Lecture 10: Training Neural Networks (Part 1)

Reminder: A3

- Due Friday, February 11

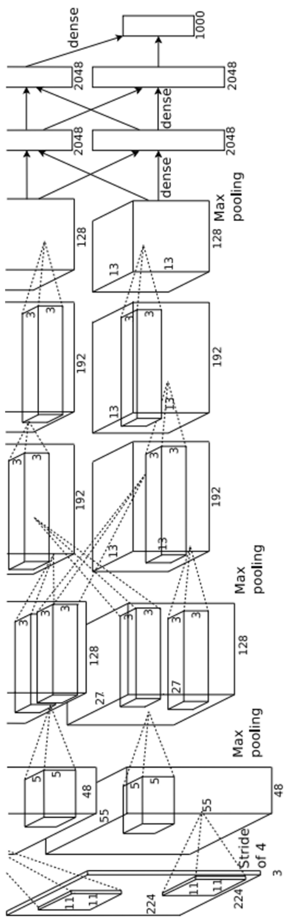
ULCS / Depth

If you are a CSE student:

- For undergrads: This course now counts as ULCS (this term only)
- For grad students: This course now counts as technical depth

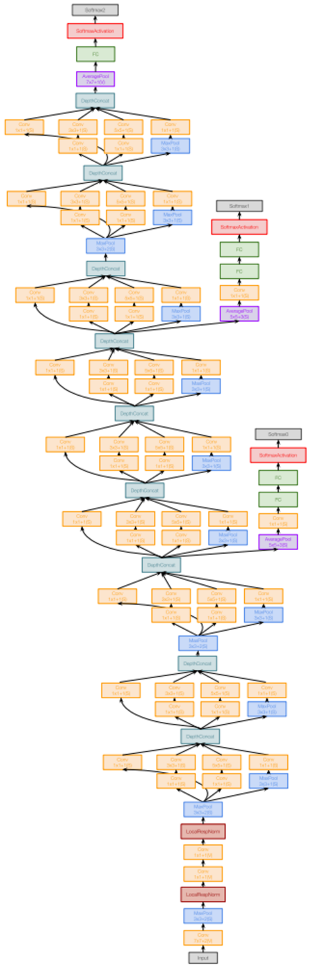
For non-CSE students: Check with your program

Last Time: CNN Architectures

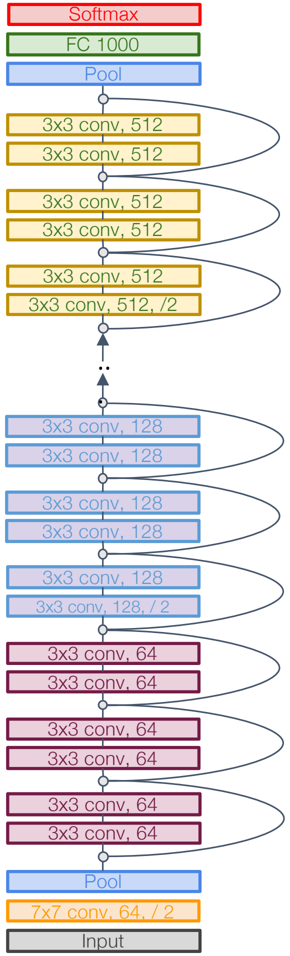


AlexNet

VGG



GoogLeNet



ResNet

Overview

1. **One time setup**
   Activation functions, data preprocessing, weight initialization, regularization
2. **Training dynamics**
   Learning rate schedules; large-batch training; hyperparameter optimization
3. **After training**
   Model ensembles, transfer learning

Overview

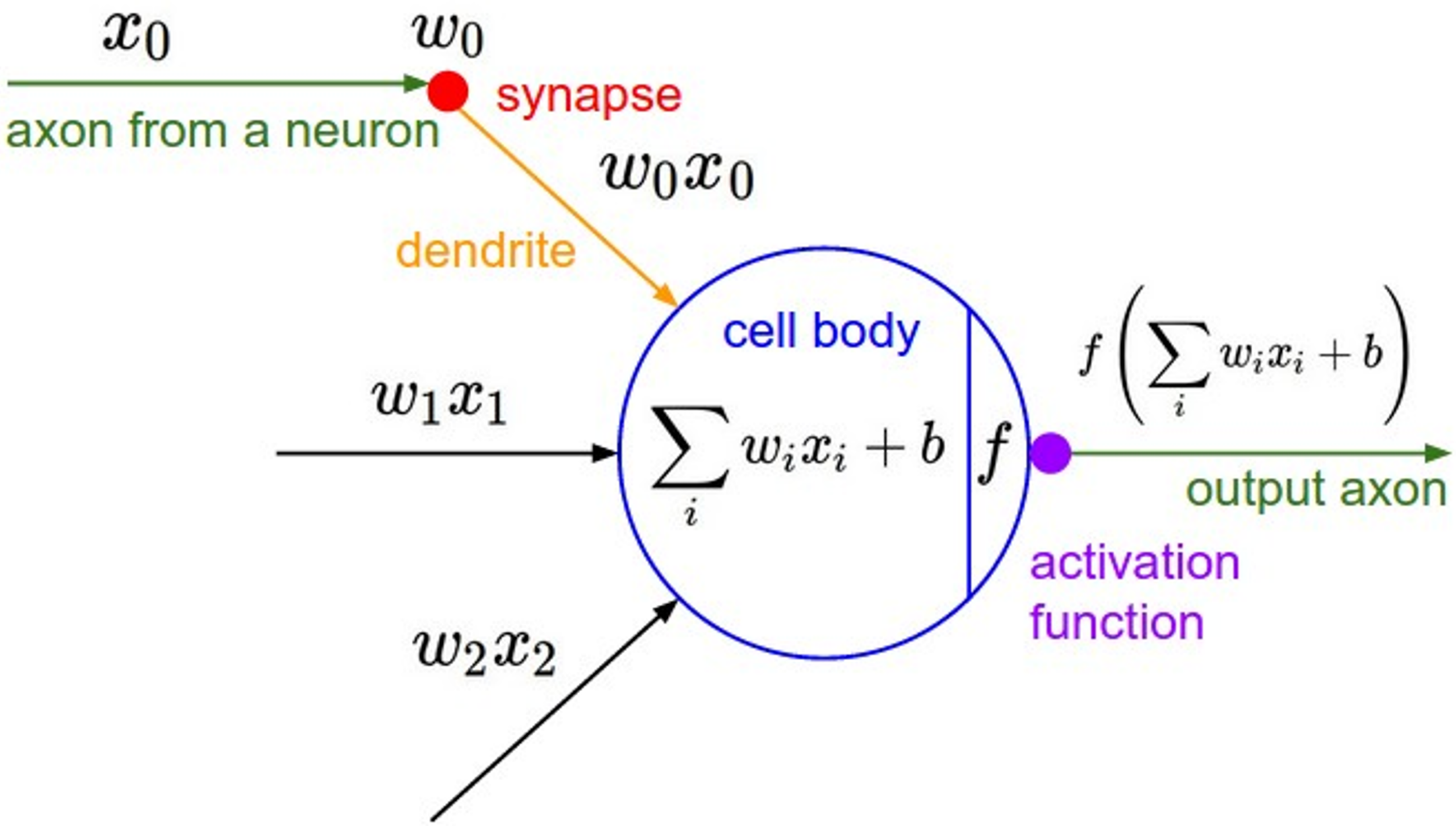
1. **One time setup**
   Activation functions, data preprocessing, weight initialization, regularization
2. **Training dynamics**
   Learning rate schedules; large-batch training; hyperparameter optimization
3. **After training**
   Model ensembles, transfer learning

Today

Next time

Activation Functions

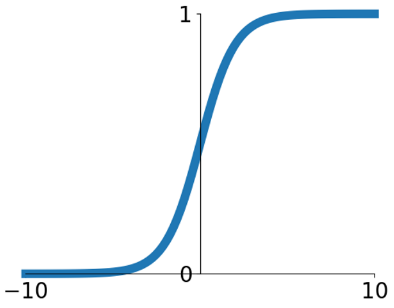
Activation Functions



Activation Functions

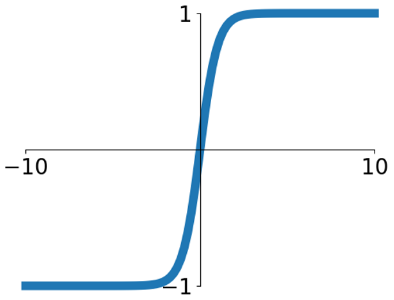
Sigmoid

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



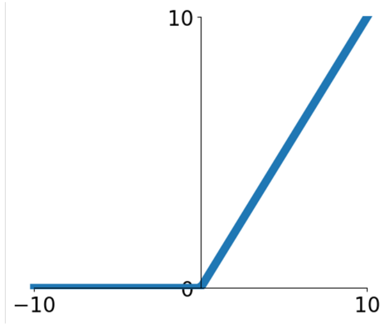
tanh

$\tanh(x)$



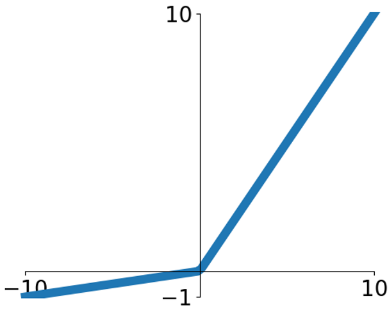
ReLU

$\max(0, x)$



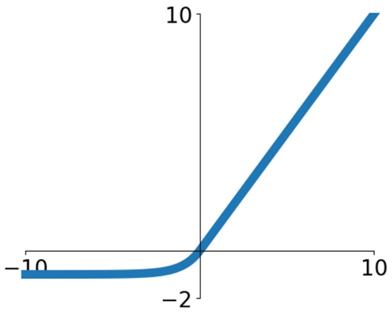
Leaky ReLU

$\max(0.1x, x)$



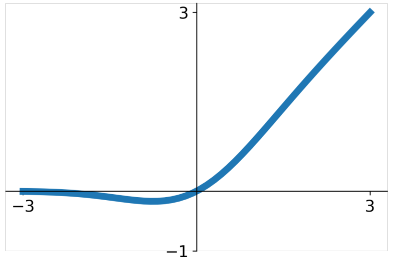
ELU

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

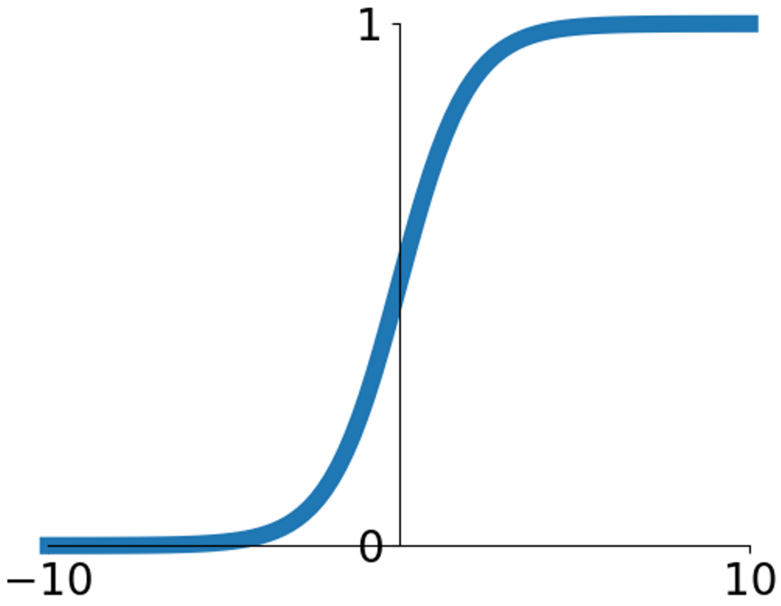


GELU

$\approx x\sigma(1.702x)$



Activation Functions: Sigmoid

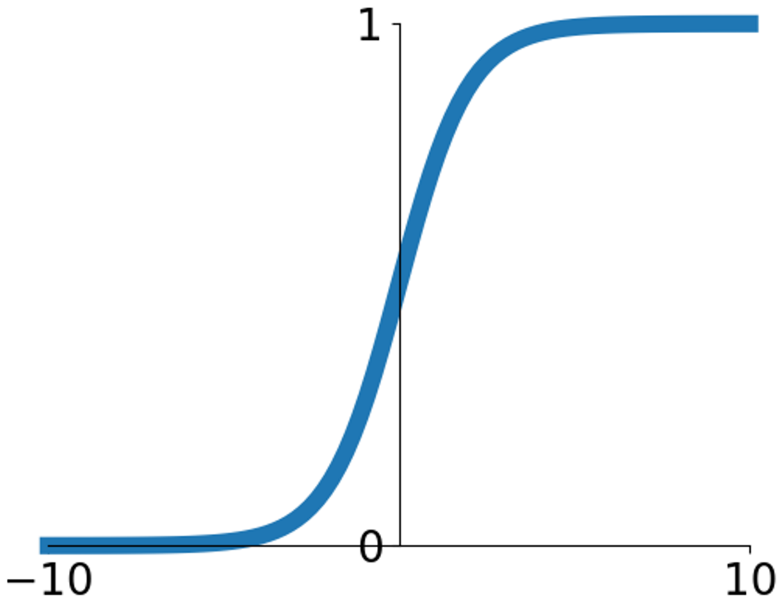


Sigmoid

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

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

Activation Functions: Sigmoid



Sigmoid

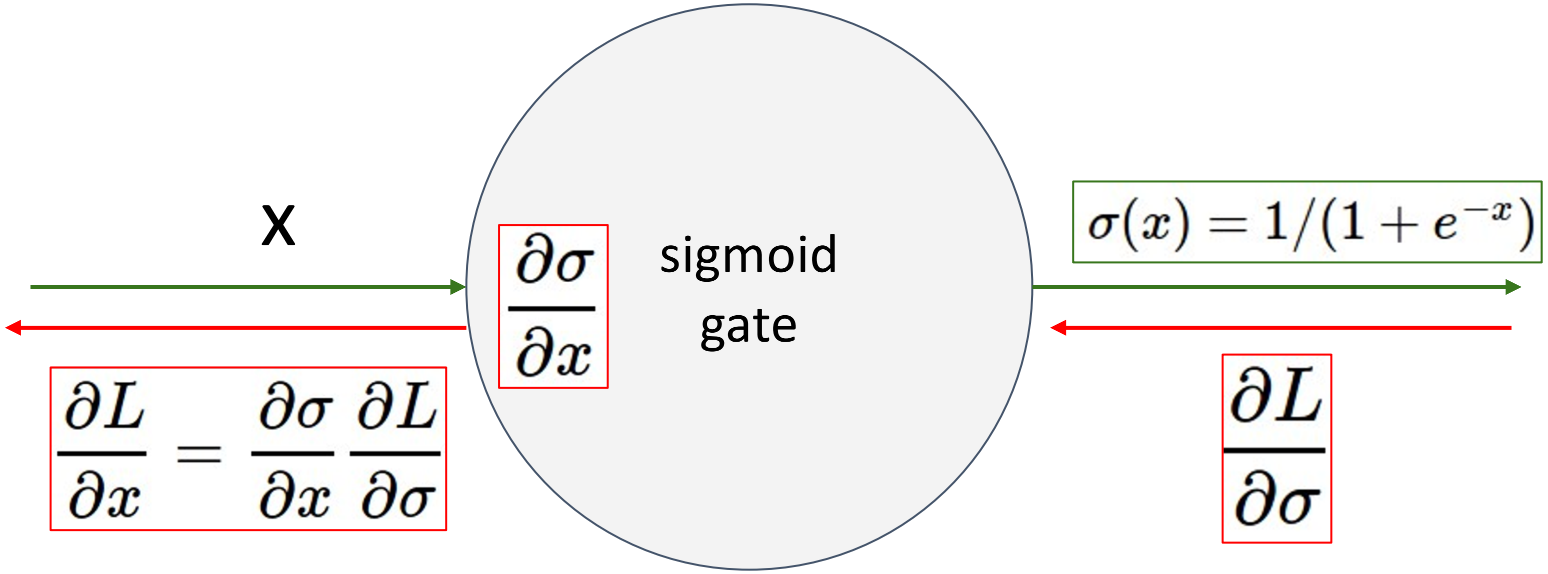
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

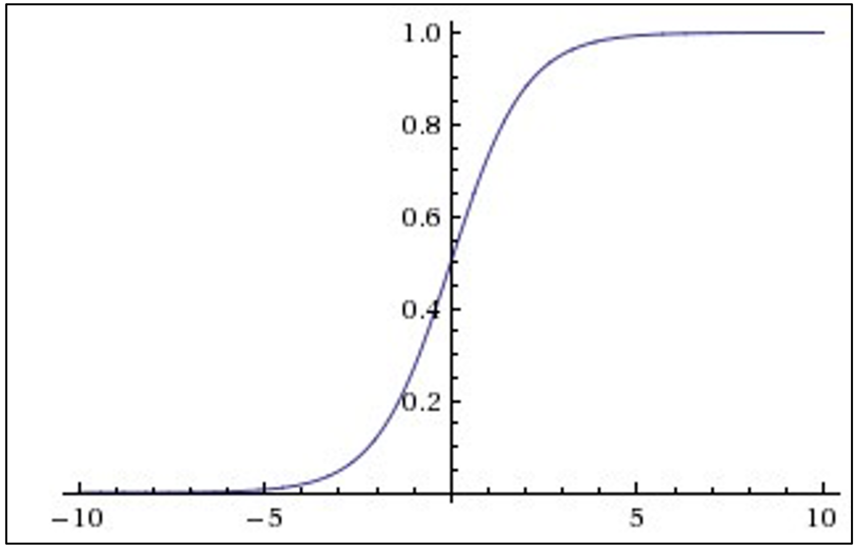
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

3 problems:

1. Saturated neurons "kill" the gradients

Activation Functions: Sigmoid



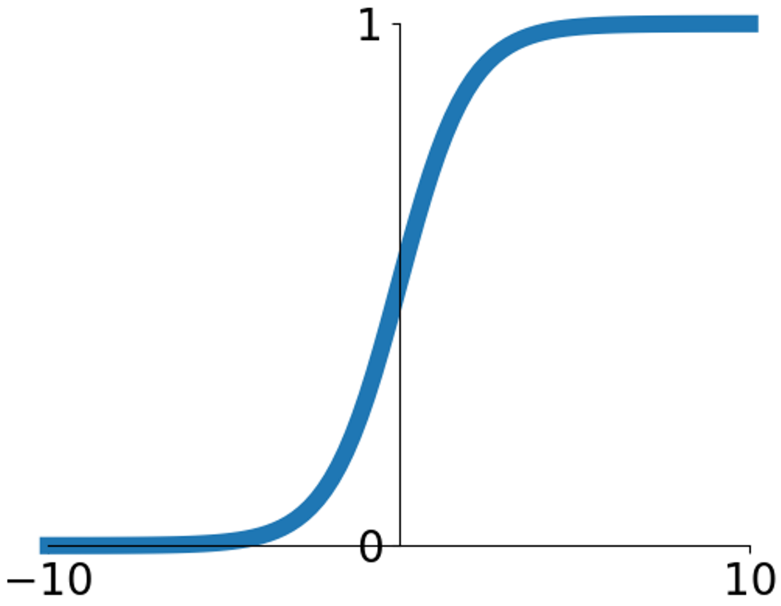


What happens when x = -10?

What happens when x = 0?

What happens when x = 10?

Activation Functions: Sigmoid



Sigmoid

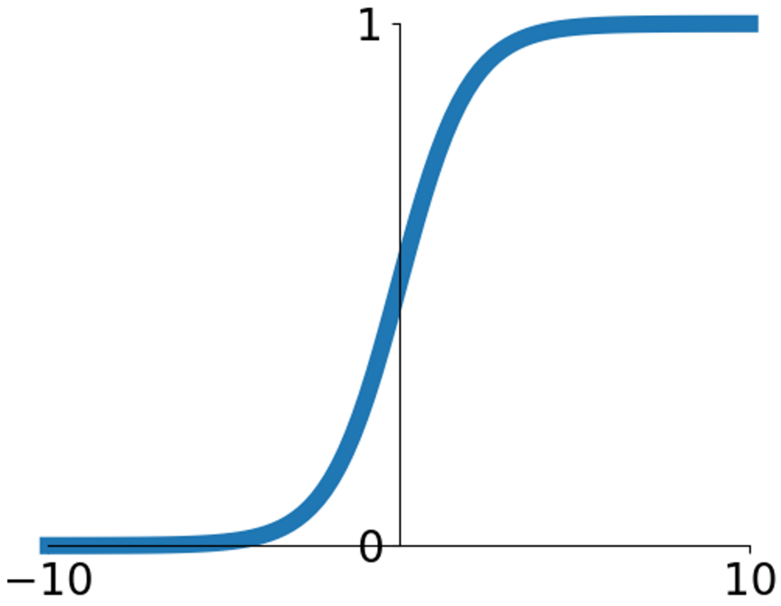
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- 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

Activation Functions: Sigmoid



Sigmoid

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

- 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 zero-centered

Consider what happens when nonlinearity is always positive

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

$h_i^{(\ell)}$ is the ith element of the hidden layer at layer ℓ (before activation)
$w^{(\ell)}, \mathrm{b}^{(\ell)}$ are the weights and bias of layer ℓ

What can we say about the gradients on $w^{(\ell)}$?

