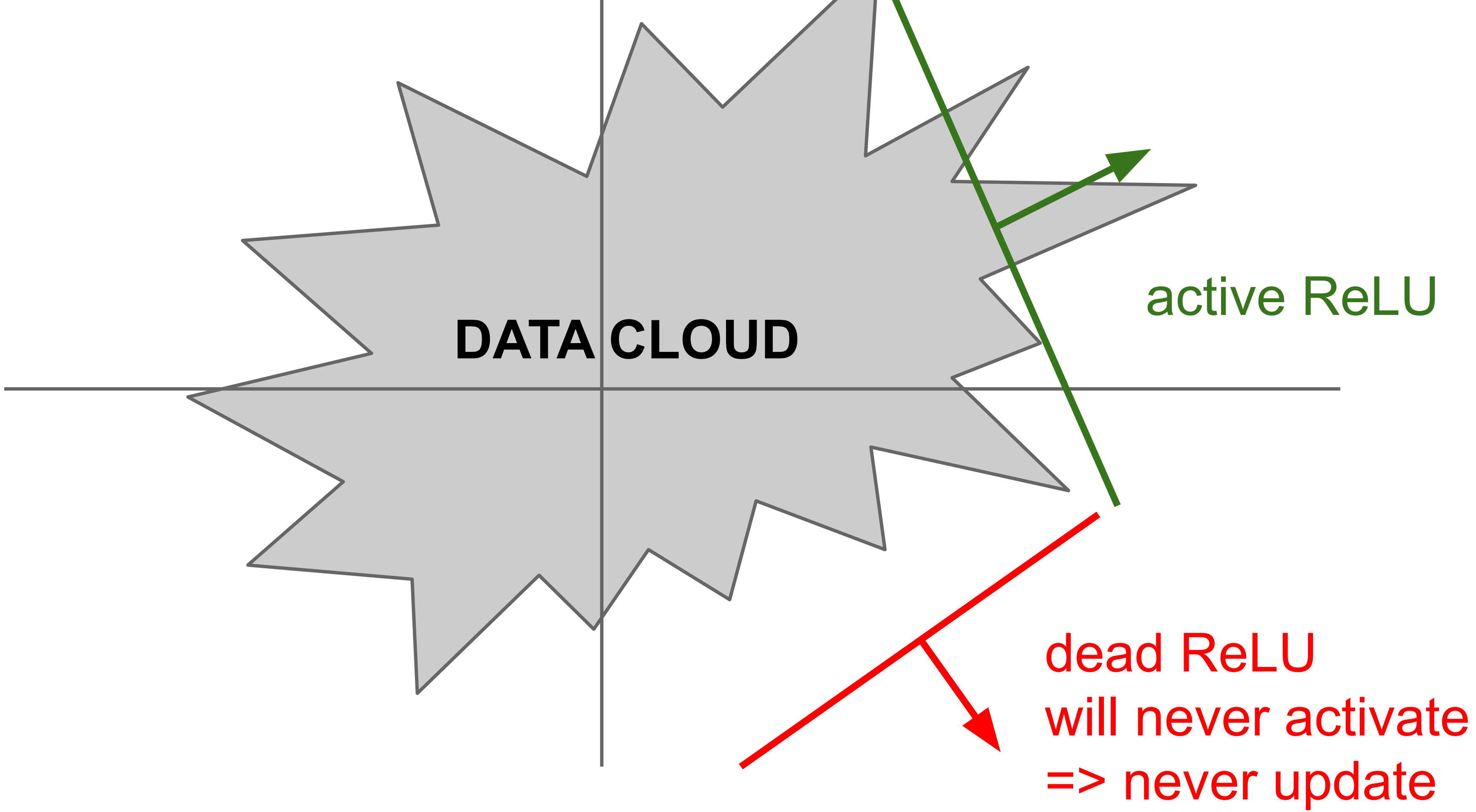
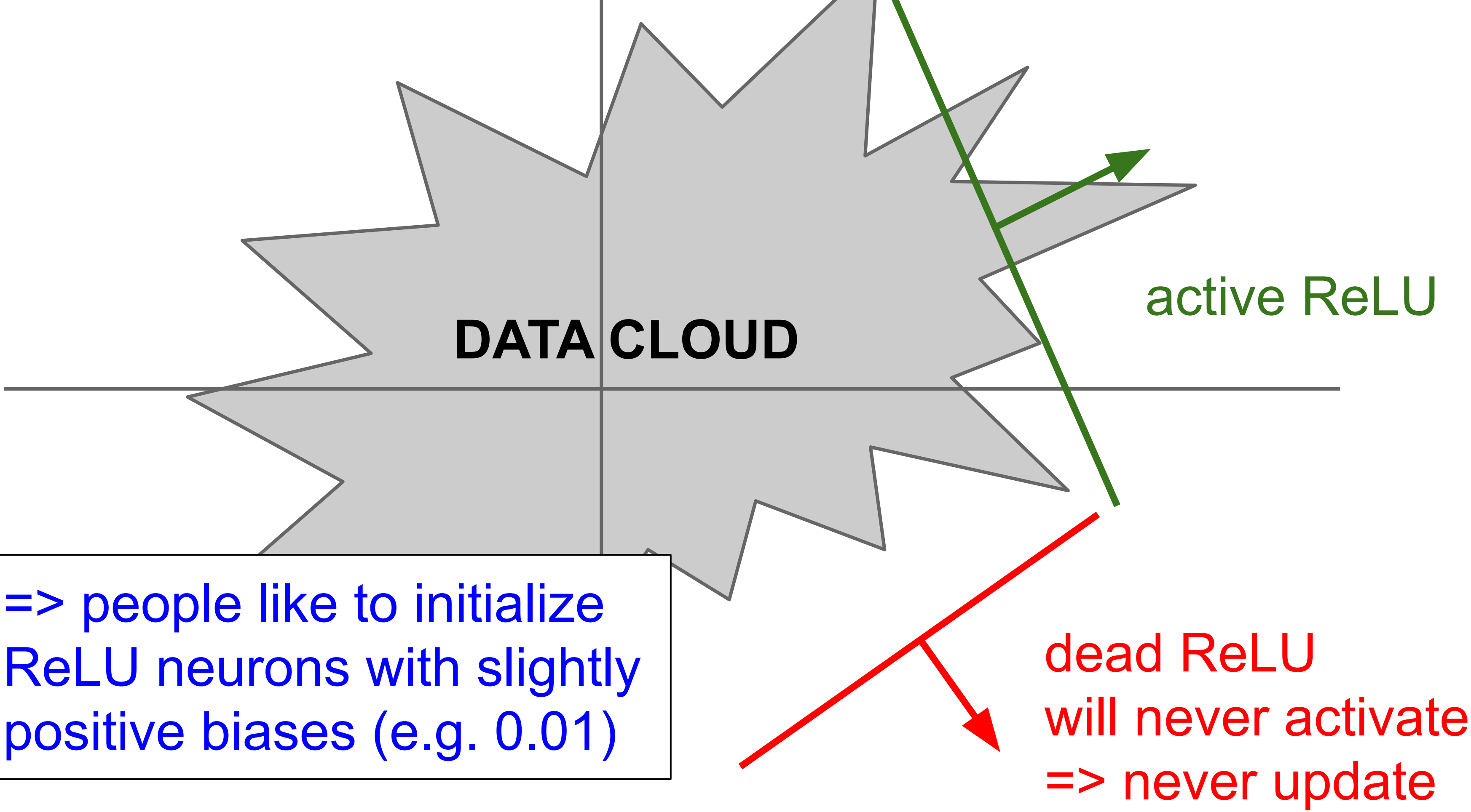
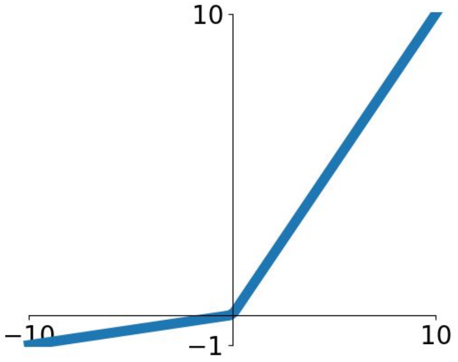

