

DeepRob

Lecture 9
Training Neural Networks I
University of Michigan and University of Minnesota







Project 2—Updates

- Instructions available on the website
 - Here: https://rpm-lab.github.io/CSCI5980-Spr23-DeepRob/

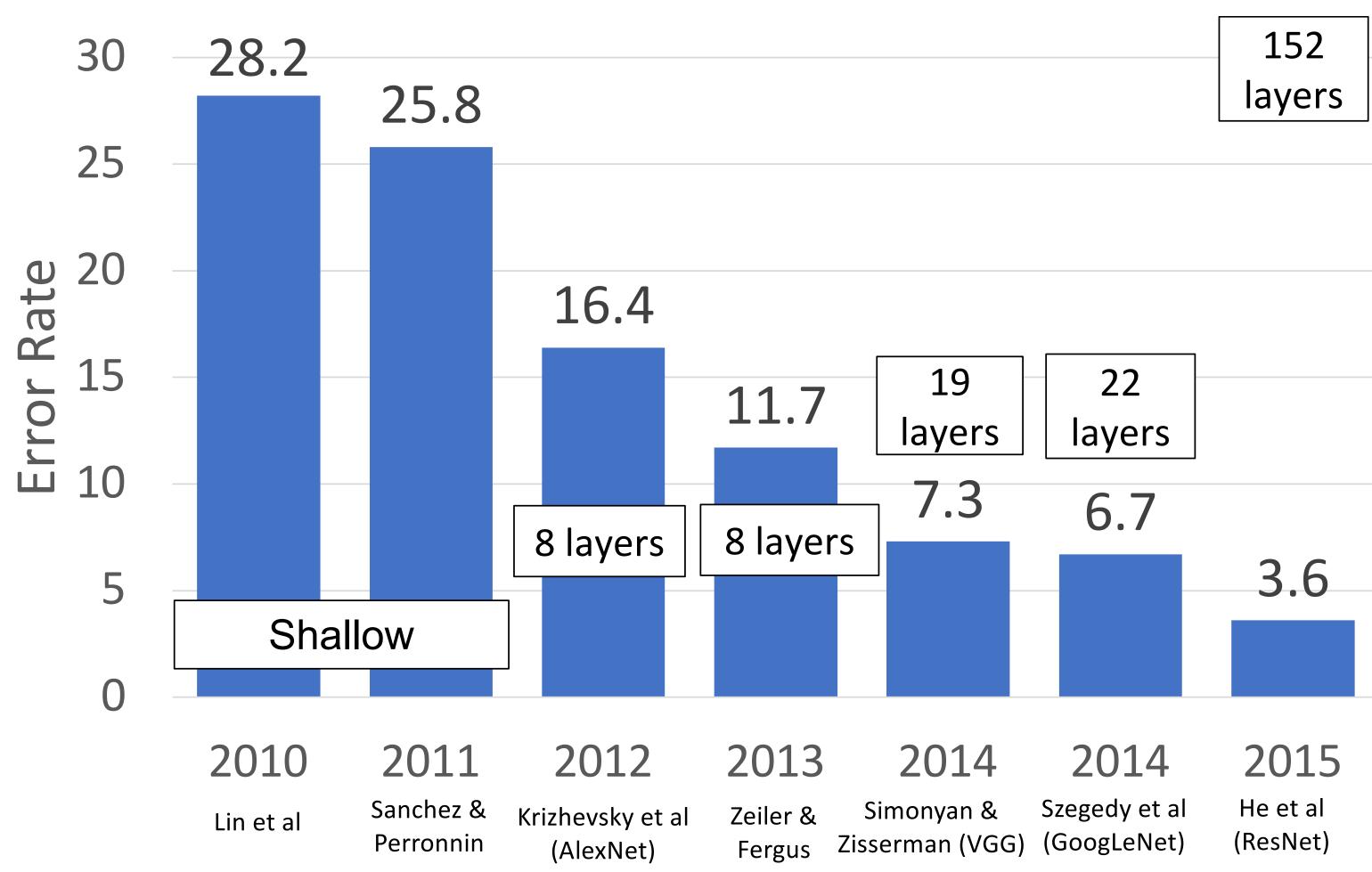
projects/project2/

- Implement two-layer neural network and generalize to FCN
- Autograder will be available today!
- Due Tuesday, February 21st 11:59 PM CT





Recap: CNN Architectures for ImageNet Classification





DR





Questions from the previous lecture

Computation for Forward pass vs Backward pass

- Backward pass in a neural network takes significantly more compute than the forward pass (computing gradients and propagating them back through the network)
- Forward pass compute time is used to compare networks as we care about the inference time (after training)

AlexNet memory requirement

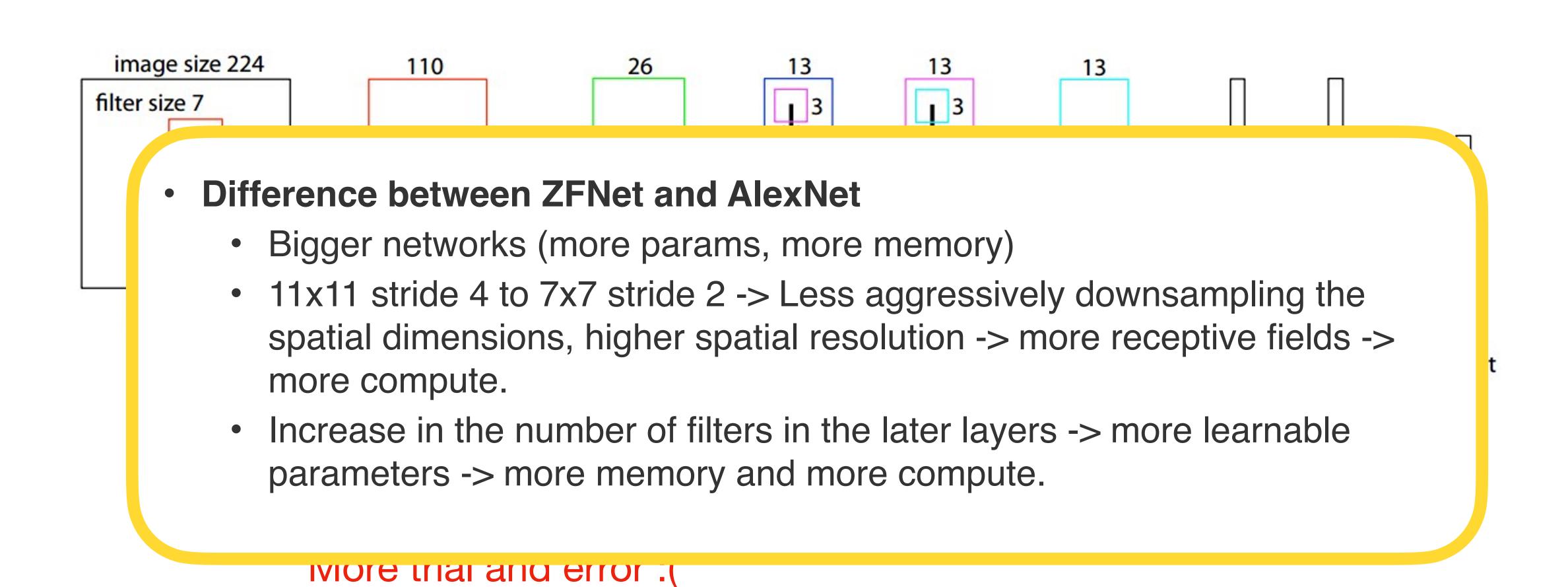
- Input size of 227 x 227 pixels
- Batch size of 128 images
- ~2.3 gigabytes for storing the activations of all the layers during the forward pass
- During training, additional memory is required to store intermediate results for backpropagation, weight updates, and other operations.







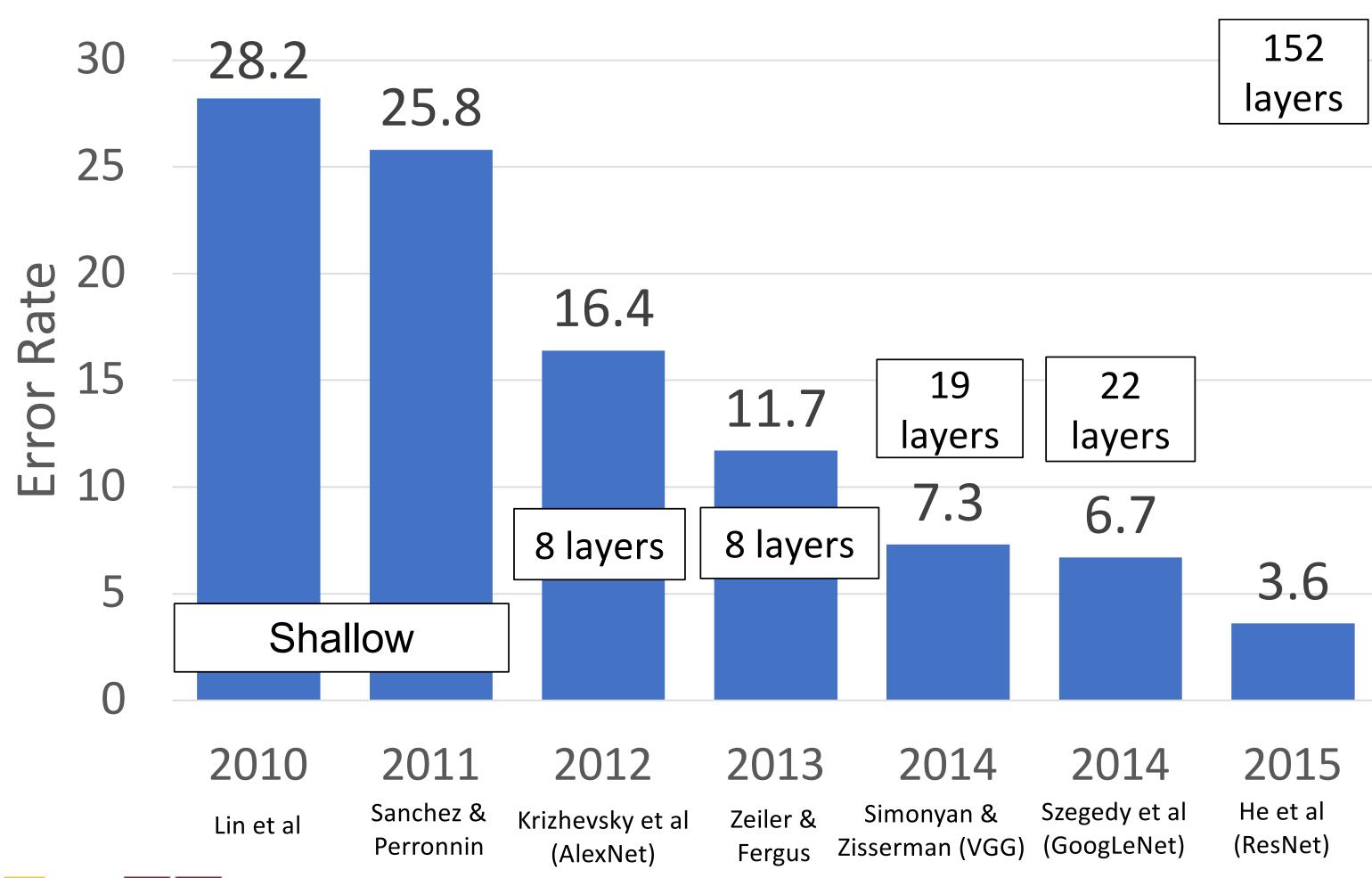
Questions from the previous lecture







Recap: CNN Architectures for ImageNet Classification





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Once we have Batch Normalization, we can train networks with 10+ layers. What happens as we go deeper?

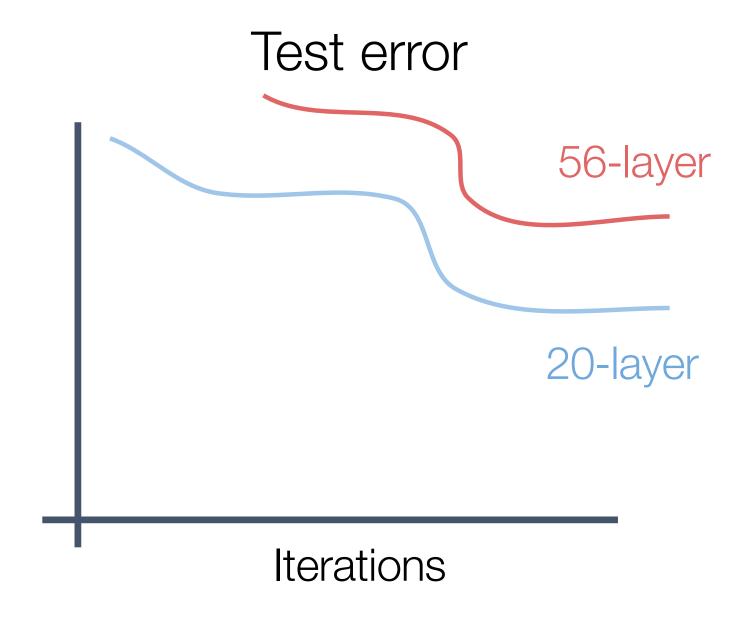






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Deeper model does worse than shallow model!





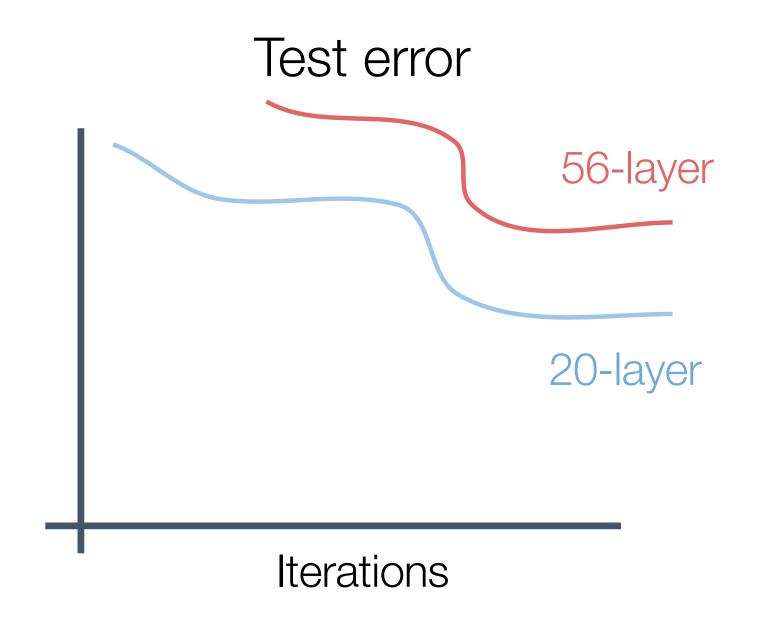




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Deeper model does worse than shallow model!

Initial guess: Deep model is **overfitting** since it is much bigger than the other model

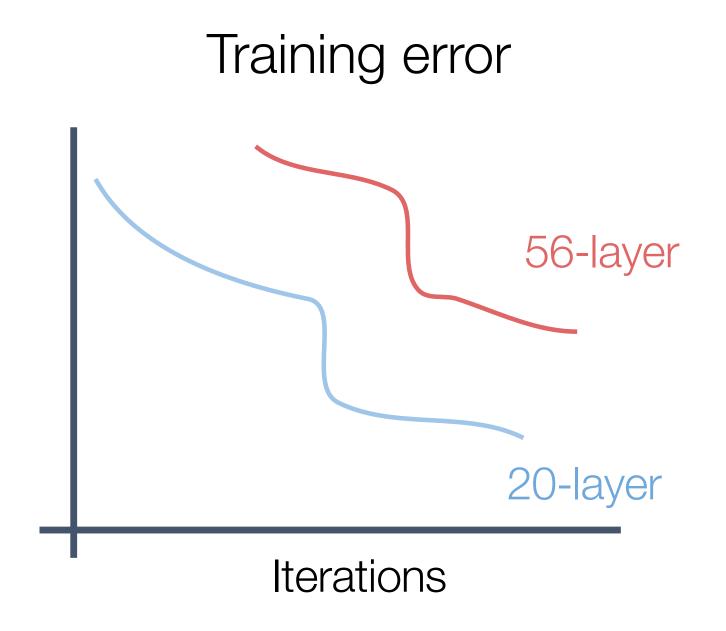


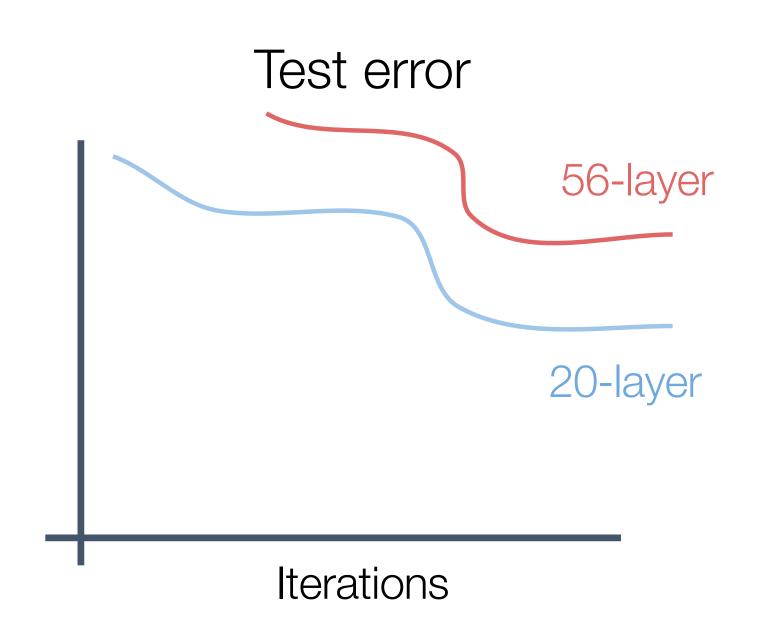






Once we have Batch Normalization, we can train networks with 10+ layers. What happens as we go deeper?





In fact the deep model seems to be **underfitting** since it also performs worse than the shallow model on the training set! It is actually **underfitting**







A deeper model can emulate a shallower model: copy layers from shallower model, set extra layers to identity

Thus deeper models should do at least as good as shallow models







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Hypothesis: This is an optimization problem. Deeper models are harder to optimize, and in particular don't learn identity functions to emulate shallow models







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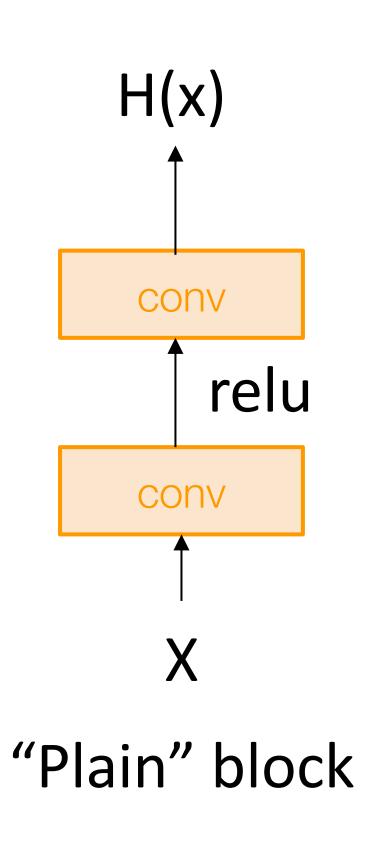
Solution: Change the network so learning identity functions with extra layers is easy!

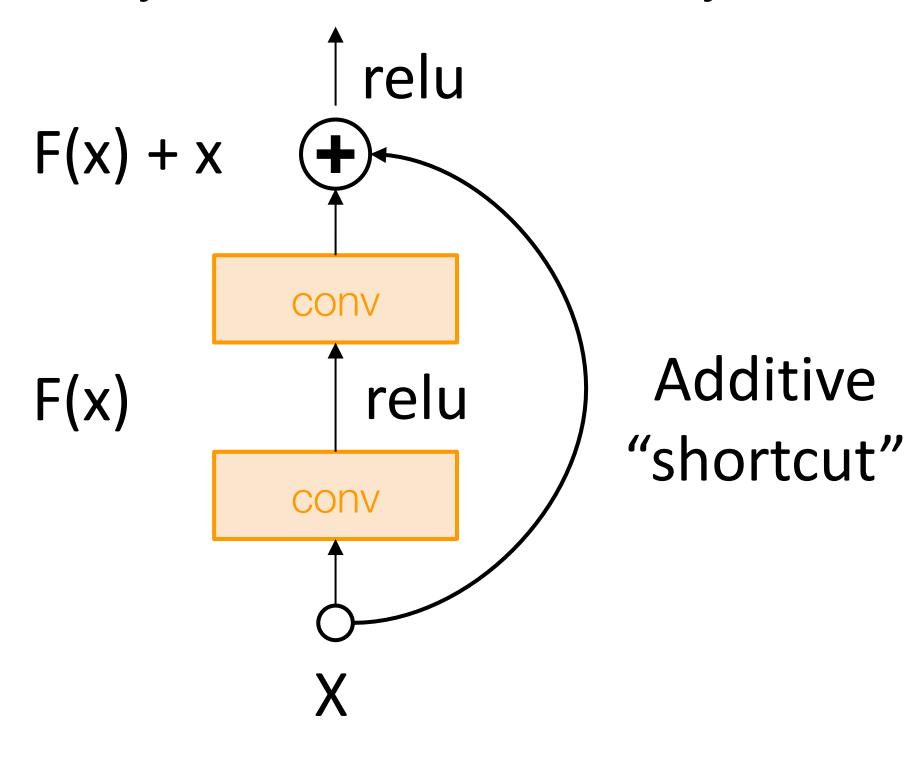






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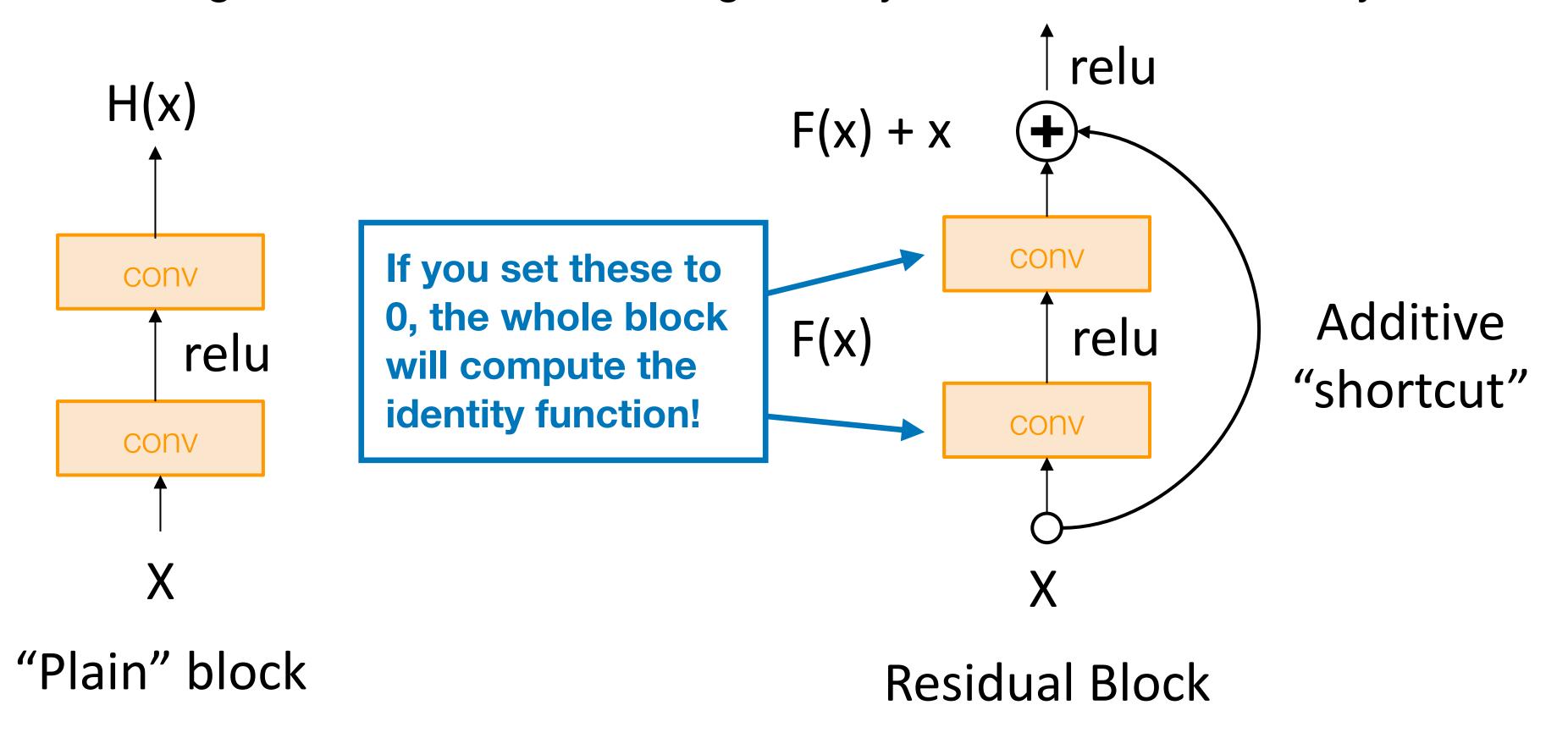
Residual Block







Solution: Change the network so learning identity functions with extra layers is easy!