Consider what happens when nonlinearity is always positive

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

Local Gradient | Upstream Gradient

$$\frac{\partial L}{\partial w_{i,j}^{(\ell)}} = \frac{\partial h_i^{(\ell)}}{\partial w_{i,j}} \cdot \frac{\partial L}{\partial h_i^{(\ell)}}$$

$h_i^{(\ell)}$ is the ith element of the hidden layer at layer ℓ (before activation)
$w^{(\ell)}, \mathrm{b}^{(\ell)}$ are the weights and bias of layer ℓ

What can we say about the gradients on $w^{(\ell)}$?

Consider what happens when nonlinearity is always positive

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

$h_i^{(\ell)}$ is the ith element of the hidden layer at layer ℓ (before activation)
$w^{(\ell)}, \mathrm{b}^{(\ell)}$ are the weights and bias of layer ℓ

Local Gradient   Upstream Gradient

$$\frac{\partial L}{\partial w_{i,j}^{(\ell)}} = \frac{\partial h_i^{(\ell)}}{\partial w_{i,j}} \cdot \frac{\partial L}{\partial h_i^{(\ell)}}$$

$$= \sigma\left(h_j^{(\ell-1)}\right) \cdot \frac{\partial L}{\partial h_i^{(\ell)}}$$

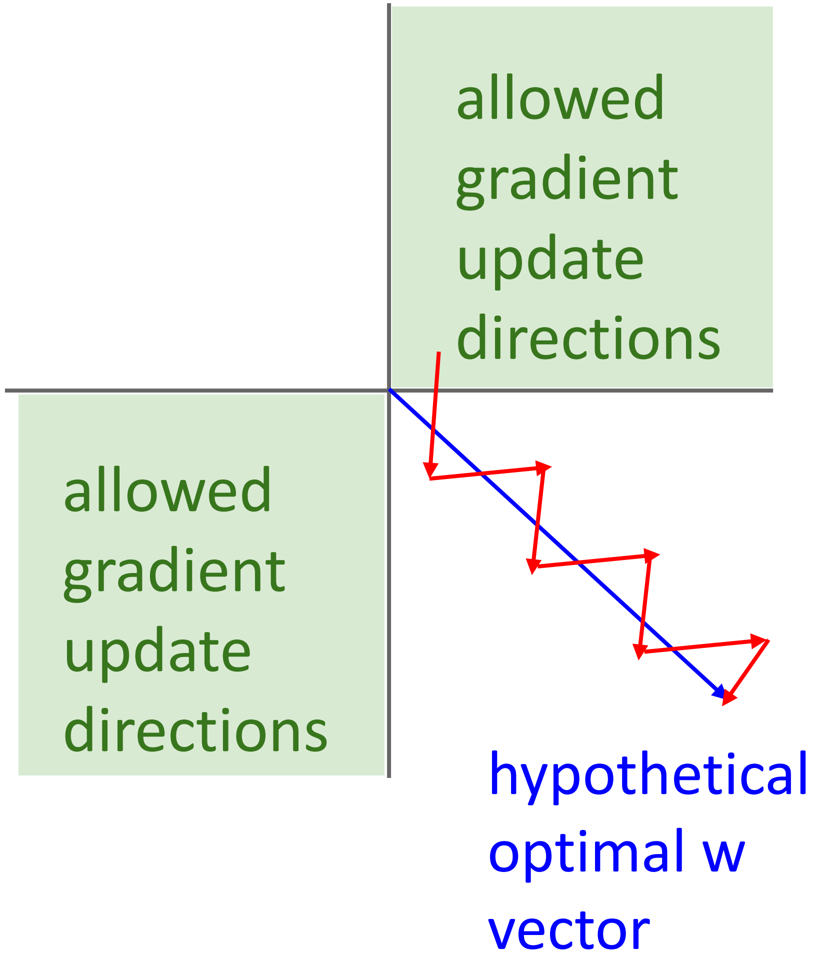
What can we say about the gradients on $w^{(\ell)}$?

Gradients on all $w_{i,j}^{(ell)}$ have the same sign as upstream gradient $\partial L / \partial h_i^{(\ell)}$

Consider what happens when nonlinearity is always positive

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

$h_i^{(\ell)}$ is the ith element of the hidden layer at layer ℓ (before activation)
$w^{(\ell)}, \mathrm{b}^{(\ell)}$ are the weights and bias of layer ℓ



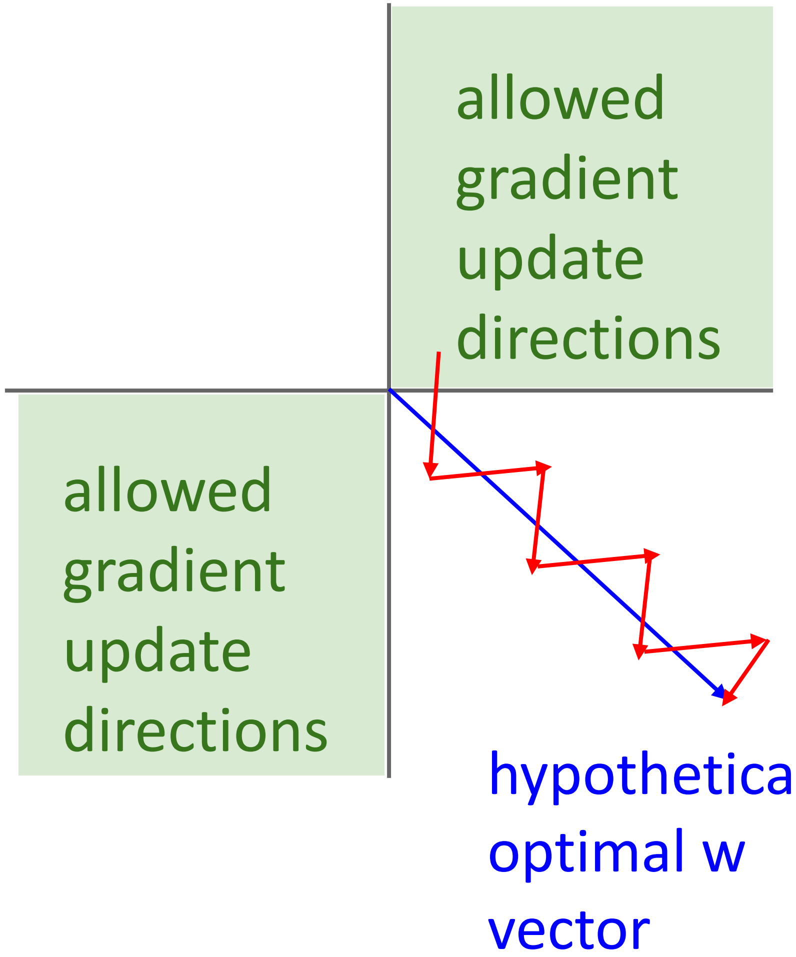
What can we say about the gradients on $w^{(\ell)}$?
Gradients on all $w_{i,j}^{(ell)}$ have the same sign as upstream gradient $\partial L / \partial h_i^{(\ell)}$

Gradients on rows of w can only point in some directions; needs to “zigzag” to move in other directions

Consider what happens when nonlinearity is always positive

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

$h_i^{(\ell)}$ is the ith element of the hidden layer at layer ℓ (before activation)
$w^{(\ell)}, \mathrm{b}^{(\ell)}$ are the weights and bias of layer ℓ

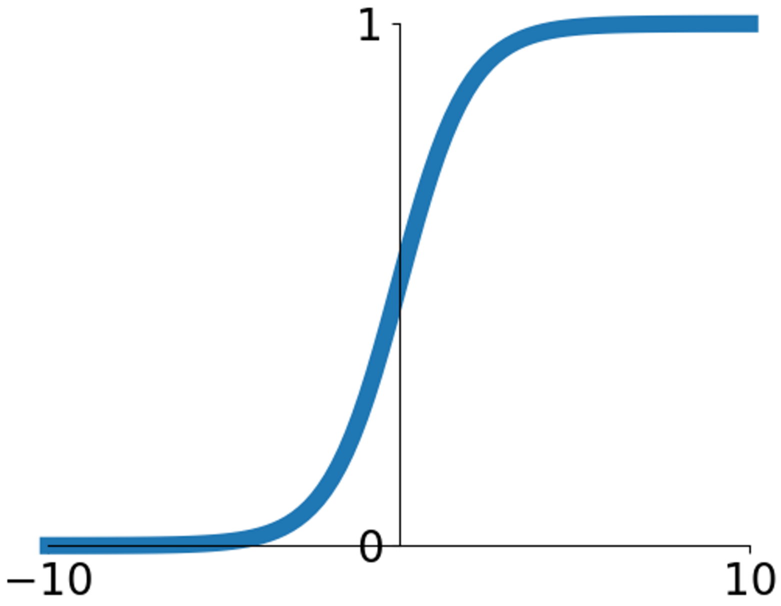


What can we say about the gradients on $w^{(\ell)}$?

Gradients on all $w_{i,j}^{(ell)}$ have the same sign as upstream gradient $\partial L / \partial h_i^{(\ell)}$

Not that bad in practice:
- Only true for a single example, minibatches help
- BatchNorm can also avoid this

Activation Functions: Sigmoid



Sigmoid

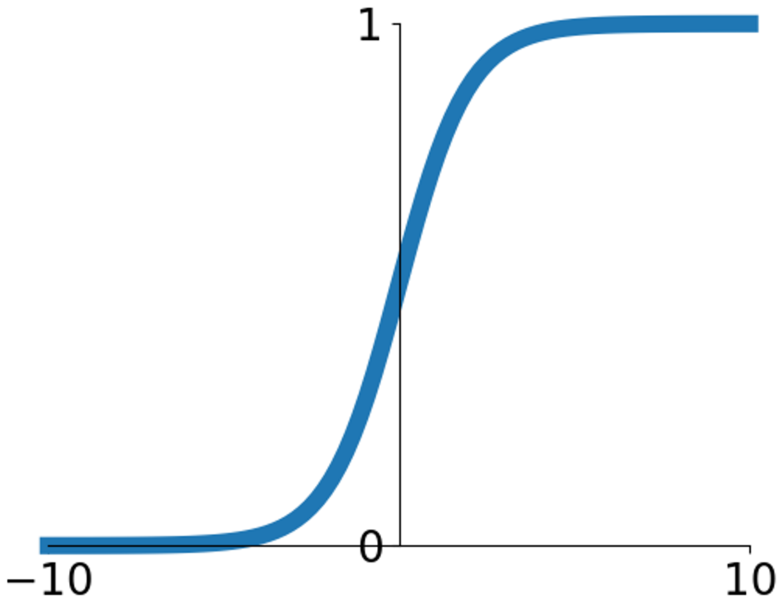
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- 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 zero-centered

Activation Functions: Sigmoid



Sigmoid

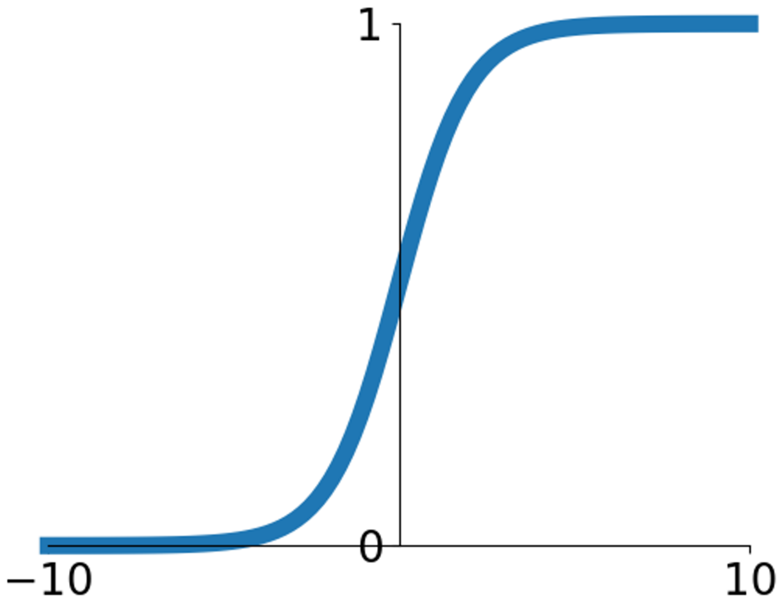
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

- 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 zero-centered
3. exp() is a bit compute expensive

Activation Functions: Sigmoid



Sigmoid

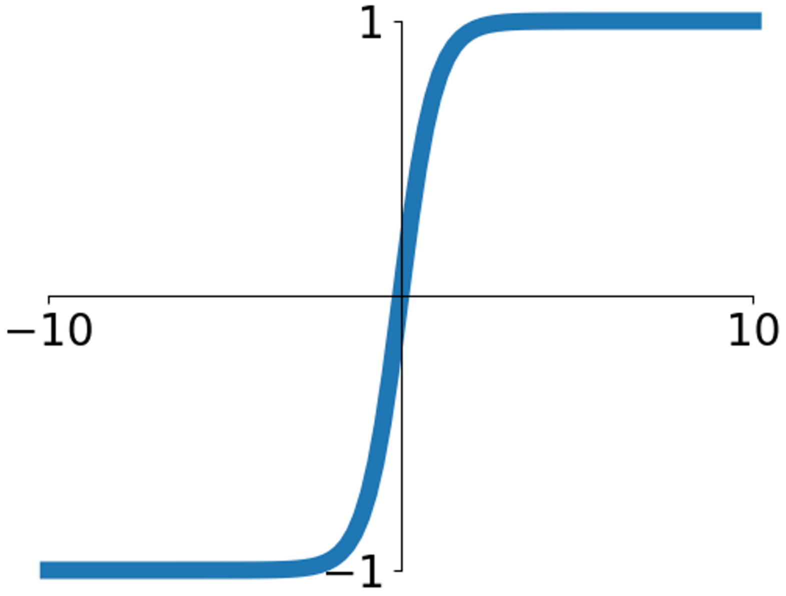
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

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

3 problems: **Worst problem in practice**

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

Activation Functions: Tanh

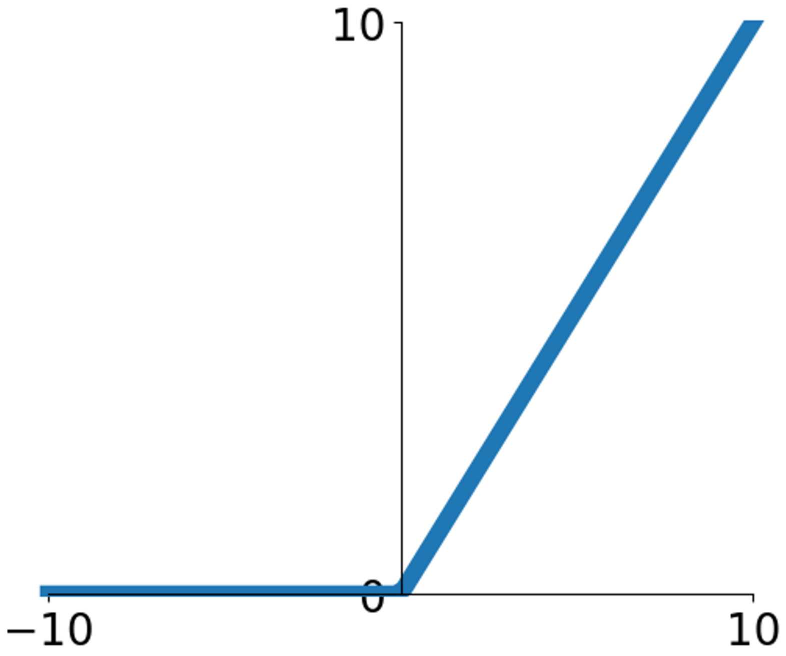


tanh(x)

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

Activation Functions: ReLU

$f(x) = \max(0,x)$



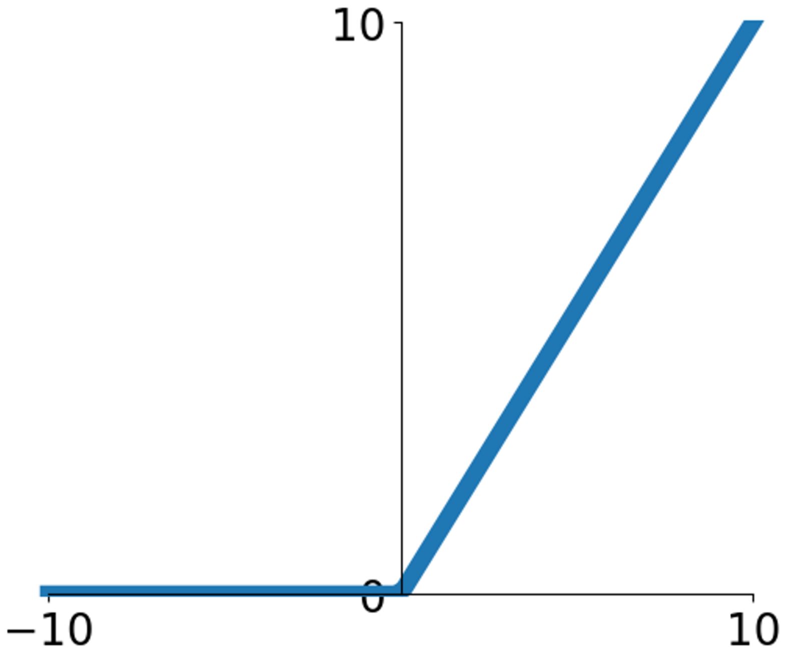
ReLU

(Rectified Linear Unit)

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

Activation Functions: ReLU

$f(x) = \max(0,x)$



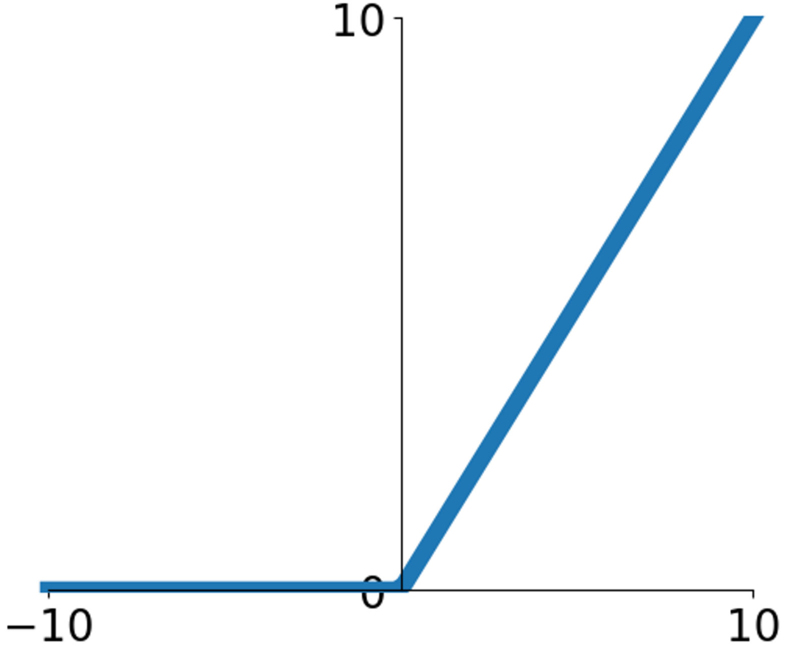
ReLU
(Rectified Linear Unit)