DATA CLOUD
active ReLU
dead ReLU
will never activate
=> never update



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

Activation Functions

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



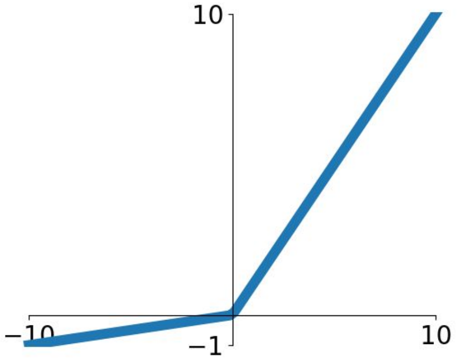
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

Activation Functions

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



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- **will not “die”.**

Leaky ReLU

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

Parametric Rectifier (PReLU)

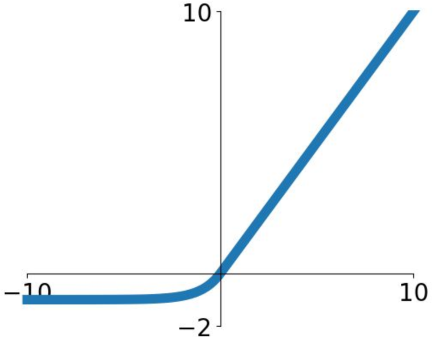
$$f(x) = \max(\alpha x, x)$$

backprop into \alpha
(parameter)

Activation Functions

[Clevert et al., 2015]

Exponential Linear Units (ELU)



- All benefits of ReLU
- Closer to zero mean outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

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

- Computation requires exp()

Maxout "Neuron"

[Goodfellow et al., 2013]

- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

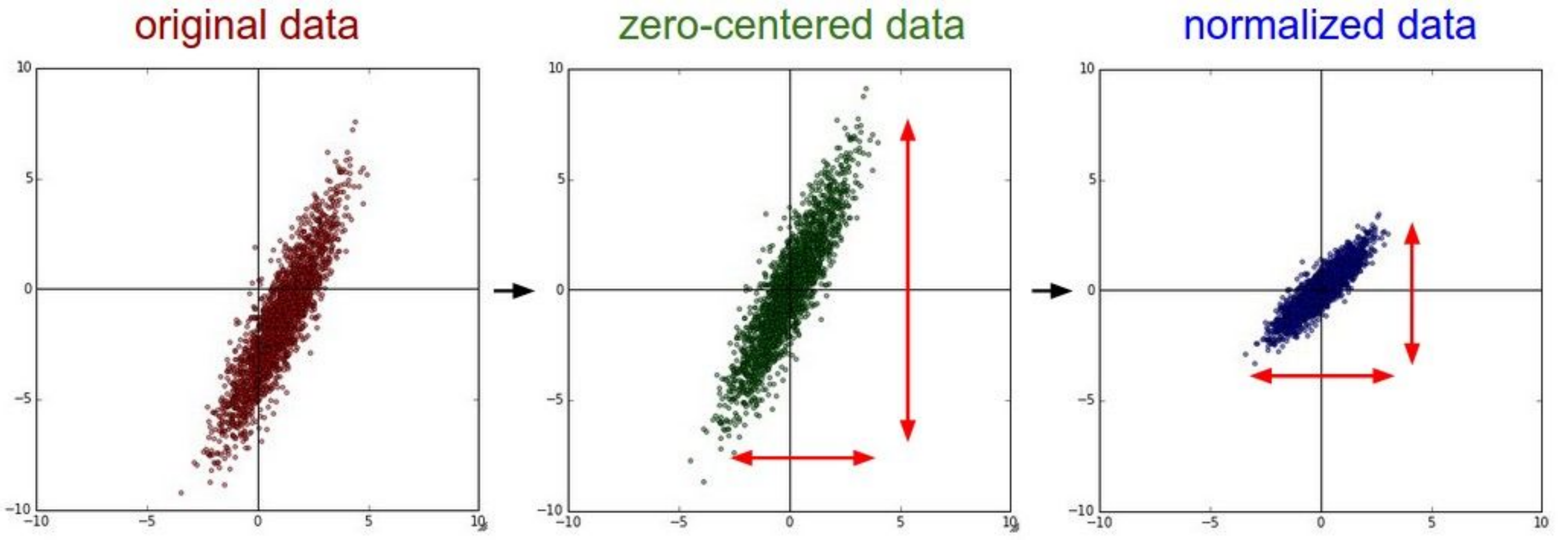
Problem: doubles the number of parameters/neuron :(