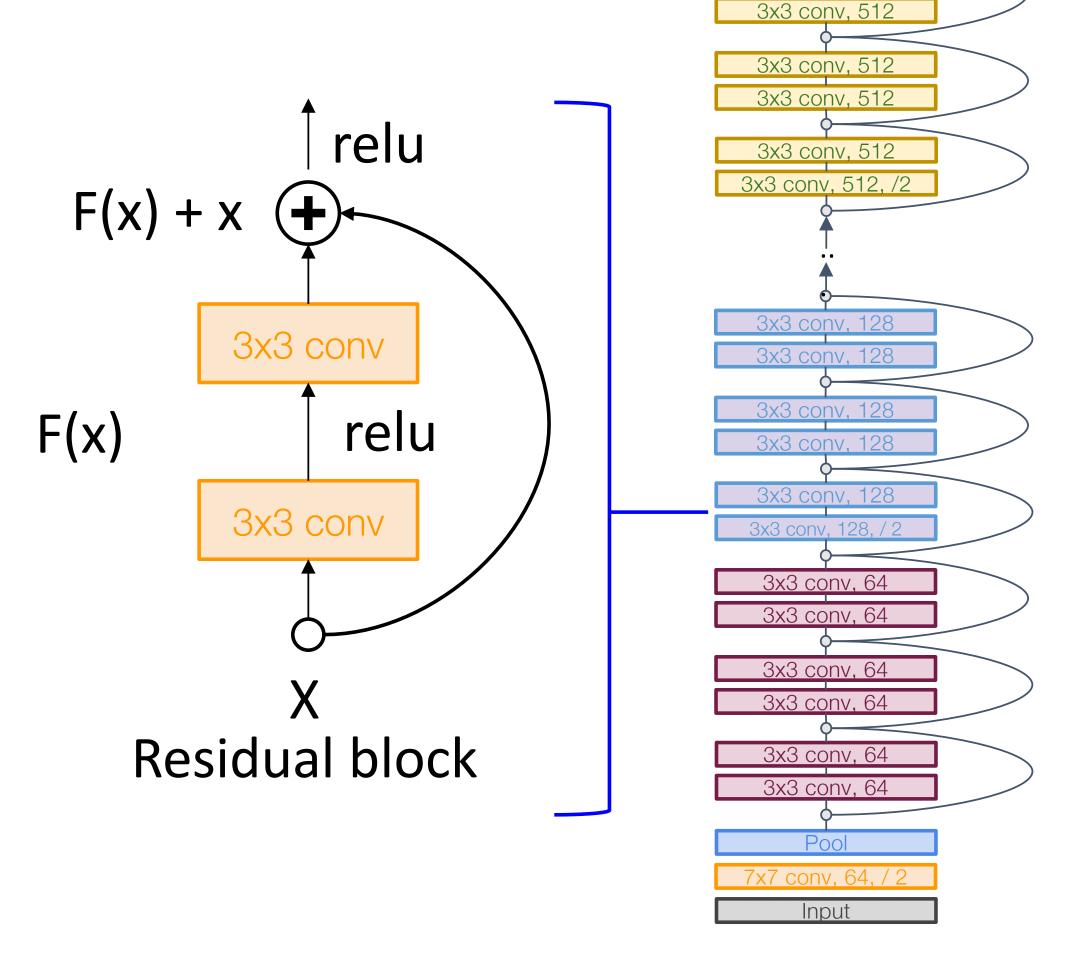








A residual network is a stack of many residual blocks







Softmax

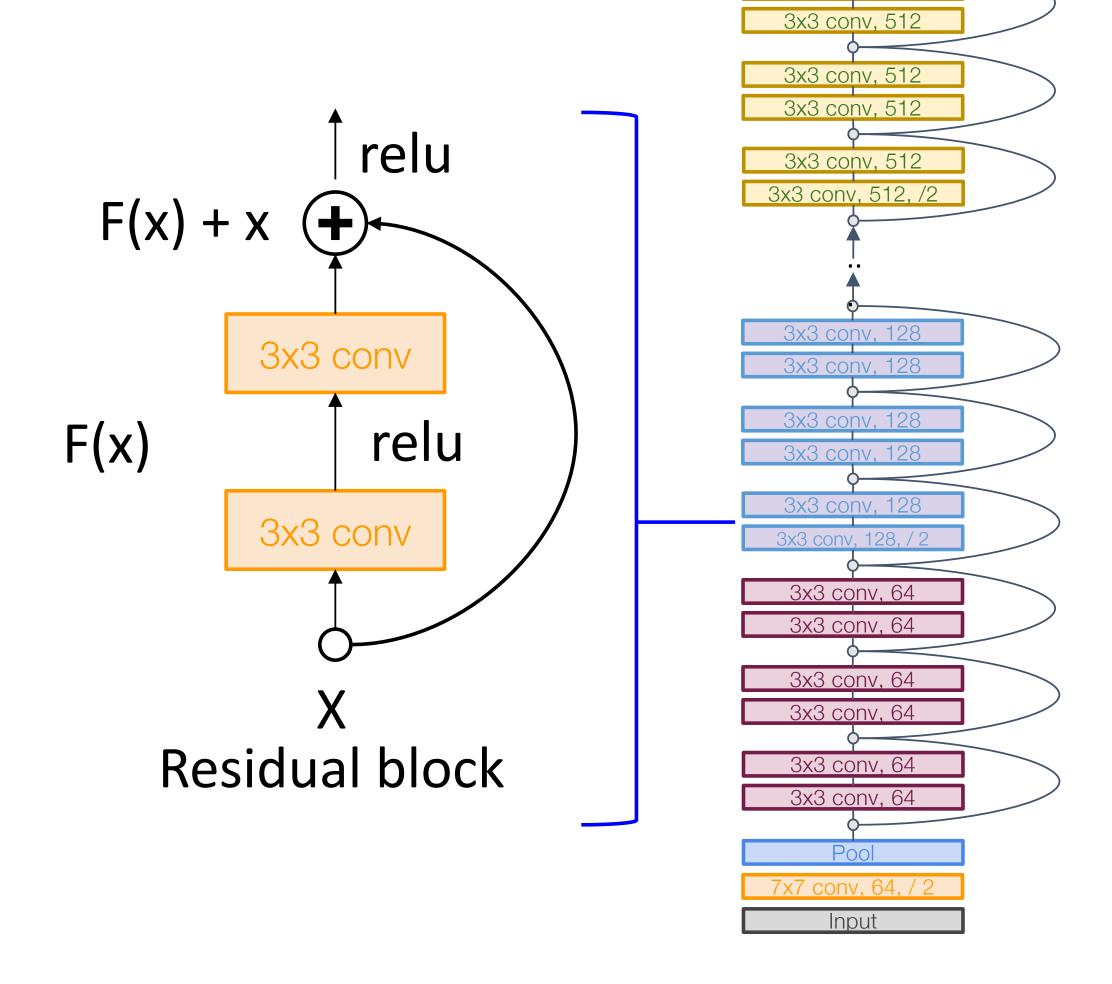
FC 1000

3x3 conv, 512



A residual network is a stack of many residual blocks

Regular design, like VGG: each residual block has two 3x3 conv







FC 1000

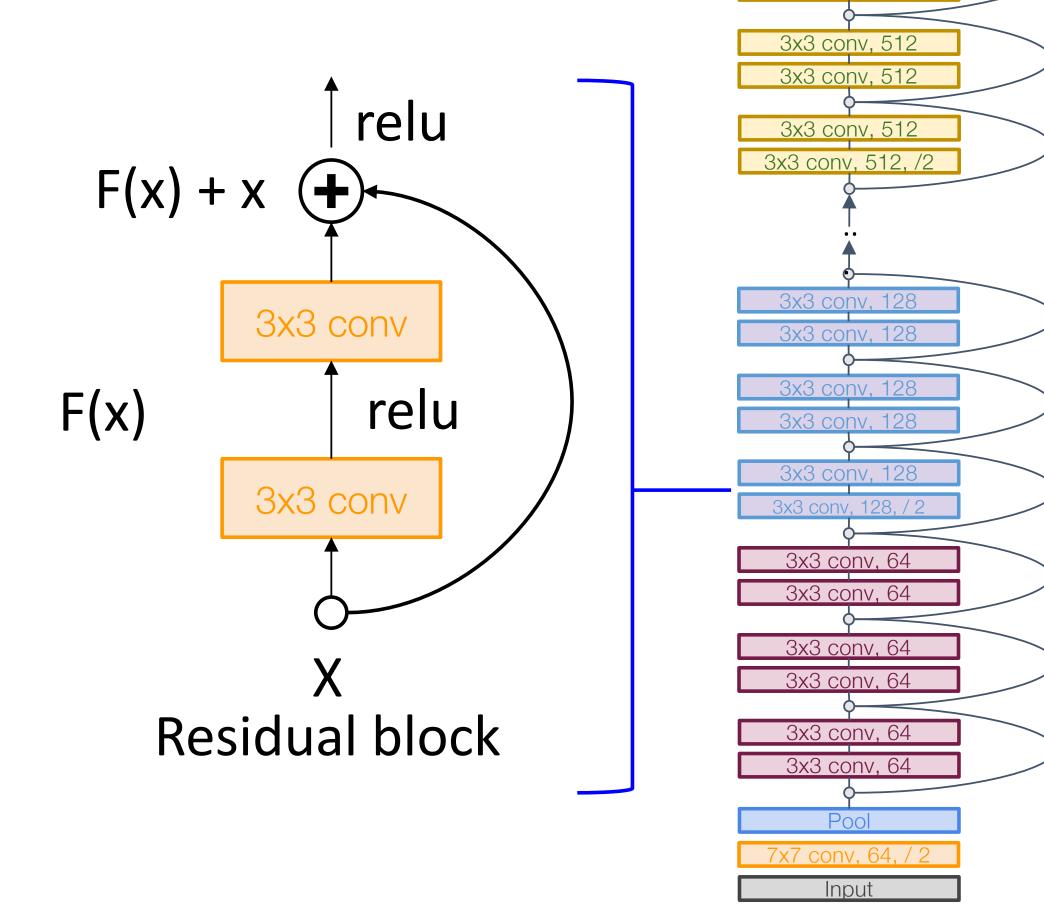
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A residual network is a stack of many residual blocks

Regular design, like VGG: each residual block has two 3x3 conv

Network is divided into **stages**: the first block of each stage halves the resolution (with stride-2 conv) and doubles the number of channels







FC 1000

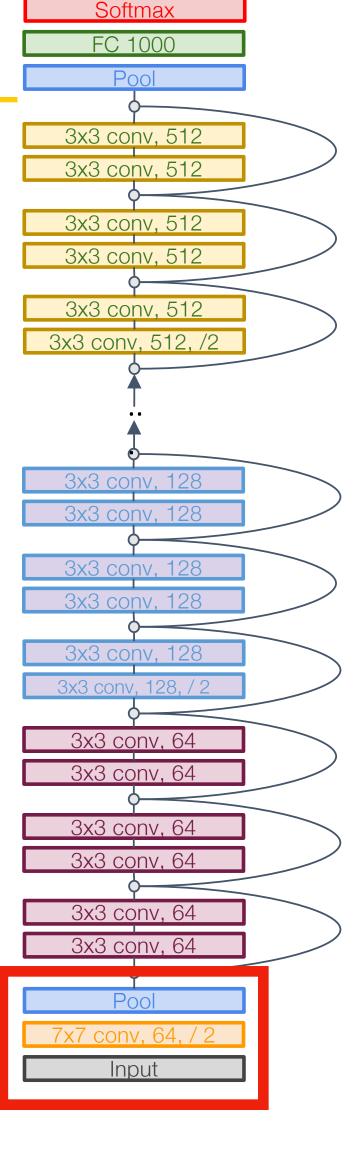
3x3 conv. 512

3x3 conv, 512



Uses the same aggressive **stem** as GoogleNet to downsample the input 4x before applying residual blocks:

	Inp	ut size	Layer				Outpu	ıt size			
Layer	С	H/W	Filters	Kernel	Stride	Pad	С	H/W	Memory (KB)	Params	Flop (M)
Conv	3	224	64	7	2	3	64	112	3136	9	118
Max-pool	64	112		3	2	1	64	56	784	0	2

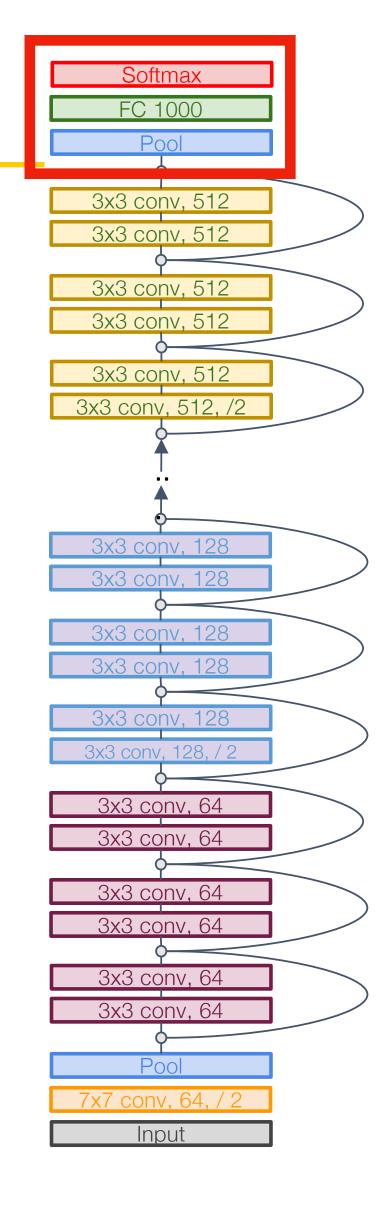








Like GoogLeNet, no big fully-connected-layers: Instead use global average pooling and a single linear layer at the end









ResNet-18:

Stem: 1 conv layer

Stage 1 (C=64): 2 res. block = 4 conv

Stage 2 (C=128): 2 res. block = 4 conv

Stage 3 (C=256): 2 res. block = 4 conv

Stage 4 (C=512): 2 res. block = 4 conv

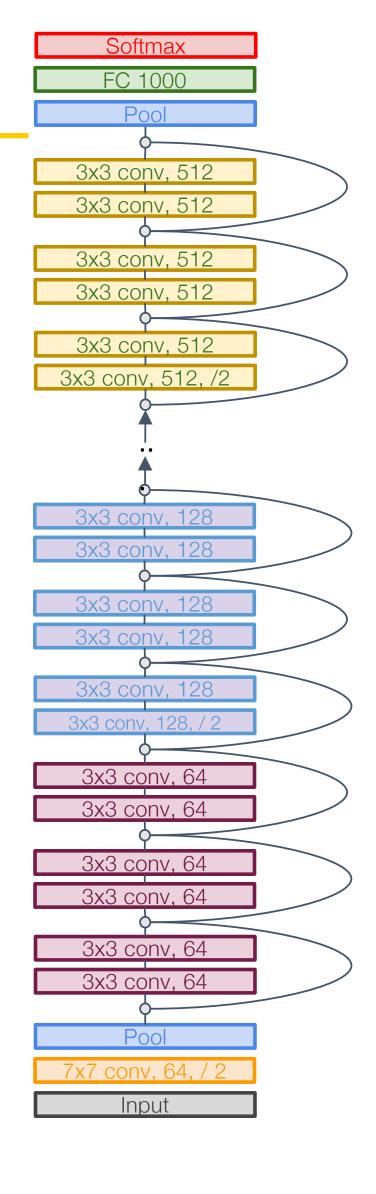
Linear

ImageNet top-5 error: 10.92

GFLOP: 1.8









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ResNet-34:

Stem: 1 conv layer

Stage 1: 3 res. block = 6 conv

Stage 2: 4 res. block = 8 conv

Stage 3: 6 res. block = 12 conv

Stage 4: 3 res. block = 6 conv

Linear

ImageNet top-5 error: 8.58

GFLOP: 3.6

VGG-16:

ImageNet top-5 error: 9.62

GFLOP: 13.6





FC 1000

3x3 conv, 512

3x3 conv, 512

3x3 conv, 512

3x3 conv, 512

3x3 conv, 512, /2

3x3 conv, 128

3x3 conv, 128

3x3 conv. 64

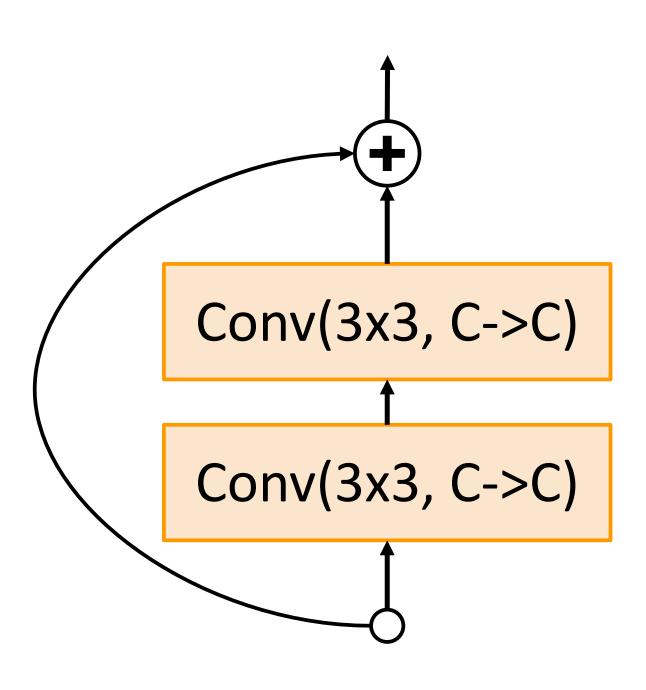
3x3 conv. 64

3x3 conv, 64

3x3 conv. 64



Residual Networks: Basic Block



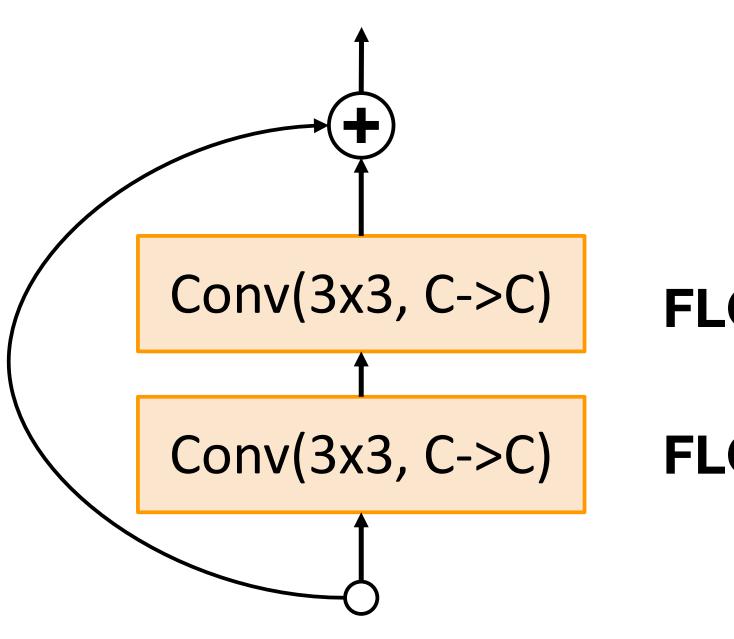
"Basic" Residual block







Residual Networks: Basic Block



FLOPs: 9HWC²

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"Basic" Residual block

Total FLOPs:

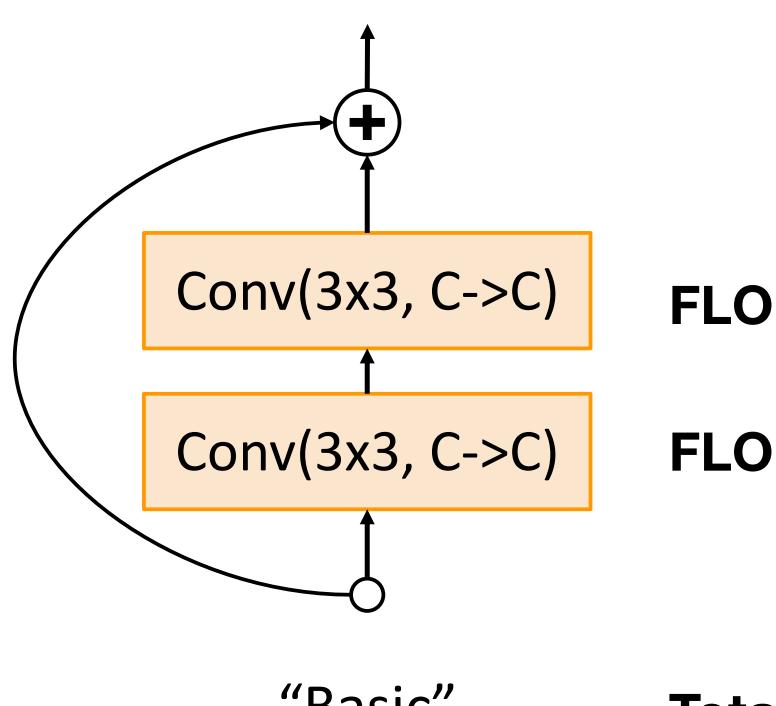
18HWC²







Residual Networks: Bottleneck Block

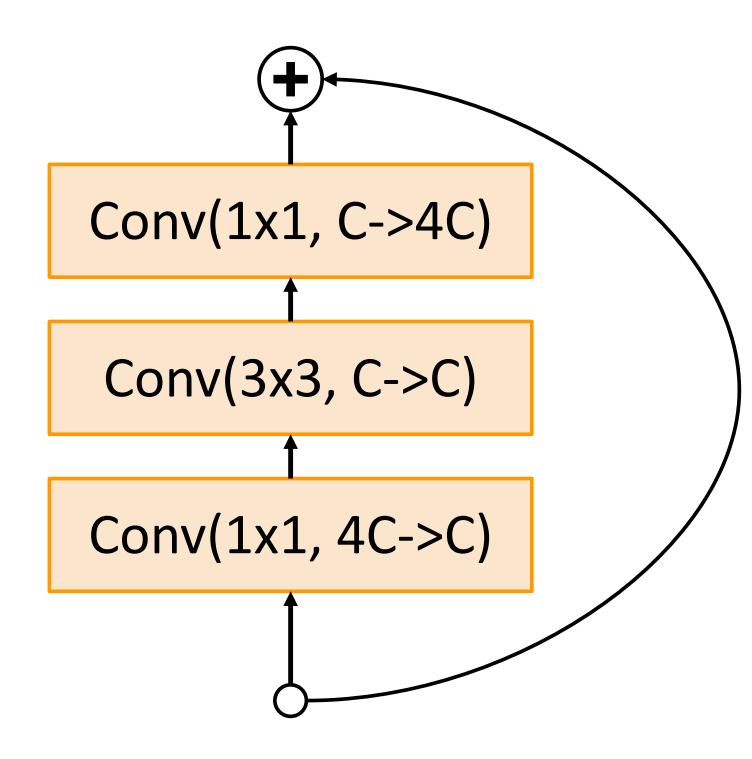


FLOPs: 9HWC²

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"Basic" Residual block

Total FLOPs: 18HWC²



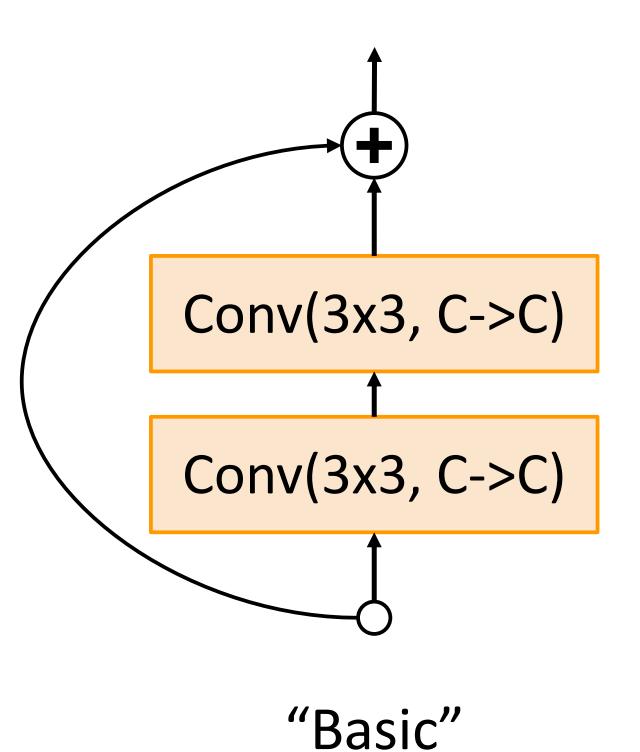
"Bottleneck" Residual block







Residual Networks: Bottleneck Block



More layers, less computational cost!

