



# DeepRob

Lecture 9  
Training Neural Networks I  
University of Minnesota





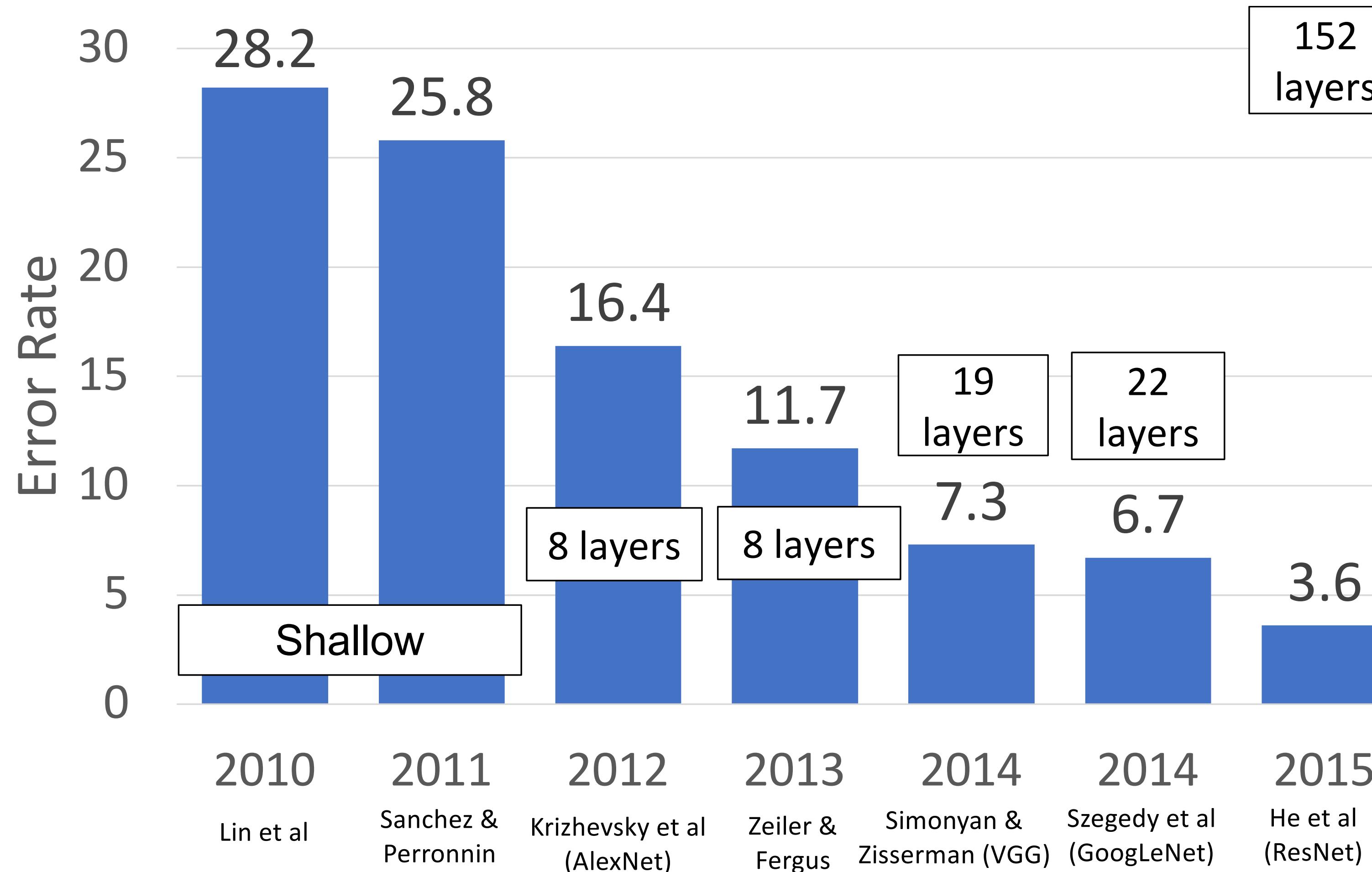
# Project 2—Updates

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- Instructions available on the website
  - Here: <https://rpm-lab.github.io/CSCI5980-F24-DeepRob/projects/project2/>
- Implement two-layer neural network and generalize to FCN
- **Autograder fixed!**
- Due Monday, October 14th, 11:59 PM CT