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

Data Preprocessing



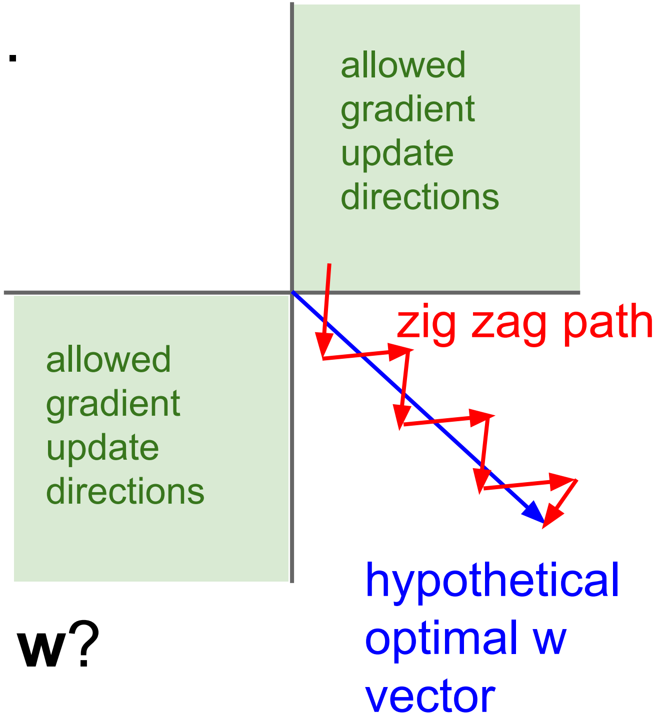
`X -= np.mean(X, axis = 0)`

`X /= np.std(X, axis = 0)`

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

Remember: Consider what happens when the input to a neuron is always positive...

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

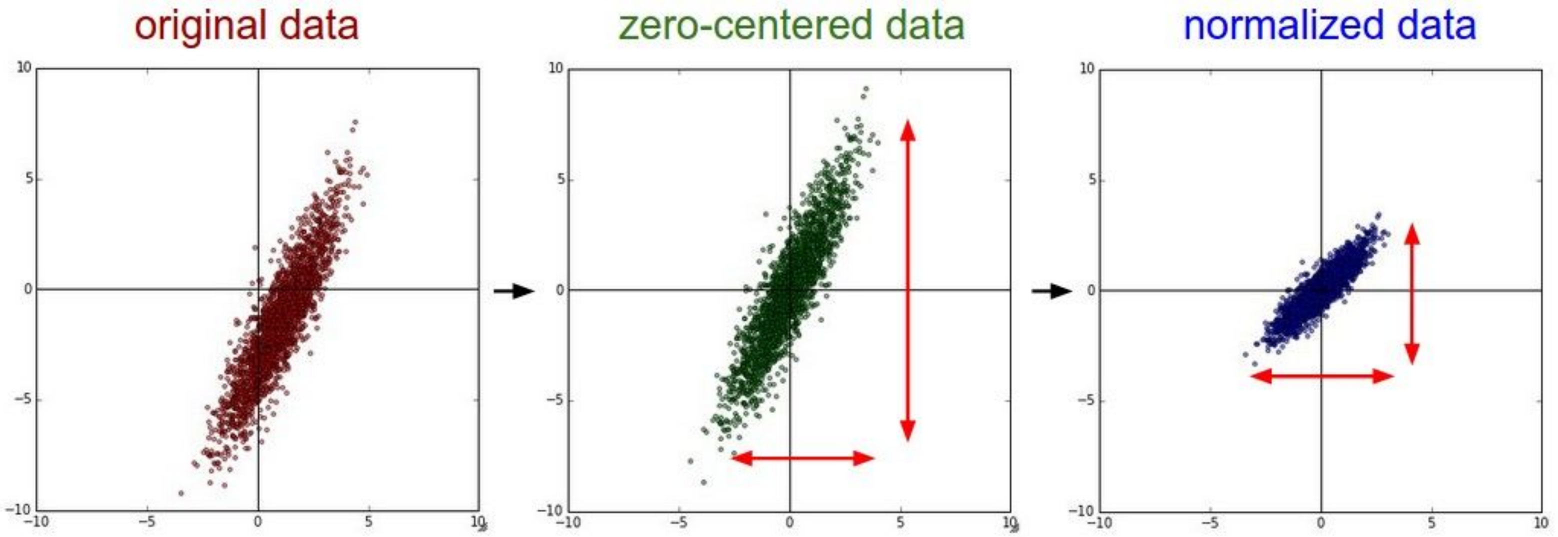


What can we say about the gradients on **w**?

Always all positive or all negative :(

(this is also why you want zero-mean data!)

Data Preprocessing

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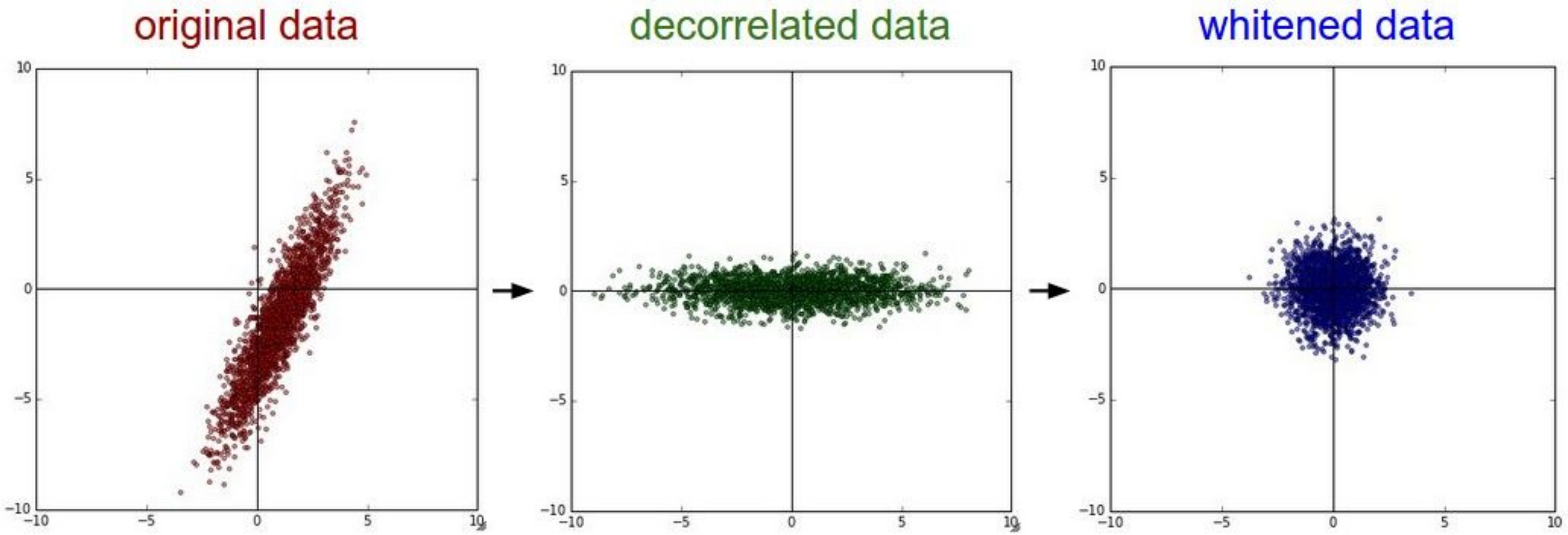
X -= np.mean(X, axis = 0)
```