FLOPs: 9HWC²

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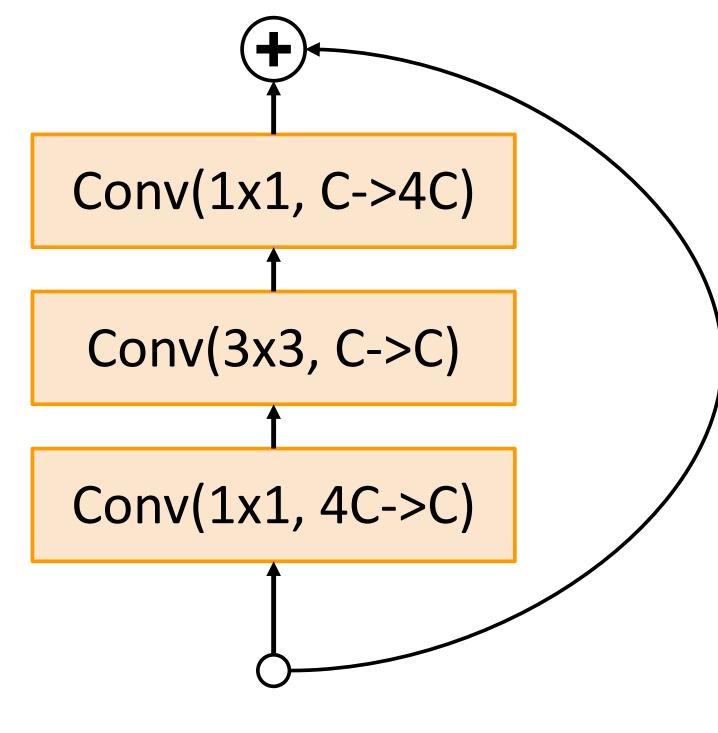
Total FLOPs: 18HWC²

FLOPs: 4HWC²

FLOPs: 9HWC²

FLOPs: 4HWC²





"Bottleneck" Residual block



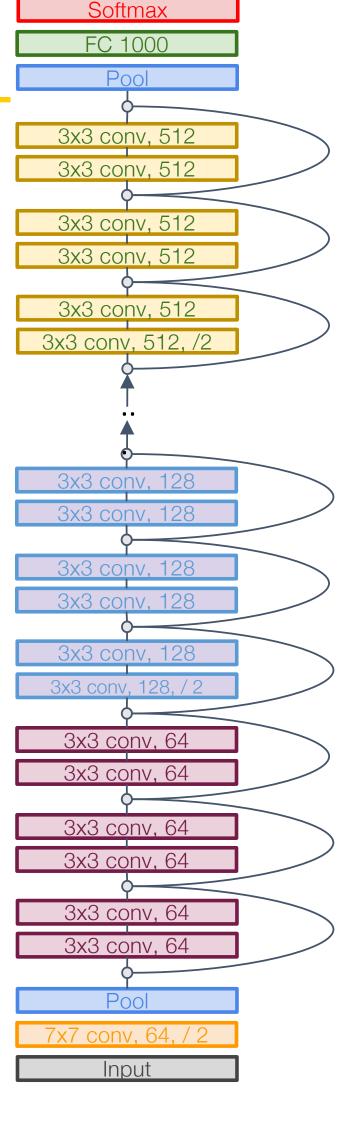


Residual block



Deeper ResNet-101 and ResNet-152 models are more accurate, but also more computationally heavy

			Stage 1		Stage 2		Stage 3		Stage 4				
	Block type	Stem layers	Block s	Layers	Block s	Layer s	Block s	Layer s	Block s	Layer s	FC Layers	GFLOP	Image Net
ResNet-18	Basic	1	2	4	2	4	2	4	2	4	1	1.8	10.92
ResNet-34	Basic	1	3	6	4	8	6	12	3	6	1	3.6	8.58
ResNet-50	Bottle	1	3	9	4	12	6	18	3	9	1	3.8	7.13
ResNet-101	Bottle	1	3	9	4	12	23	69	3	9	1	7.6	6.44
ResNet-152	Bottle	1	3	9	8	24	36	108	3	9	1	11.3	5.94









- Able to train very deep networks
- Deeper networks do better than shallow networks (as expected)
- Swept 1st place in all ILSVRC and COCO 2015 competitions
- Still widely used today

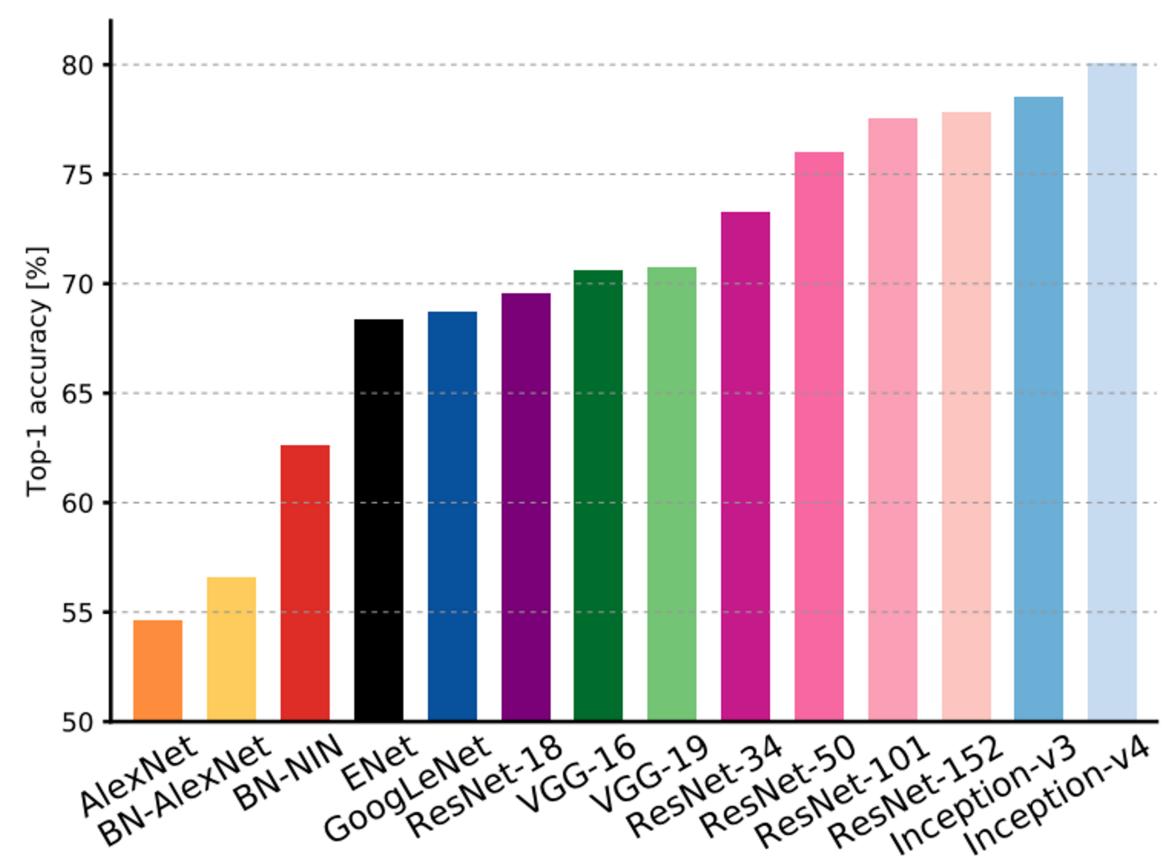
MSRA @ ILSVRC & COCO 2015 Competitions

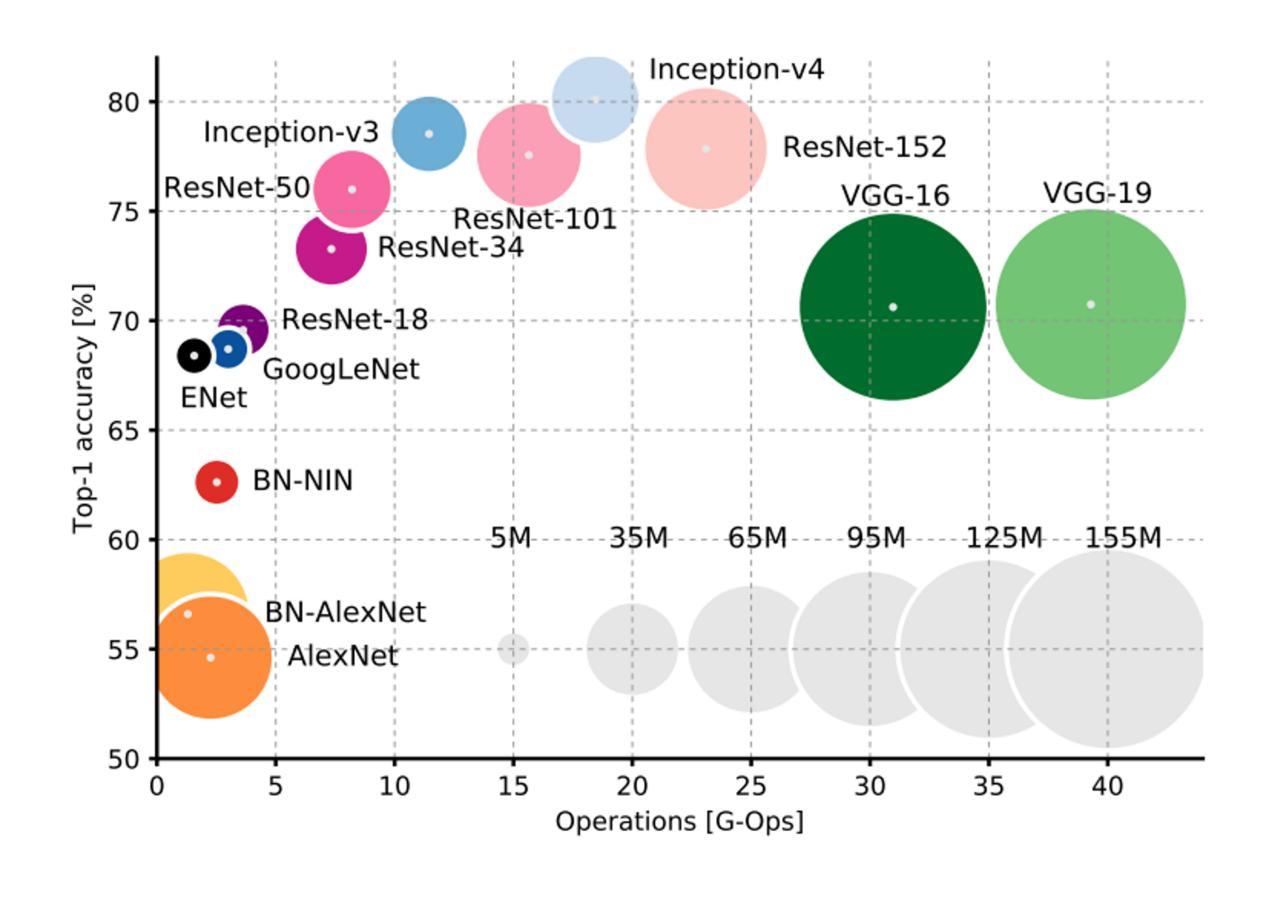
- 1st places in all five main tracks
 - ImageNet Classification: "Ultra-deep" (quote Yann) 152-layer nets
 - ImageNet Detection: 16% better than 2nd
 - ImageNet Localization: 27% better than 2nd
 - COCO Detection: 11% better than 2nd
 - COCO Segmentation: 12% better than 2nd







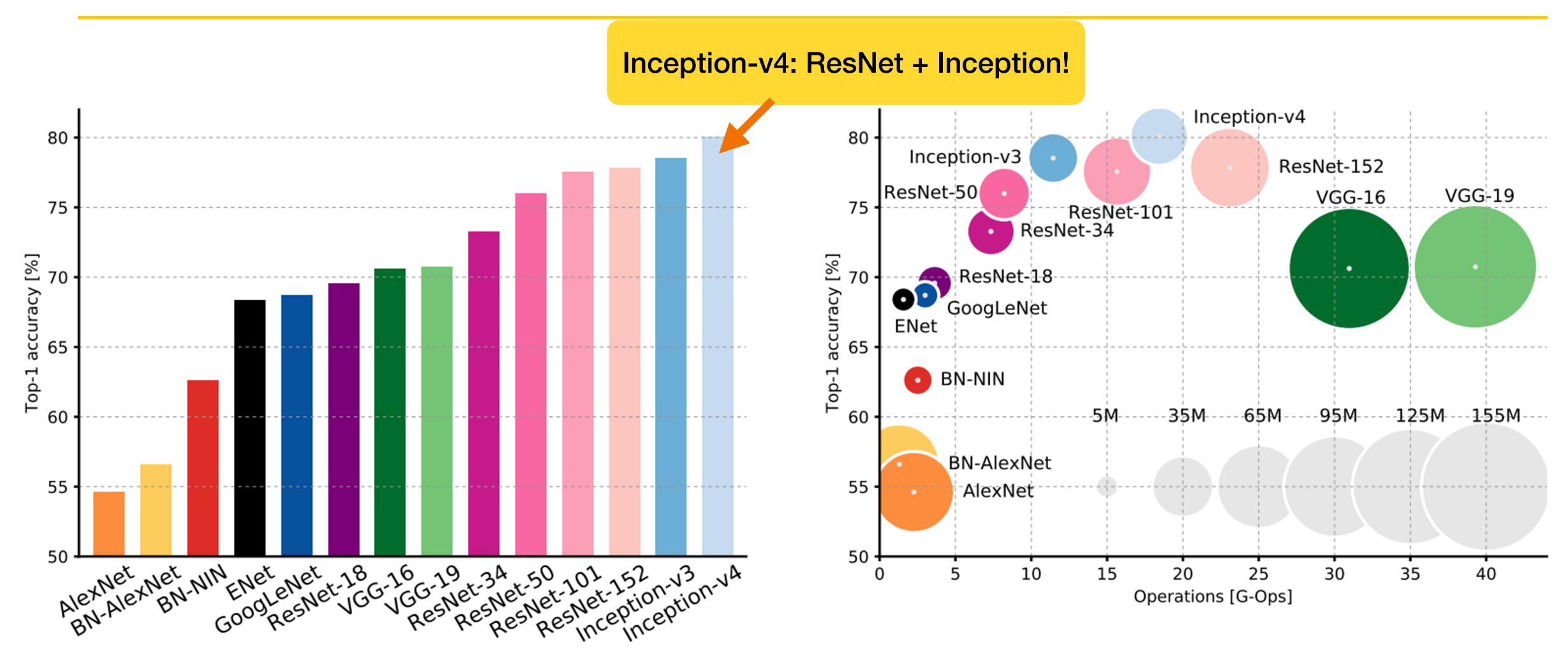










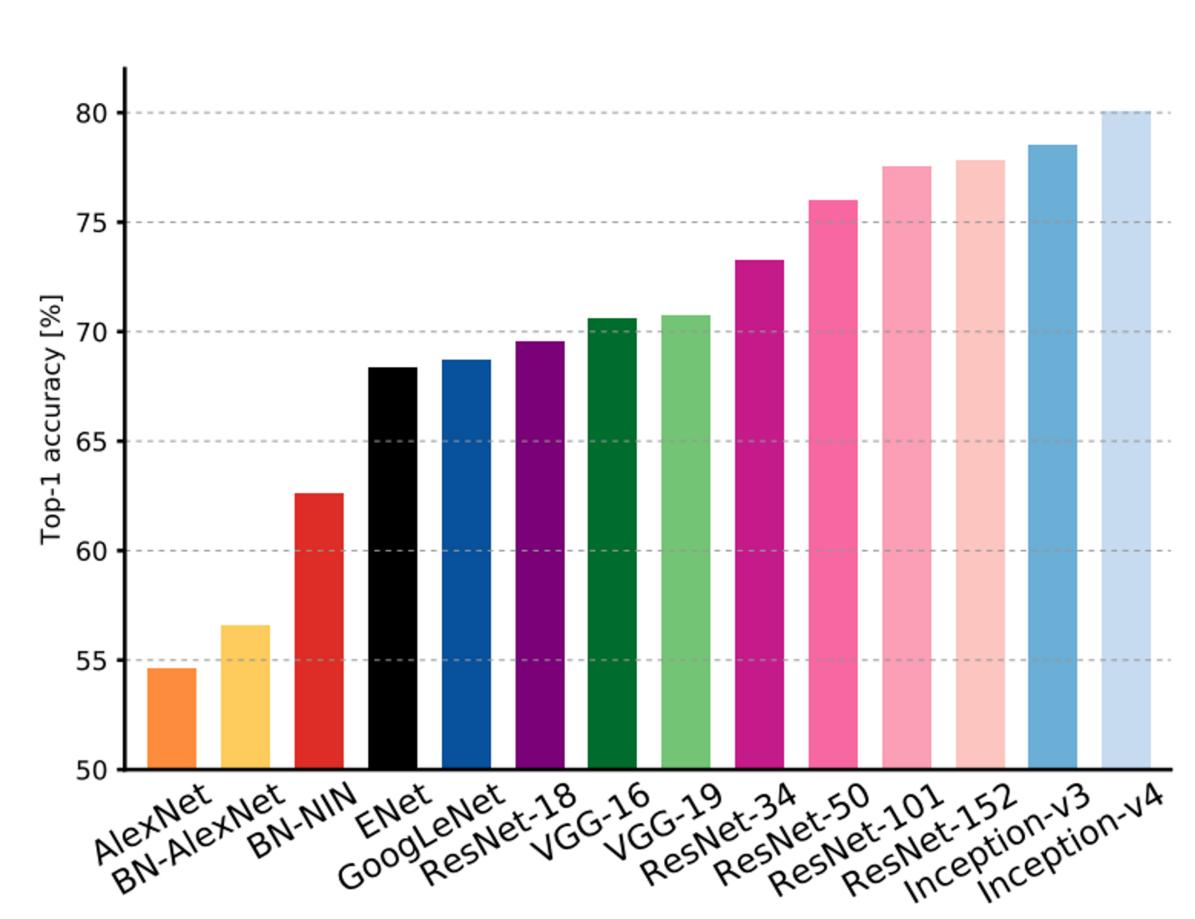


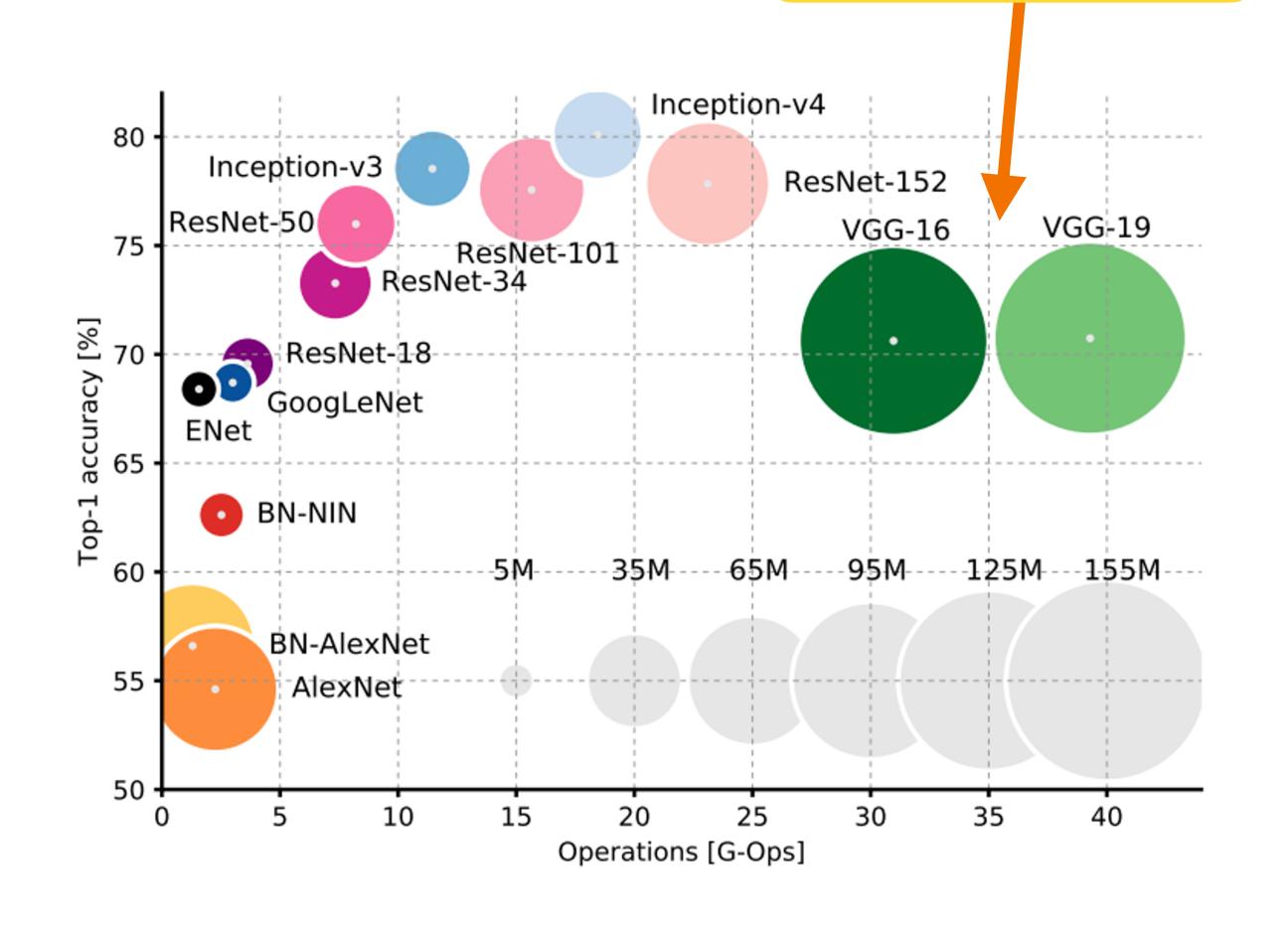










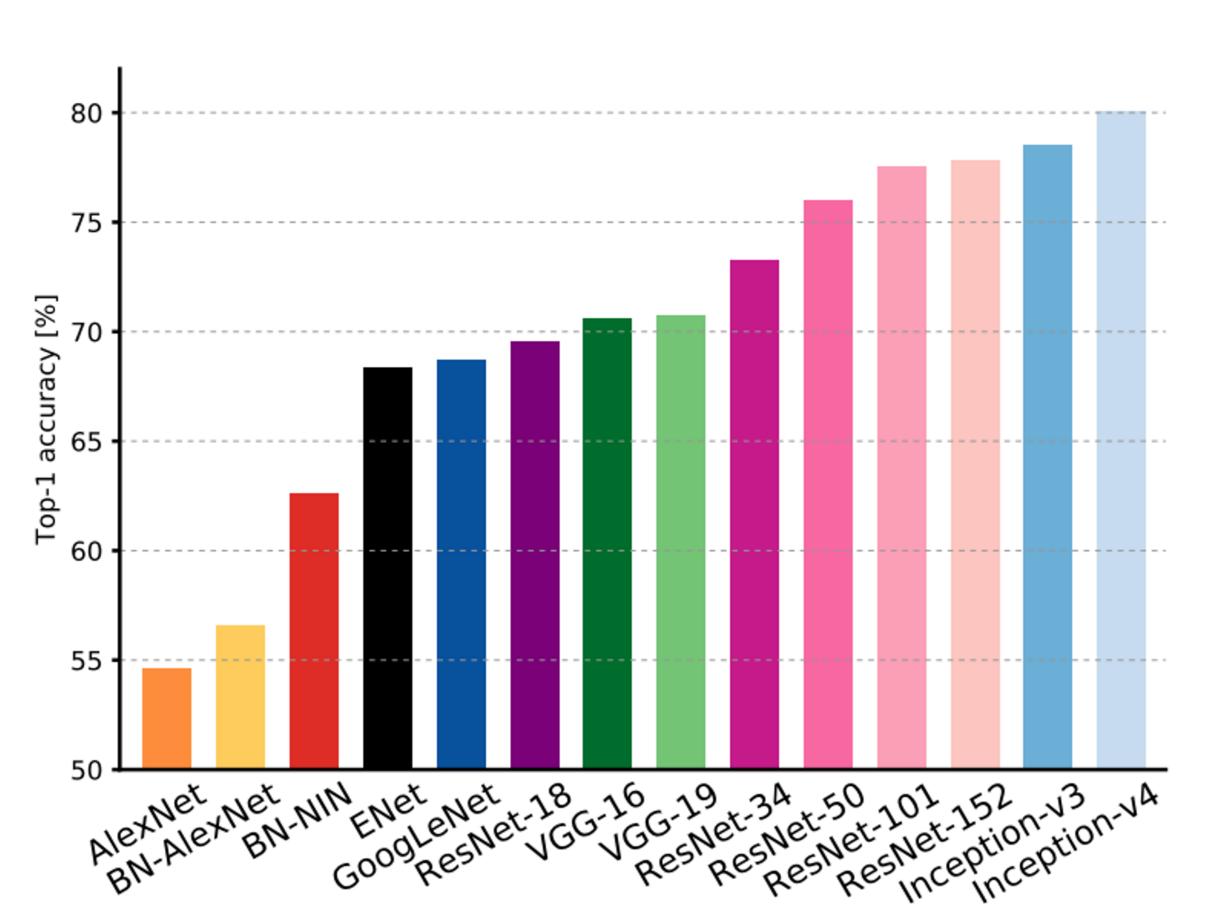


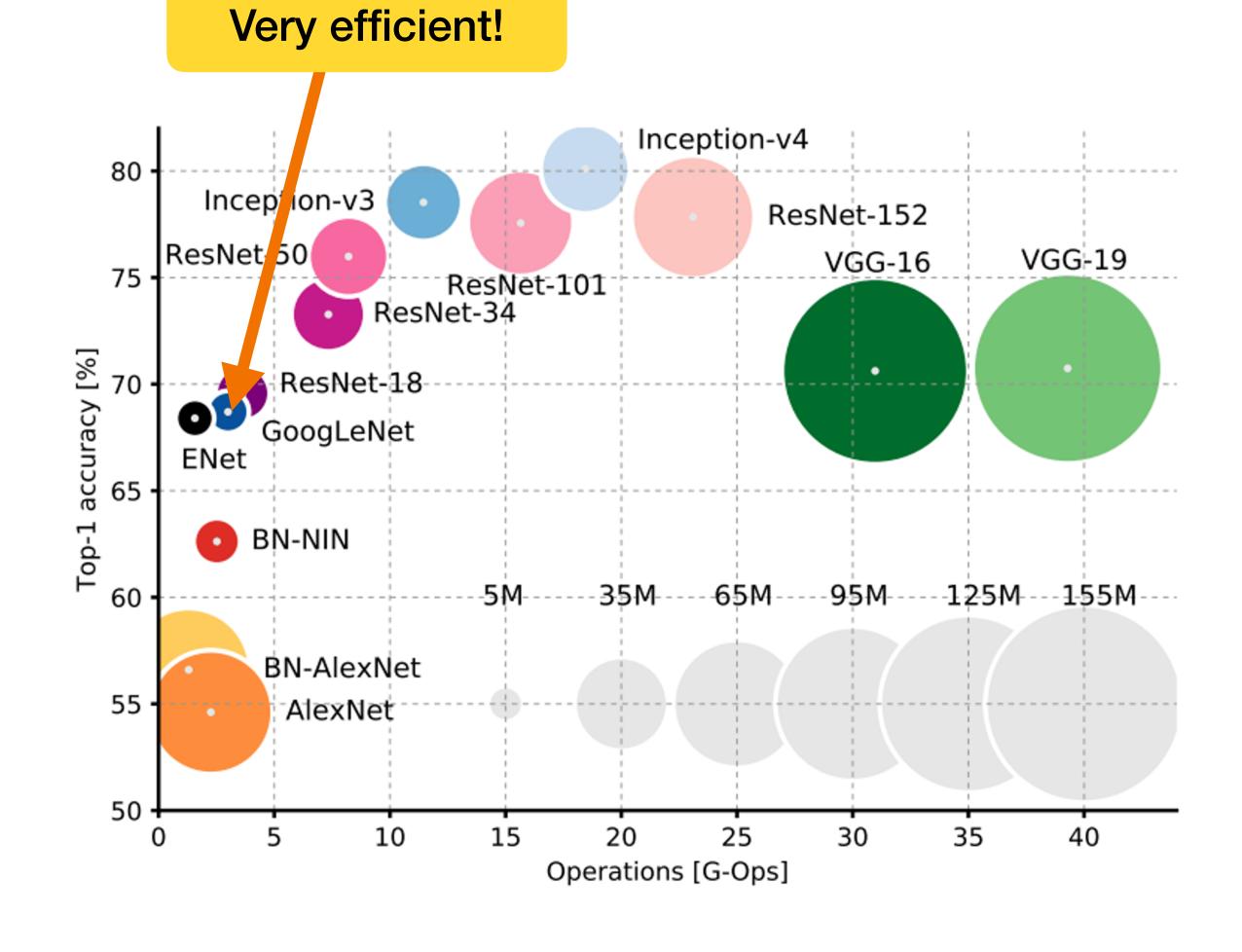






GoogLeNet:

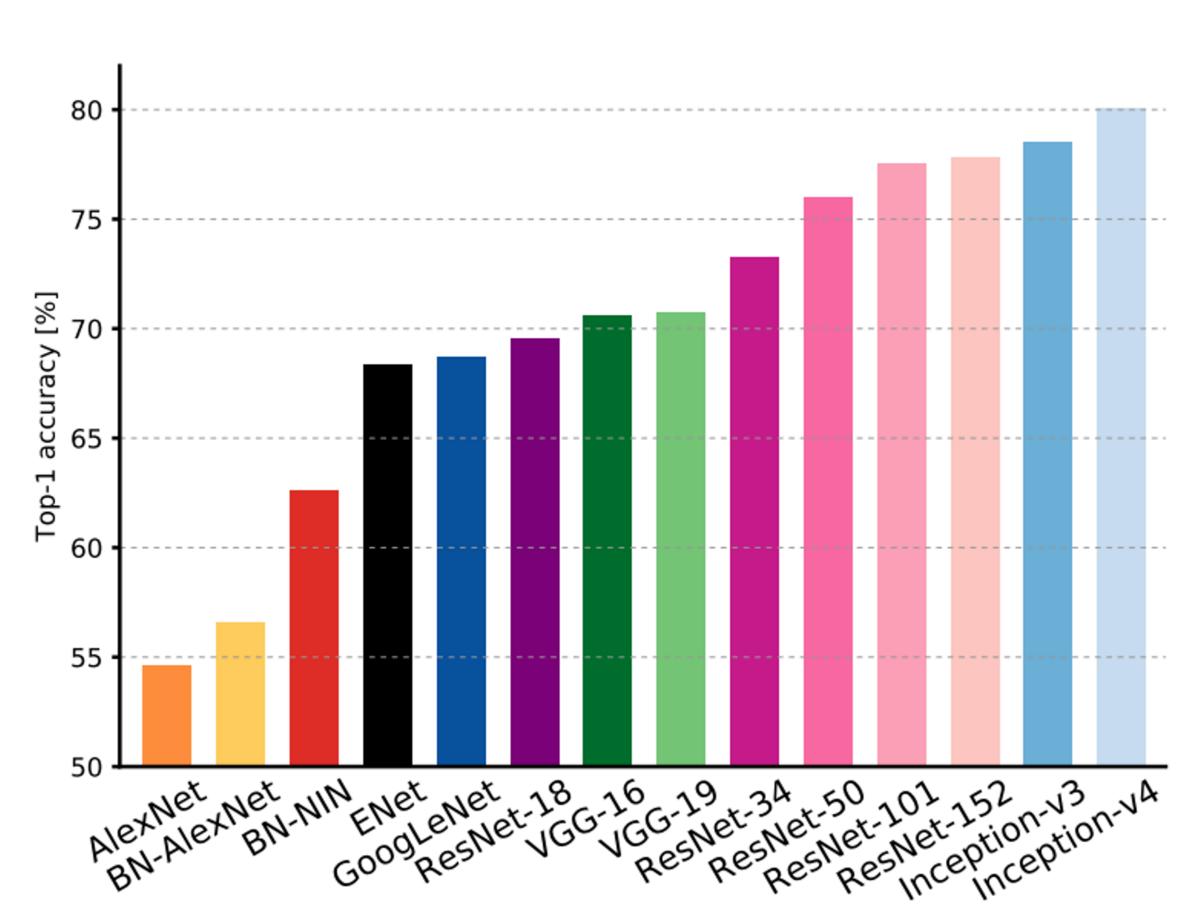


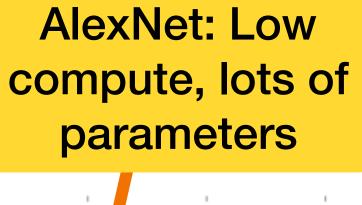


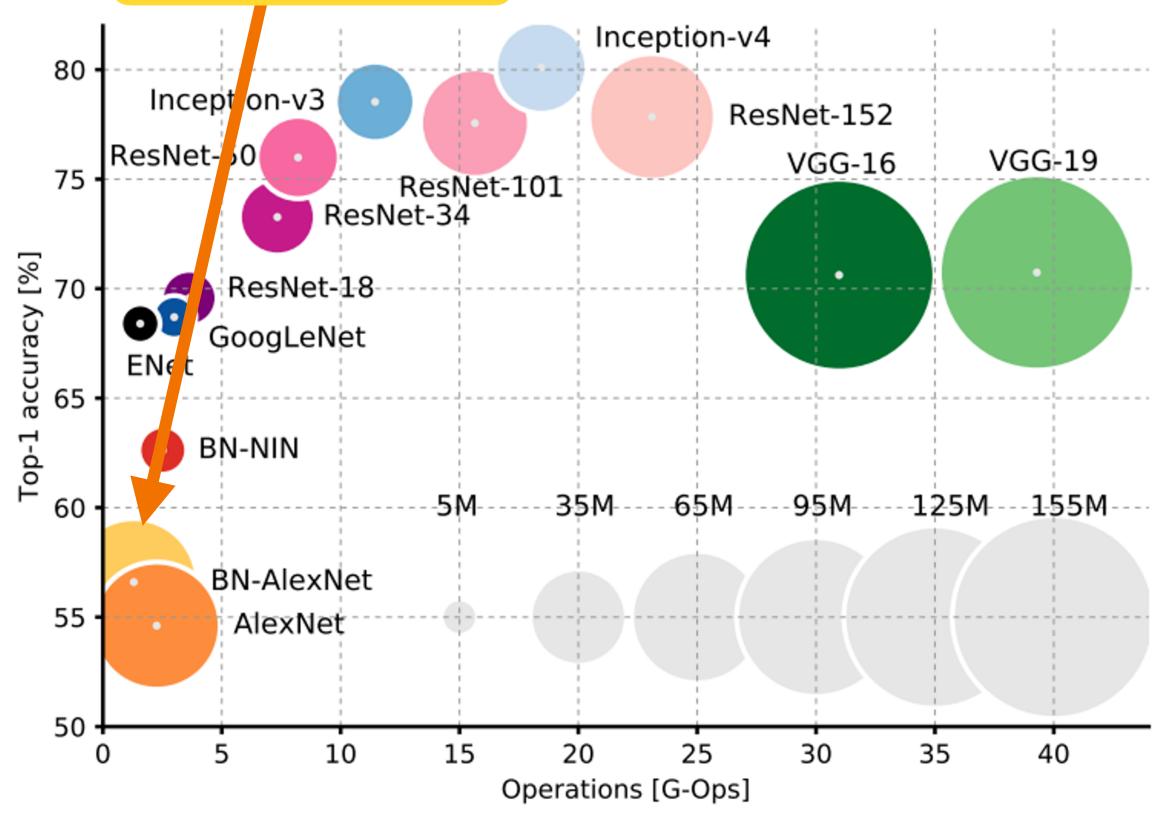










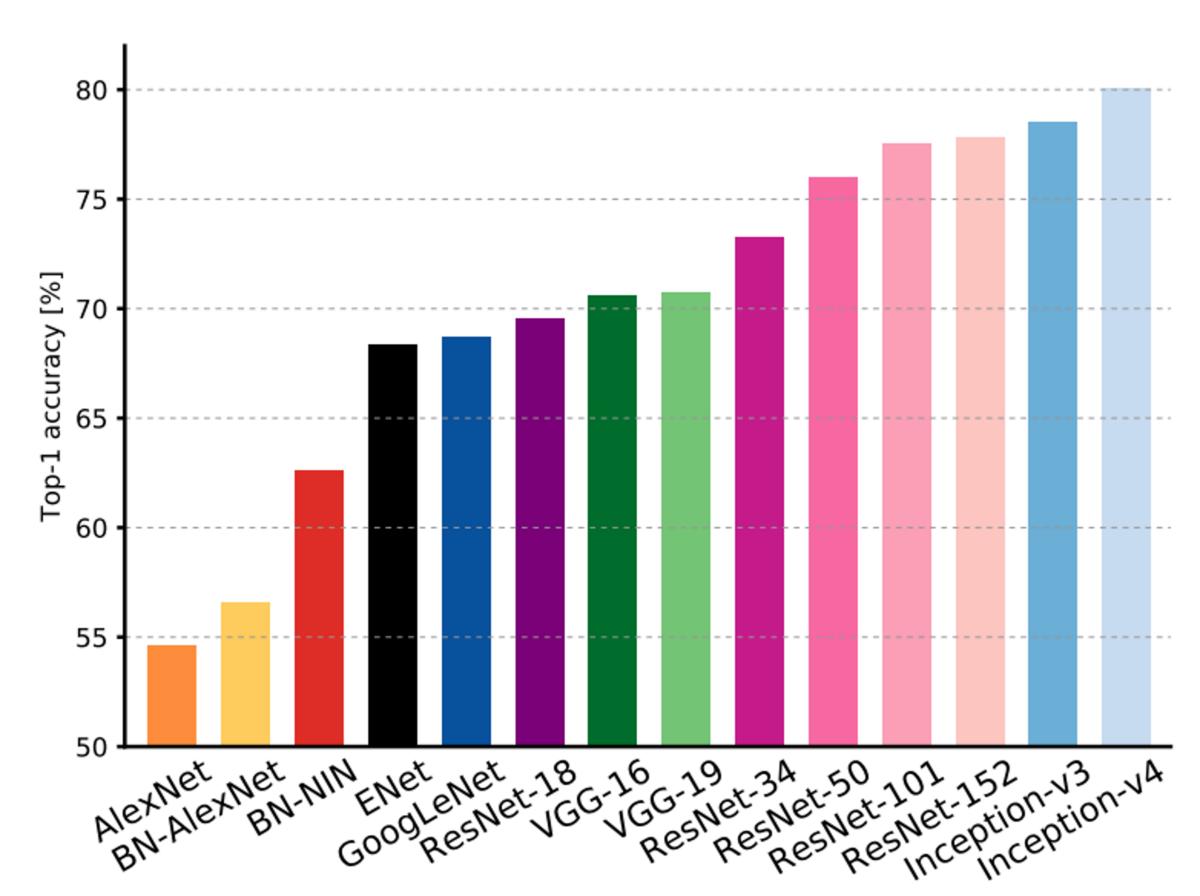


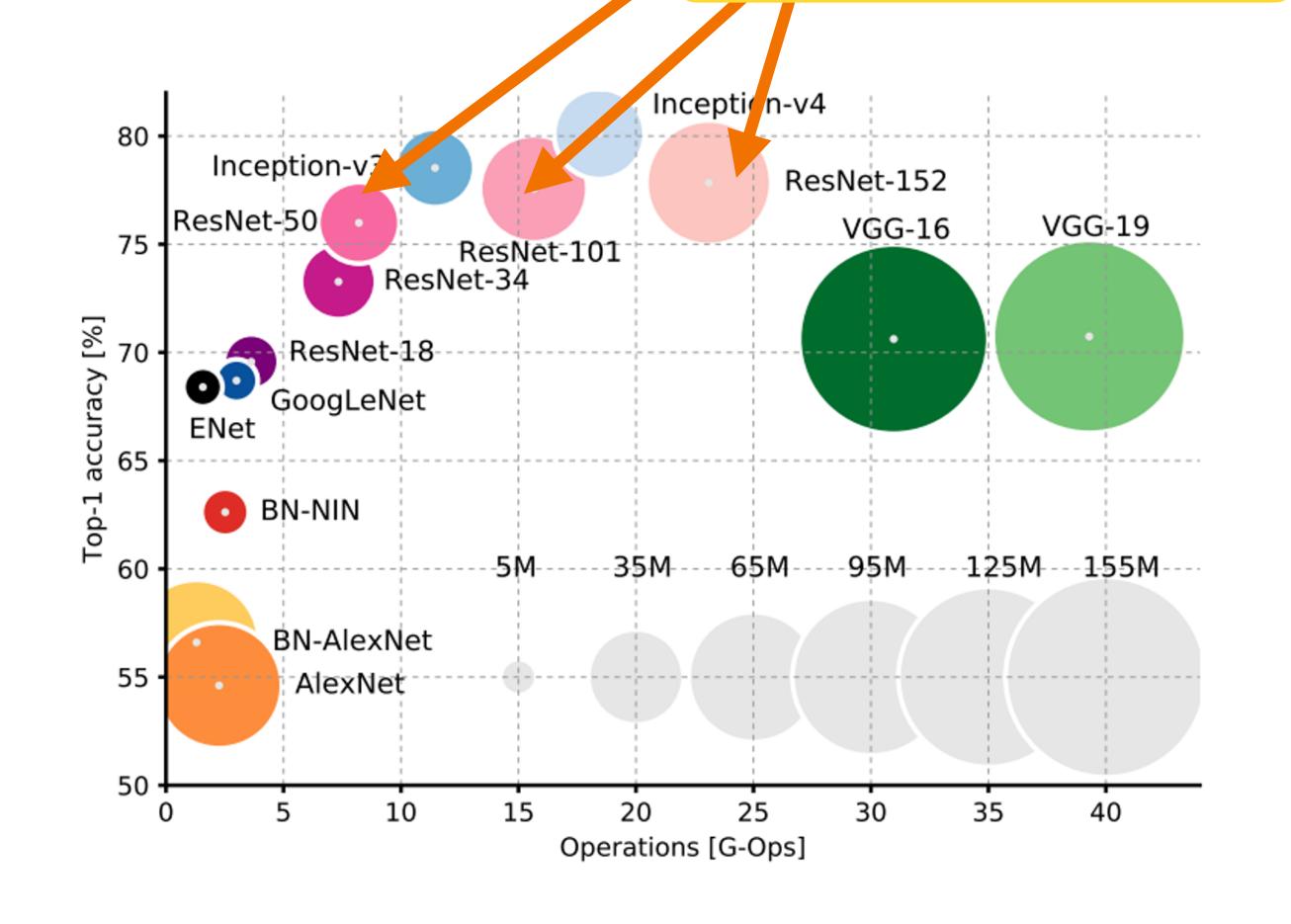






ResNet: Simple design, moderate efficiency, high accuracy



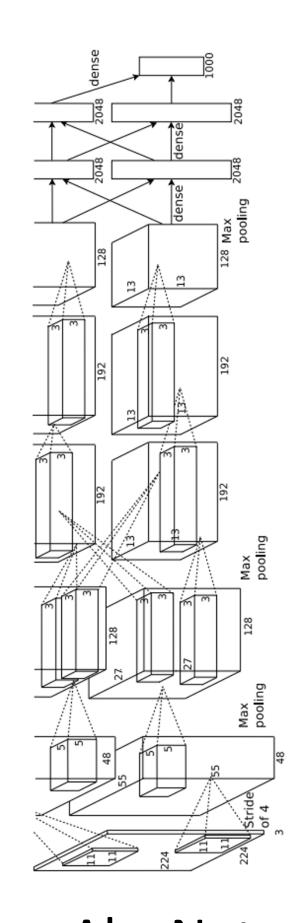




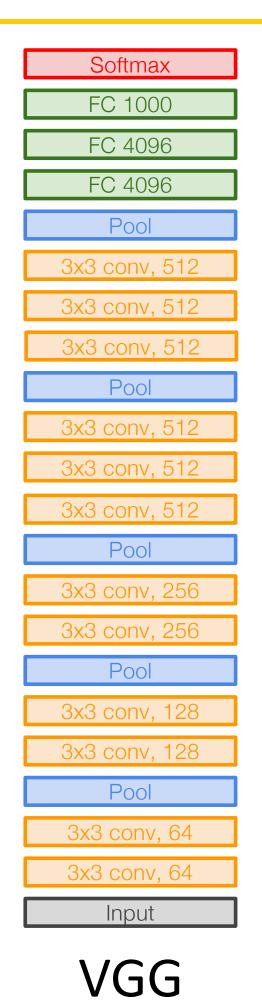


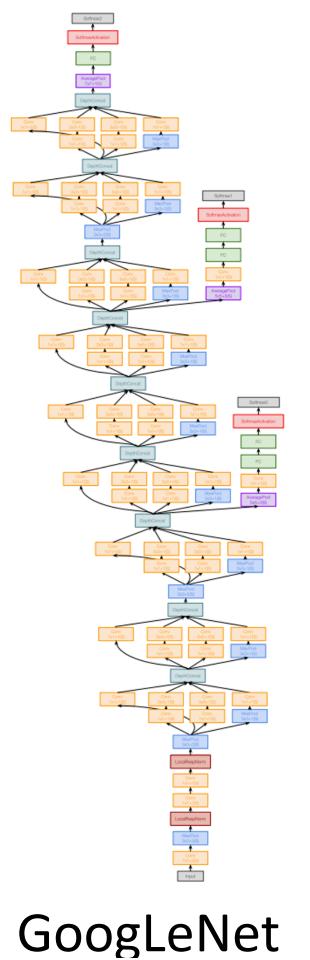


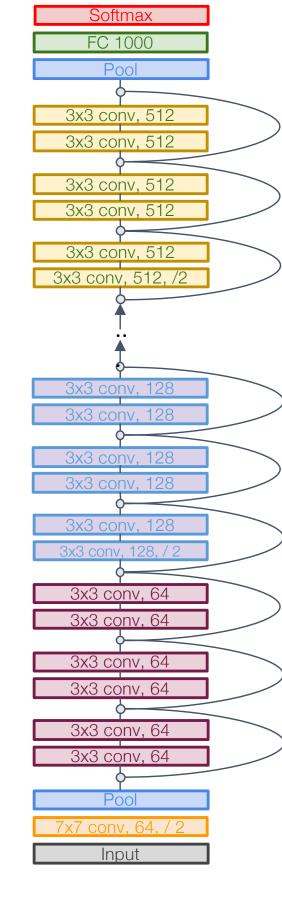
Recap



AlexNet











LeNet ResNet



Overview

1. One time setup:

Today

- Activation functions, data preprocessing, weight initialization, regularization
- 2. Training dynamics:

Next time

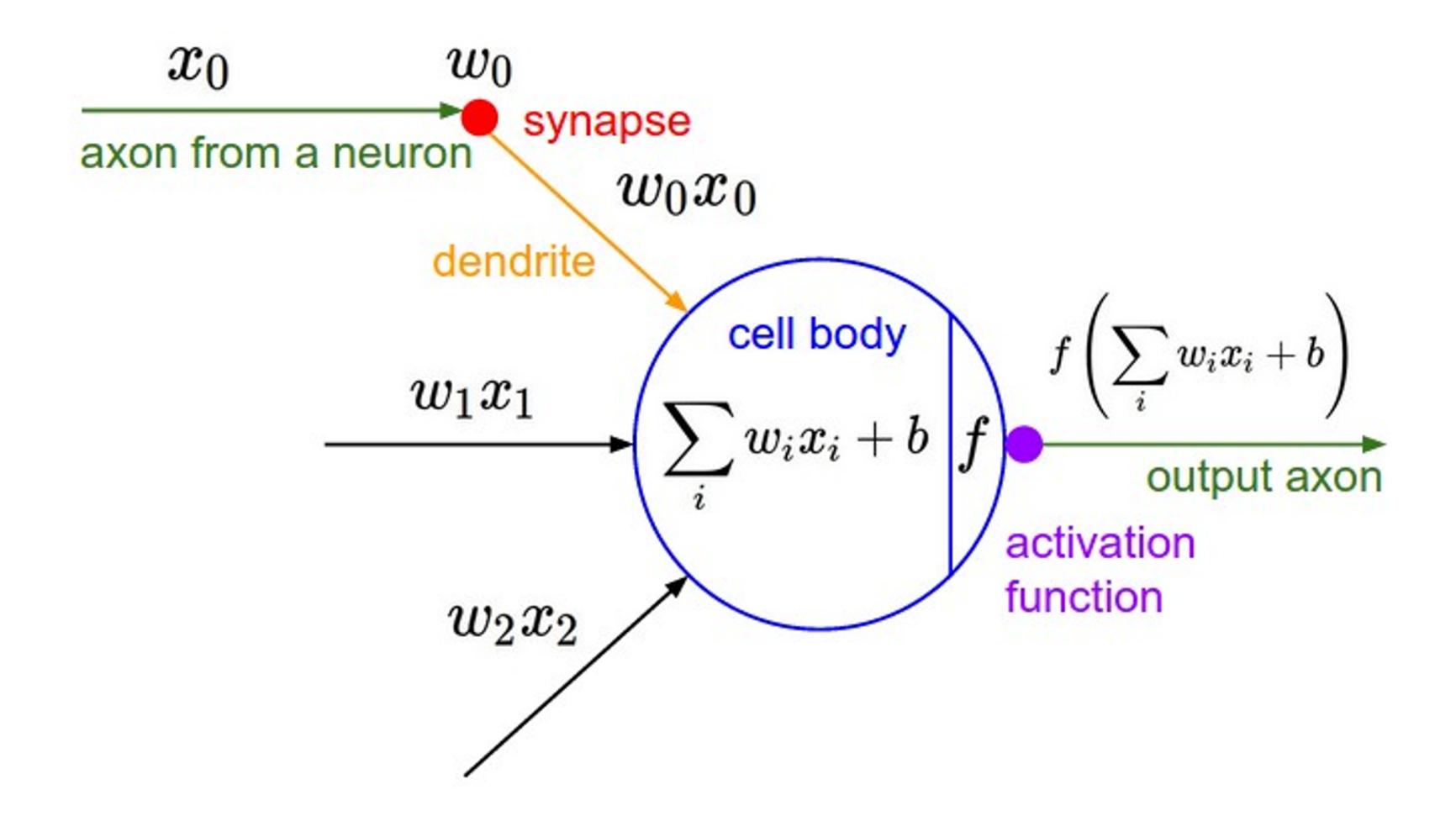
- Learning rate schedules; large-batch training; hyperparameter optimization
- 3. After training:
 - Model ensembles, transfer learning







Activation Functions





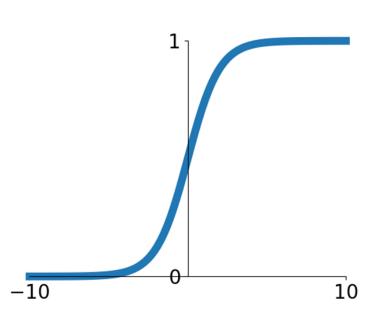




Activation Functions

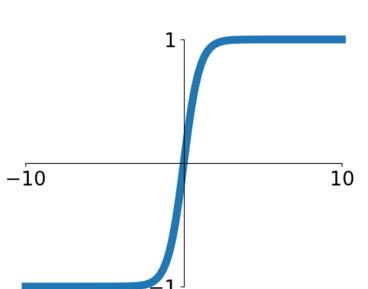
Sigmoid

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



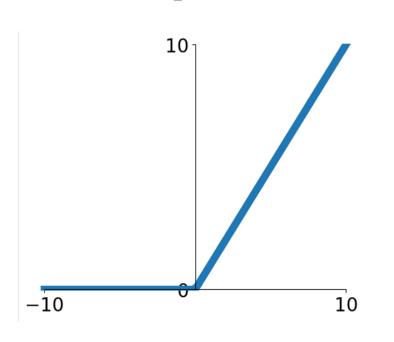
tanh

tanh(x)



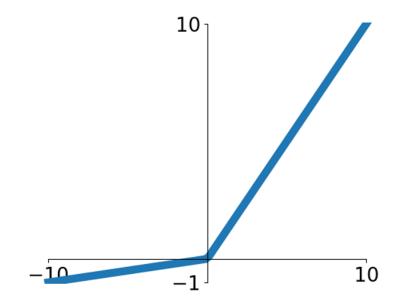
ReLU

max(0,x)



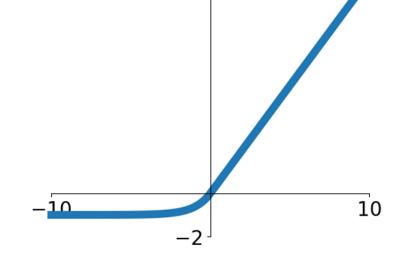
Leaky ReLU

max(0.1x, x)



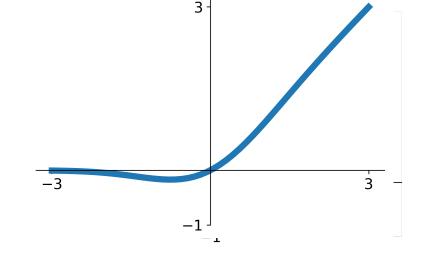
ELU

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



GELU

$$\approx x\alpha(1.702x)$$



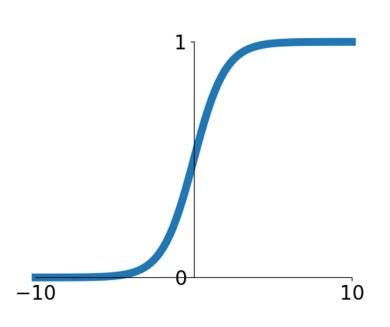






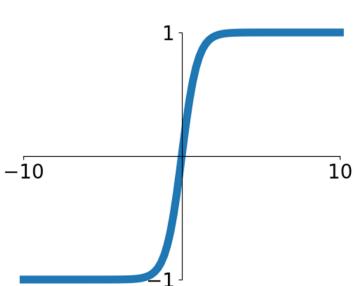
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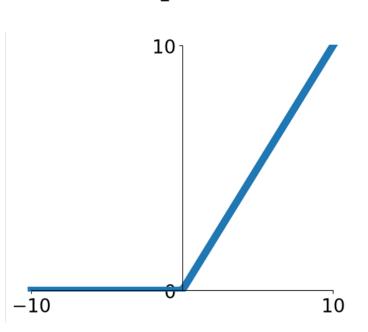
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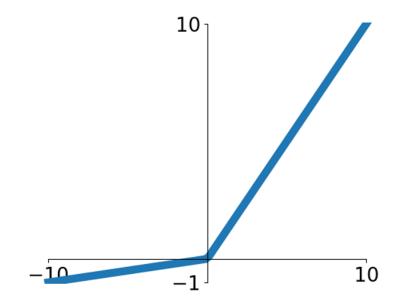
ReLU