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

- Not zero-centered output

Activation Functions: ReLU

$f(x) = \max(0,x)$



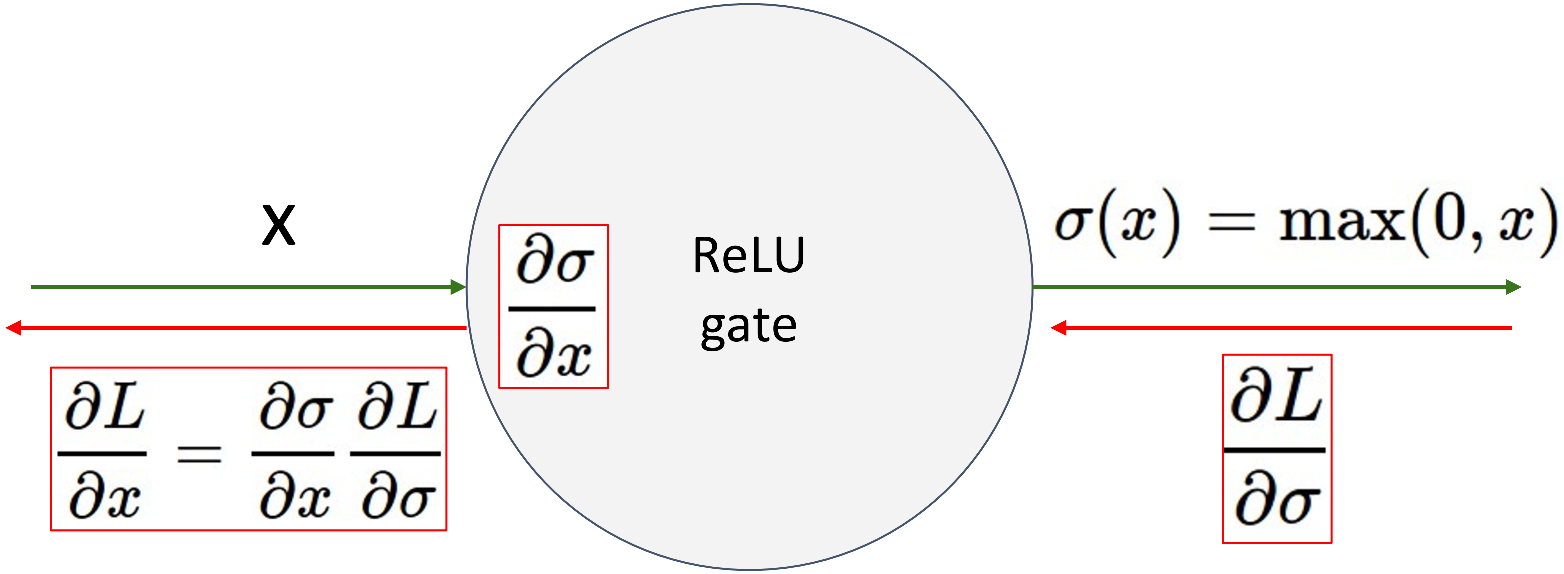
ReLU
(Rectified Linear Unit)

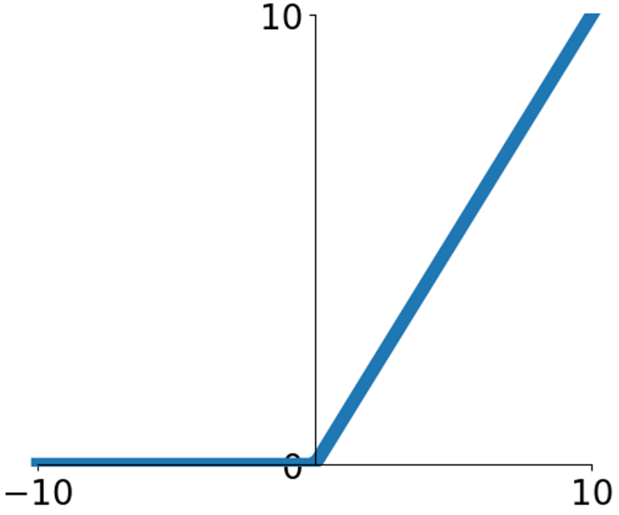
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

- Not zero-centered output
- An annoyance:

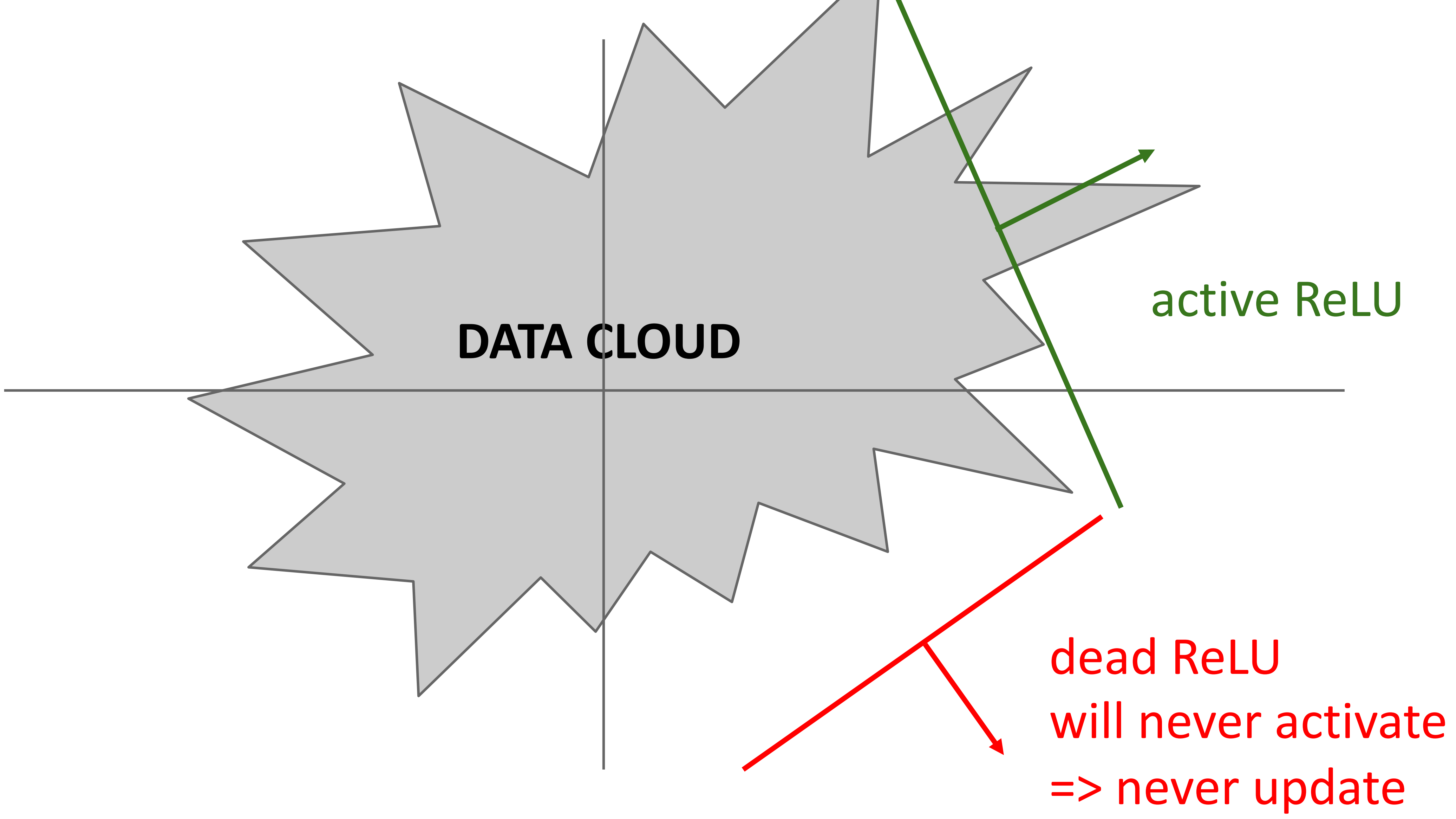
hint: what is the gradient when $x < 0$?

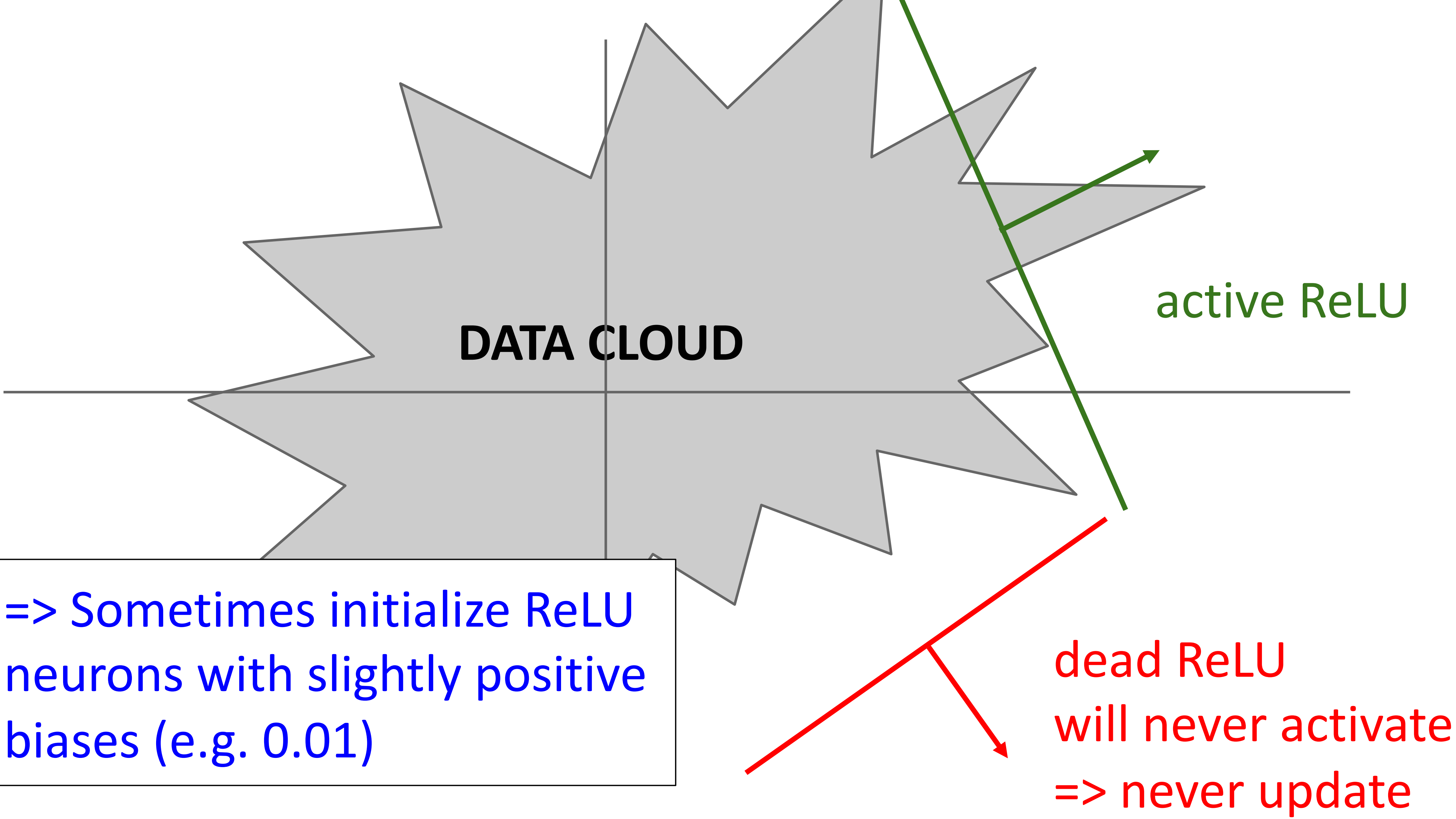
Activation Functions: ReLU





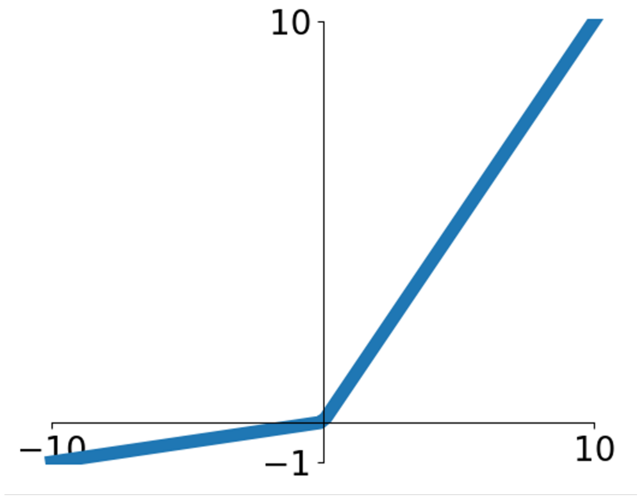
What happens when x = -10?
What happens when x = 0?
What happens when x = 10?


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



=> Sometimes initialize ReLU neurons with slightly positive biases (e.g. 0.01)

Activation Functions: Leaky ReLU



Leaky ReLU

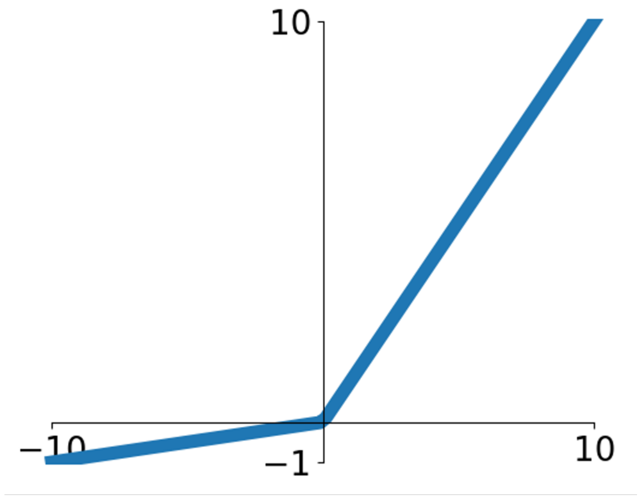
$f(x) = \max(\alpha x, x)$

α is a hyperparameter, often $\alpha = 0.1$

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

Maas et al, "Rectifier Nonlinearities Improve Neural Network Acoustic Models", ICML 2013

Activation Functions: Leaky ReLU



Leaky ReLU

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

α is a hyperparameter, often $\alpha = 0.1$

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

Parametric ReLU (PReLU)

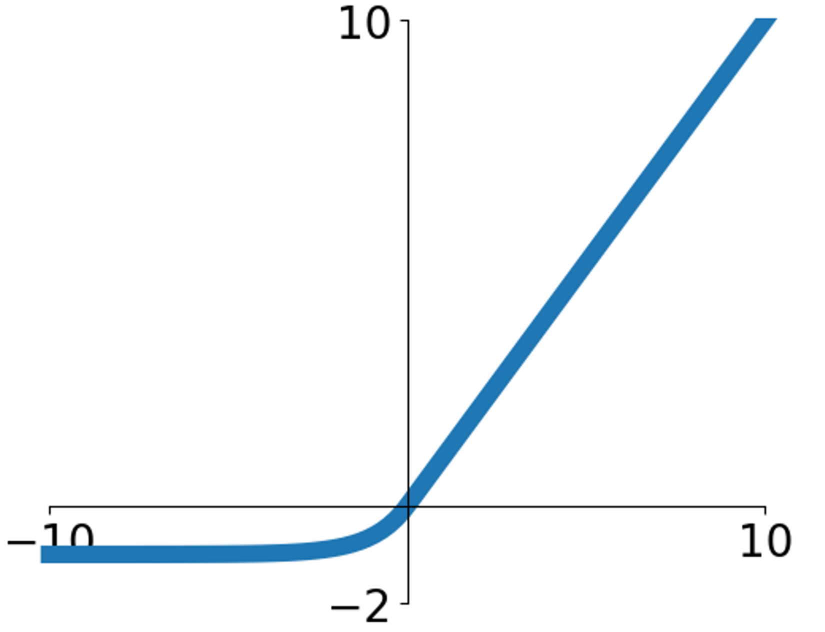
$f(x) = \max(\alpha x, x)$

α is learned via backprop

Maas et al, "Rectifier Nonlinearities Improve Neural Network Acoustic Models", ICML 2013

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

Activation Functions: Exponential Linear Unit (ELU)



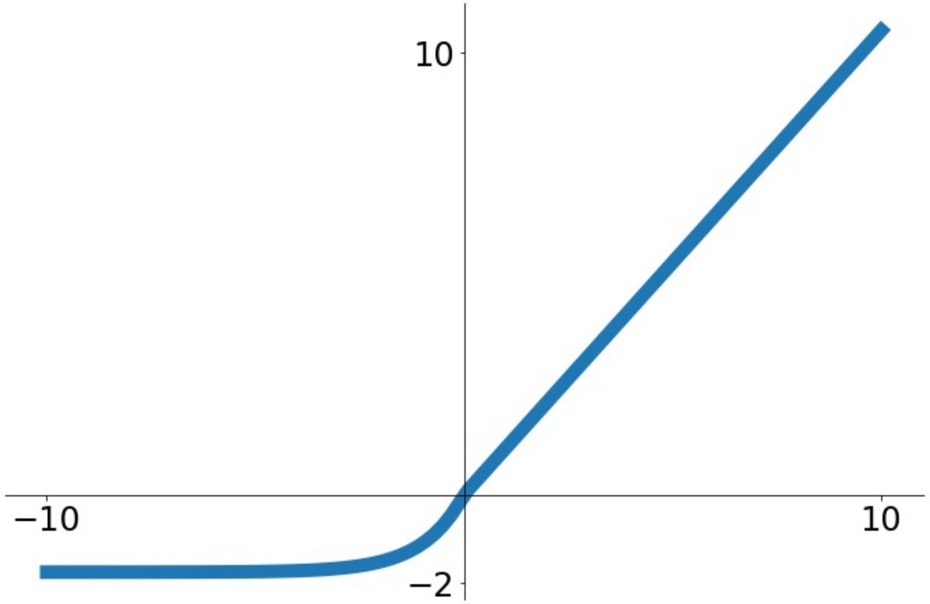
$$f(x) = \begin{cases} x & if\ x > 0 \\ \alpha(e^x - 1) & if\ x \leq 0 \end{cases}$$

(Default alpha=1)

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

- Computation requires exp()

Activation Functions: Scaled Exponential Linear Unit (SELU)



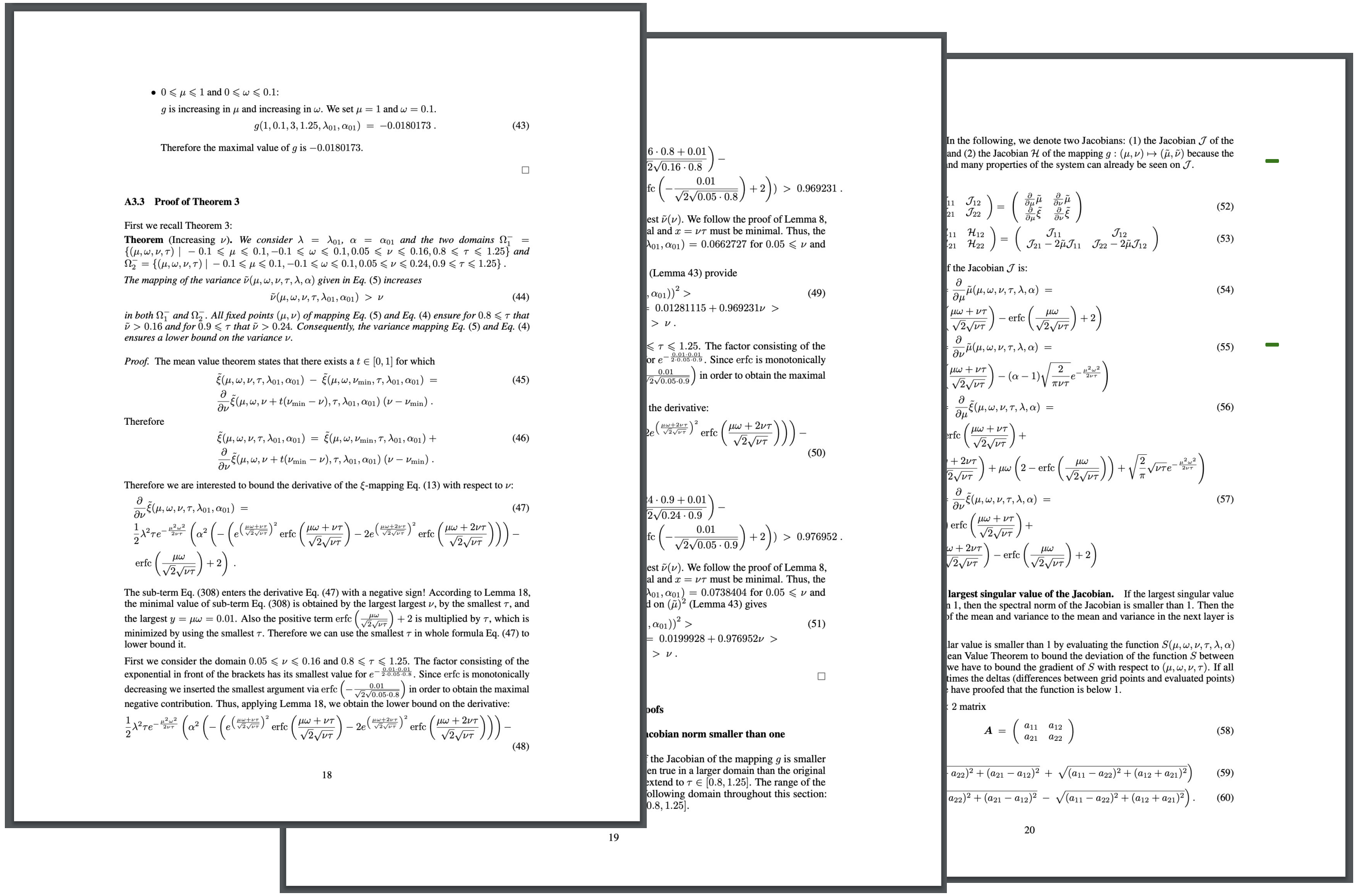
- Scaled version of ELU that works better for deep networks
- "Self-Normalizing" property; can train deep SELU networks without BatchNorm

$$selu(x) = \begin{cases} \lambda x & if\ x > 0 \\ \lambda\alpha(e^x - 1) & if\ x \leq 0 \end{cases}$$

$$\alpha = 1.6732632423543772848170429916717$$
$$\lambda = 1.0507009873554804934193349852946$$