```
X /= np.std(X, axis = 0)
```

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

Data Preprocessing

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

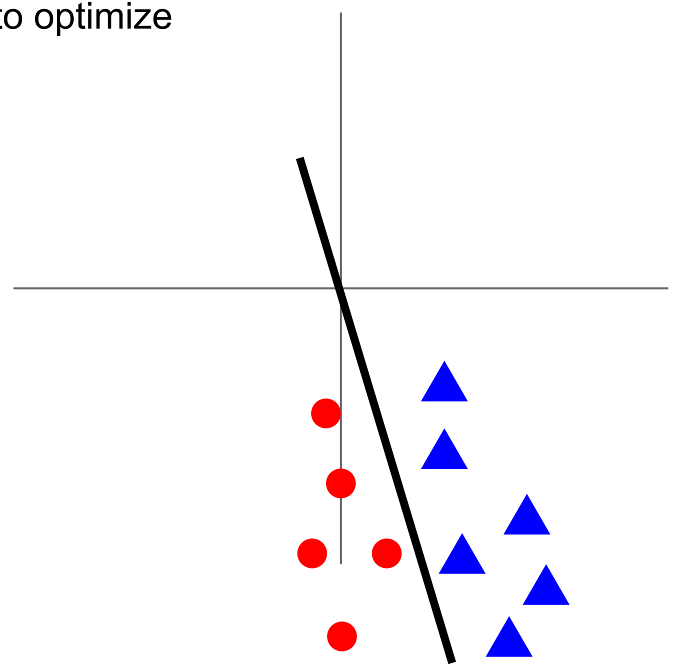


(data has diagonal covariance matrix)

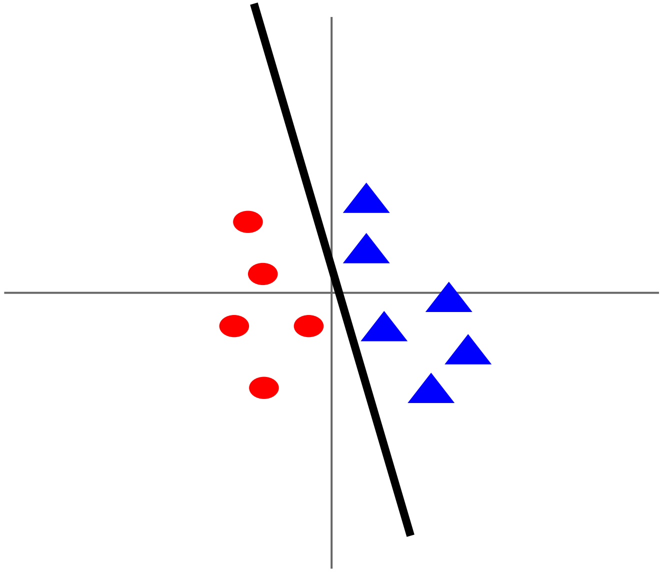
(covariance matrix is the identity matrix)

Data Preprocessing

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize



After normalization: less sensitive to small changes in weights; easier to optimize



TLDR: In practice for Images: center only

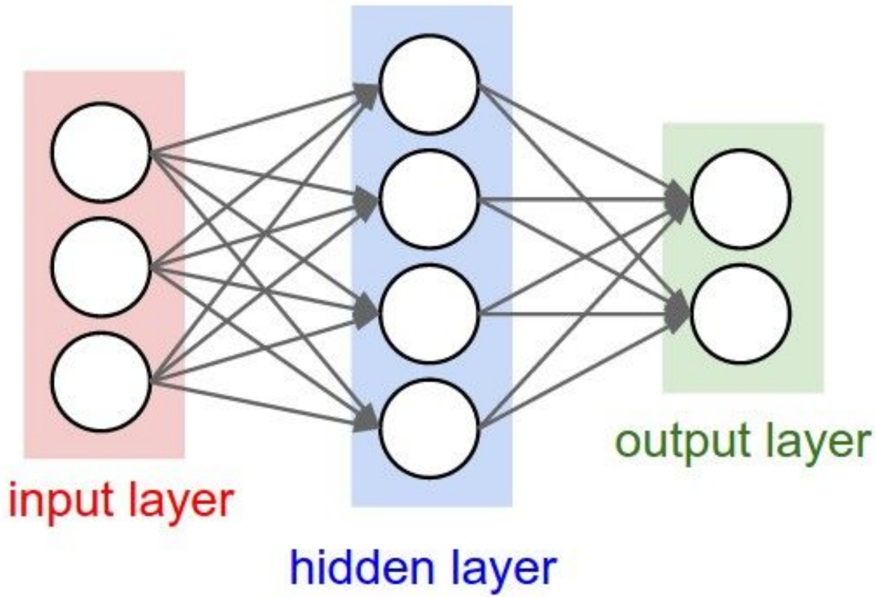
e.g. consider CIFAR-10 example with [32,32,3] images

- 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)
- Subtract per-channel mean and
  Divide by per-channel std (e.g. ResNet)
  (mean along each channel = 3 numbers)

Not common to do PCA or whitening

Weight Initialization

- Q: what happens when W=constant init is used?



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

```
W = 0.01 * np.random.randn(Din, Dout)
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(gaussian with zero mean and 1e-2 standard deviation)

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```

Works ~okay for small networks, but problems with deeper networks.