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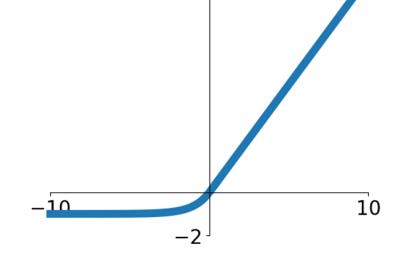
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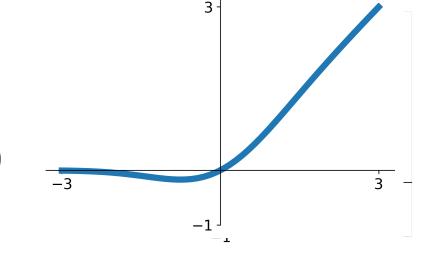
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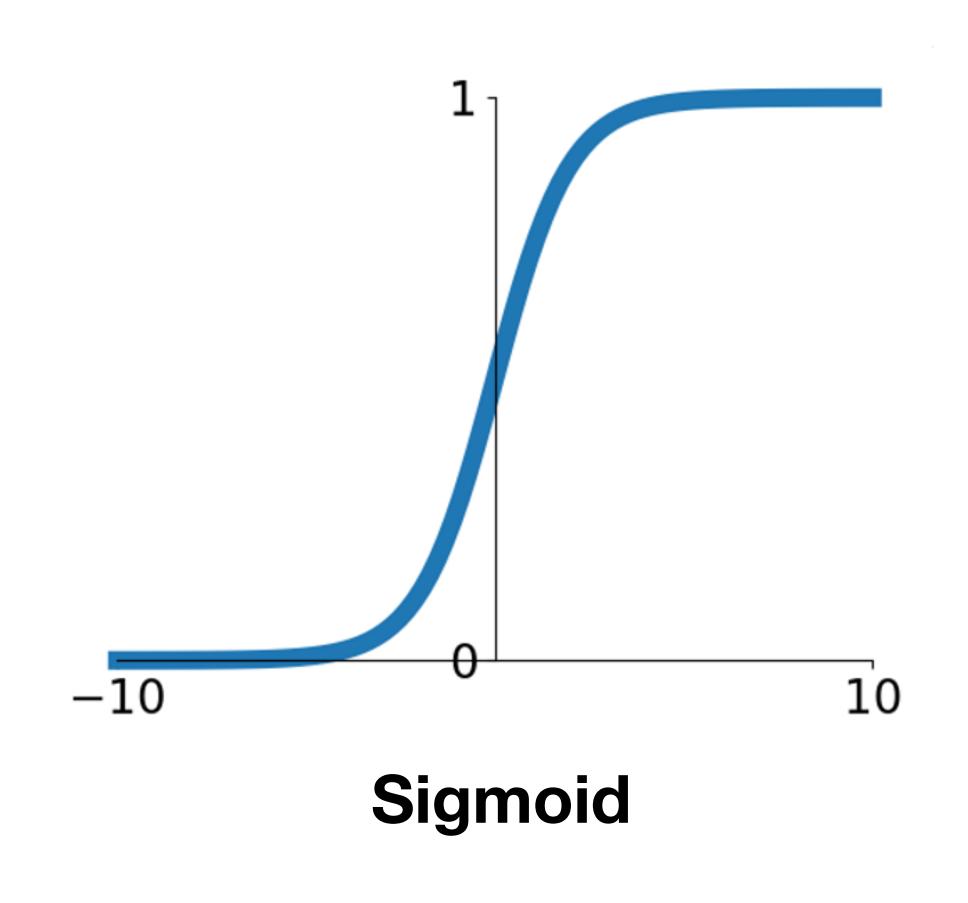
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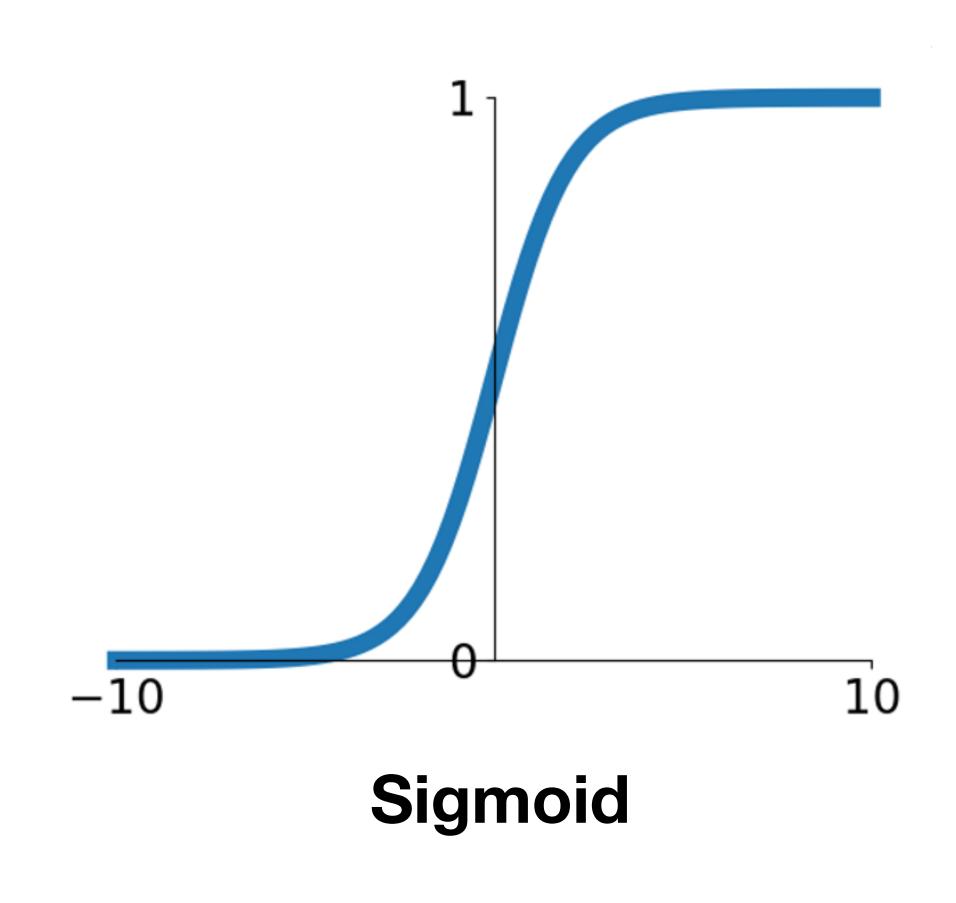
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- Squashes numbers to range [0, 1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron









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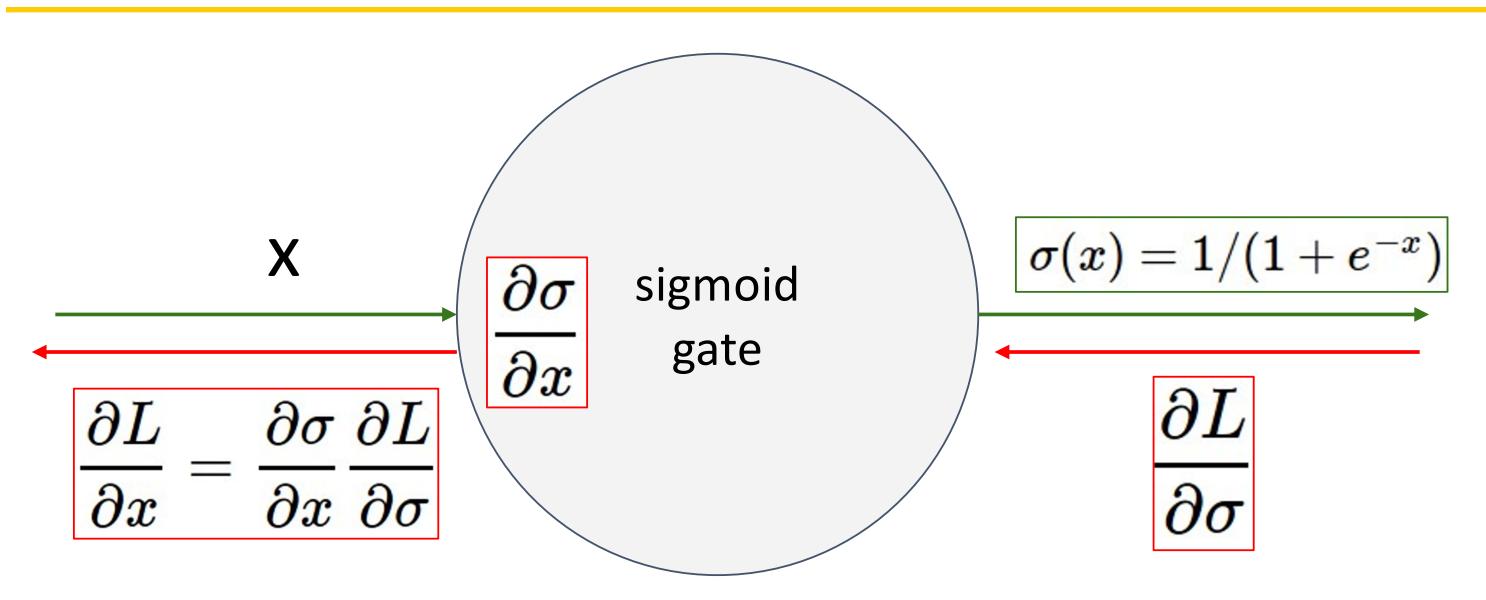
3 problems:

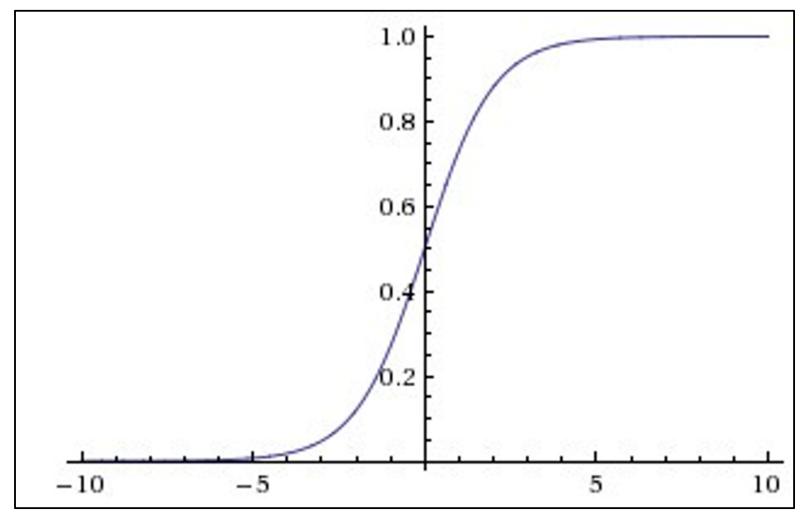
1. Saturated neurons "kill" the gradients









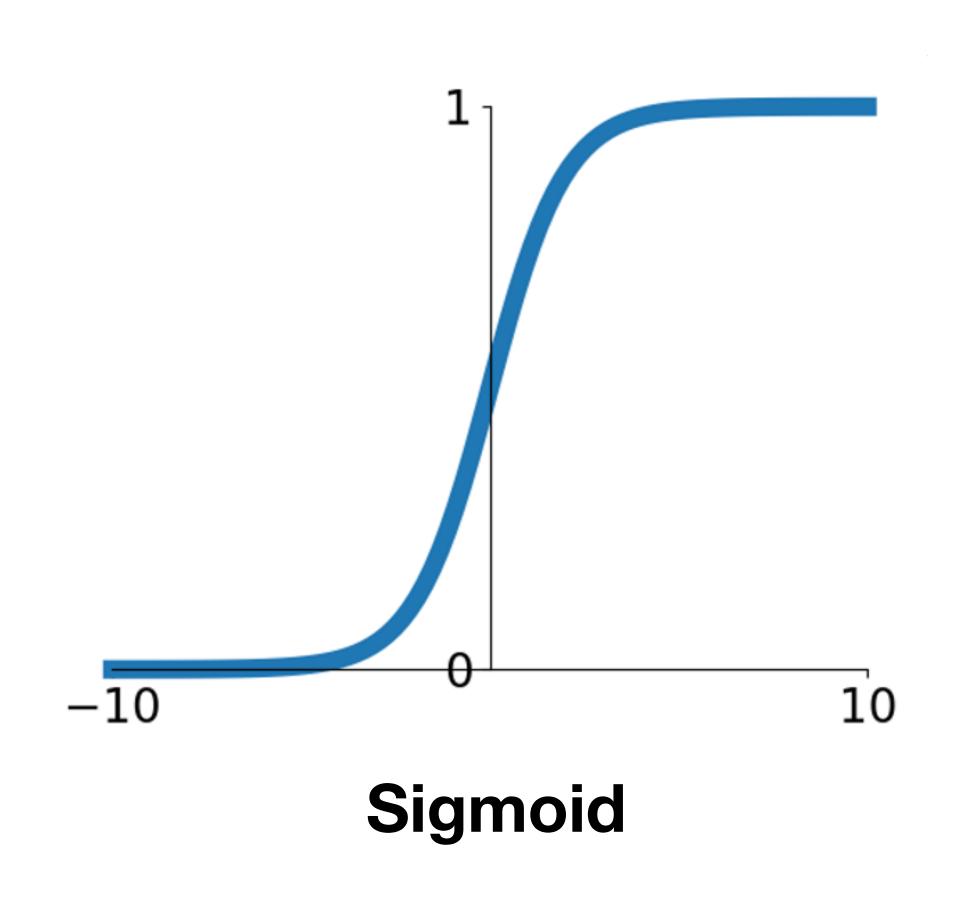


- What happens when x = -10?
- What happens when x = 0?
- What happens when x = 10?









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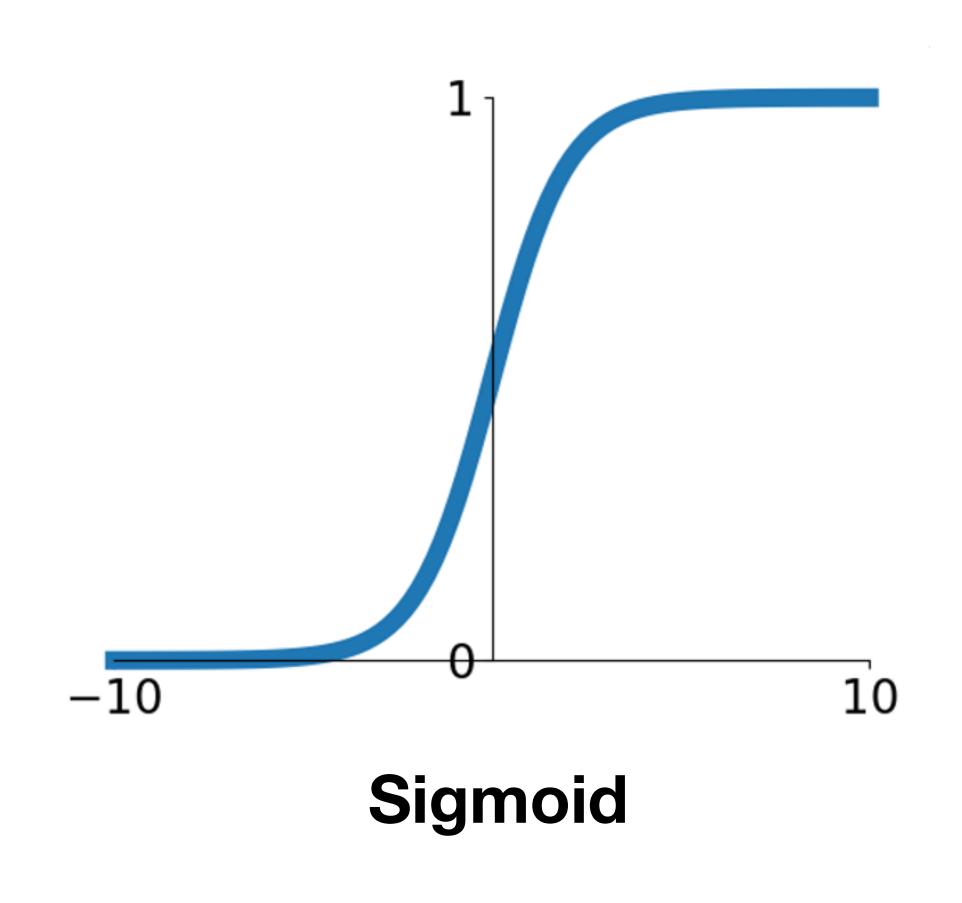
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3 problems:

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







Consider what happens when nonlinearity is always positive

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

 $h_i^{(\ell)}$ is the *i*th element of the hidden layer at layer ℓ (before activation) $w^{(\ell)}, b^{(\ell)}$ 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

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

Upstream Local gradient gradient

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







Consider what happens when nonlinearity is always positive

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



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

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







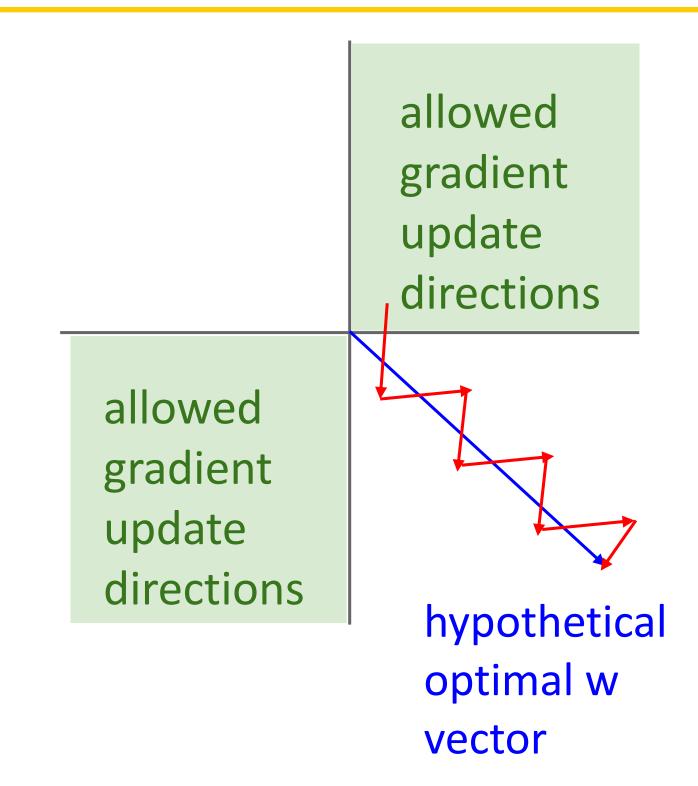
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What can we say about the gradients on $w^{(\ell)}$?

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

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

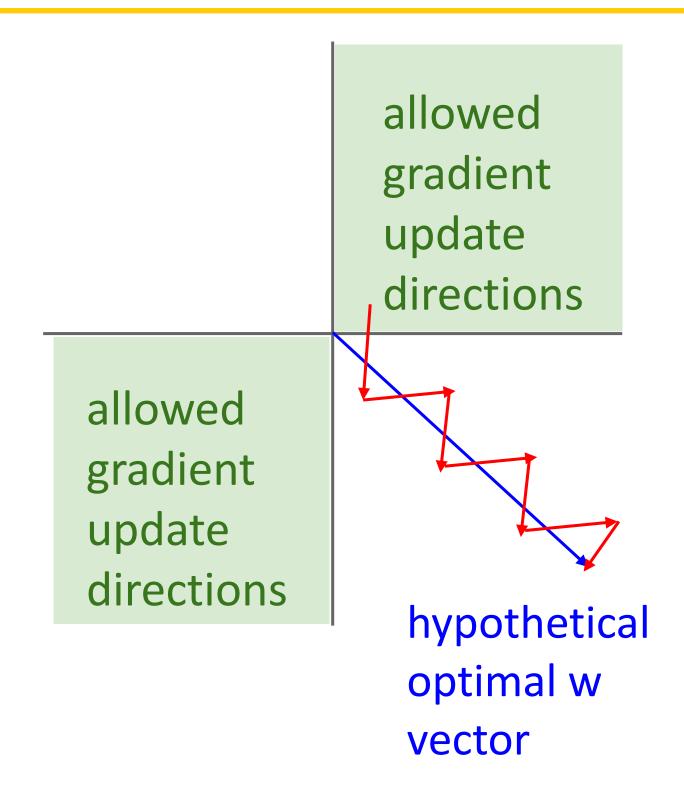
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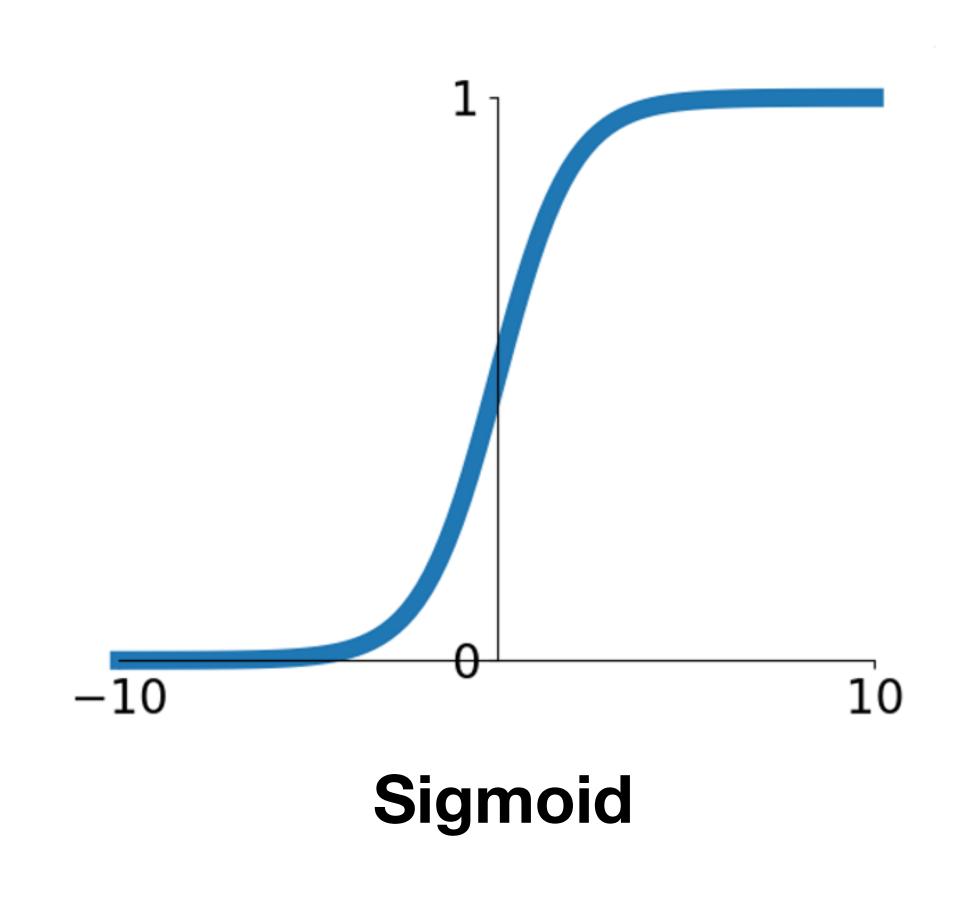




Not that bad in practice:

- Only true for a single example, mini batches help
- BatchNorm can also avoid this





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

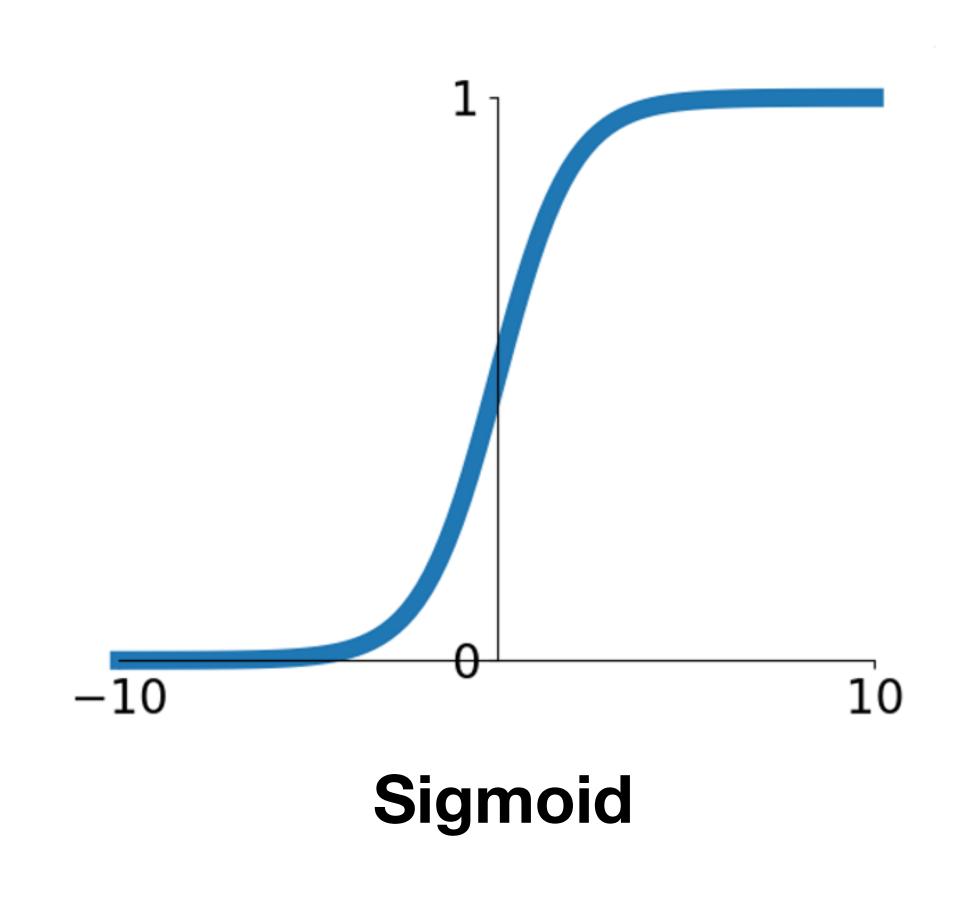
3 problems:

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









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

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

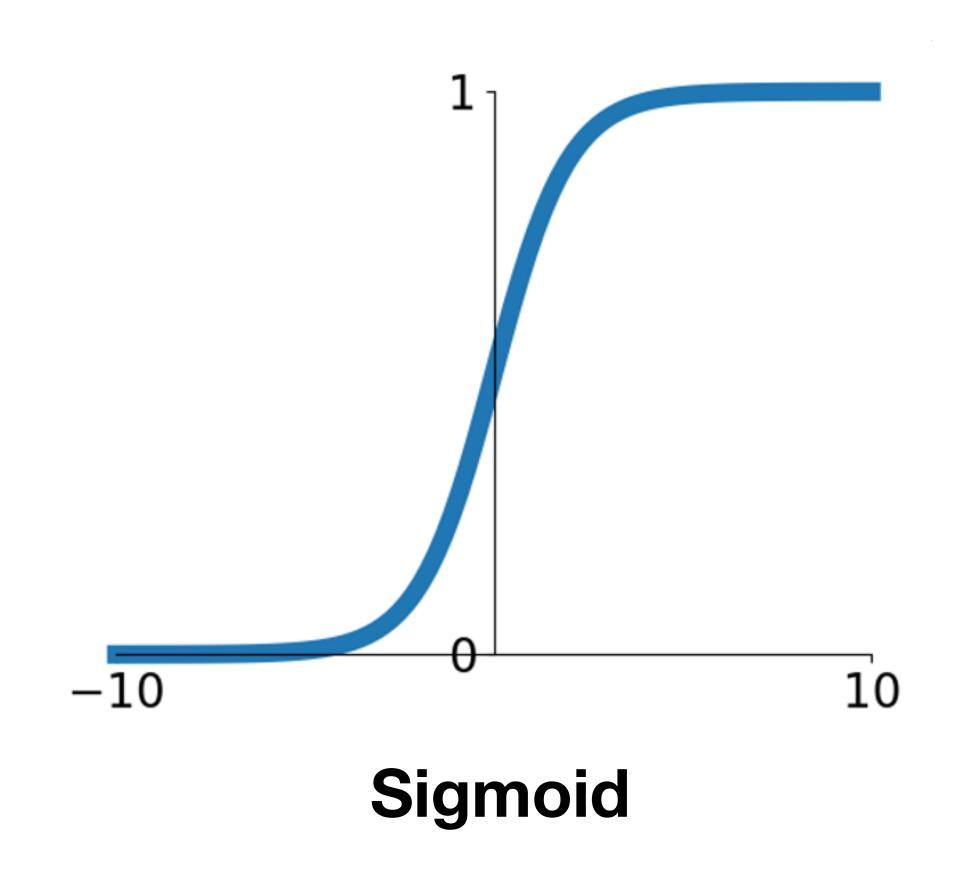
3 problems:

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









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

- 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

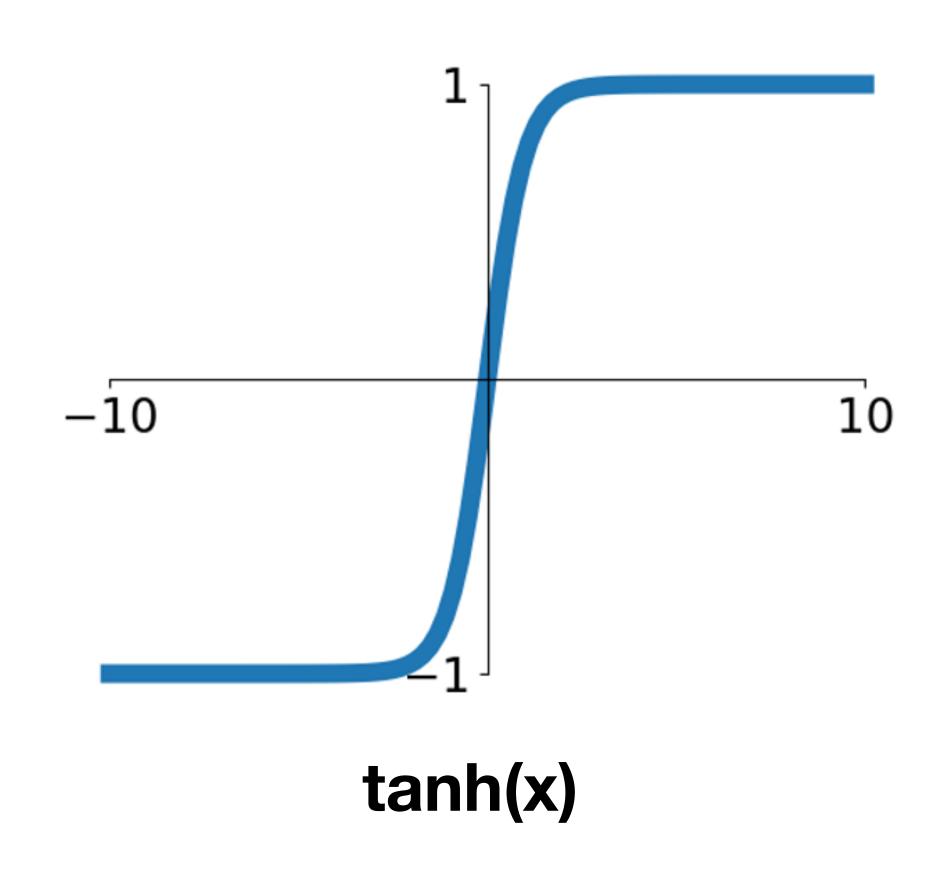
- 1. Saturated neurons "kill" the gradients
- 2. Sigmoid outputs are not zero-centered
- 3. exp() is a bit compute expensive







Activation Functions: tanh



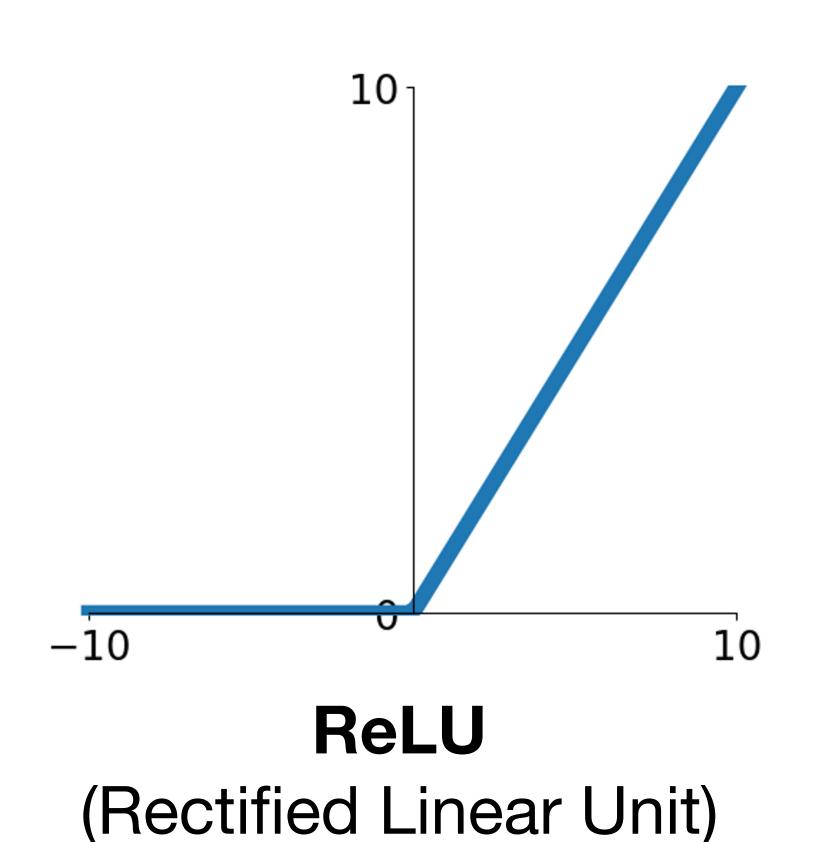
- Squashes numbers to range [-1, 1]
- Zero centered (nice)
- Still kills gradients when saturated :(







Activation Functions: ReLU



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

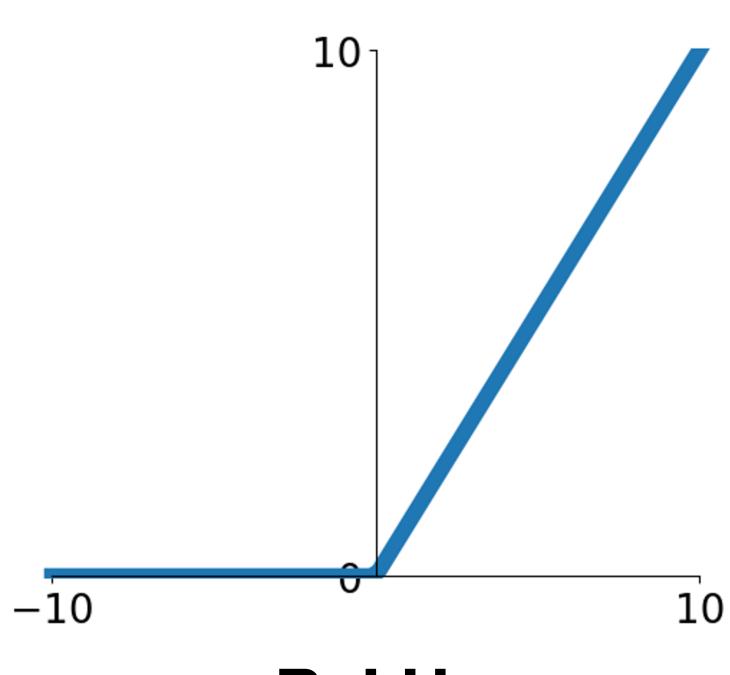
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid and tanh in practice (e.g. 6x)







Activation Functions: ReLU



ReLU
(Rectified Linear Unit)

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

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

- Not zero-centered output
- An annoyance:

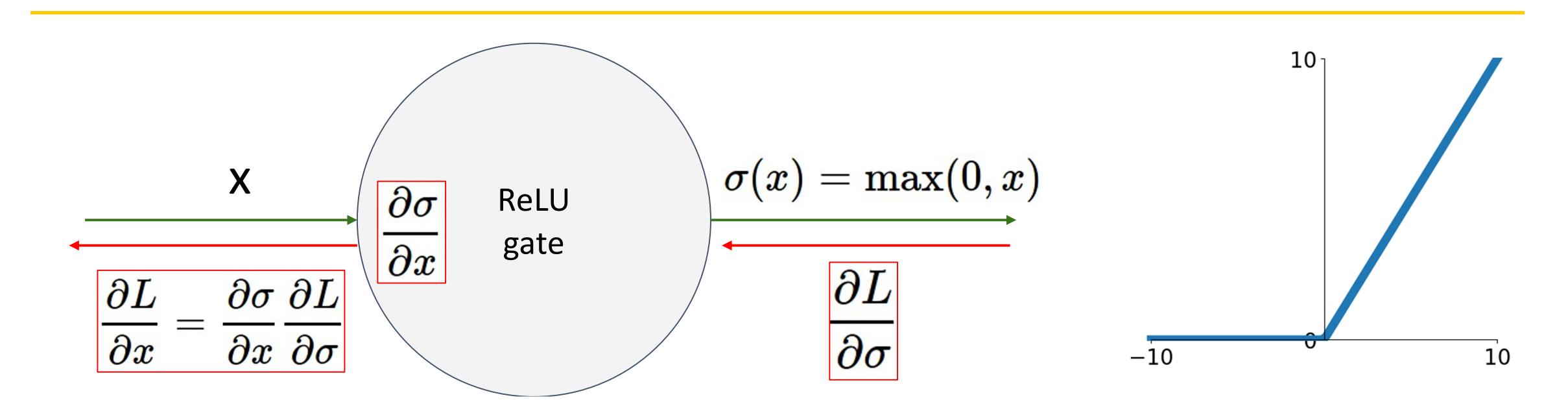
Hint: what is the gradient when x<0?







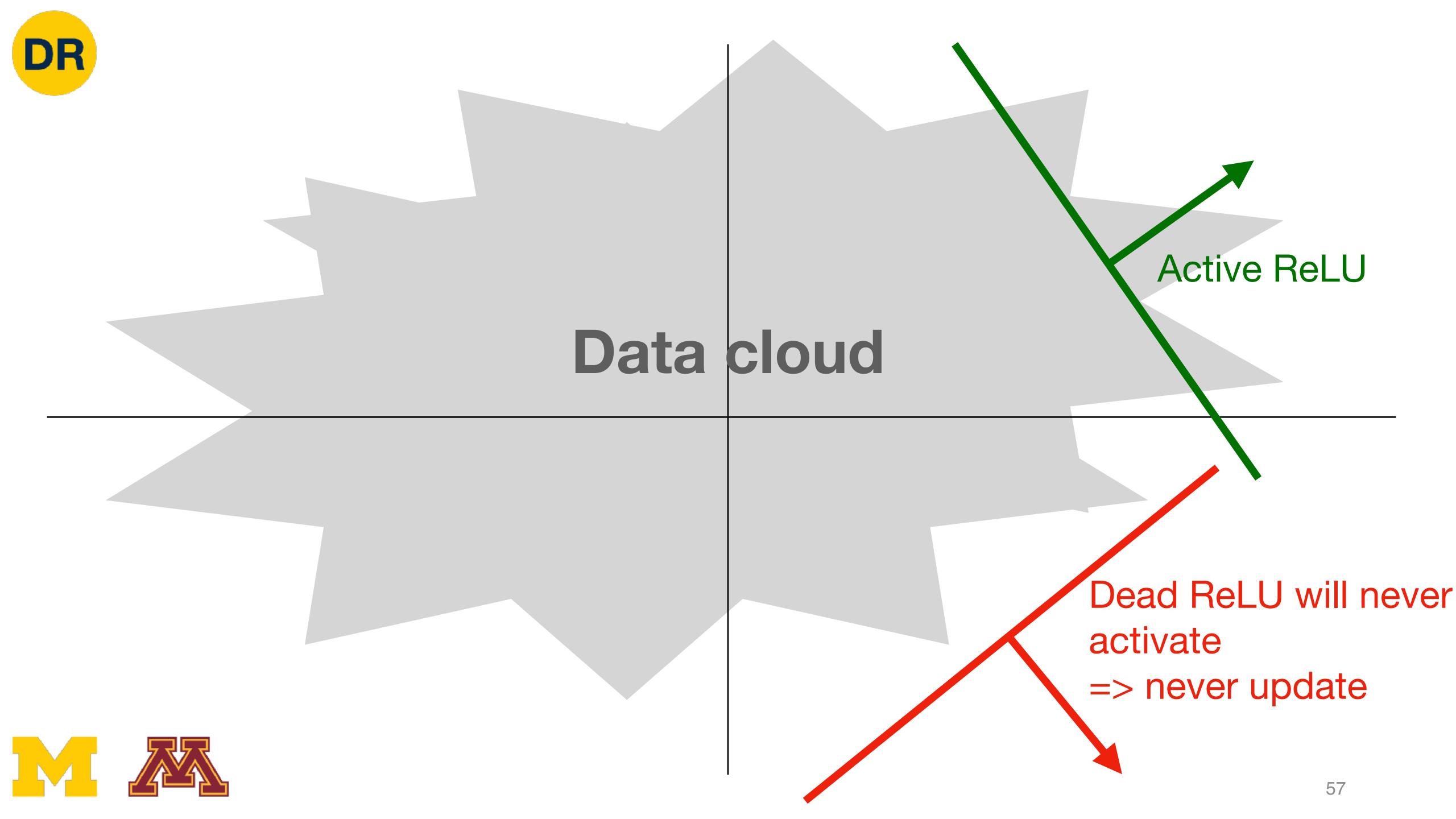
Activation Functions: ReLU

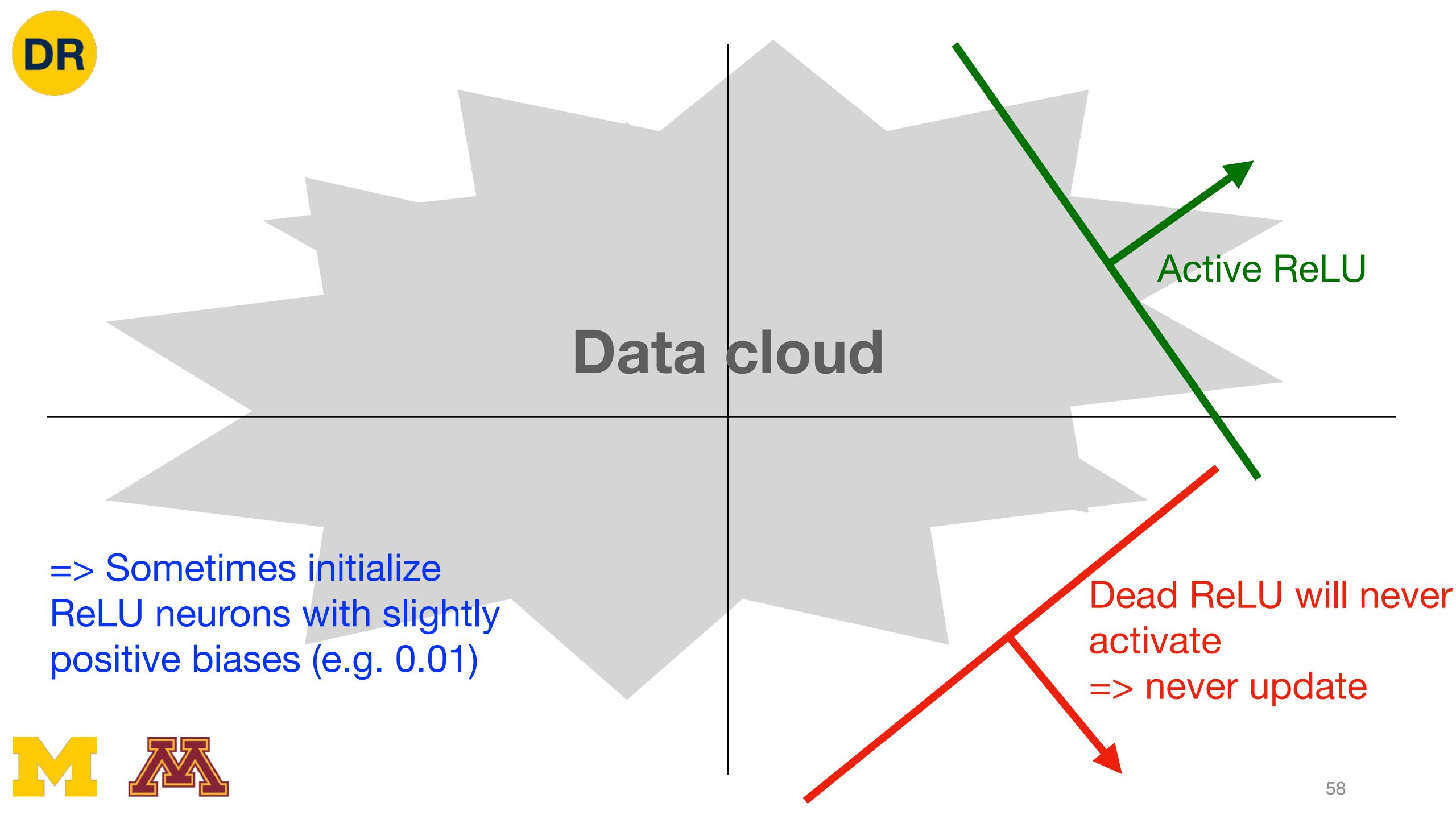


- What happens when x = -10?
- What happens when x = 0?
- What happens when x = 10?



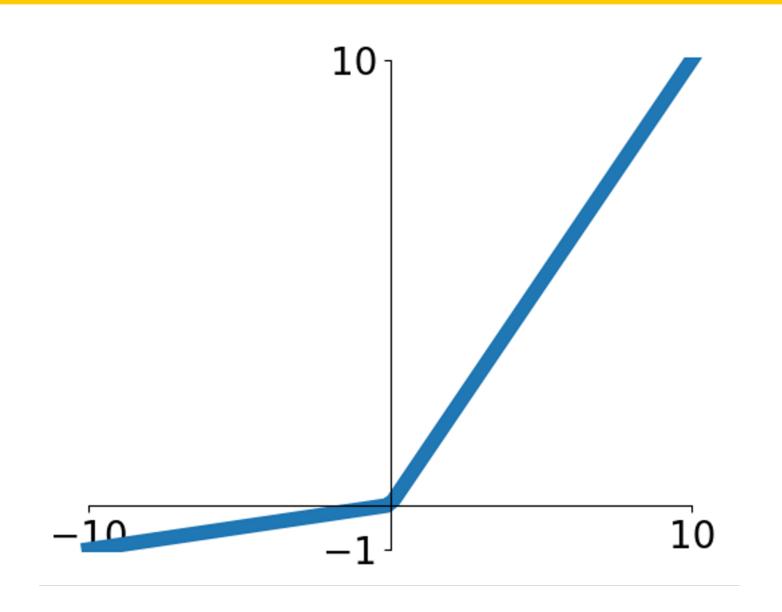








Activation Functions: Leaky ReLU



Leaky ReLU

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

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

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

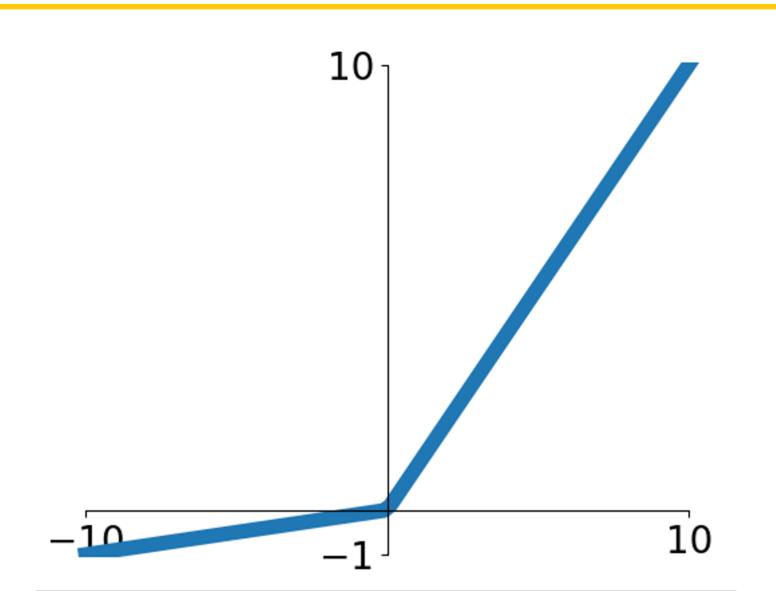




- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid and tanh in practice (e.g. 6x)
- Will not "die"



Activation Functions: Leaky ReLU



Leaky ReLU

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

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

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



- Computationally efficient
- Converges much faster than sigmoid and tanh in practice (e.g. 6x)
- Will not "die"

Parametric ReLU (PReLU)

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

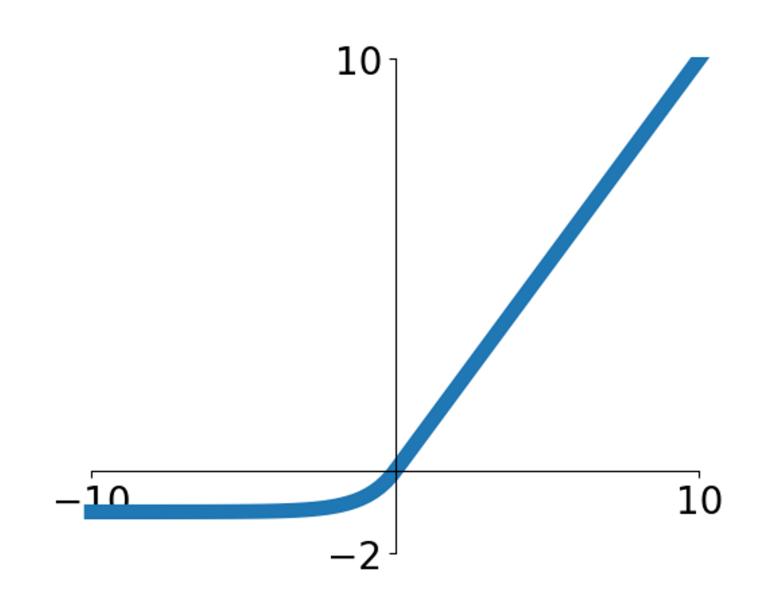
 α is learned via backprop

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





Activation Functions: Exponential Linear Unit (ELU)



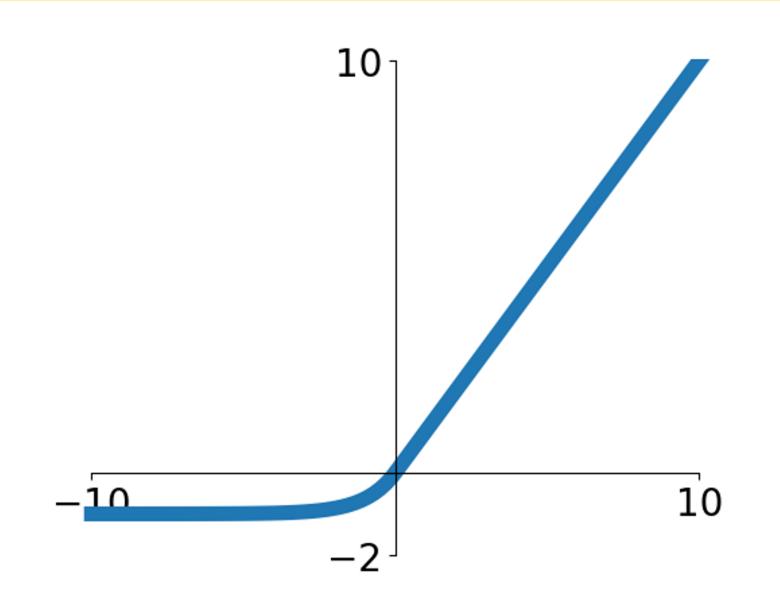
$$f(x) = \begin{cases} x & \text{if } x > 0\\ \alpha(e^x - 1) & \text{if } x \le 0 \end{cases}$$
(Default $\alpha = 1$)

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





Activation Functions: Exponential Linear Unit (ELU)



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

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

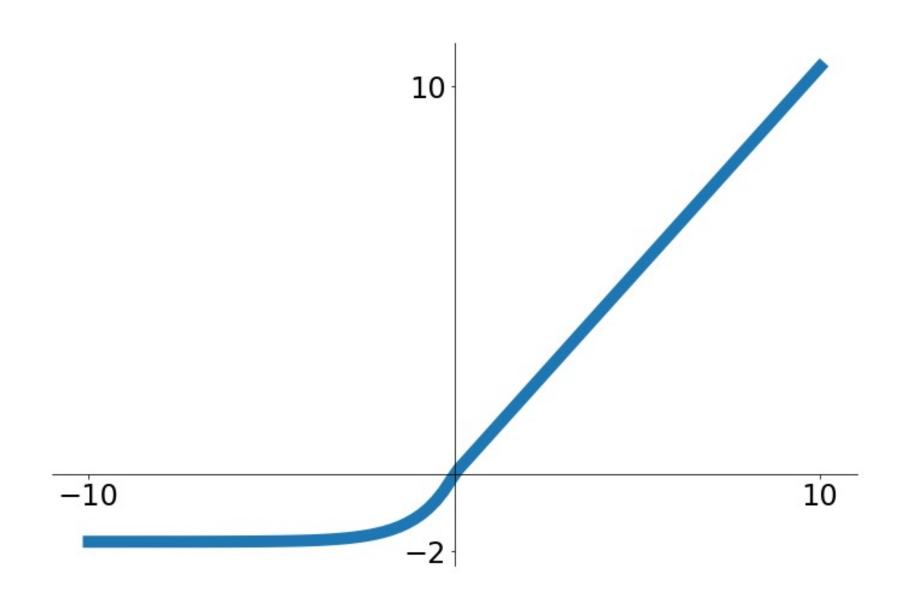
- Computation requires exp()







Activation Functions: Scale Exponential Linear Unit (SELU)



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

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

 $\alpha = 1.6732632423543772848170429916717$

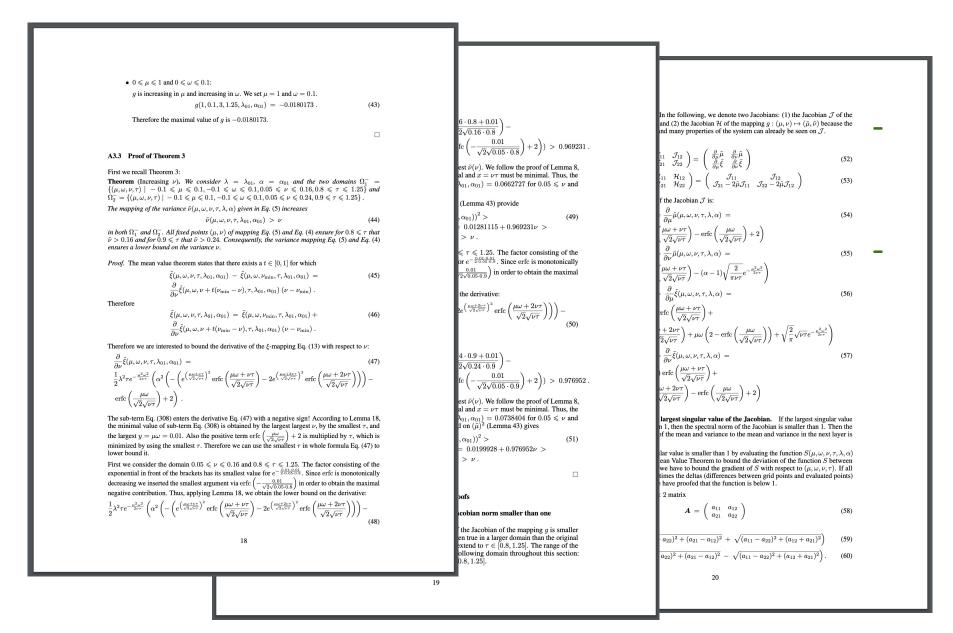
 $\lambda = 1.0507009873554804934193349852946$







Activation Functions: Scale Exponential Linear Unit (SELU)



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

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

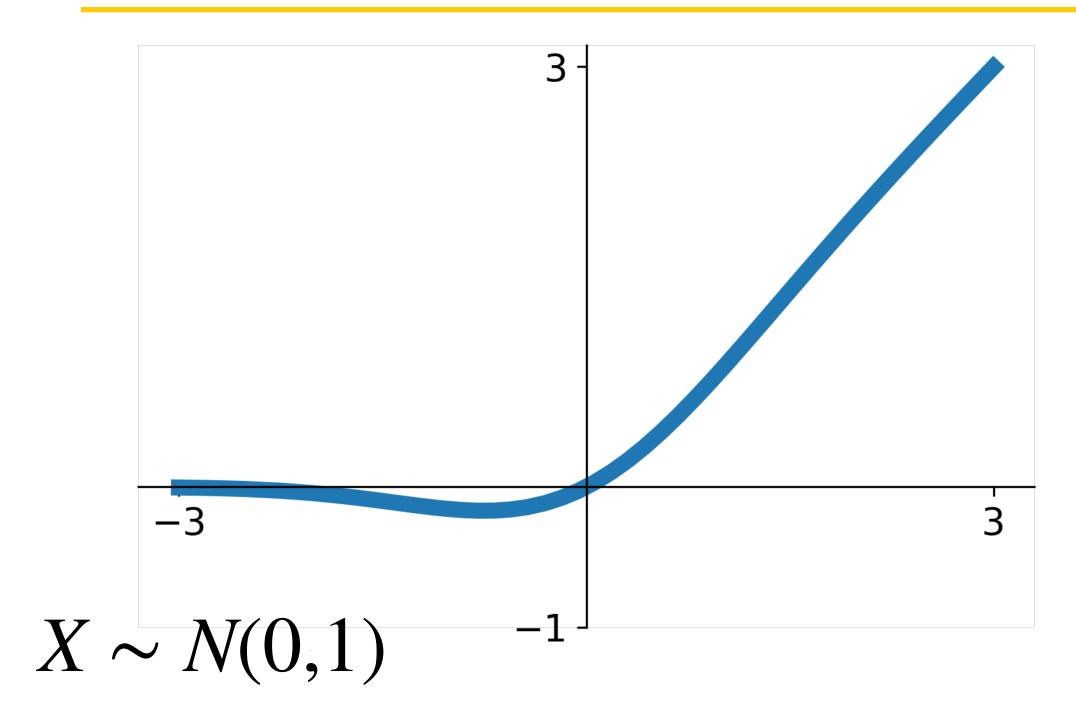
- Derivation takes 91 pages of math in appendix...