Klambauer et al, Self-Normalizing Neural Networks, ICLR 2017

Activation Functions: Scaled Exponential Linear Unit (SELU)



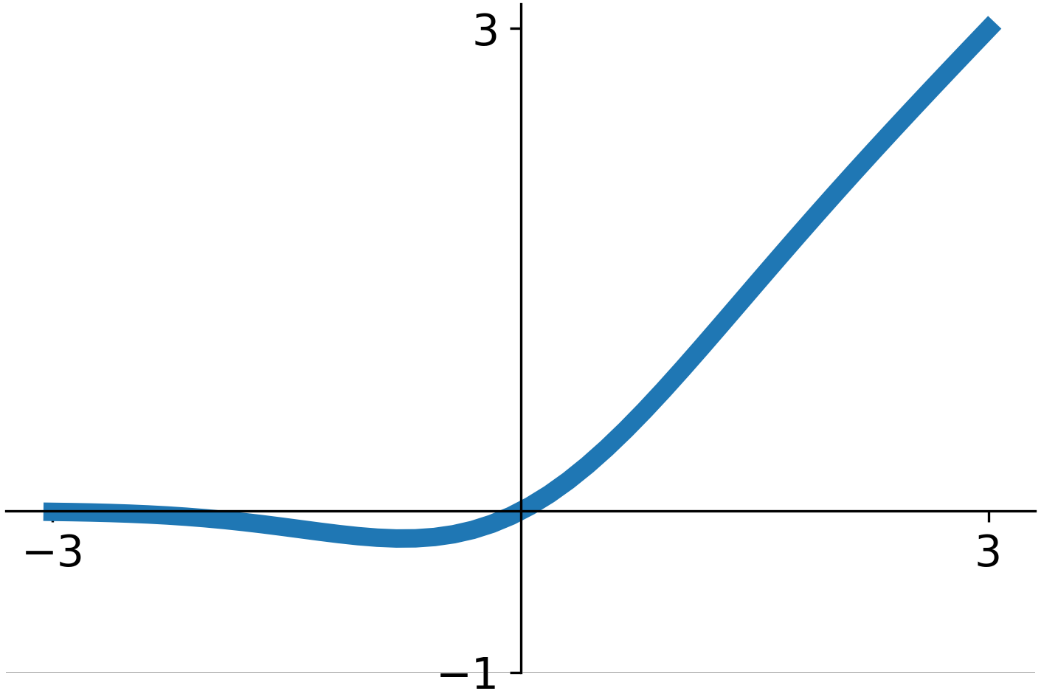
- Scaled version of ELU that works better for deep networks
- "Self-Normalizing" property; can train deep SELU networks without BatchNorm

Derivation takes 91 pages of math in appendix…

$$\alpha = 1.6732632423543772848170429916717$$
$$\lambda = 1.0507009873554804934193349852946$$

Klambauer et al, Self-Normalizing Neural Networks, ICLR 2017

Activation Functions: Gaussian Error Linear Unit (GELU)



$$X \sim N(0,1)$$

$$gelu(x) = xP(X \le x) = \frac{x}{2}\left(1 + \mathrm{erf}\left(x/\sqrt{2}\right)\right)$$

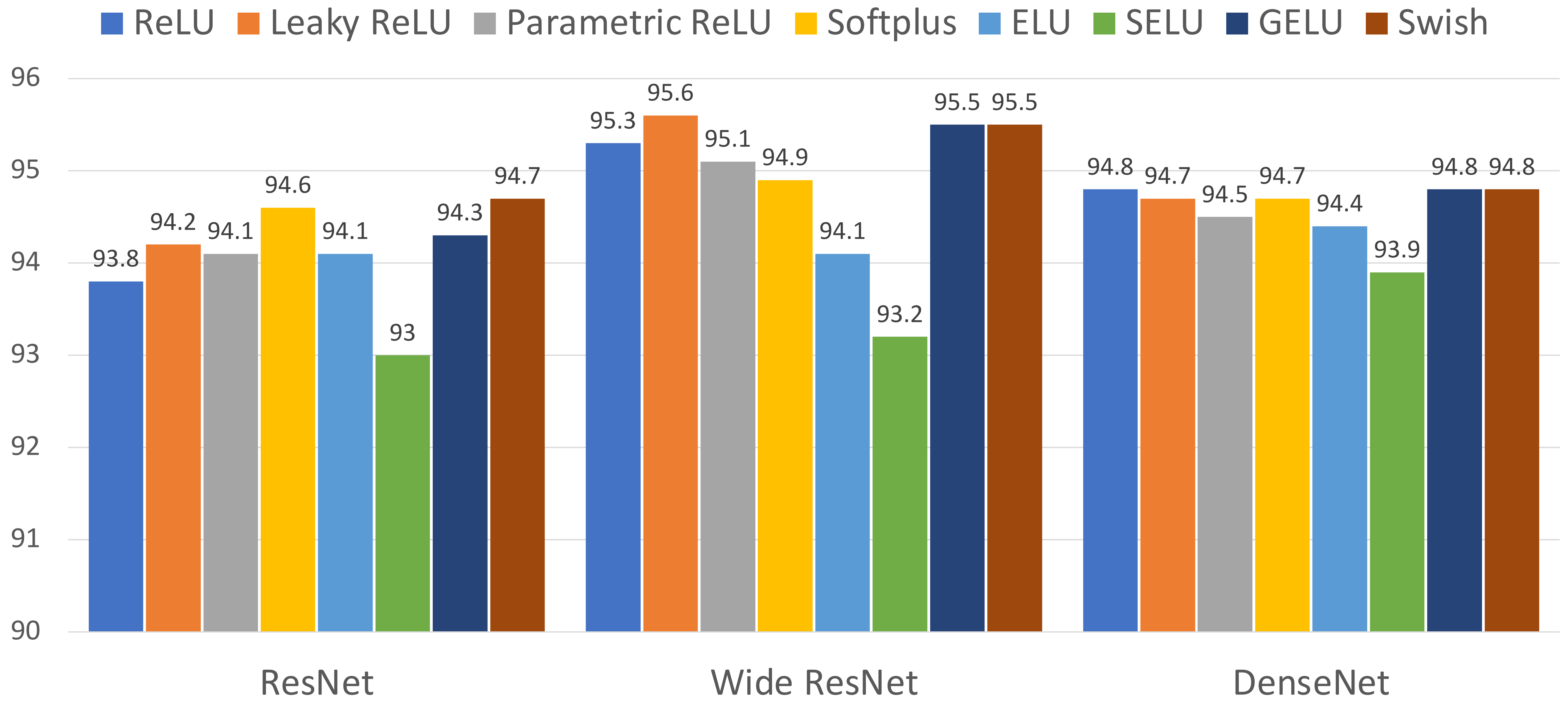
$$\approx x\sigma(1.702x)$$

- **Idea**: Multiply input by 0 or 1 at random; large values more likely to be multiplied by 1, small values more likely to be multiplied by 0 (data-dependent dropout)
- Take expectation over randomness
- Very common in Transformers (BERT, GPT, ViT)

Hendrycks and Gimpel, Gaussian Error Linear Units (GELUs), 2016

Accuracy on CIFAR10

Ramachandran et al, "Searching for activation functions", ICLR Workshop 2018



Activation Functions: Summary

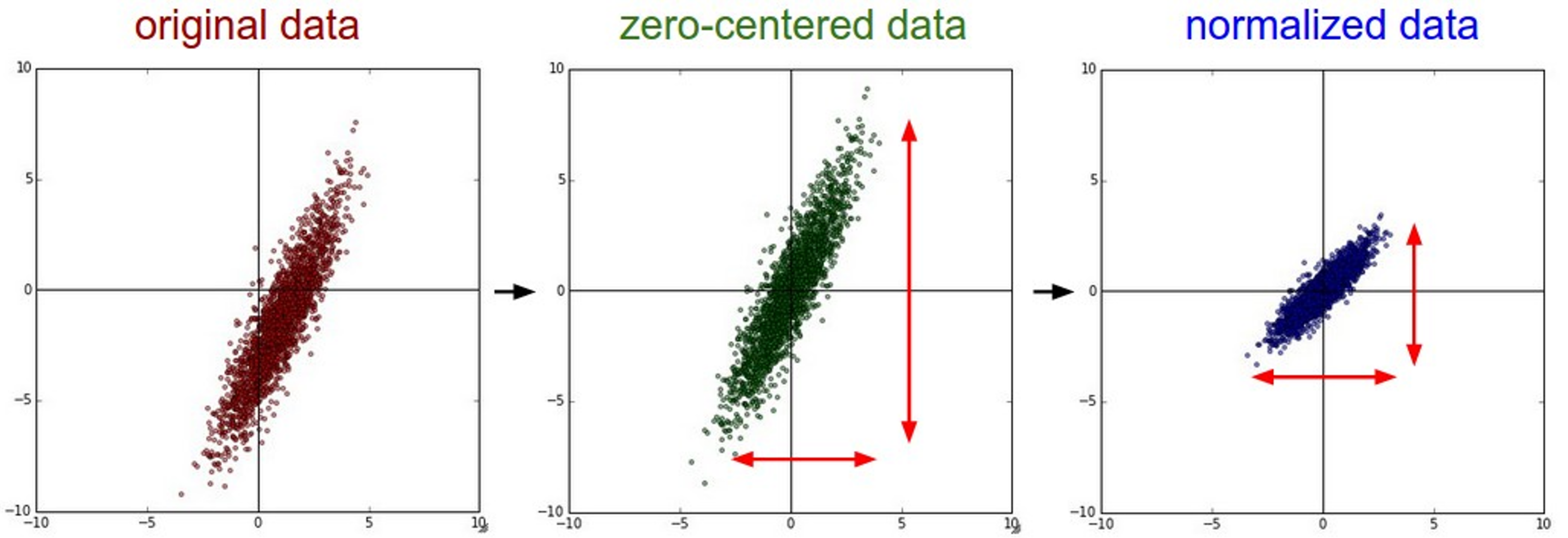
- Don’t think too hard. Just use ReLU
- Try out Leaky ReLU / ELU / SELU / GELU
  if you need to squeeze that last 0.1%
- Don’t use sigmoid or tanh

Some (very) recent architectures use GeLU instead of ReLU, but the gains are minimal

Dosovitskiy et al, “An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale”, ICLR 2021
Liu et al, “A ConvNet for the 2020s”, arXiv 2022

Data Preprocessing

Data Preprocessing



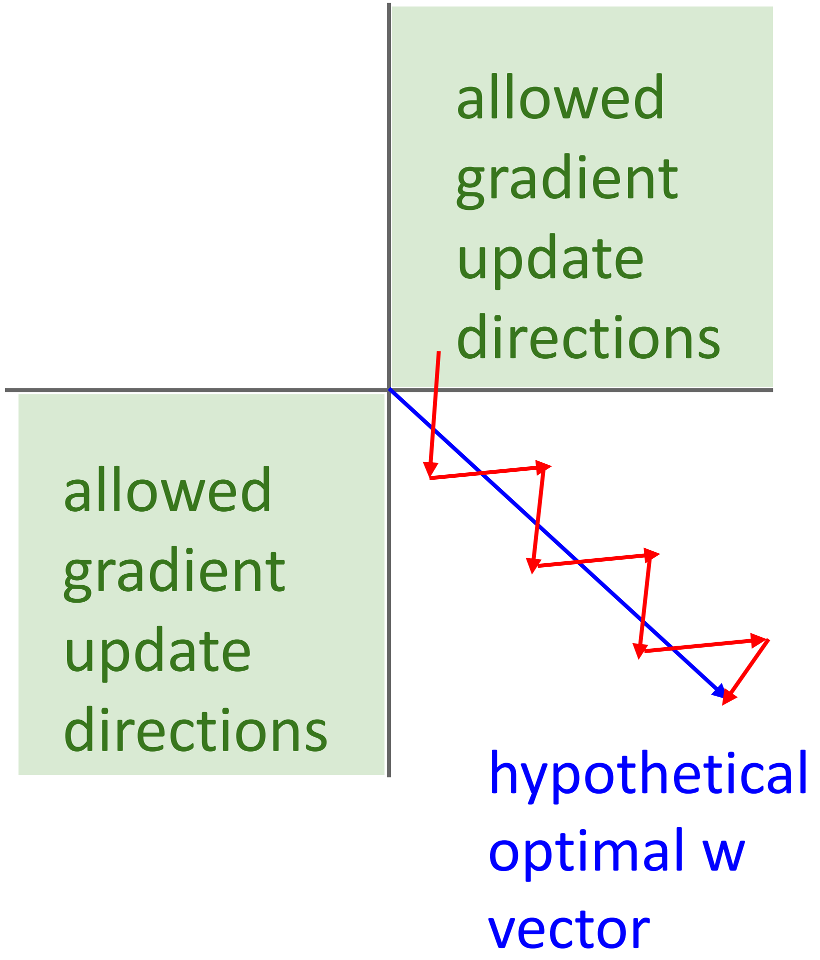

```
X -= np.mean(X, axis = 0)
```

```
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...

$$h_i^{(\ell)} = \sum_j w_{i,j}^{(\ell)} \sigma\left(h_j^{(\ell-1)}\right) + b_i^{(\ell)}$$

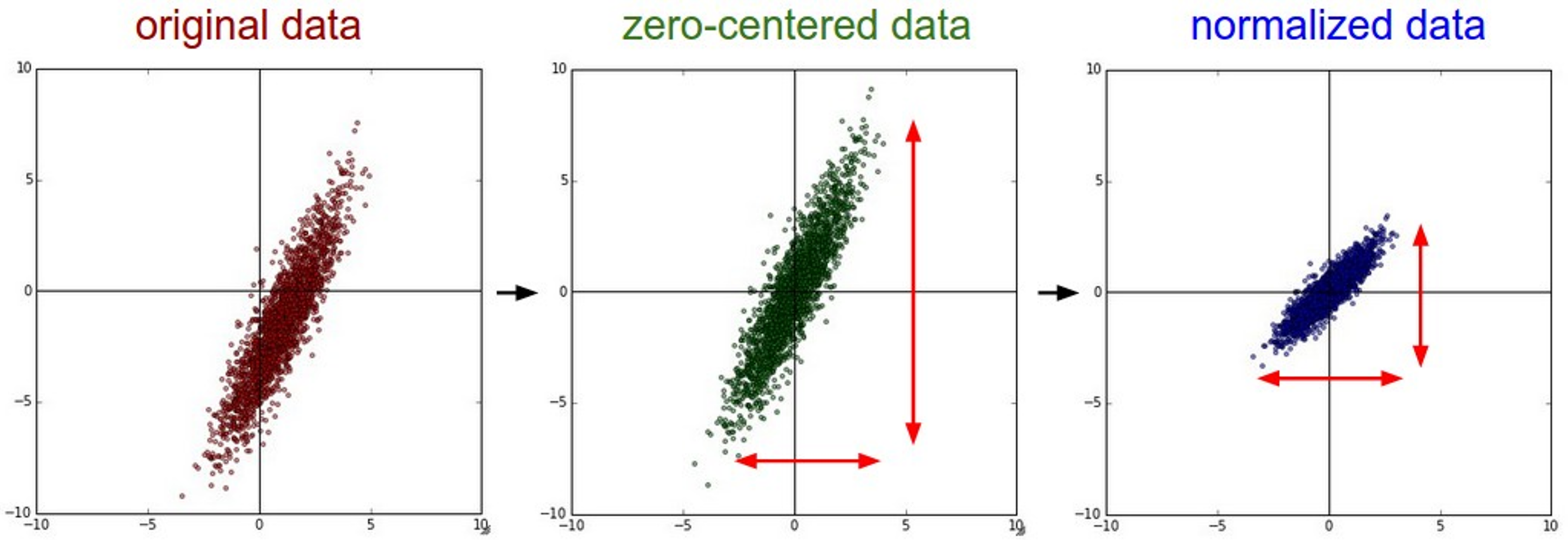


What can we say about the gradients on **w**?

Always all positive or all negative :(

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

Data Preprocessing



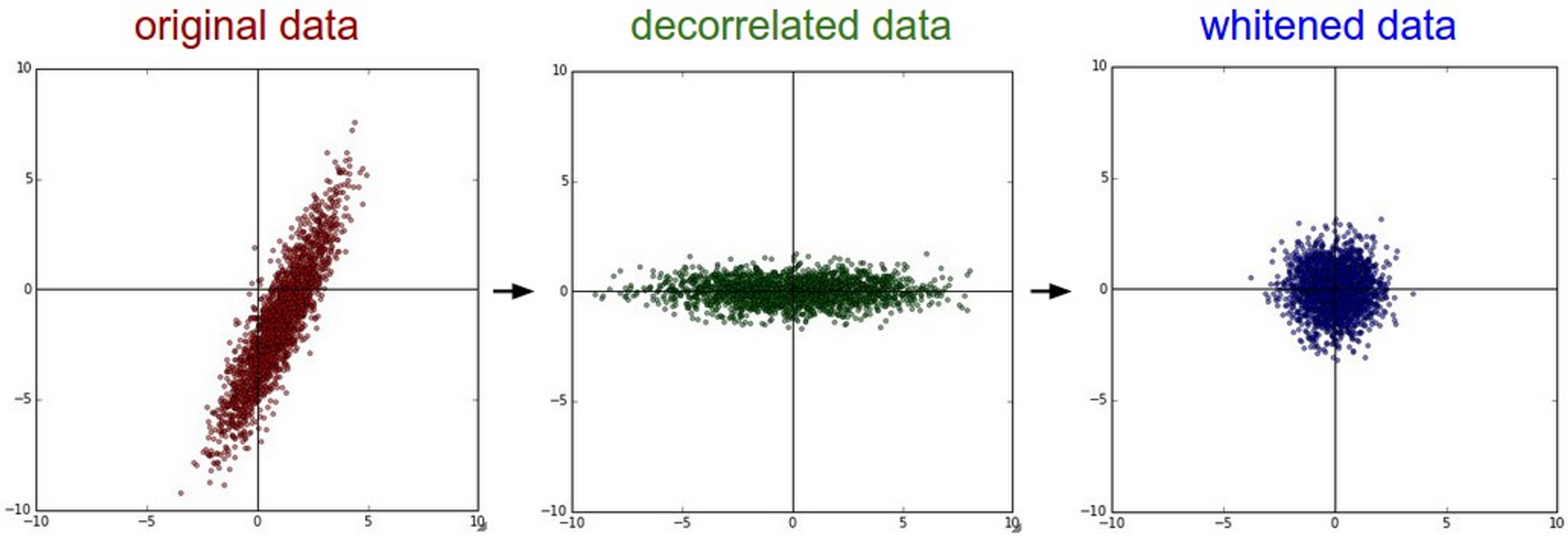