# Recap: CNN Architectures for ImageNet Classification





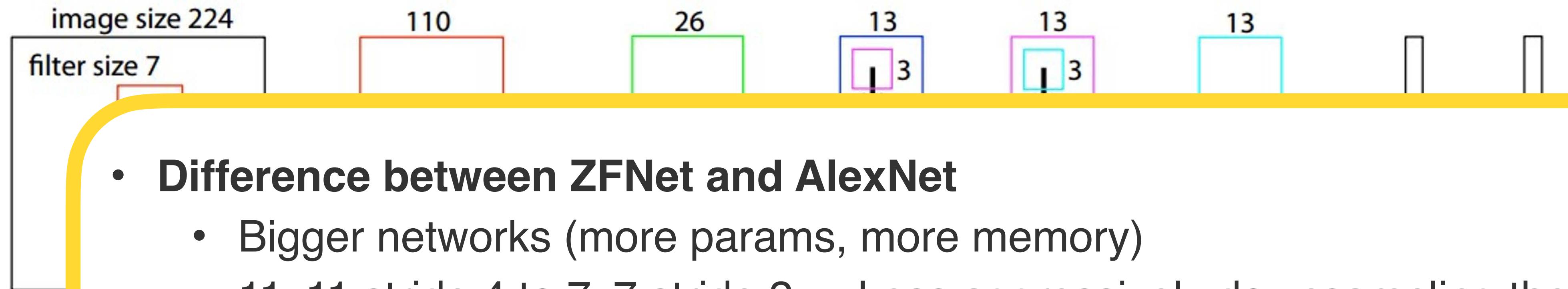
# Questions from the previous lecture

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- **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

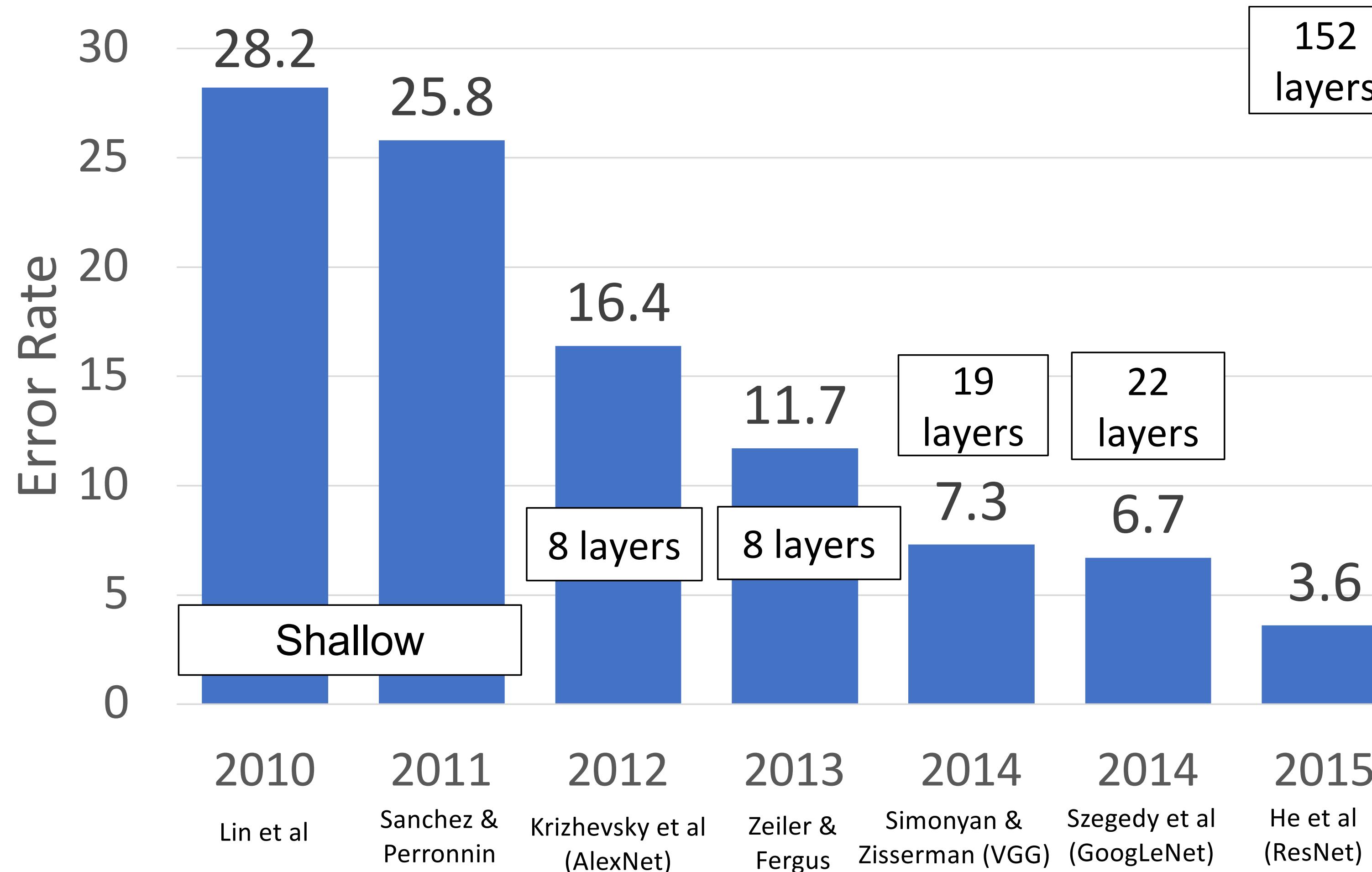


- **Difference between ZFNet and AlexNet**
  - Bigger networks (more params, more memory)
  - 11x11 stride 4 to 7x7 stride 2 -> Less aggressively downsampling the spatial dimensions, higher spatial resolution -> more receptive fields -> more compute.
  - Increase in the number of filters in the later layers -> more learnable parameters -> more memory and more compute.