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





Activation Functions: Gaussian Error Linear Unit (GELU)



$$gelu(x) = xP(X \le x) = \frac{x}{2}(1 + erf(x/\sqrt{2}))$$
$$\approx x\sigma(1.702x)$$

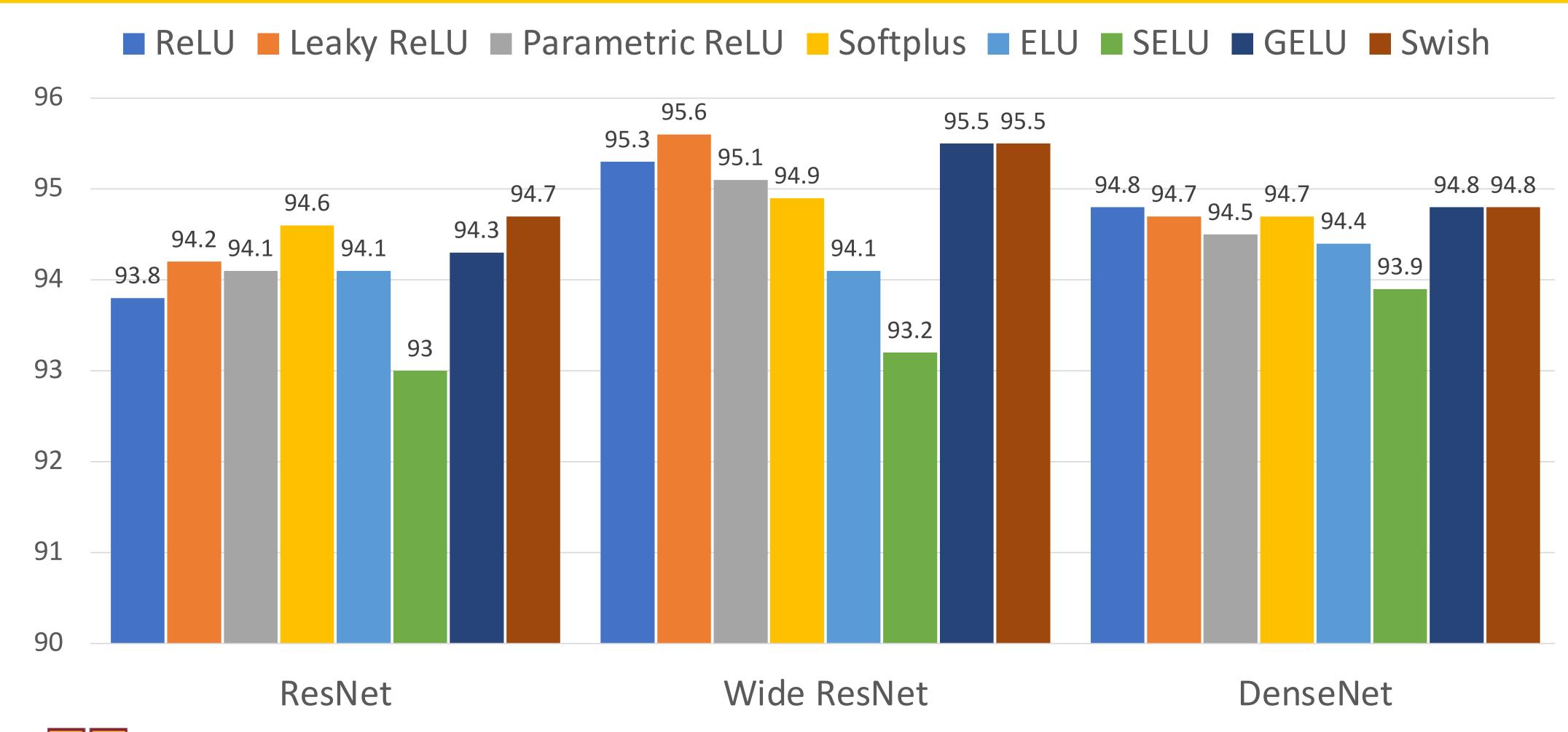
- Idea: Multiply input by 0 or 1 at random; large values more likely to be multiplied by 1, small values more likely to be multiplied by 0 (datadependent dropout)
- Take expectation over randomness
- Very common in Transformers (BERT, GPT, ViT)







Accuracy on CIFAR10









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



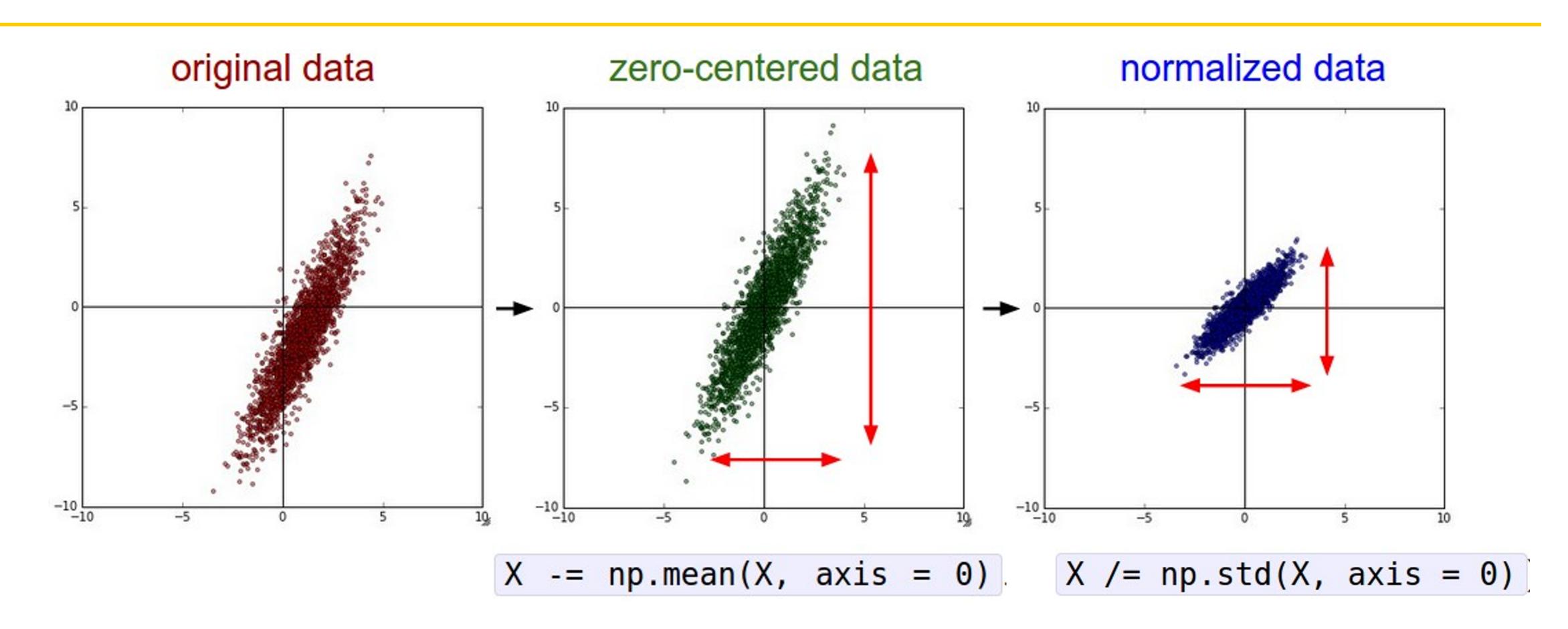












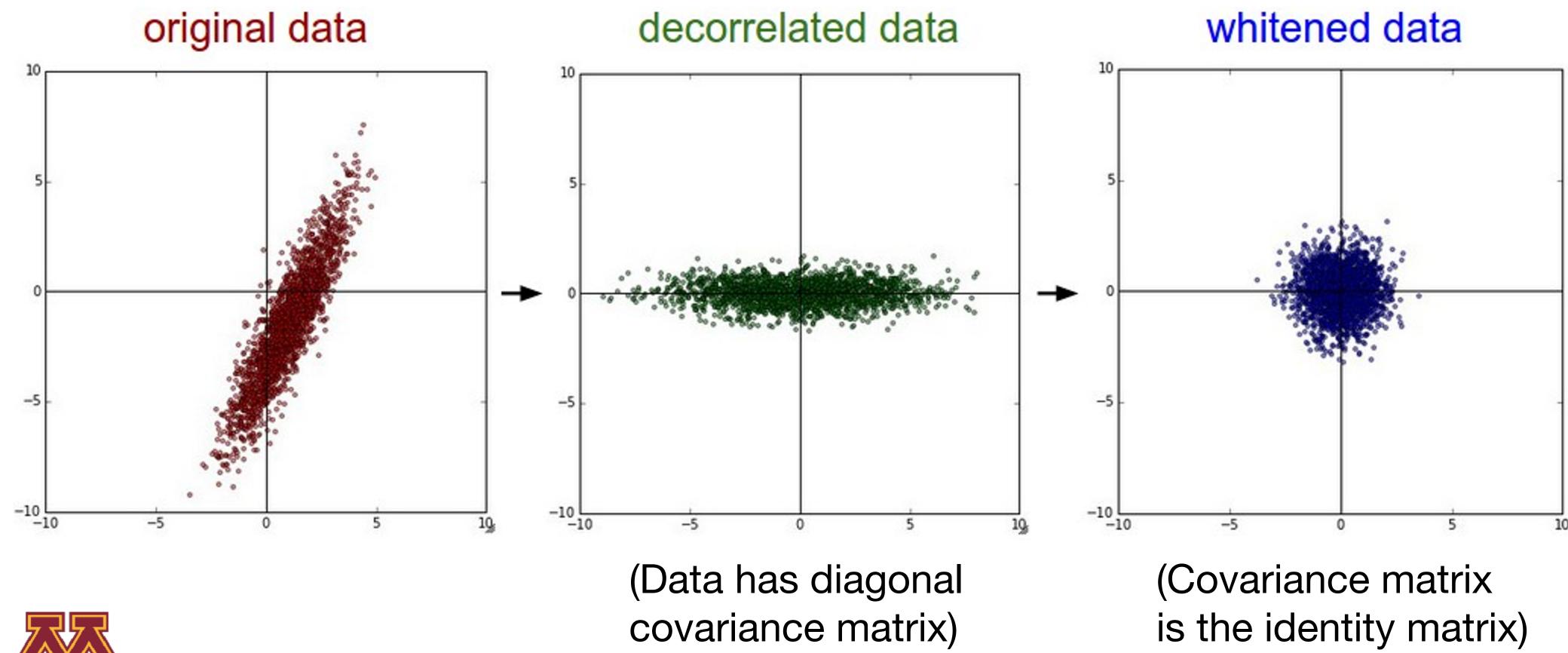
(Assume X[NxD] is data matrix, each example in a row)







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



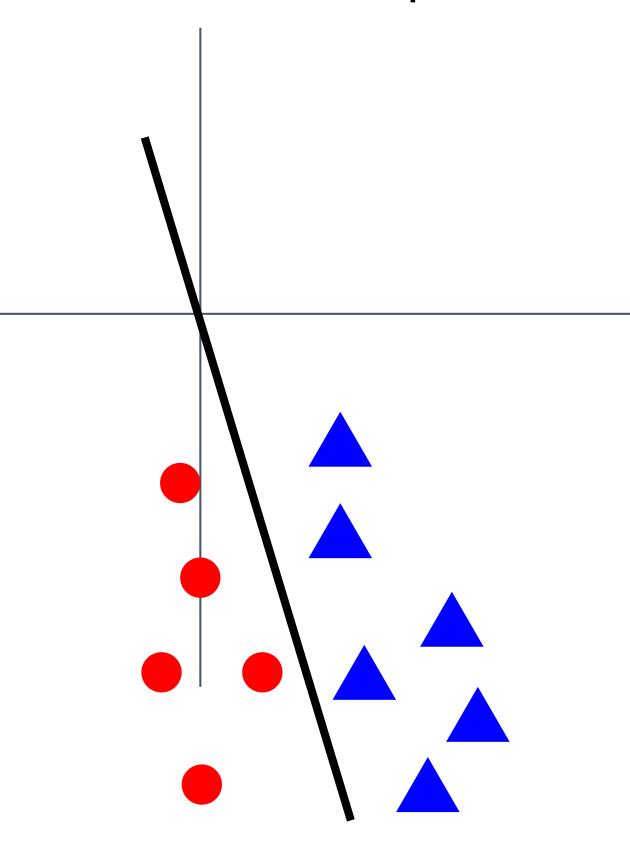


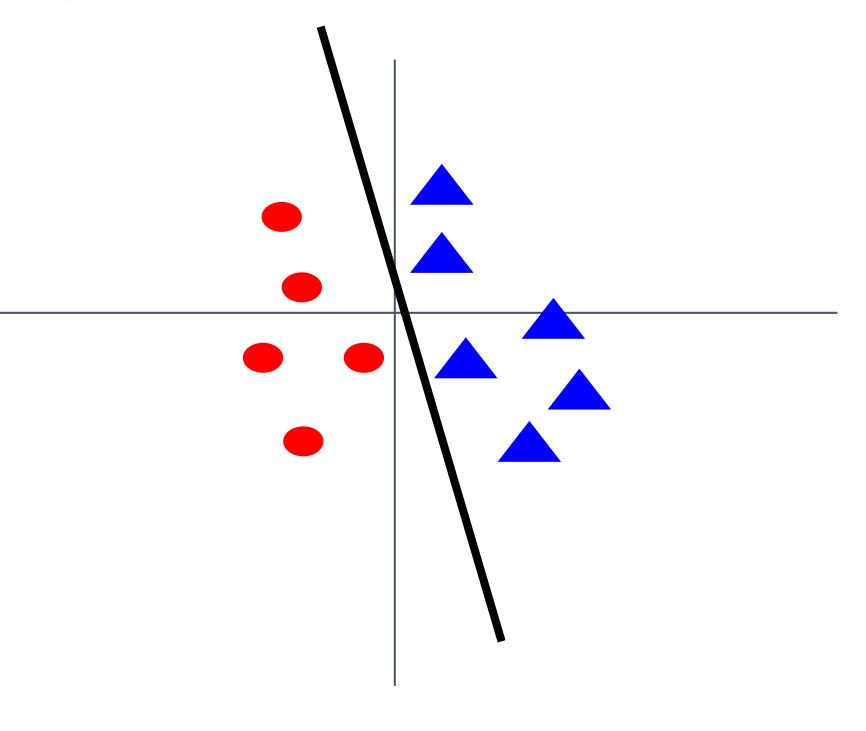




Before normalization: Classification loss very sensitive to changes in weight matrix; hard to optimize

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 perchannel std (e.g. ResNet)
 (mean along each channel = 3 numbers)

Not common to do PCA or whitening



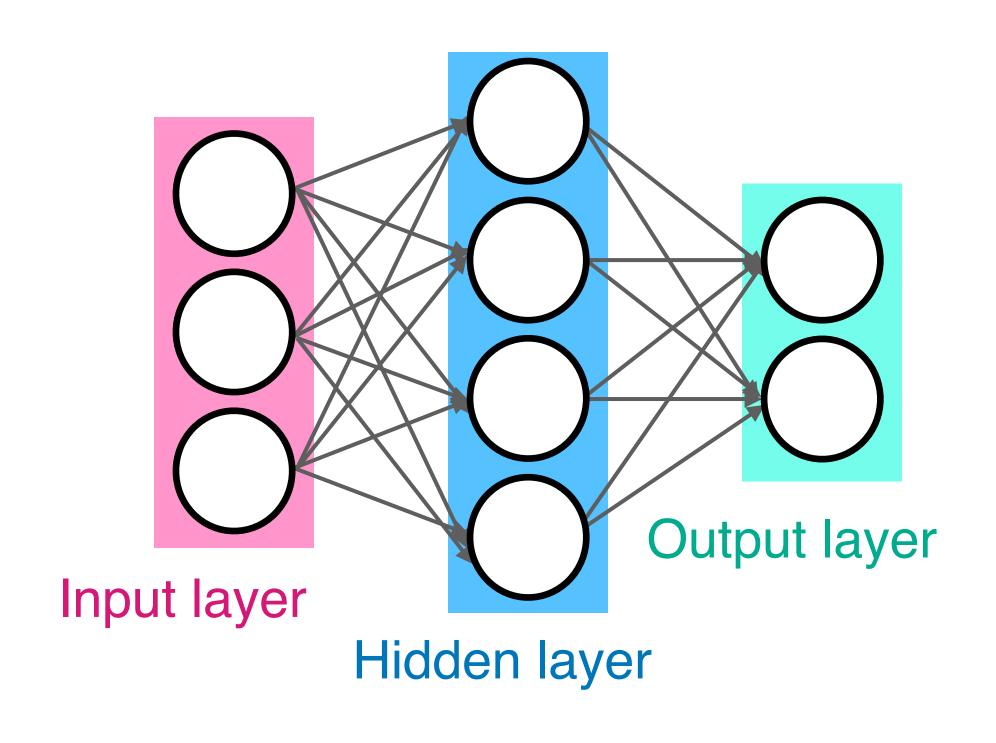












Q: What happens if we initialize all W=0, b=0?

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







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

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







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.







```
dims = [4096] * 7 Forward pass for a 6-layer
                   net with hidden size 4096
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)
```



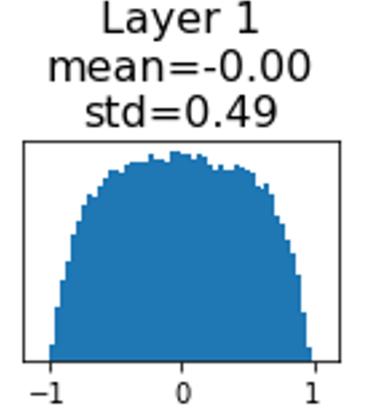


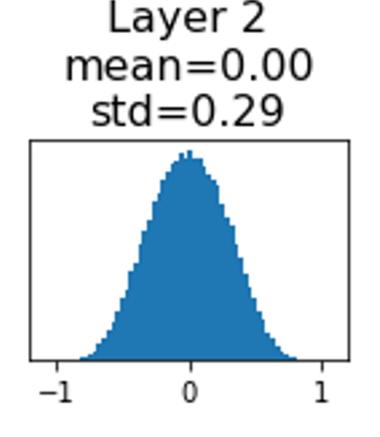


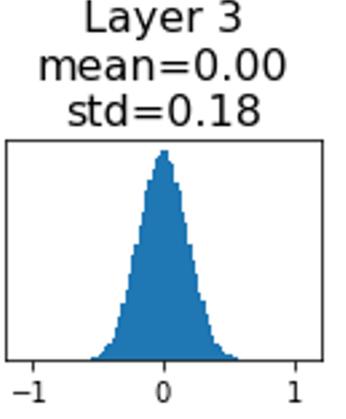
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dims = [4096] * 7 Forward pass for a 6-layer
hs = [] net with hidden size 4096
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

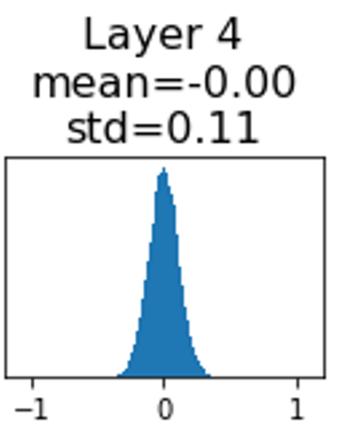
All activations tend to zero for deeper network layers

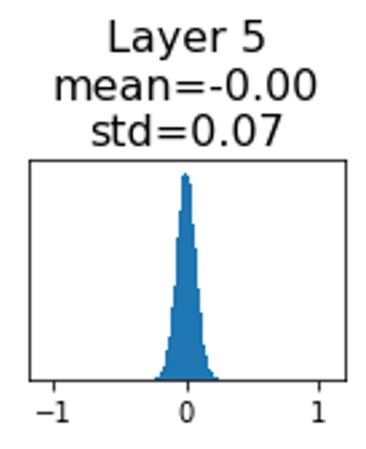
Q: What do the gradients dL/dW look like?

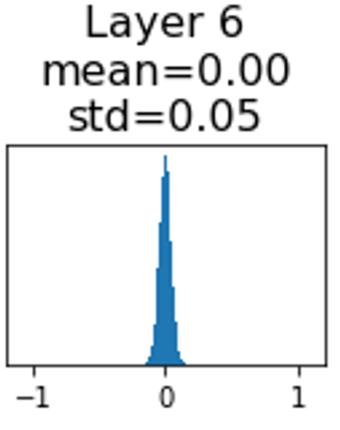
















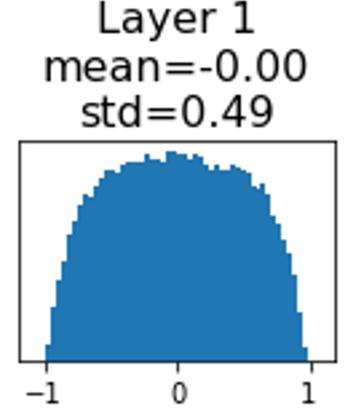


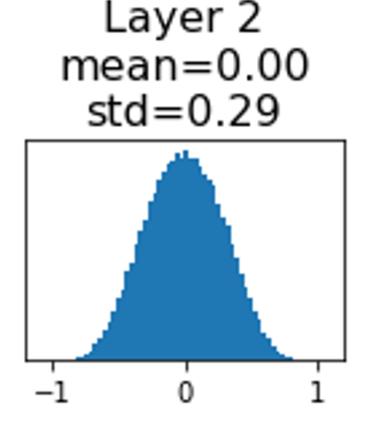
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    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

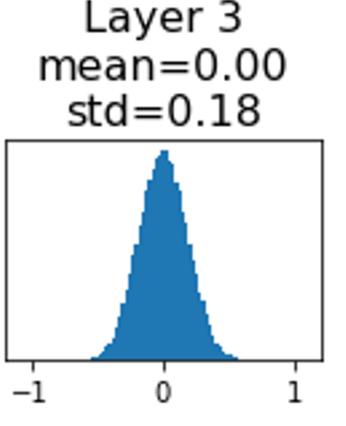
All activations tend to zero for deeper network layers

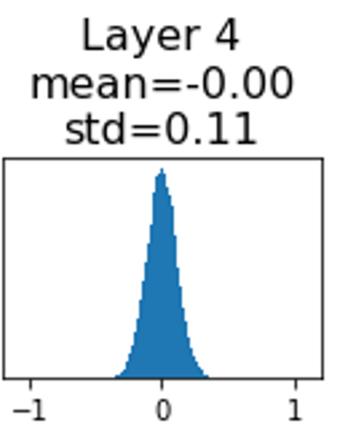
Q: What do the gradients dL/dW look like?

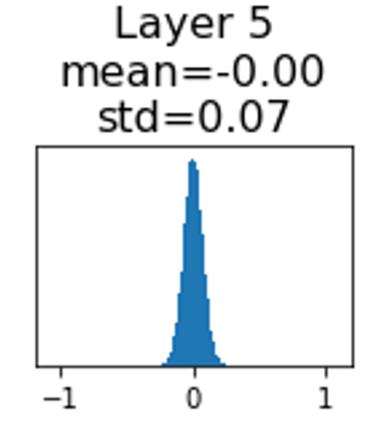
A: All zero, no learning:(

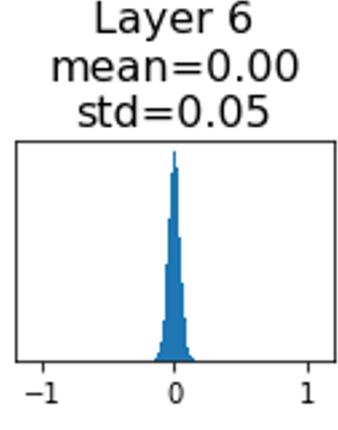












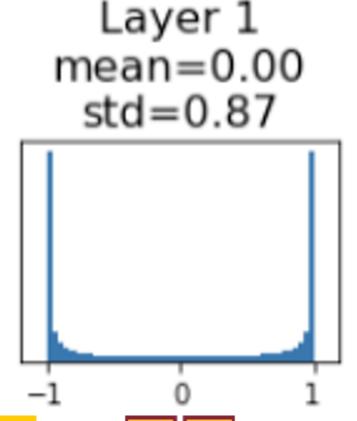


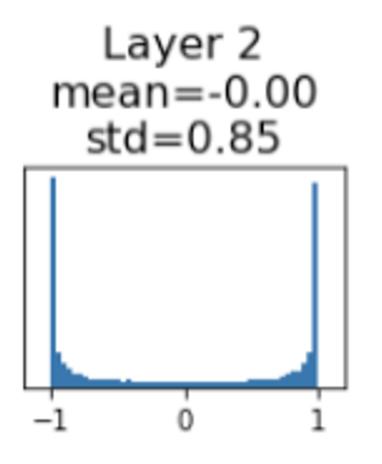


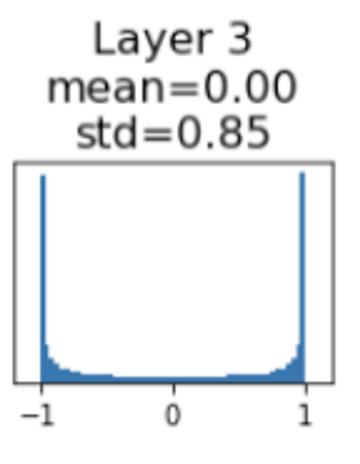


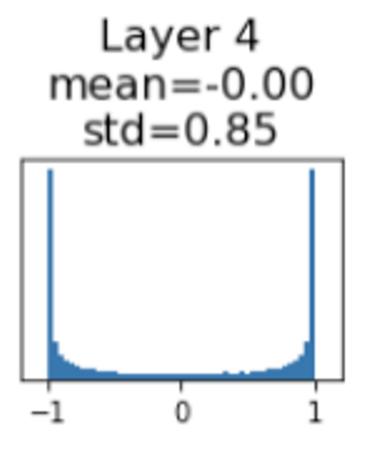
All activations saturate

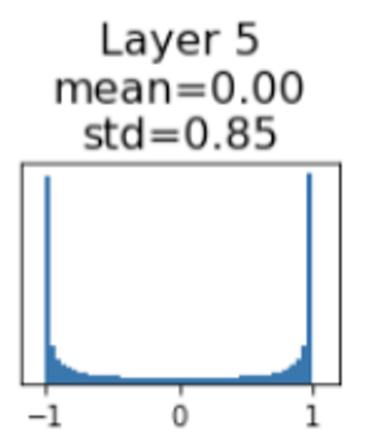
Q: What do the gradients look like?