```
X -= np.mean(X, axis = 0)
```

```
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

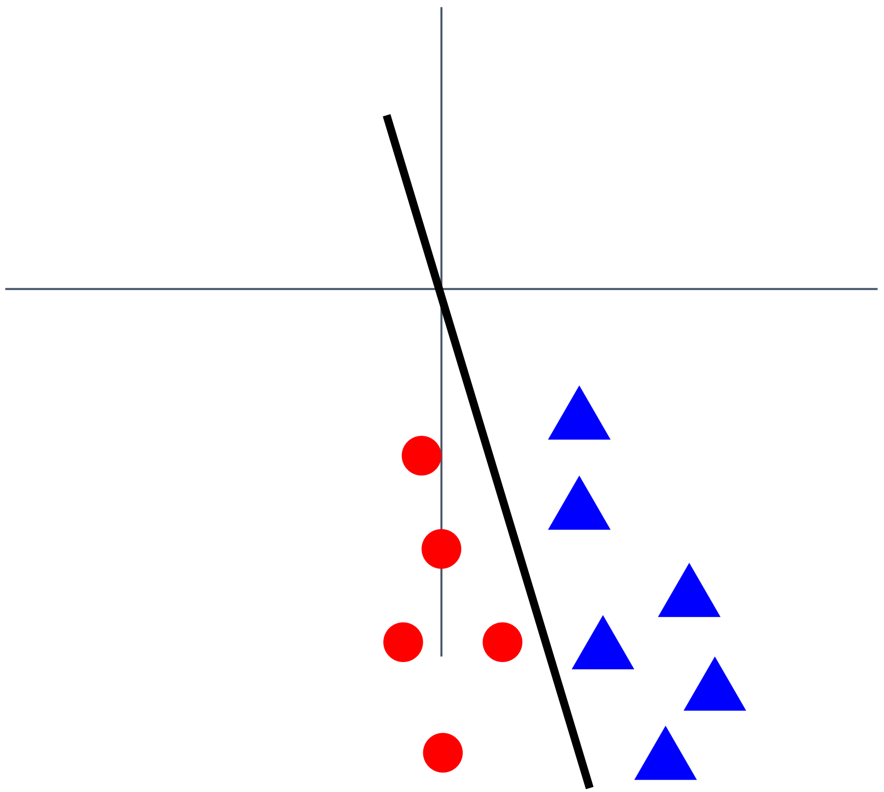


(data has diagonal covariance matrix)

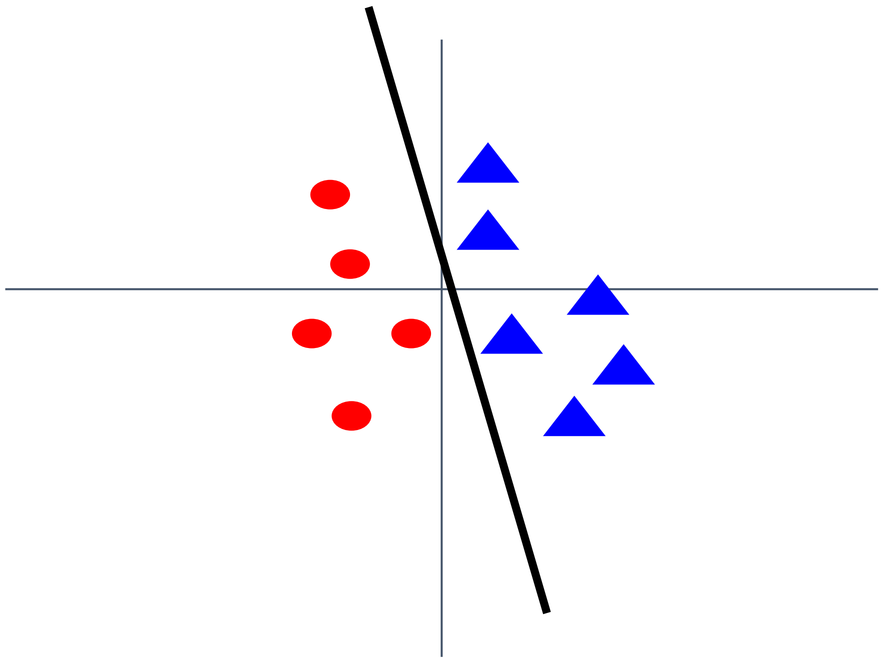
(covariance matrix is the identity matrix)

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



Data Preprocessing for Images

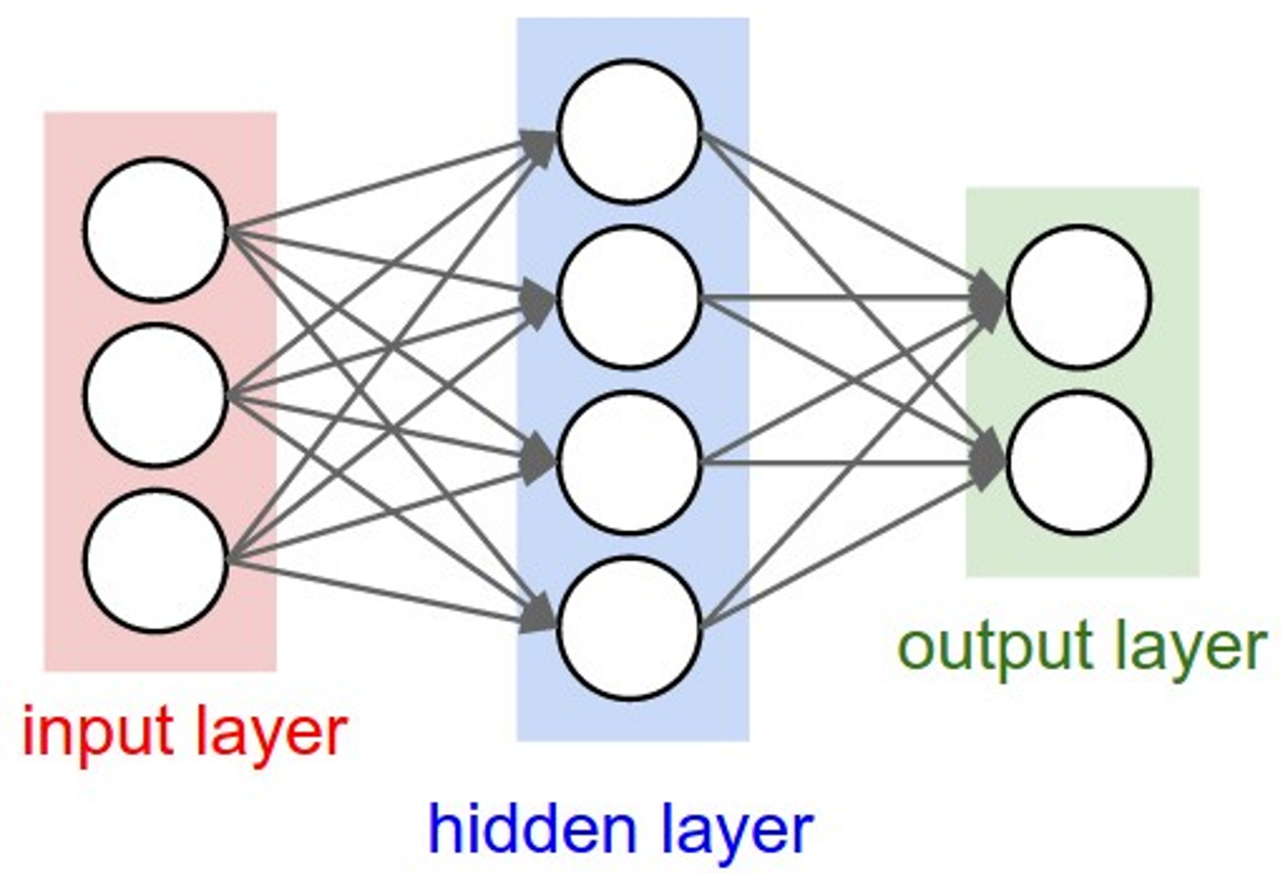
e.g. consider CIFAR-10 example with [32,32,3] images

- 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

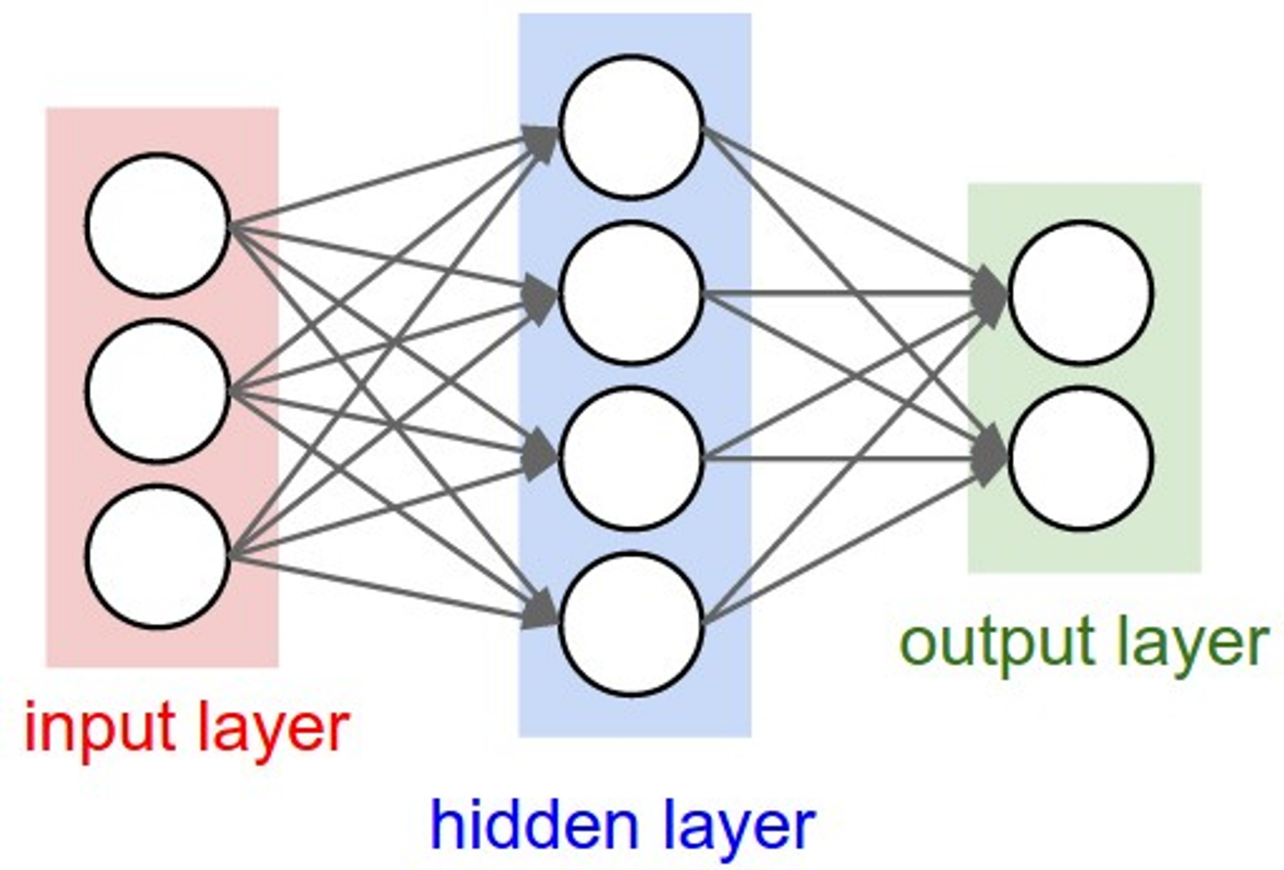
Weight Initialization

Weight Initialization



Q: What happens if we initialize all W=0, b=0?

Weight Initialization



Q: What happens if we initialize all W=0, b=0?

A: All outputs are 0, all gradients are the same! No “symmetry breaking”

Weight Initialization

Next idea: **small random numbers**
(Gaussian with zero mean, std=0.01)

```
W = 0.01 * np.random.randn(Din, Dout)
```

Weight Initialization

Next idea: **small random numbers**
(Gaussian with zero mean, std=0.01)

```
W = 0.01 * np.random.randn(Din, Dout)
```

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

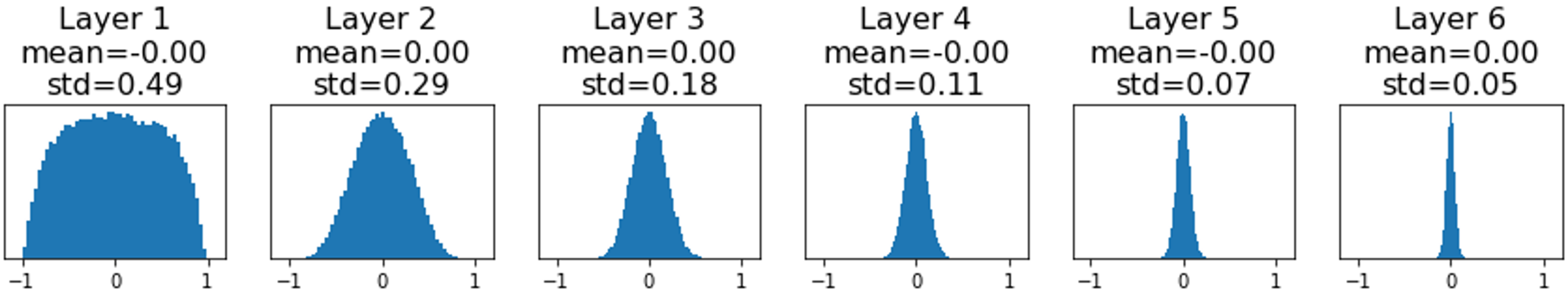
Weight Initialization: Activation Statistics

```
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

All activations tend to zero for deeper network layers

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



Weight Initialization: Activation Statistics

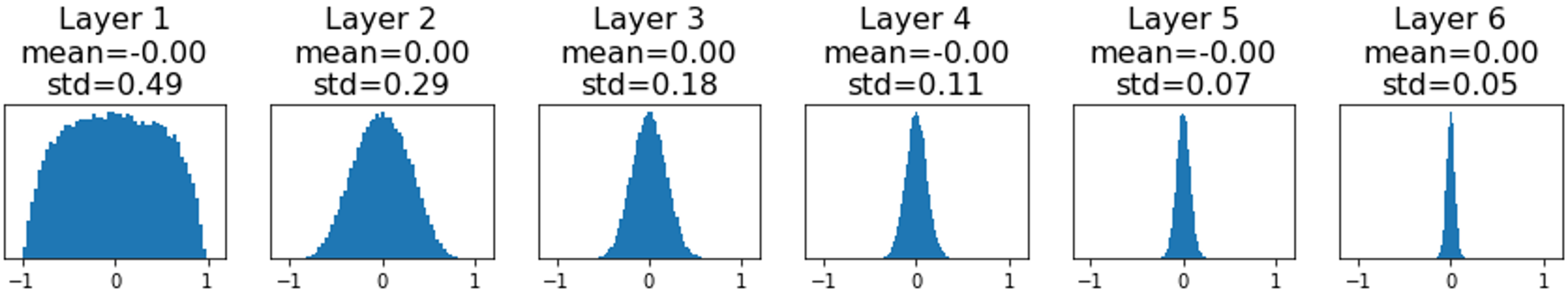
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

A: All zero, no learning =(



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 = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Increase std of initial weights from 0.01 to 0.05

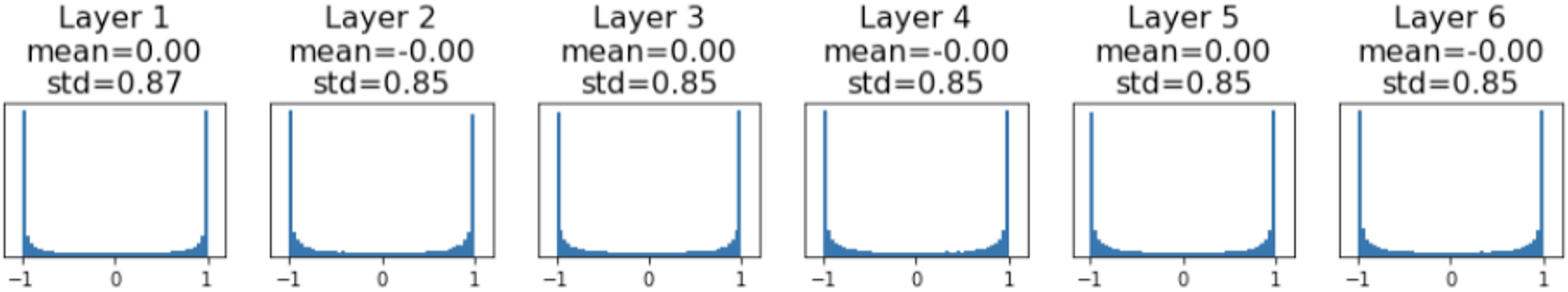
Weight Initialization: Activation Statistics

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?



Weight Initialization: Activation Statistics

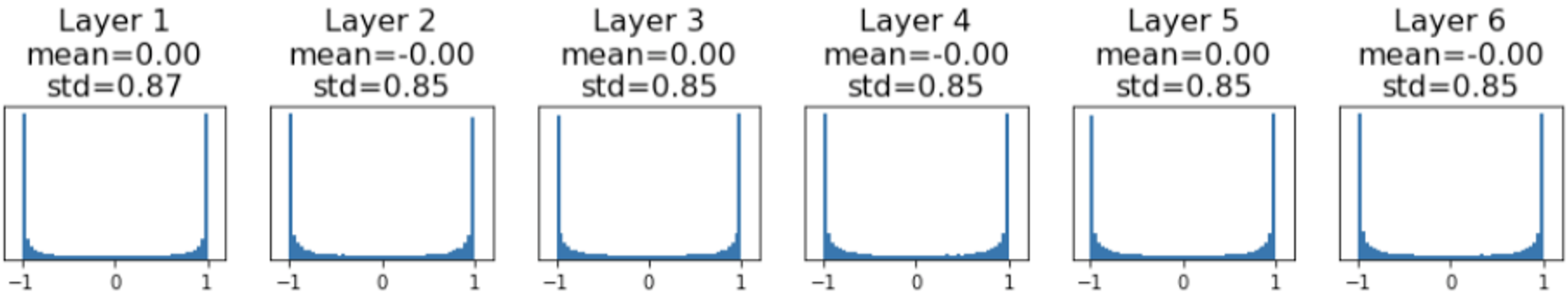
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

A: Local gradients all zero, no learning =(



Weight Initialization: Xavier 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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

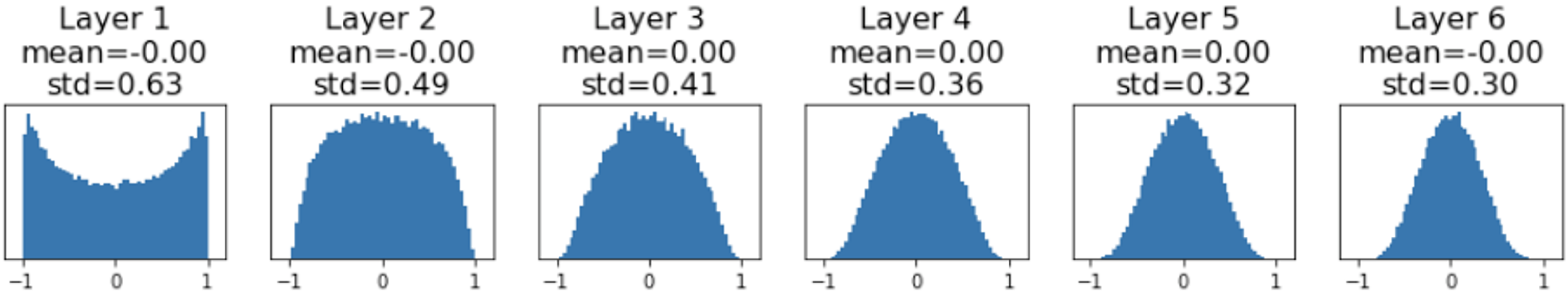
Glorot and Bengio, "Understanding the difficulty of training deep feedforward neural networks", AISTAT 2010

Weight Initialization: Xavier 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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

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



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

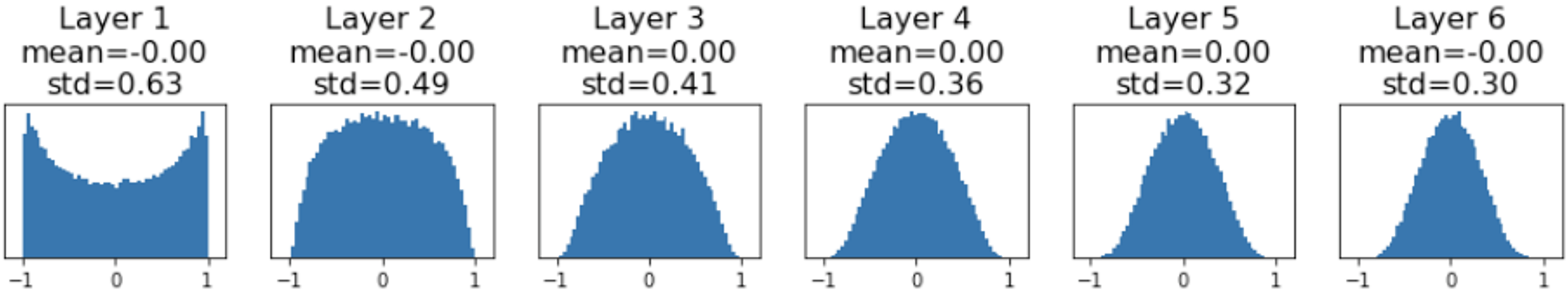
Weight Initialization: Xavier Initialization