Weight Initialization: Activation statistics

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Forward pass for a 6-layer net with hidden size 4096

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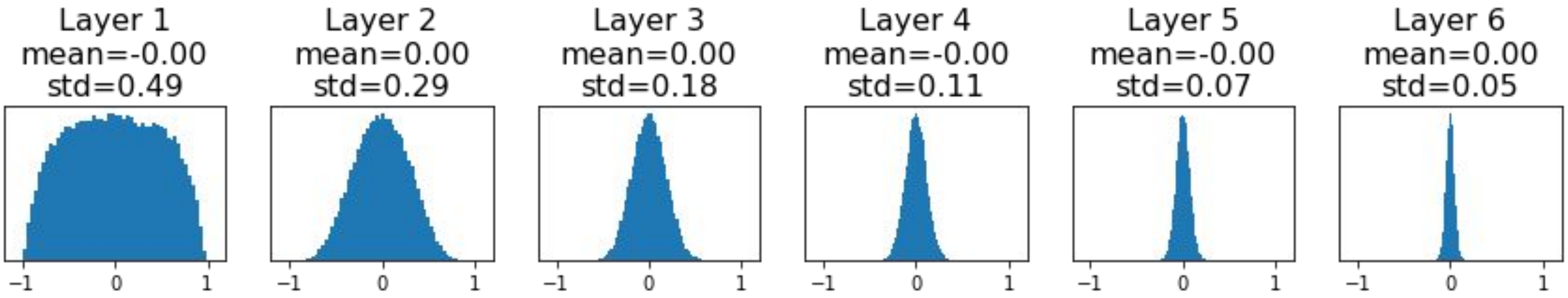
All activations tend to zero for deeper network layers

Q: What do the gradients dL/dW look like?



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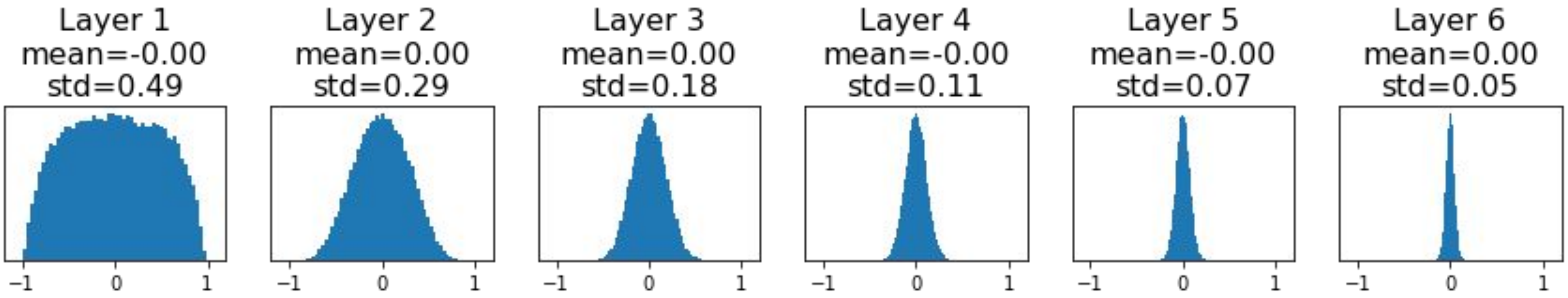
Q: What do the gradients dL/dW look like?

A: All zero, no learning =(



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Increase std of initial weights from 0.01 to 0.05

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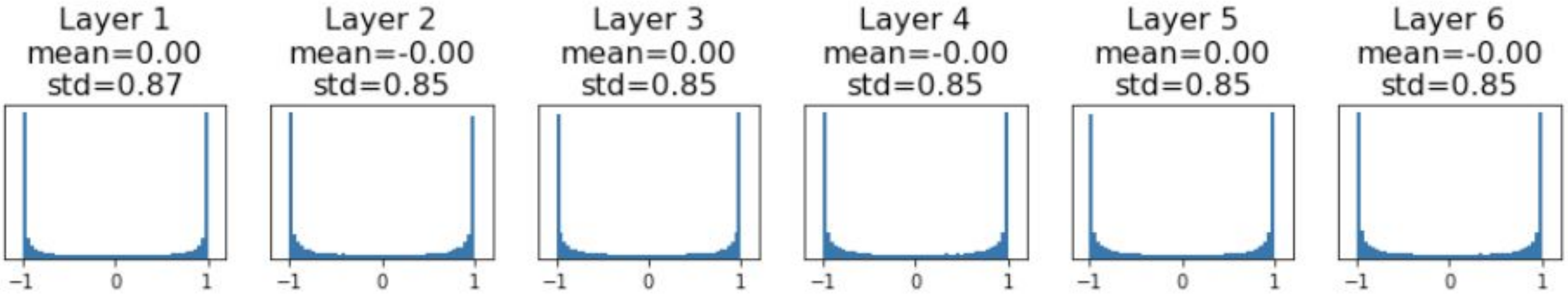
All activations saturate

Q: What do the gradients look like?



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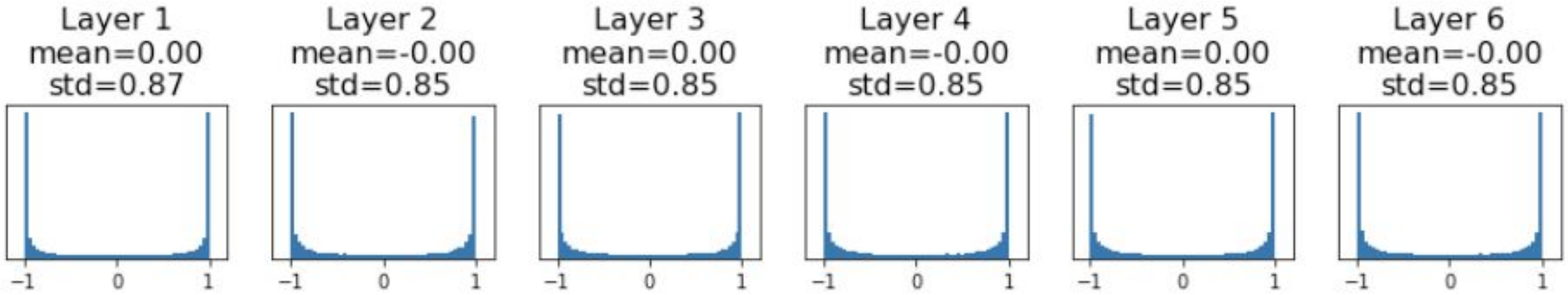
A: Local gradients all zero, no learning =(



Weight Initialization: "Xavier" Initialization

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"Xavier" initialization:
std = 1/sqrt(Din)

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

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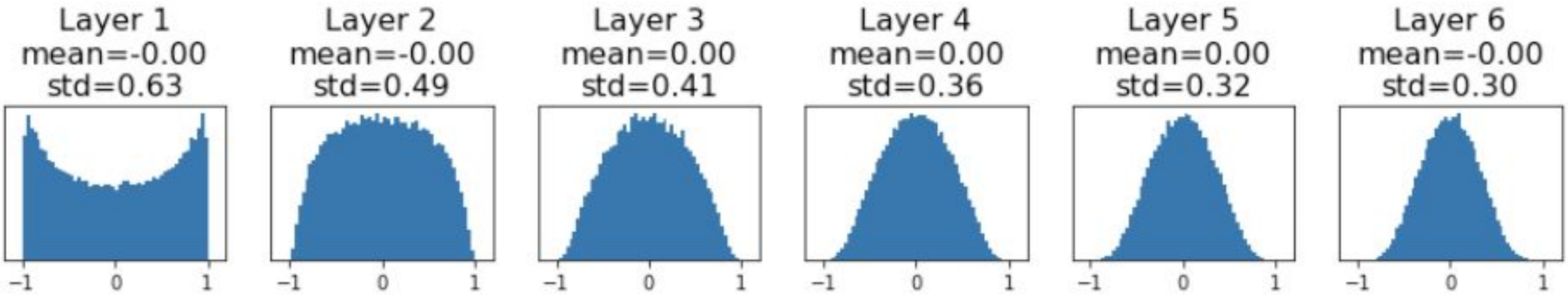
“Just right”: Activations are nicely scaled for all layers!