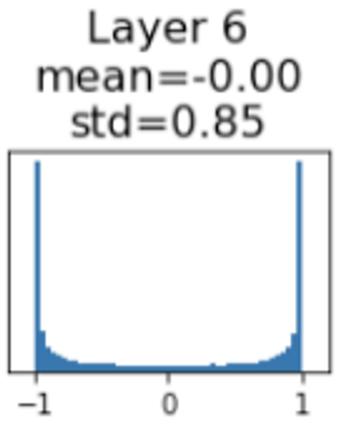














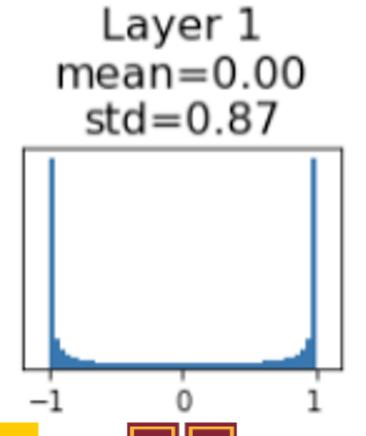


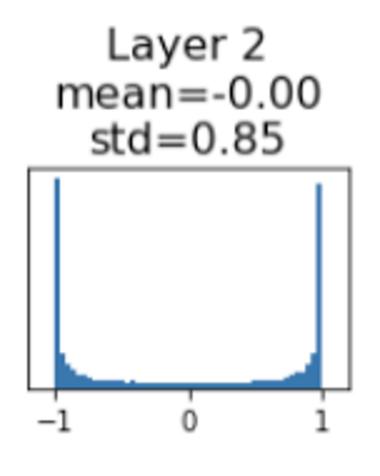


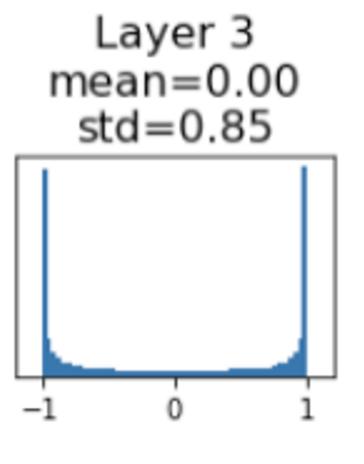
All activations saturate

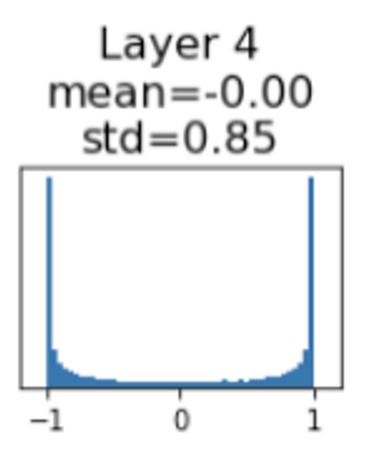
Q: What do the gradients look like?

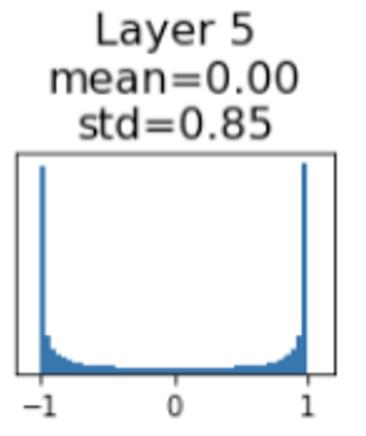
A: Local gradients all zero, no learning:

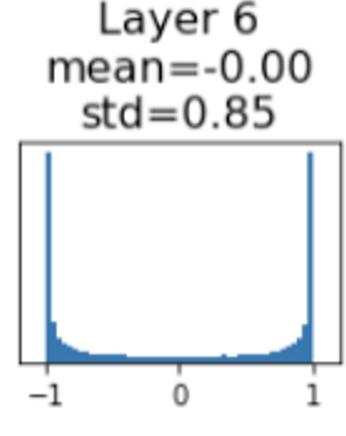


















Weight initialization: Xavier Initialization

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

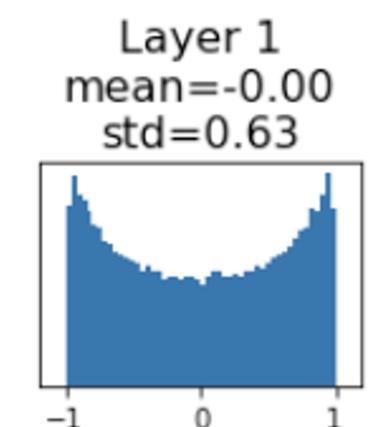


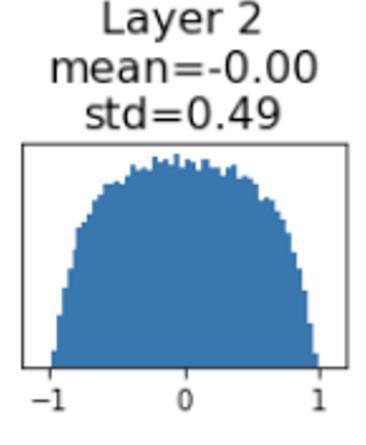


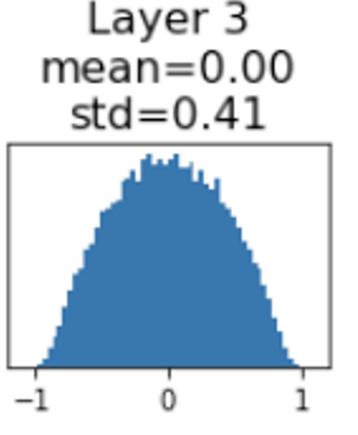


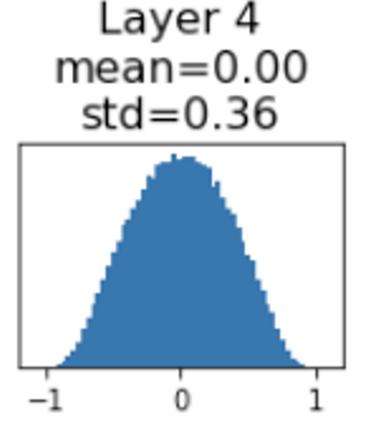
Weight initialization: Xavier Initialization

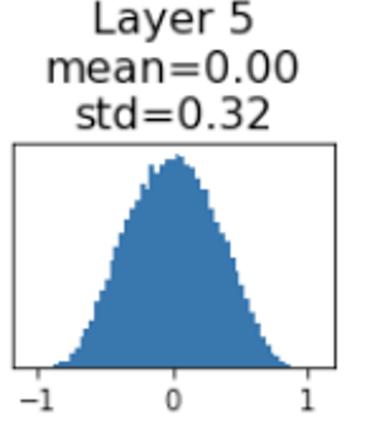
"Just right": Activations are nicely scaled for all layers!

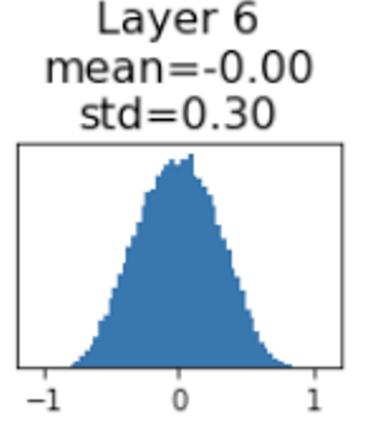














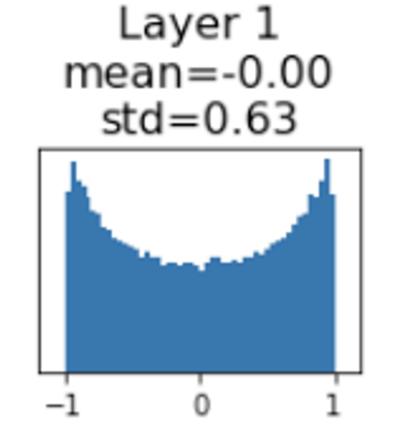


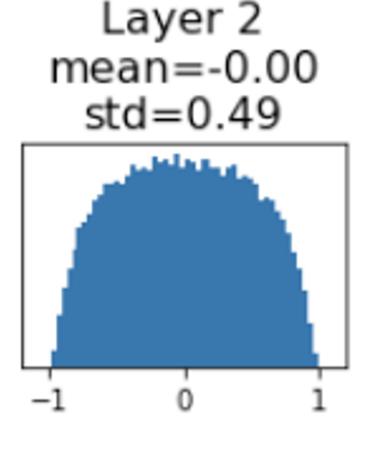


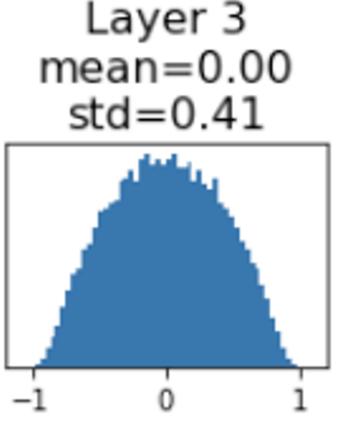
Weight initialization: Xavier Initialization

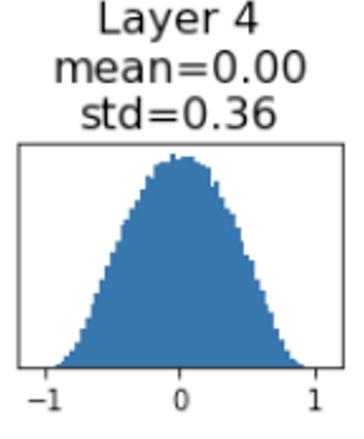
"Just right": Activations are nicely scaled for all layers!

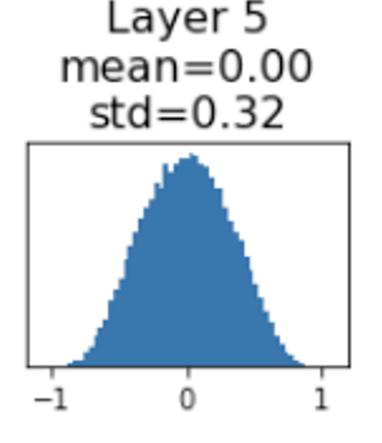
For conv layers, Din is kernel_size² x input_channels

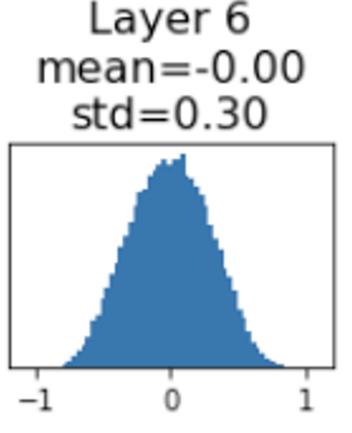


















Weight initialization: What about ReLU?

```
dims = [4096] * 7
                     Change from tanh to ReLU
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)
```

Xavier assumes zero centered activation function





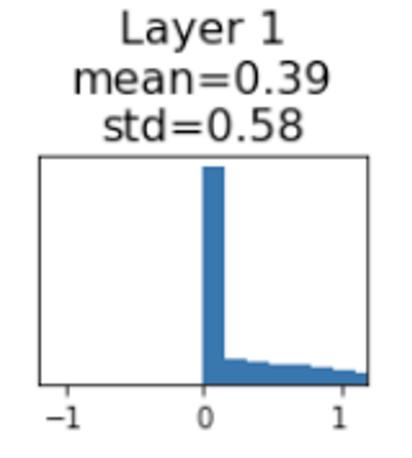


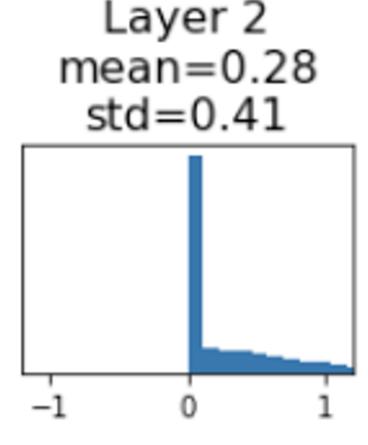
Weight initialization: What about ReLU?

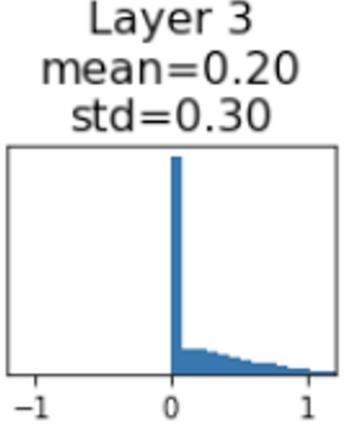
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dims = [4096] * 7
                     Change from tanh to ReLU
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x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x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

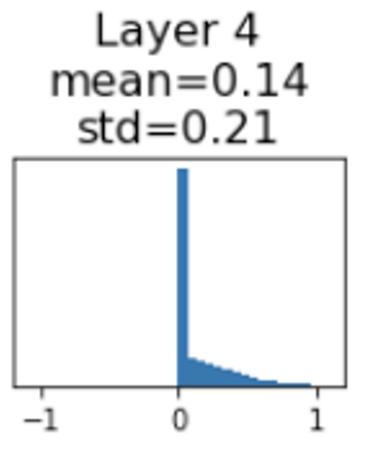
Xavier assumes zero centered activation function

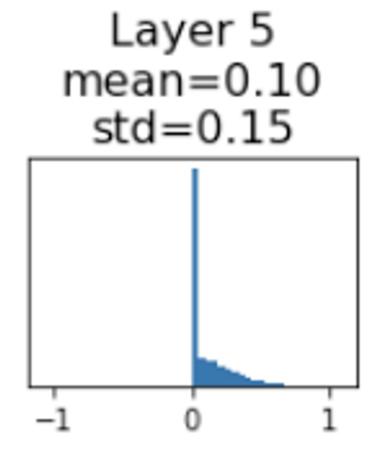
Activations collapse to zero again, no learning:(

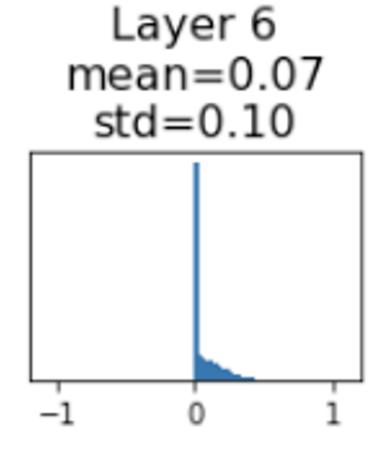












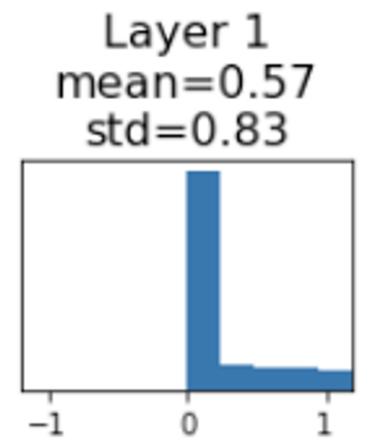


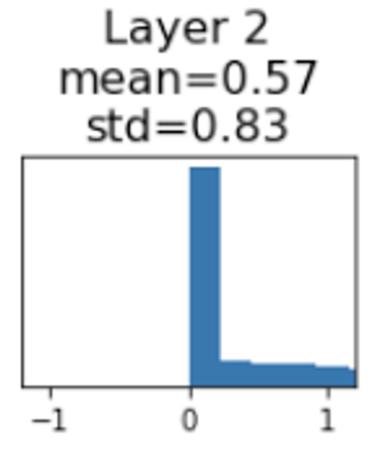


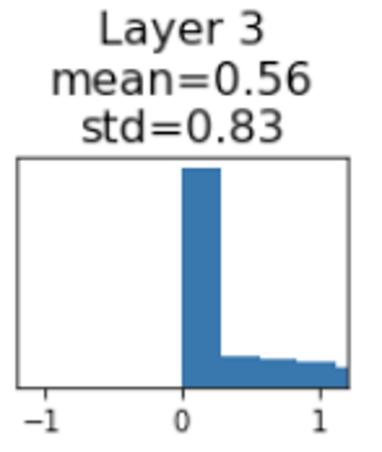
Weight initialization: Kaiming / MSRA initialization

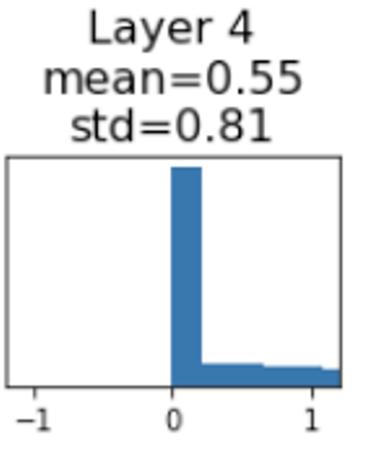
```
dims = [4096] * 7 ReLU correction: std = sqrt(2 / Din)
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

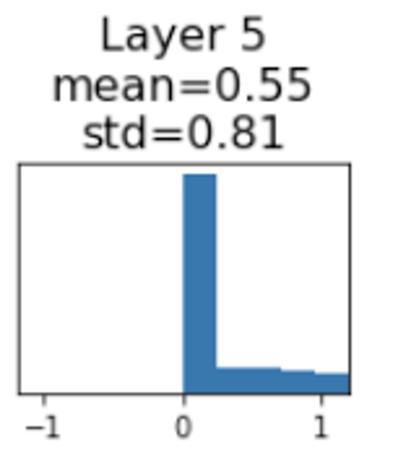
"Just right" - activations nicely scaled for all layers

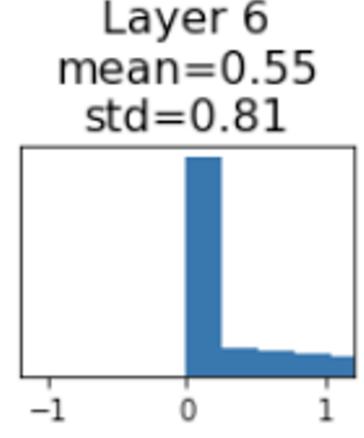










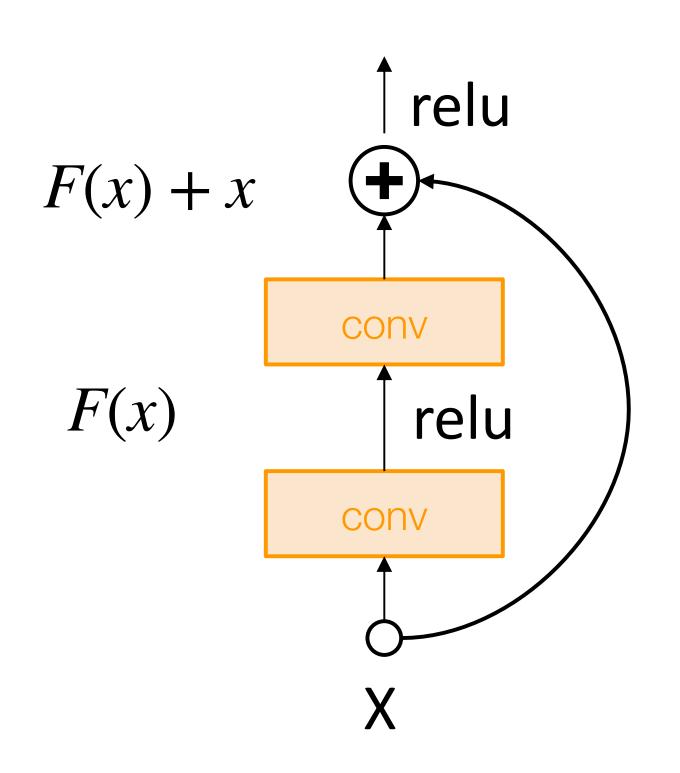








Weight initialization: Residual Networks



Residual Block

If we initialize with MSRA: then Var(F(x)) = Var(x)

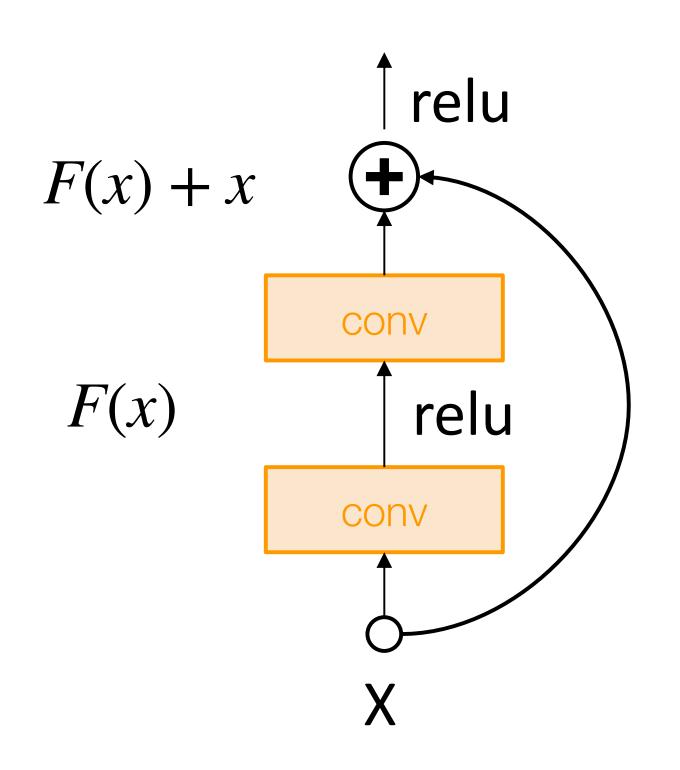
But then Var(F(x) + x) > Var(x) variance grows with each block!







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(F(x) + x) = Var(x)





Proper initialization is an active area of research

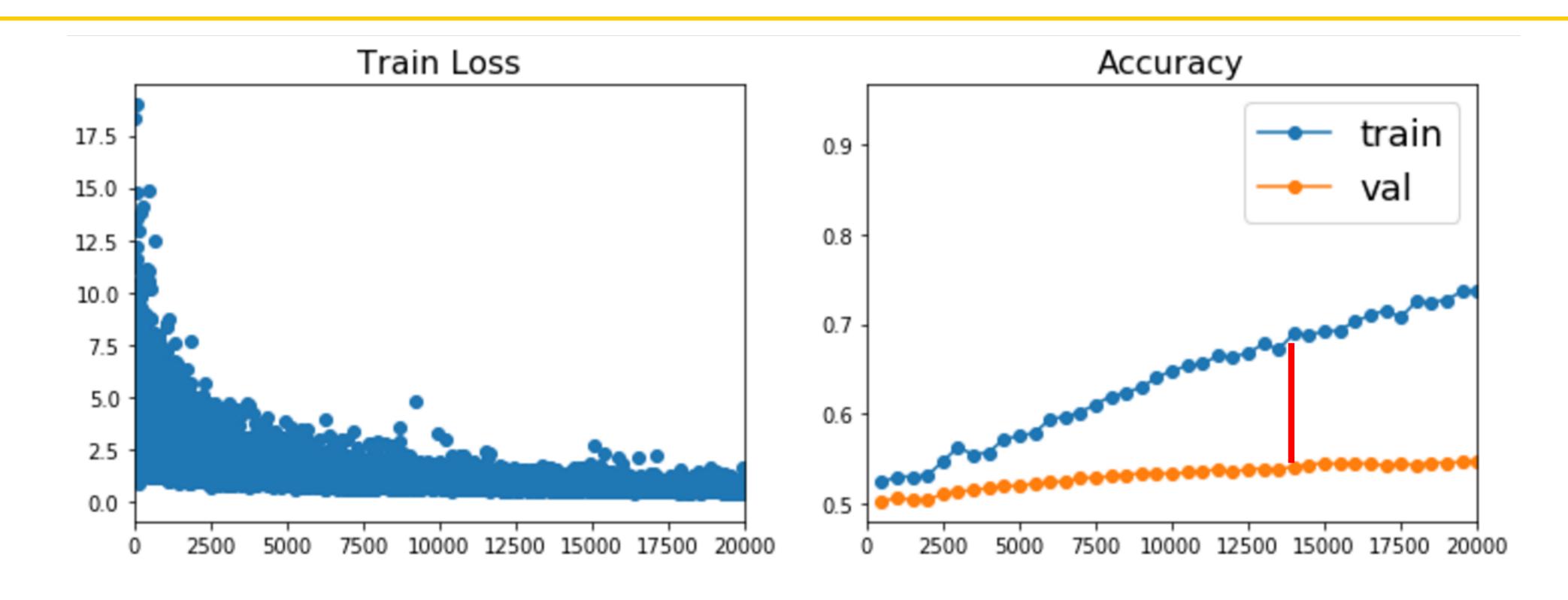
- Understanding the difficulty of training deep feedforward neural networks by Glorot and Bengio, 2010
- Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013
- Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 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





DR

Now your model is training ... but it overfits!



Regularization







Summary

1. One time setup:

Today

Activation functions, data preprocessing, weight initialization, regularization

2. Training dynamics:

Next time

 Learning rate schedules; large-batch training; hyperparameter optimization

3. After training:

• Model ensembles, transfer learning







Next Time: Training Neural Networks II







DeepRob

Lecture 9 **Training Neural Networks I University of Michigan and University of Minnesota**