```
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(Din)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

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

For conv layers, Din is kernel_size^2 * input_channels



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

Weight Initialization: Xavier Initialization

“Xavier” initialization:
std = 1/sqrt(Din)

Derivation: Variance of output = Variance of input

y = Wx

$$y_i = \sum_{j=1}^{Din} x_j w_j$$

Weight Initialization: Xavier Initialization

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

Derivation: Variance of output = Variance of input

y = Wx

$$y_i = \sum_{j=1}^{Din} x_j w_j$$

$\mathrm{Var}(y_i) = \mathrm{Din} * \mathrm{Var}(x_i w_i)$

[Assume x, w are iid]

Weight Initialization: Xavier Initialization

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

Derivation: Variance of output = Variance of input

y = Wx

$$y_i = \sum_{j=1}^{Din} x_j w_j$$

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

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

Weight Initialization: Xavier Initialization

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

Derivation: Variance of output = Variance of input

y = Wx

$$y_i = \sum_{j=1}^{Din} x_j w_j$$

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

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

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

Weight Initialization: Xavier Initialization

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

Derivation: Variance of output = Variance of input

$$y = Wx \qquad\qquad y_i = \sum_{j=1}^{Din} x_j w_j$$

$\mathrm{Var}(y_i) = \mathrm{Din} * \mathrm{Var}(x_i w_i)$ [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 independent]

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

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

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

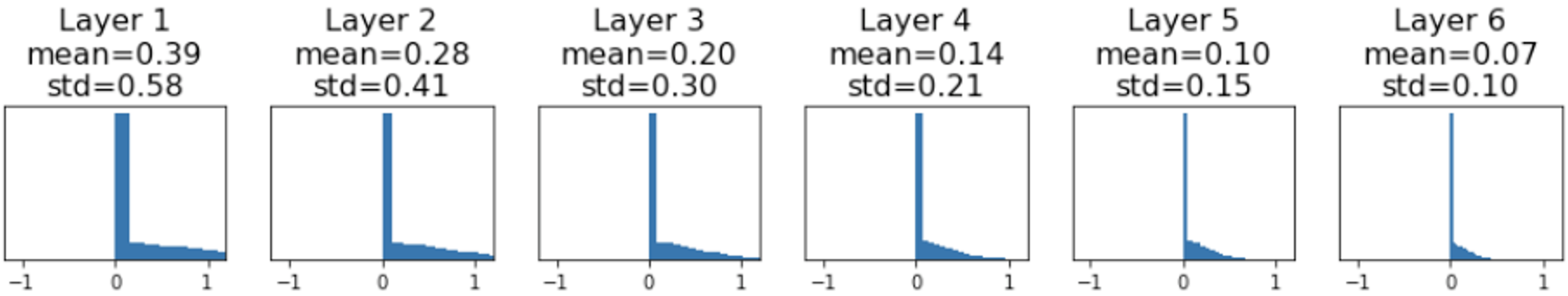
Weight Initialization: What about ReLU?

```
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 =(

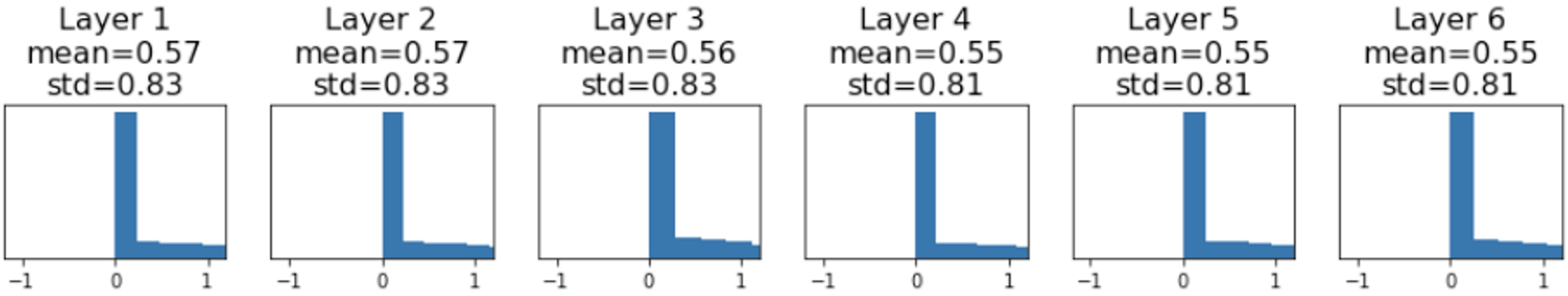


Weight Initialization: Kaiming / MSRA Initialization

```
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(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

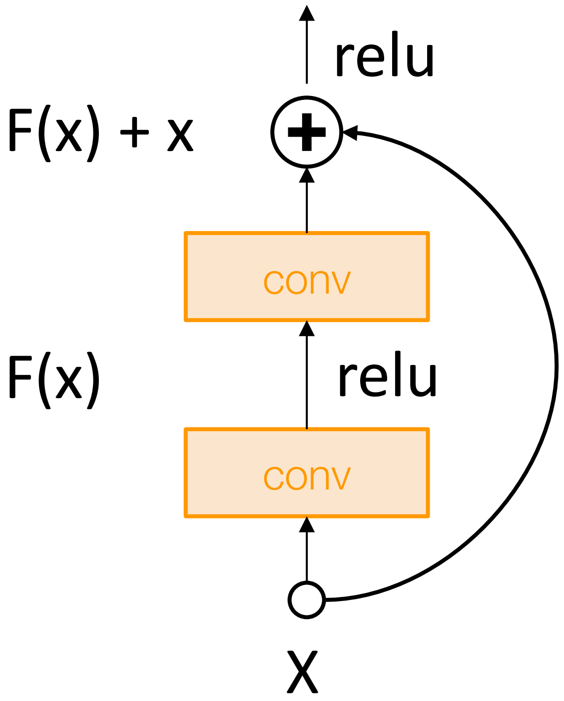
ReLU correction: std = sqrt(2 / Din)

”Just right” – activations nicely scaled for all layers



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

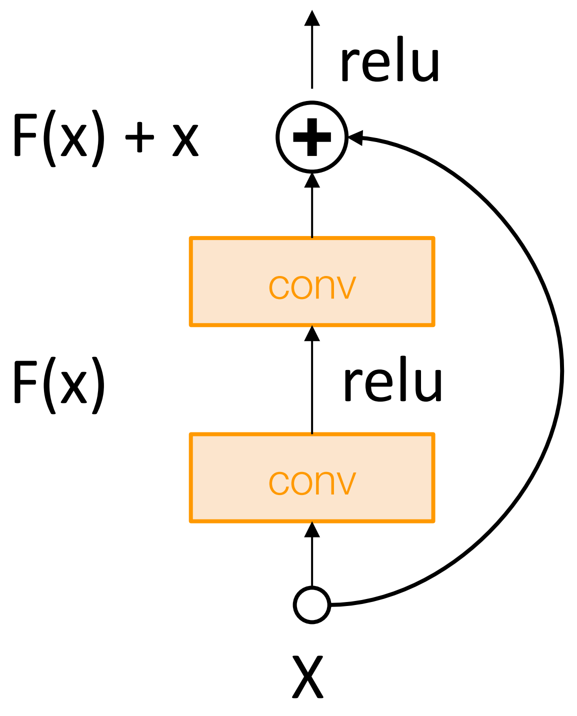
Weight Initialization: Residual Networks



Residual Block

If we initialize with MSRA:
then Var(F(x)) = Var(x)
But then Var(F(x) + x) > Var(x)
variance grows with each block!

Weight Initialization: Residual Networks



Residual Block

If we initialize with MSRA:
then Var(F(x)) = Var(x)
But then Var(F(x) + x) > Var(x)
variance grows with each block!

Solution: Initialize first conv with MSRA, initialize second conv to zero. Then Var(x + F(x)) = Var(x)

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

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

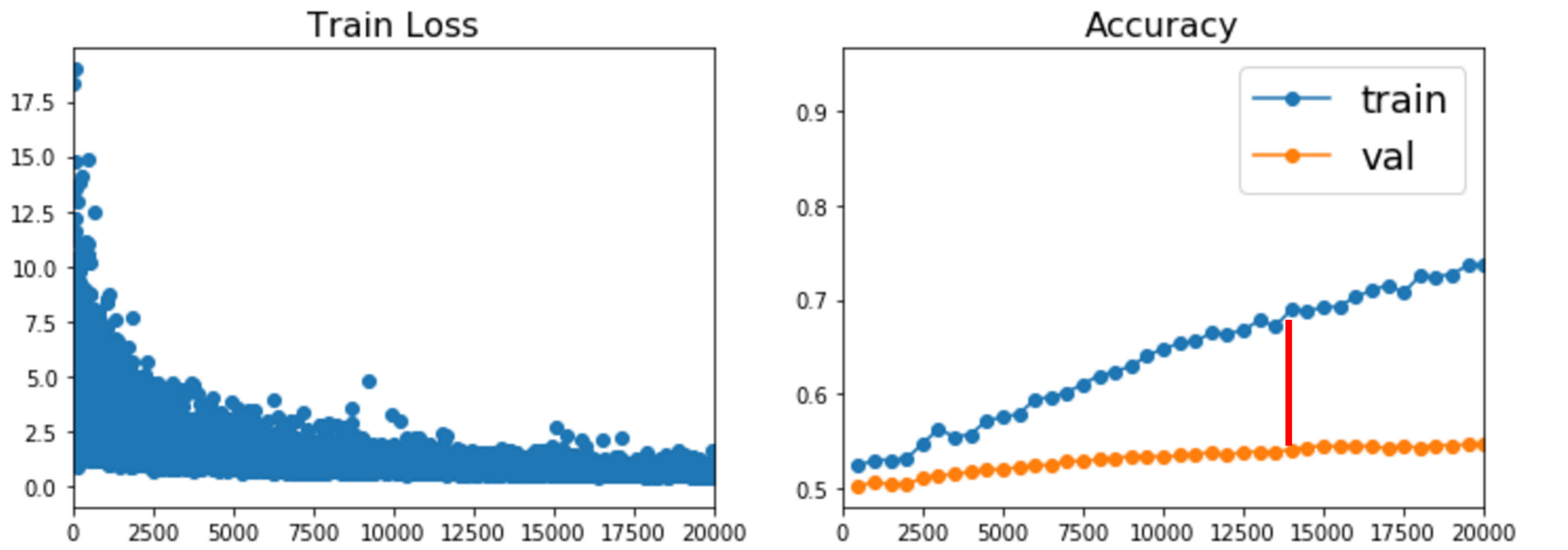
Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

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

Now your model is training … but it overfits!



Regularization

Regularization: Add term to the loss

$$L = \frac{1}{N}\sum_{i=1}^{N}\sum_{j\neq y_i}\max(0, f(x_i;W)_j - f(x_i;W)_{y_i} + 1) + \boxed{\lambda R(W)}$$

In common use:

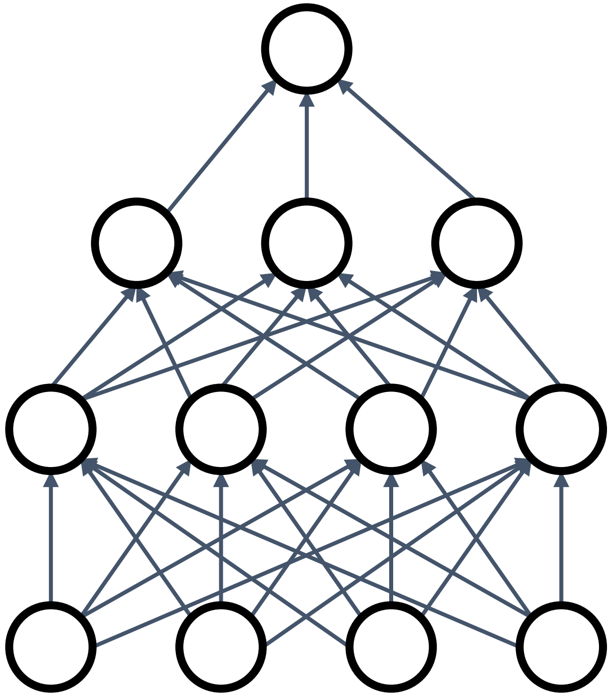
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

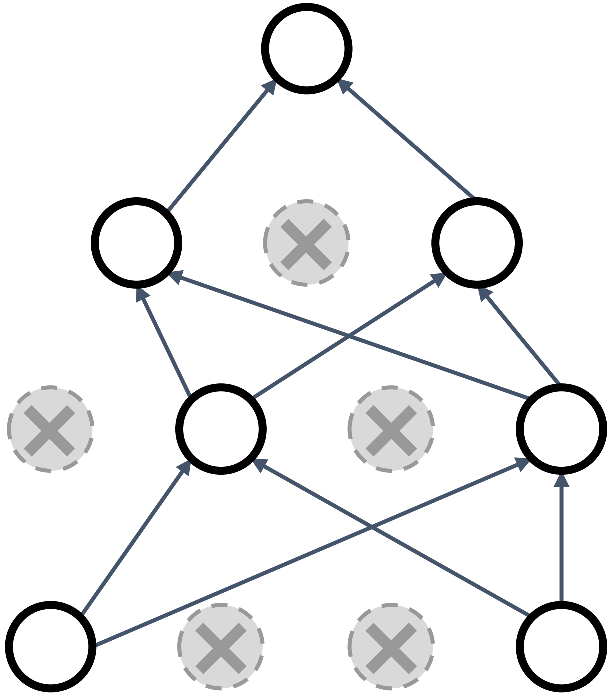
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Regularization: Dropout

In each forward pass, randomly set some neurons to zero
Probability of dropping is a hyperparameter; 0.5 is common



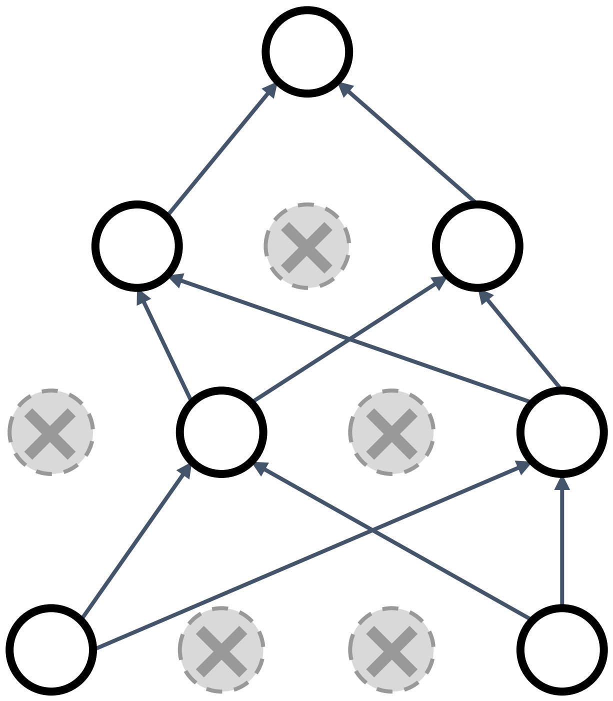


Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

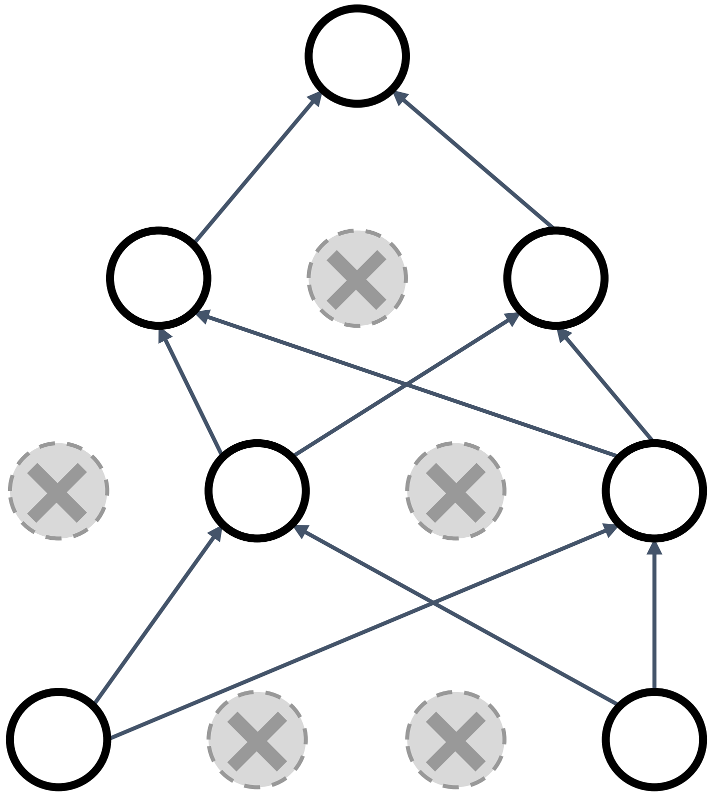
Regularization: Dropout

```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)
```

Example forward pass with a 3-layer network using dropout

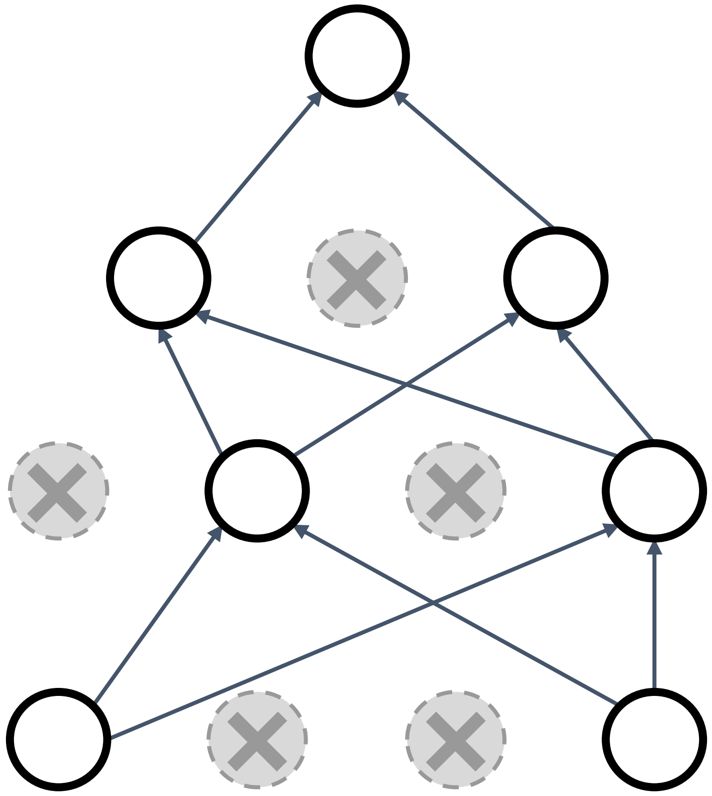


Regularization: Dropout



Forces the network to have a redundant representation; Prevents **co-adaptation** of features

Regularization: Dropout



Another interpretation:

Dropout is training a large **ensemble** of models (that share parameters).