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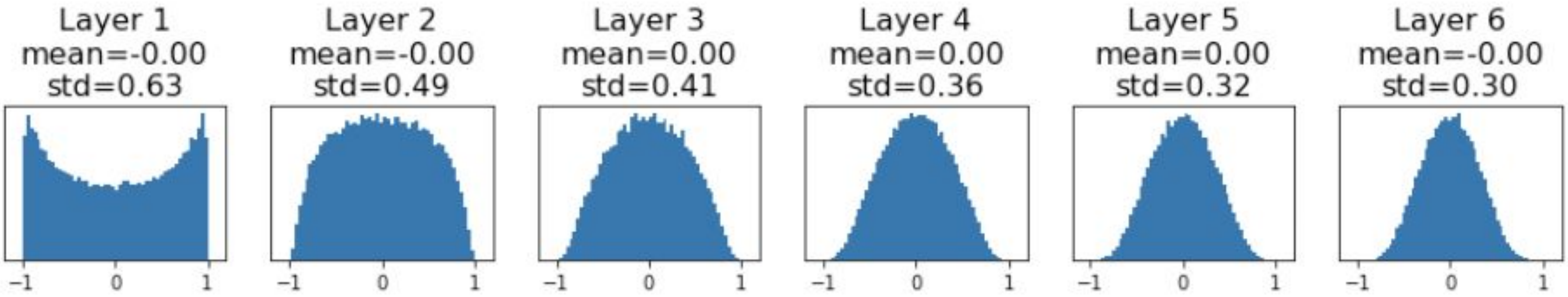

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For conv layers, Din is $\text{kernel\_size}^2 * \text{input\_channels}$

$y = Wx$
$h = f(y)$

Derivation:

$\mathrm{Var}(y_i) = \mathrm{Din} * \mathrm{Var}(x_i w_i)$ [Assume x, w are iid]

$= \mathrm{Din} * (E[x_i^2]E[w_i^2] - E[x_i]^2 E[w_i]^2)$ [Assume x, w independant]

$= \mathrm{Din} * \mathrm{Var}(x_i) * \mathrm{Var}(w_i)$ [Assume x, w are zero-mean]

If $\mathrm{Var}(w_i) = 1/\mathrm{Din}$ then $\mathrm{Var}(y_i) = \mathrm{Var}(x_i)$

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

Weight Initialization: What about ReLU?

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

Change from tanh to ReLU

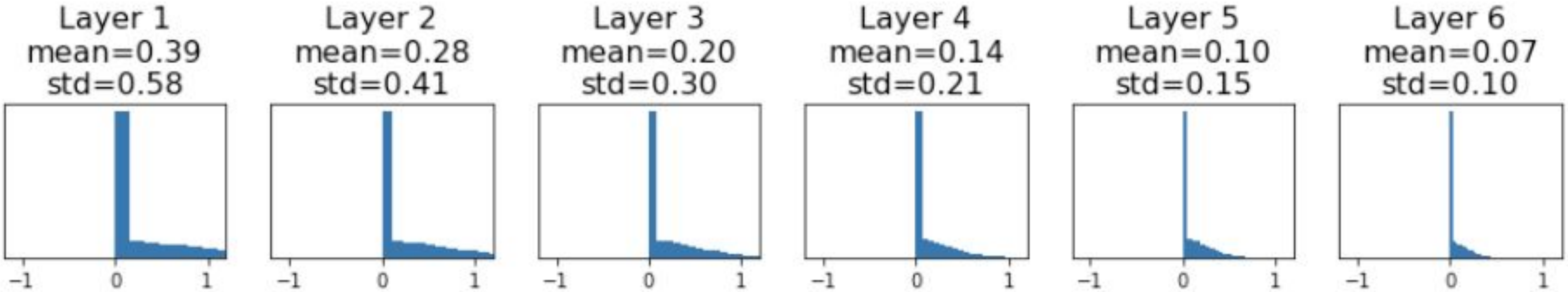
Weight Initialization: What about ReLU?

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

Change from tanh to ReLU

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning =(

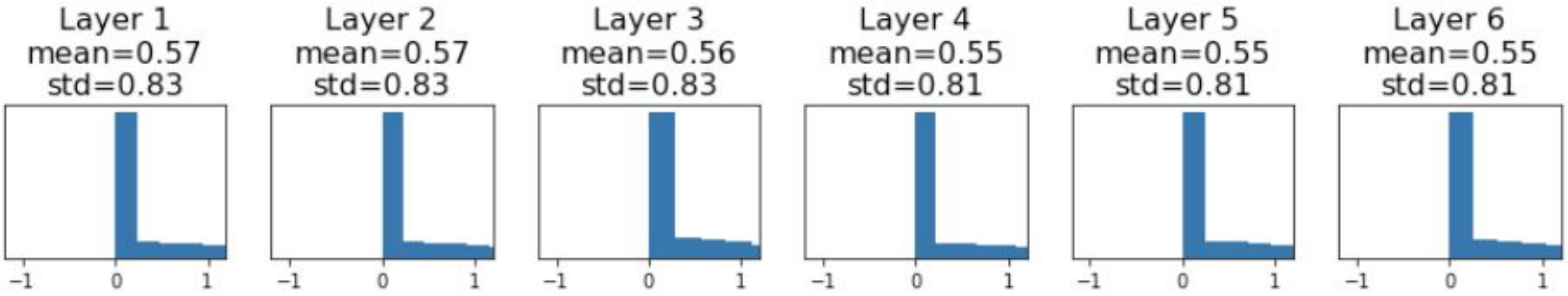


Weight Initialization: Kaiming / MSRA Initialization

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) * np.sqrt(2/Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

ReLU correction: std = sqrt(2 / Din)

"Just right": Activations are nicely scaled for all layers!



He et al, "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification", ICCV 2015

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

Fixup Initialization: Residual Learning Without Normalization, Zhang et al, 2019

The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks, Frankle and Carbin, 2019

Batch Normalization

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want zero-mean unit-variance activations? just make them so."

consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

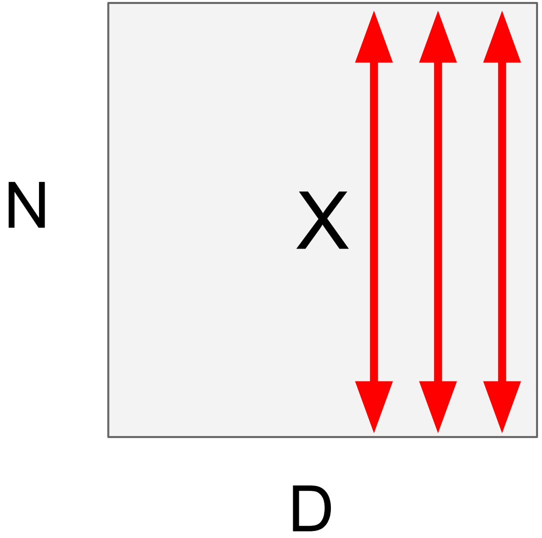
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



$$\mu_j = \frac{1}{N} \sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

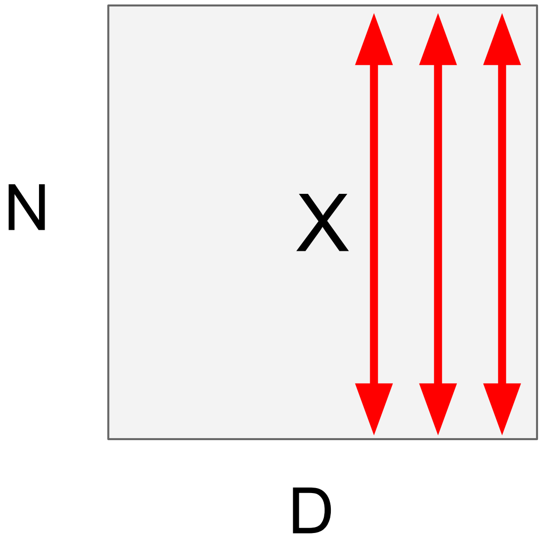
$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



$$\mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j}$$ Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{i,j} - \mu_j)^2$$ Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$ Normalized x, Shape is N x D

Problem: What if zero-mean, unit variance is too hard of a constraint?

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

$$\mu_j = \frac{1}{N} \sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization: Test-Time

Estimates depend on minibatch; can't do this at test-time!

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

$$\mu_j = \frac{1}{N}\sum_{i=1}^{N} x_{i,j}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \frac{1}{N}\sum_{i=1}^{N}(x_{i,j} - \mu_j)^2$$

Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization: Test-Time

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

During testing batchnorm becomes a linear operator! Can be fused with the previous fully-connected or conv layer

$\mu_j =$ (Running) average of values seen during training — Per-channel mean, shape is D

$\sigma_j^2 =$ (Running) average of values seen during training — Per-channel var, shape is D

$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x, Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output, Shape is N x D

Batch Normalization: Test-Time

Input: $x : N \times D$

Learnable scale and shift parameters:

$\gamma, \beta : D$

Learning $\gamma = \sigma$,
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$$\hat{x}_{i,j} = \frac{x_{i,j} - \mu_j}{\sqrt{\sigma_j^2 + \varepsilon}}$$

Normalized x,
Shape is N x D

$$y_{i,j} = \gamma_j \hat{x}_{i,j} + \beta_j$$

Output,
Shape is N x D

Batch Normalization for ConvNets

Batch Normalization for **fully-connected** networks

$$\mathbf{x}: N \times D$$

Normalize $\downarrow$

$$\boldsymbol{\mu}, \boldsymbol{\sigma}: 1 \times D$$

$$\gamma, \beta: 1 \times D$$

$$\mathbf{y} = \gamma(\mathbf{x} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \beta$$

Batch Normalization for **convolutional** networks (Spatial Batchnorm, BatchNorm2D)

$$\mathbf{x}: N \times C \times H \times W$$

Normalize $\downarrow \quad \downarrow \quad \downarrow$

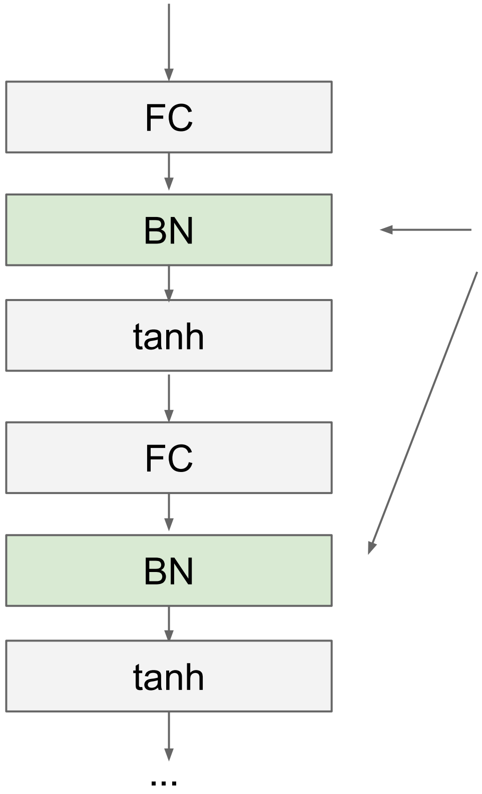
$$\boldsymbol{\mu}, \boldsymbol{\sigma}: 1 \times C \times 1 \times 1$$

$$\gamma, \beta: 1 \times C \times 1 \times 1$$

$$\mathbf{y} = \gamma(\mathbf{x} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \beta$$

Batch Normalization

[Ioffe and Szegedy, 2015]

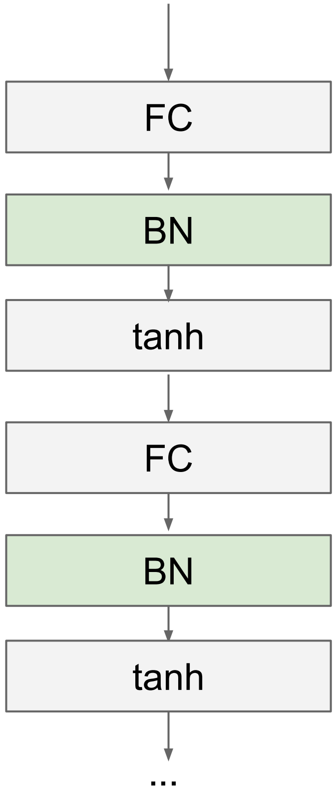


Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

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

Batch Normalization

[Ioffe and Szegedy, 2015]



- Makes deep networks **much** easier to train!
- Improves gradient flow
- Allows higher learning rates, faster convergence
- Networks become more robust to initialization
- Acts as regularization during training
- Zero overhead at test-time: can be fused with conv!
- Behaves differently during training and testing: this is a very common source of bugs!