Each binary mask is one model

An FC layer with 4096 units has $2^{4096} \sim 10^{1233}$ possible masks!
Only $\sim 10^{82}$ atoms in the universe...

Dropout: Test Time

Dropout makes our output random!

Output (label)

Input (image)

$$\boldsymbol{y} = f_W(\boldsymbol{x}, \boldsymbol{z})$$

Random mask

Want to "average out" the randomness at test-time

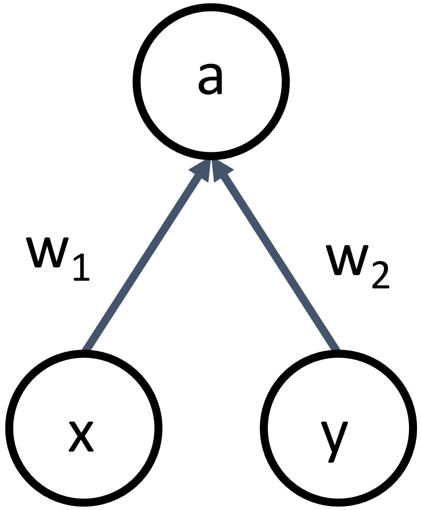
$$y = f(x) = E_z[f(x,z)] = \int p(z) f(x,z) dz$$

But this integral seems hard …

Dropout: Test Time

Want to approximate the integral

$$y = f(x) = E_z[f(x,z)] = \int p(z) f(x,z) dz$$



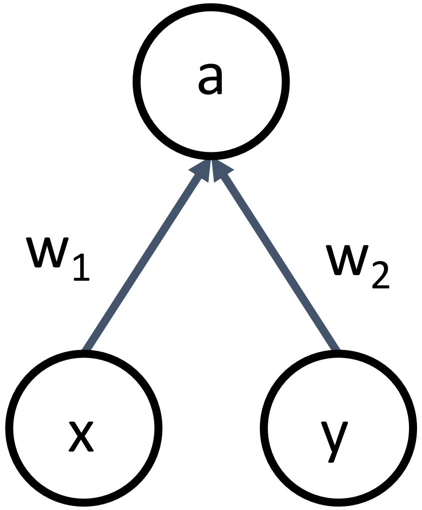
Consider a single neuron:

At test time we have: $E[a] = w_1 x + w_2 y$

Dropout: Test Time

Want to approximate the integral

$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$



Consider a single neuron:

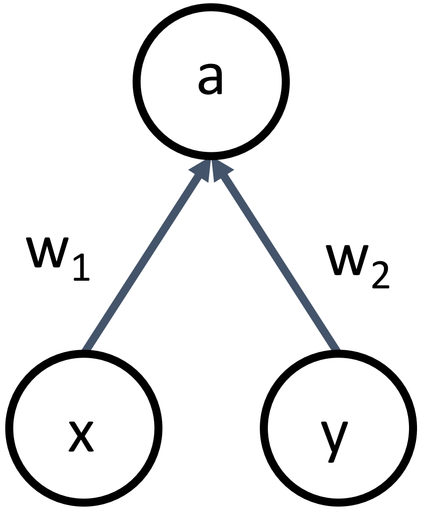
At test time we have: $E[a] = w_1x + w_2y$

During training we have: $E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) = \frac{1}{2}(w_1x + w_2y)$

Dropout: Test Time

Want to approximate the integral

$$y = f(x) = E_z[f(x, z)] = \int p(z) f(x, z) dz$$



Consider a single neuron:

At test time we have: $E[a] = w_1x + w_2y$

During training we have: $E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) = \frac{1}{2}(w_1x + w_2y)$

At test time, drop nothing and **multiply** by dropout probability

Dropout: Test Time

```
def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

At test time all neurons are active always

=> We must scale the activations so that for each neuron:

<u>output at test time</u> = <u>expected output at training time</u>

Dropout Summary

```
""" Vanilla Dropout: Not recommended implementation (see notes below) """

p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  """ X contains the data """

  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) * p # NOTE: scale the activations
  H2 = np.maximum(0, np.dot(W2, H1) + b2) * p # NOTE: scale the activations
  out = np.dot(W3, H2) + b3
```

drop in forward pass

scale at test time

More common: "Inverted dropout"

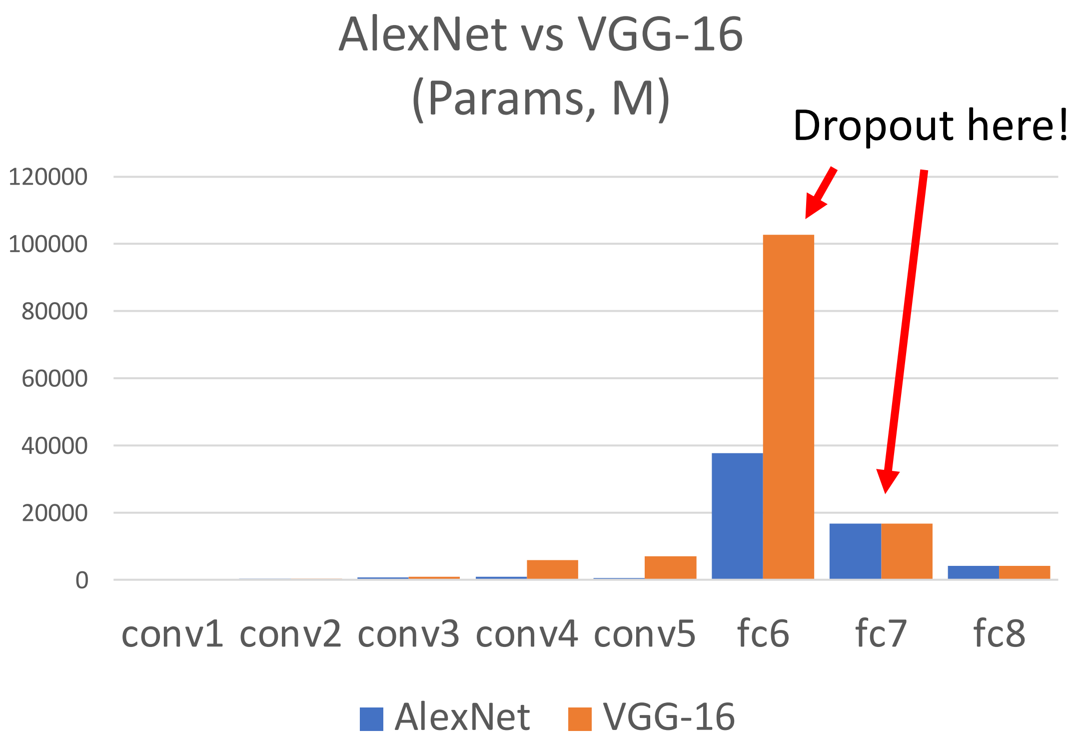
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

def train_step(X):
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = (np.random.rand(*H1.shape) < p) / p # first dropout mask. Notice /p!
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = (np.random.rand(*H2.shape) < p) / p # second dropout mask. Notice /p!
  H2 *= U2 # drop!
  out = np.dot(W3, H2) + b3

  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)

def predict(X):
  # ensembled forward pass
  H1 = np.maximum(0, np.dot(W1, X) + b1) # no scaling necessary
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  out = np.dot(W3, H2) + b3
```

Drop and scale during training

test time is unchanged!

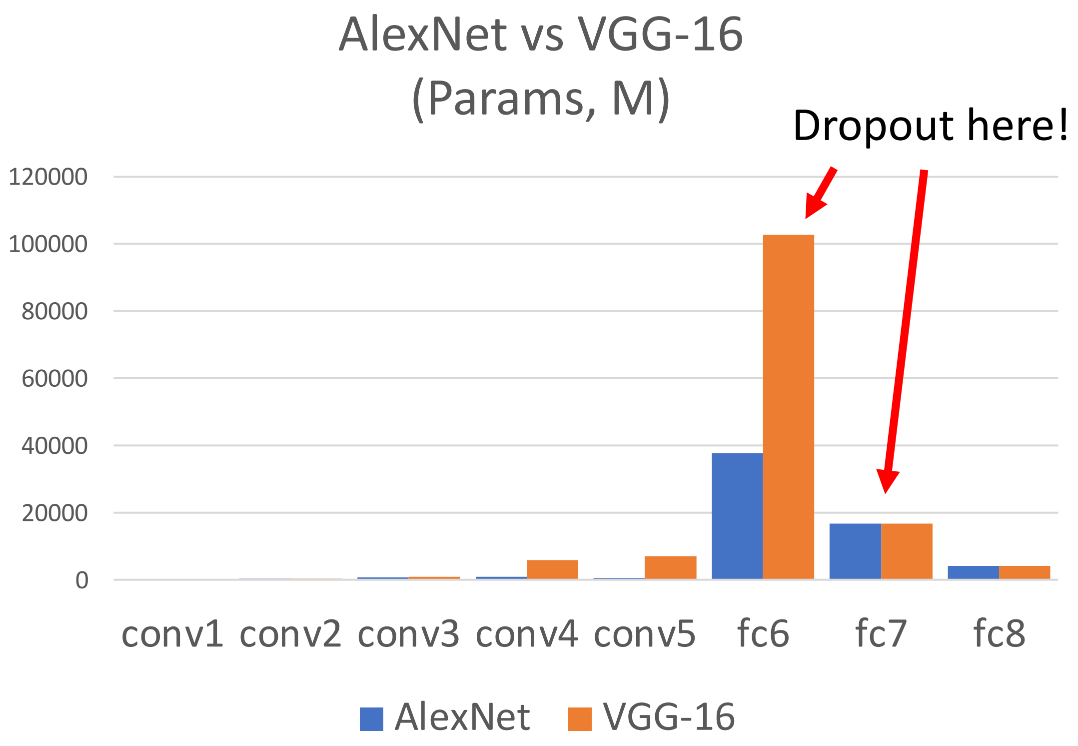
Dropout architectures

Recall AlexNet, VGG have most of their parameters in **fully-connected layers**; usually Dropout is applied there



Dropout architectures

Recall AlexNet, VGG have most of their parameters in **fully-connected layers**; usually Dropout is applied there



Later architectures (GoogLeNet, ResNet, etc) use global average pooling instead of fully-connected layers: they don't use dropout at all!

Regularization: A common pattern

Training: Add some kind of randomness

$$y = f_W(x, z)$$

Testing: Average out randomness (sometimes approximate)

$$y = f(x) = E_z[f(x, z)] = \int p(z) f(x, z) dz$$

Regularization: A common pattern

Training: Add some kind of randomness

$$y = f_W(x, z)$$

Testing: Average out randomness (sometimes approximate)

$$y = f(x) = E_z[f(x, z)] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Regularization: A common pattern

Training: Add some kind of randomness

$$y = f_W(x, z)$$

For ResNet and later, often L2 and Batch Normalization are the only regularizers!

Testing: Average out randomness (sometimes approximate)

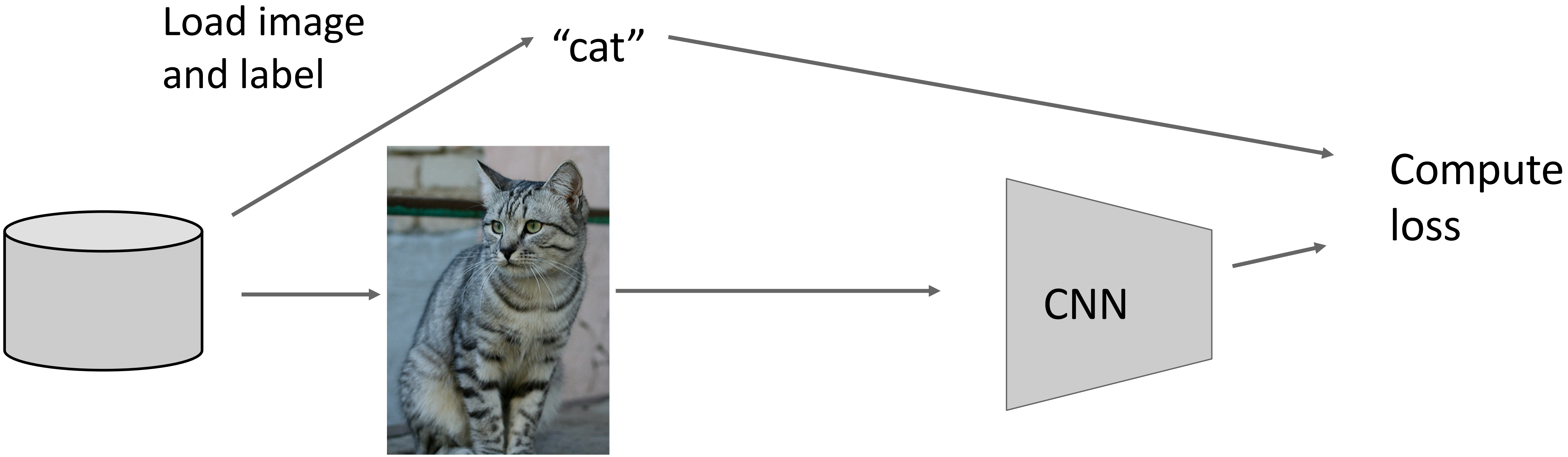
$$y = f(x) = E_z[f(x, z)] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

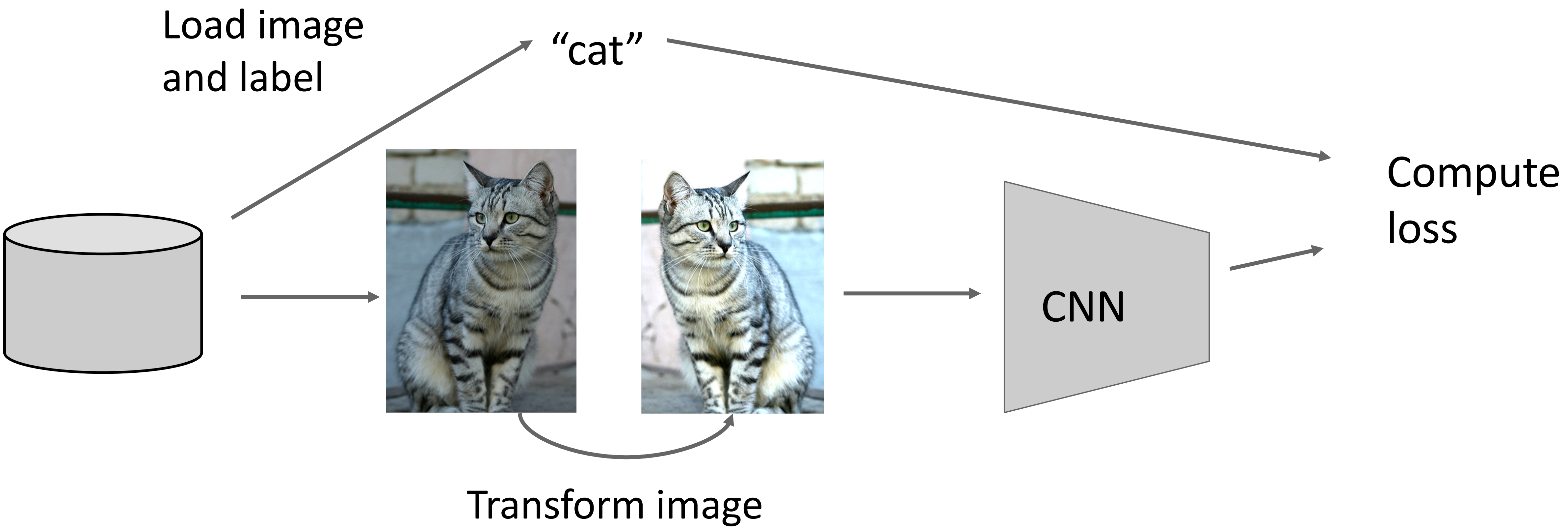
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Data Augmentation



Data Augmentation



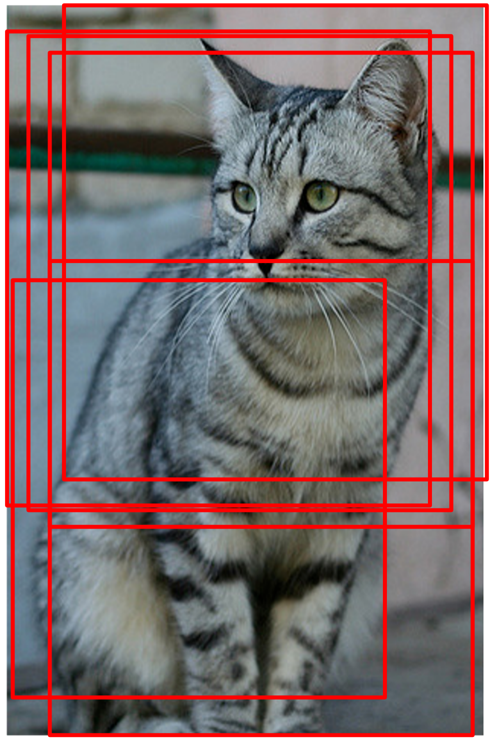
Data Augmentation: Horizontal Flips

Data Augmentation: Random Crops and Scales

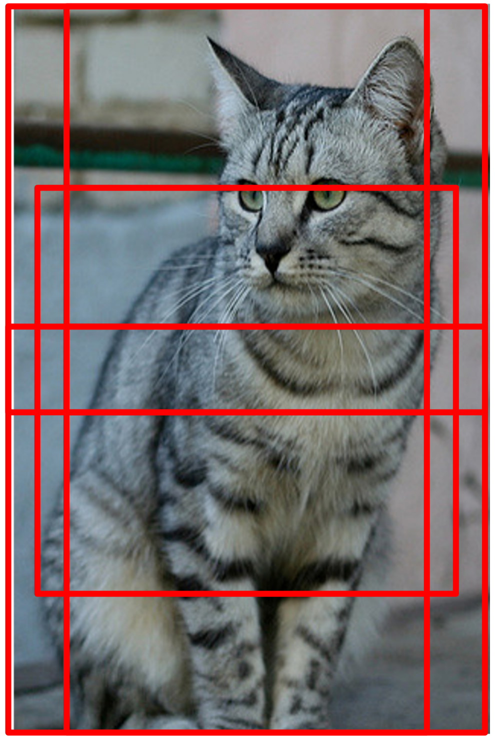
Training: sample random crops / scales

ResNet:

1. Pick random L in range [256, 480]
2. Resize training image, short side = L
3. Sample random 224 x 224 patch



Data Augmentation: Random Crops and Scales



Training: sample random crops / scales

ResNet:

1. Pick random L in range [256, 480]
2. Resize training image, short side = L
3. Sample random 224 x 224 patch

Testing: average a fixed set of crops

ResNet:

1. Resize image at 5 scales: {224, 256, 384, 480, 640}
2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips

Data Augmentation: Color Jitter

Simple: Randomize contrast and brightness

More Complex:

1. Apply PCA to all [R, G, B] pixels in training set
2. Sample a "color offset" along principal component directions
3. Add offset to all pixels of a training image

(Used in AlexNet, ResNet, etc)

Data Augmentation: RandAugment

Apply random combinations of transforms:

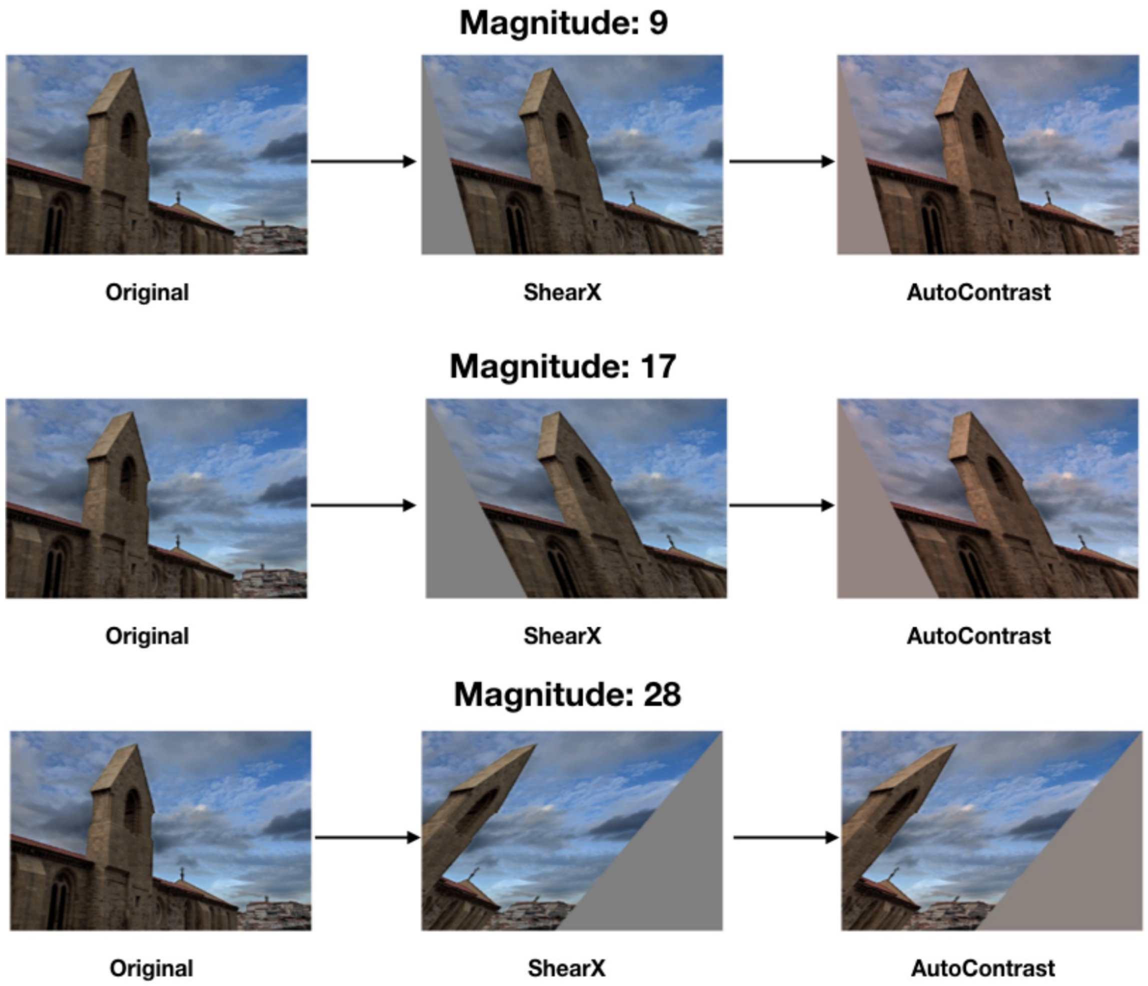
- **Geometric**: Rotate, translate, shear
- **Color**: Sharpen, contrast, brightness, solarize, posterize, color

```
transforms = [
'Identity', 'AutoContrast', 'Equalize',
'Rotate', 'Solarize', 'Color', 'Posterize',
'Contrast', 'Brightness', 'Sharpness',
'ShearX', 'ShearY', 'TranslateX', 'TranslateY']

def randaugment(N, M):
"""Generate a set of distortions.

  Args:
    N: Number of augmentation transformations to
         apply sequentially.
    M: Magnitude for all the transformations.
"""

 sampled_ops = np.random.choice(transforms, N)
 return [(op, M) for op in sampled_ops]
```

Cubuk et al, "RandAugment: Practical augmented data augmentation with a reduced search space", NeurIPS 2020

Data Augmentation: RandAugment

Apply random combinations of transforms:
- **Geometric**: Rotate, translate, shear
- **Color**: Sharpen, contrast, brightness, solarize, posterize, color



Cubuk et al, "RandAugment: Practical augmented data augmentation with a reduced search space", NeurIPS 2020

Data Augmentation: Get creative for your problem!

Data augmentation encodes **invariances** in your model

Think for your problem: what changes to the image should **not** change the network output?

May be different for different tasks!

Regularization: A common pattern

Training: Add some randomness
Testing: Marginalize over randomness

Examples:
Dropout
Batch Normalization
Data Augmentation

Wan et al, “Regularization of Neural Networks using DropConnect”, ICML 2013

Regularization: DropConnect

Training: Drop random connections between neurons (set weight=0)

Testing: Use all the connections

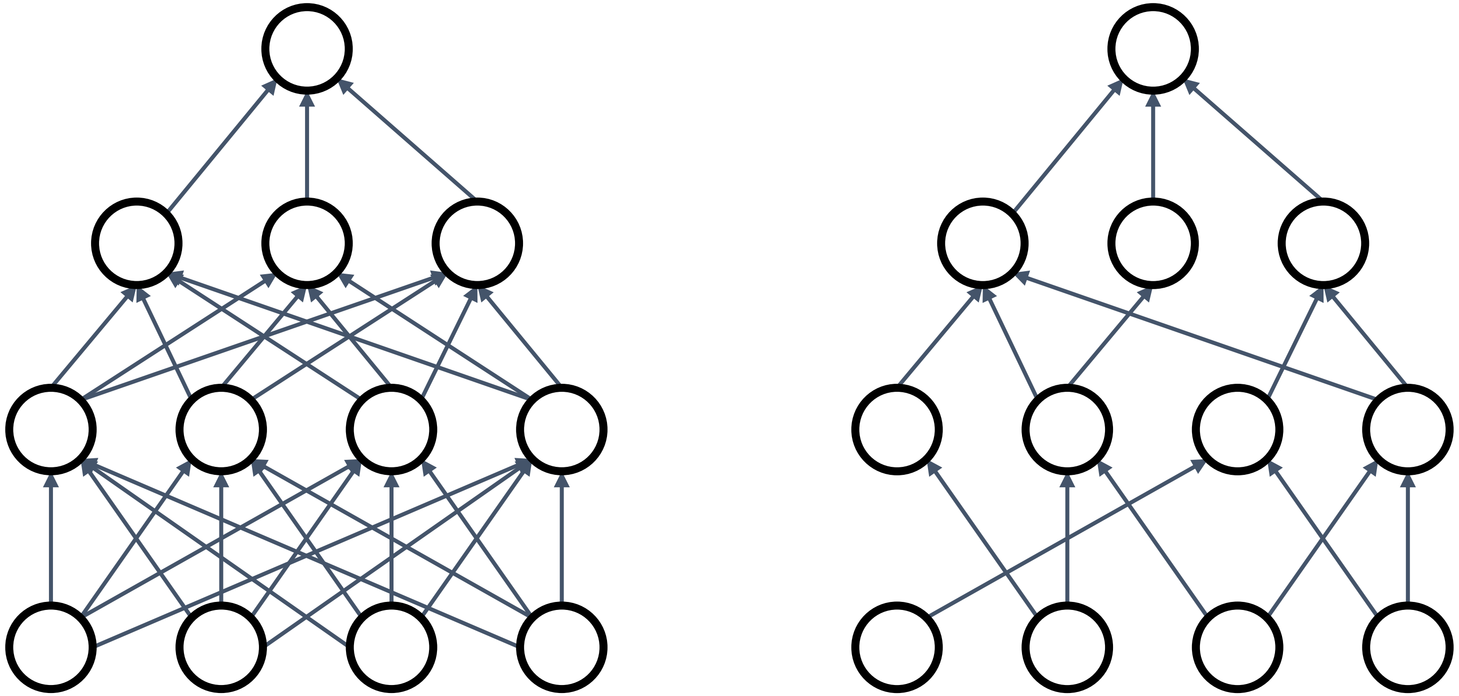
Examples:

Dropout

Batch Normalization

Data Augmentation

DropConnect

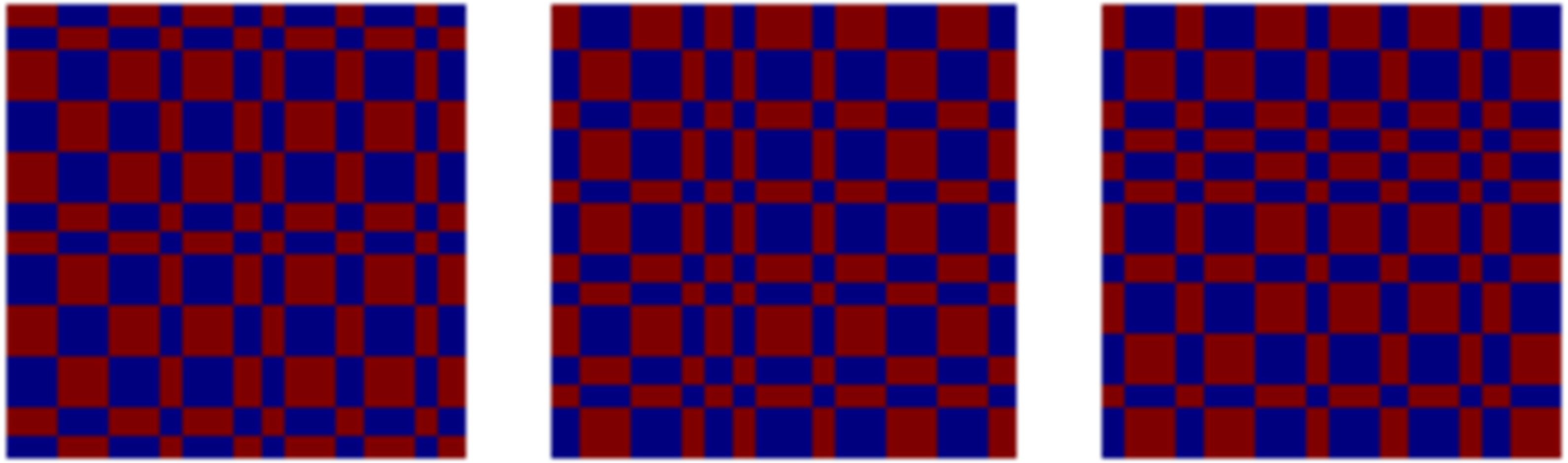


Wan et al, "Regularization of Neural Networks using DropConnect", ICML 2013

Regularization: Fractional Pooling

Training: Use randomized pooling regions
Testing: Average predictions over different samples

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling

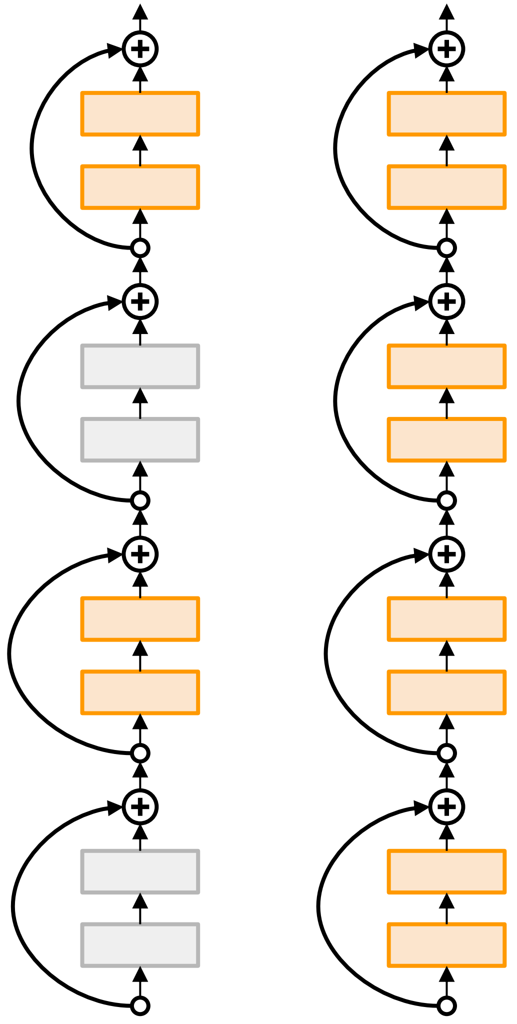


Graham, "Fractional Max Pooling", arXiv 2014

Regularization: Stochastic Depth

Training: Skip some residual blocks in ResNet

Testing: Use the whole network



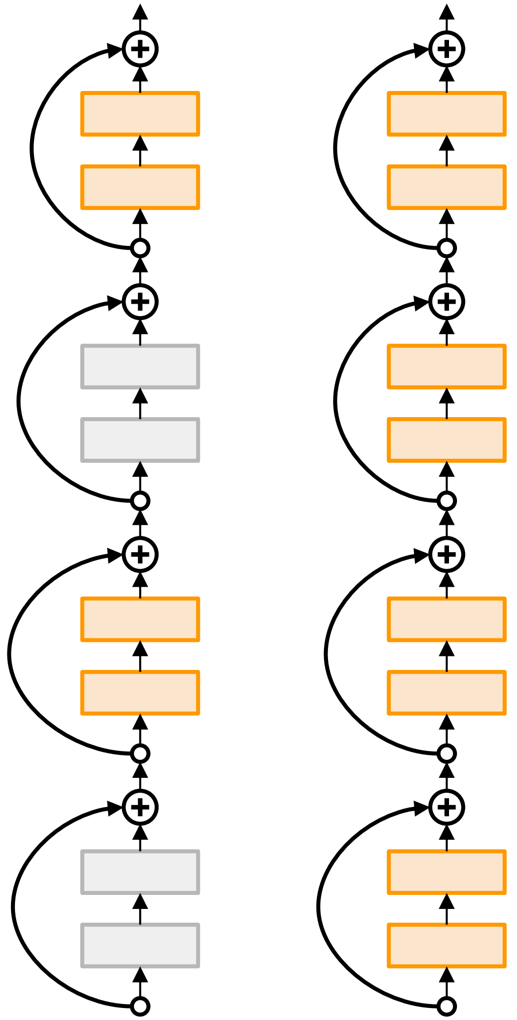
Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth

Huang et al, "Deep Networks with Stochastic Depth", ECCV 2016

Regularization: Stochastic Depth

Training: Skip some residual blocks in ResNet
Testing: Use the whole network



Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth

Starting to become common in recent architectures!

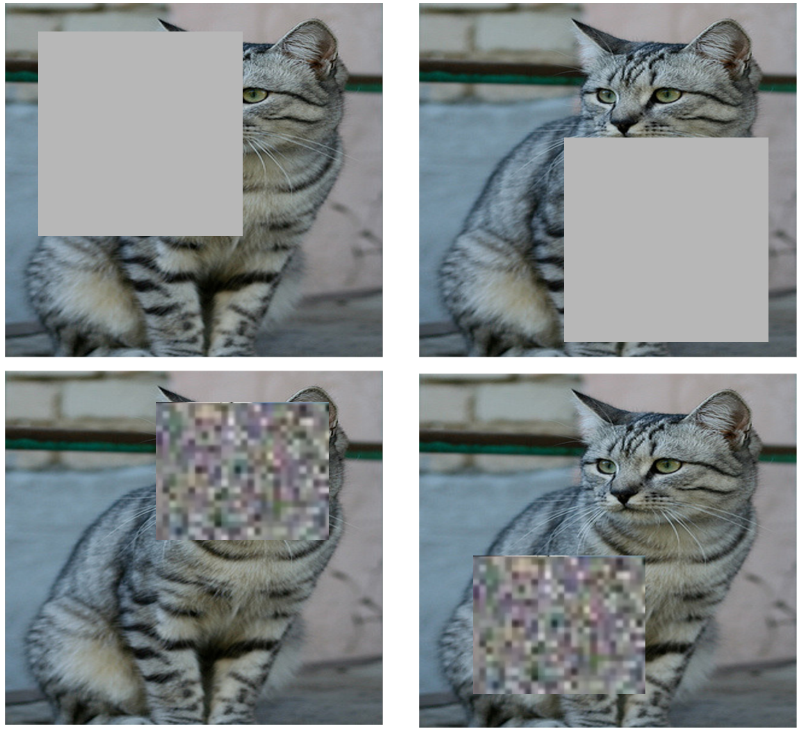
- Pham et al, "Very Deep Self-Attention Networks for End-to-End Speech Recognition", INTERSPEECH 2019
- Tan and Le, "EfficientNetV2: Smaller Models and Faster Training", ICML 2021
- Fan et al, "Multiscale Vision Transformers", ICCV 2021
- Bello et al, "Revisiting ResNets: Improved Training and Scaling Strategies", NeurIPS 2021
- Steiner et al, "How to train your ViT? Data, Augmentation, and Regularization in Vision Transformers", arXiv 2021

Huang et al, "Deep Networks with Stochastic Depth", ECCV 2016

Regularization: CutOut

Training: Set random images regions to 0
Testing: Use the whole image

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing



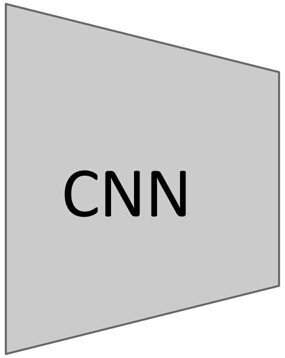
Replace random regions with mean value or random values

DeVries and Taylor, “Improved Regularization of Convolutional Neural Networks with Cutout”, arXiv 2017
Zhong et al, “Random Erasing Data Augmentation”, AAAI 2020

Regularization: Mixup

Training: Train on random blends of images
Testing: Use original images

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing
Mixup



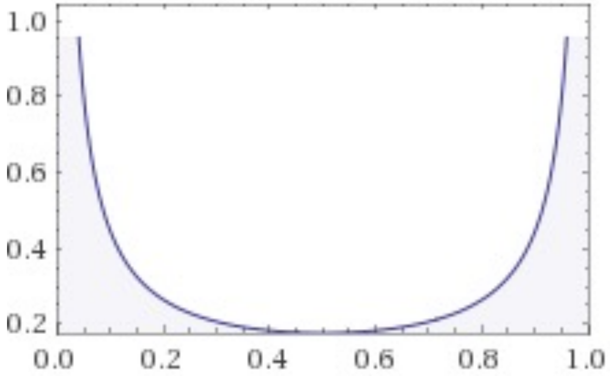
Target label:
cat: 0.4
dog: 0.6

Randomly blend the pixels of pairs of training images, e.g. 40% cat, 60% dog

Zhang et al, "*mixup*: Beyond Empirical Risk Minimization", ICLR 2018

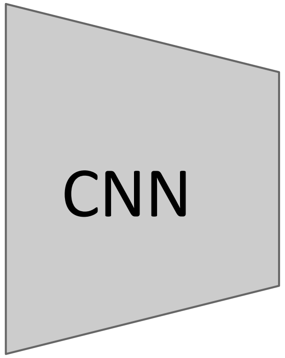
Regularization: Mixup

Training: Train on random blends of images
Testing: Use original images



Sample blend probability from a beta distribution Beta(a, b) with a=b≈0 so blend weights are close to 0/1

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing
Mixup



Target label:
cat: 0.4
dog: 0.6

Randomly blend the pixels of pairs of training images, e.g. 40% cat, 60% dog

Zhang et al, "*mixup*: Beyond Empirical Risk Minimization", ICLR 2018

Yun et al, "CutMix: Regularization Strategies to Train Strong Classifiers with Localizable Features", ICCV 2019

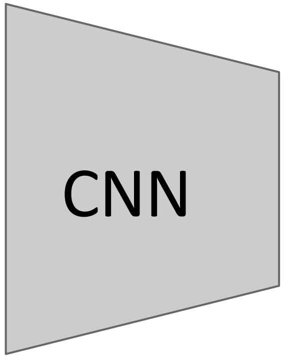
Regularization: CutMix

Training: Train on random blends of images

Testing: Use original images

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing
Mixup / CutMix



Target label:
cat: 0.6
dog: 0.4

Replace random crops of one image with another: e.g. 60% of pixels from cat, 40% from dog

Regularization: Label Smoothing

Szegedy et al, "Rethinking the Inception Architecture for Computer Vision", CVPR 2015

Training: Train on random blends of images

Testing: Use original images

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing
Mixup / CutMix
Label Smoothing

Target Distribution

Standard Training	Label Smoothing
Cat: 100%	Cat: 90%
Dog: 0%	Dog: 5%
Fish: 0%	Fish: 5%

Set target distribution to be $1 - \frac{K-1}{K}\epsilon$ on the correct category and ϵ/K on all other categories, with K categories and $\epsilon \in (0,1)$. Loss is cross-entropy between predicted and target distribution.

Regularization: Summary

Training: Train on random blends of images
Testing: Use original images

Examples:
Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout / Random Erasing
Mixup / CutMix
Label Smoothing

- Use DropOut for large fully-connected layers
- Data augmentation always a good idea
- Use BatchNorm for CNNs (but not ViTs)
- Try Cutout, MixUp, CutMix, Stochastic Depth, Label Smoothing to squeeze out a bit of extra performance

Summary

1. **One time setup**
   Activation functions, data preprocessing, weight initialization, regularization

Today

2. **Training dynamics**
   Learning rate schedules; large-batch training; hyperparameter optimization
3. **After training**
   Model ensembles, transfer learning

Next time

Next time:
Training Neural Networks
(part 2)