Layer Normalization

Batch Normalization for fully-connected networks

$\mathbf{x}: N \times D$

Normalize

$\boldsymbol{\mu}, \boldsymbol{\sigma}: 1 \times D$

$\gamma, \beta: 1 \times D$

$\mathbf{y} = \gamma(\mathbf{x} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \beta$

Layer Normalization for fully-connected networks
Same behavior at train and test!
Can be used in recurrent networks

$\mathbf{x}: N \times D$

Normalize

$\boldsymbol{\mu}, \boldsymbol{\sigma}: N \times 1$

$\gamma, \beta: 1 \times D$

$\mathbf{y} = \gamma(\mathbf{x} - \boldsymbol{\mu}) / \boldsymbol{\sigma} + \beta$

Ba, Kiros, and Hinton, “Layer Normalization”, arXiv 2016

Instance Normalization

Batch Normalization for convolutional networks

$$\mathbf{x}: N \times C \times H \times W$$

Normalize

$$\boldsymbol{\mu}, \boldsymbol{\sigma}: 1 \times C \times 1 \times 1$$

$$\gamma, \beta: 1 \times C \times 1 \times 1$$

$$y = \gamma(x - \mu) / \sigma + \beta$$

Instance Normalization for convolutional networks
Same behavior at train / test!

$$\mathbf{x}: N \times C \times H \times W$$

Normalize

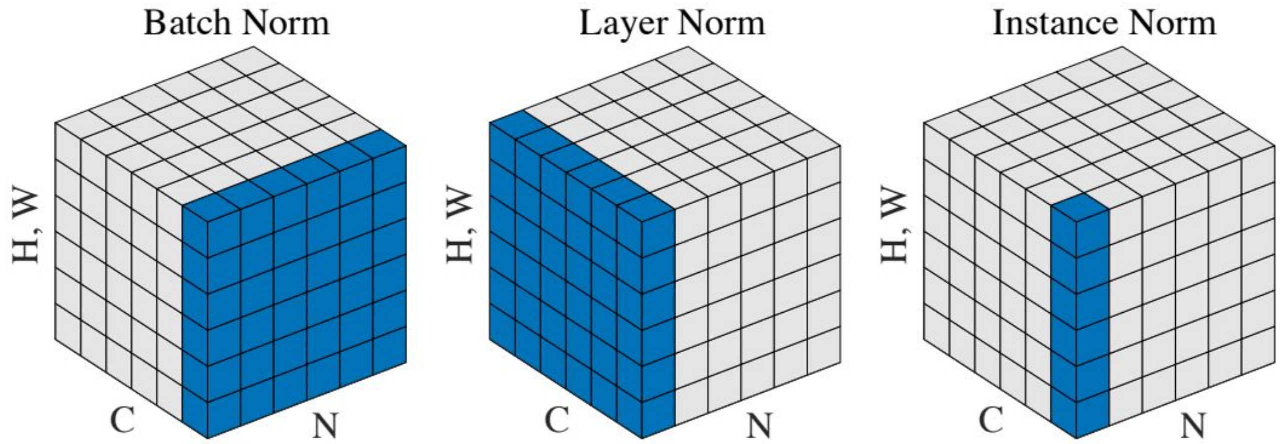
$$\boldsymbol{\mu}, \boldsymbol{\sigma}: N \times C \times 1 \times 1$$

$$\gamma, \beta: 1 \times C \times 1 \times 1$$

$$y = \gamma(x - \mu) / \sigma + \beta$$

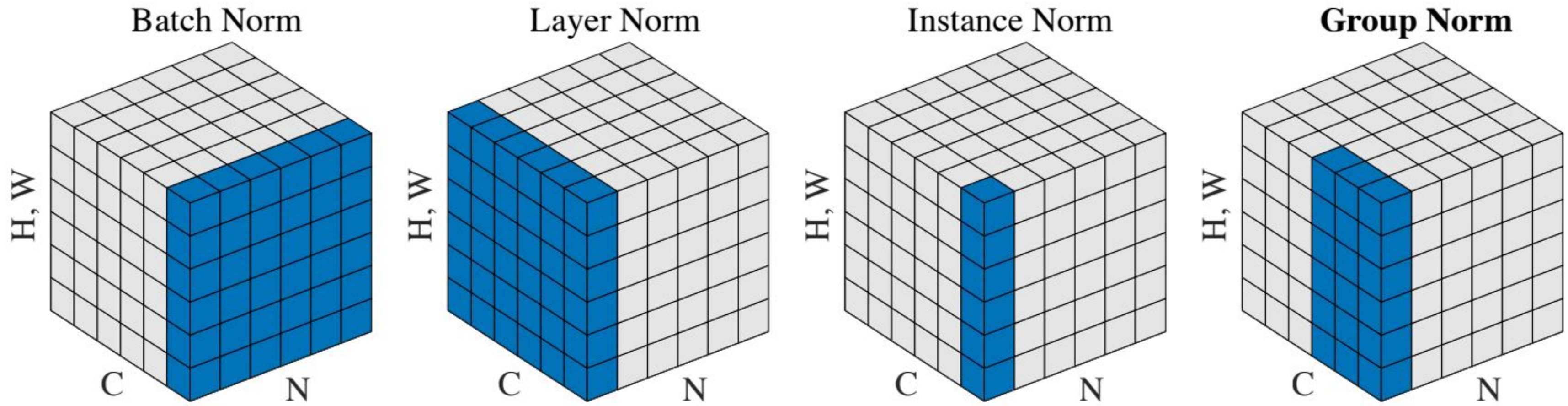
Ulyanov et al, Improved Texture Networks: Maximizing Quality and Diversity in Feed-forward Stylization and Texture Synthesis, CVPR 2017

Comparison of Normalization Layers



Wu and He, “Group Normalization”, ECCV 2018

Group Normalization



Wu and He, "Group Normalization", ECCV 2018

Summary

TLDRs

We looked in detail at:

- Activation Functions (use ReLU)
- Data Preprocessing (images: subtract mean)
- Weight Initialization (use Xavier/He init)
- Batch Normalization (use)