more trial and error :)



# Recap: CNN Architectures for ImageNet Classification





# Residual Networks

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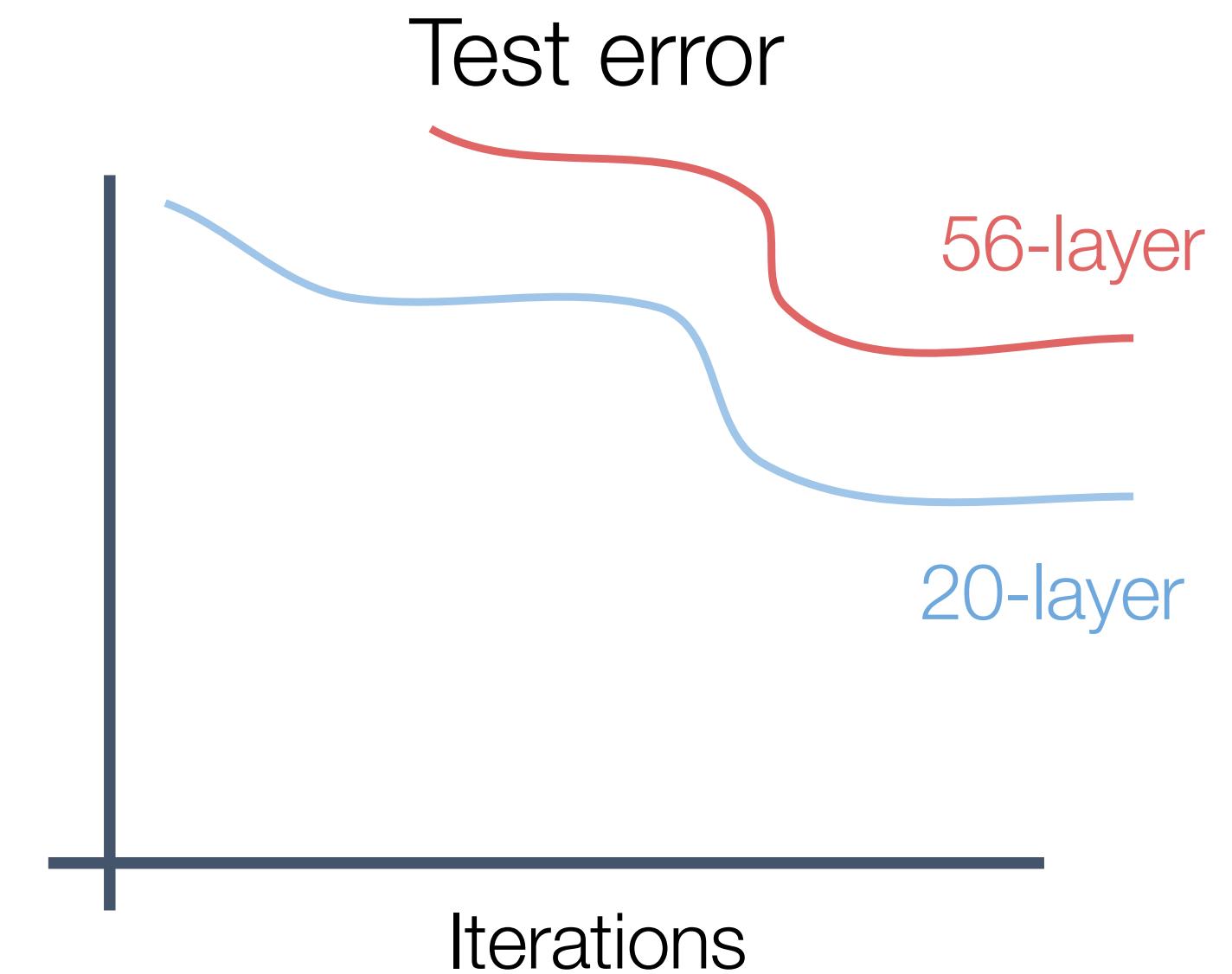
Once we have Batch Normalization, we can train networks with 10+ layers.  
What happens as we go deeper?



# Residual Networks

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

Deeper model does worse than shallow model!

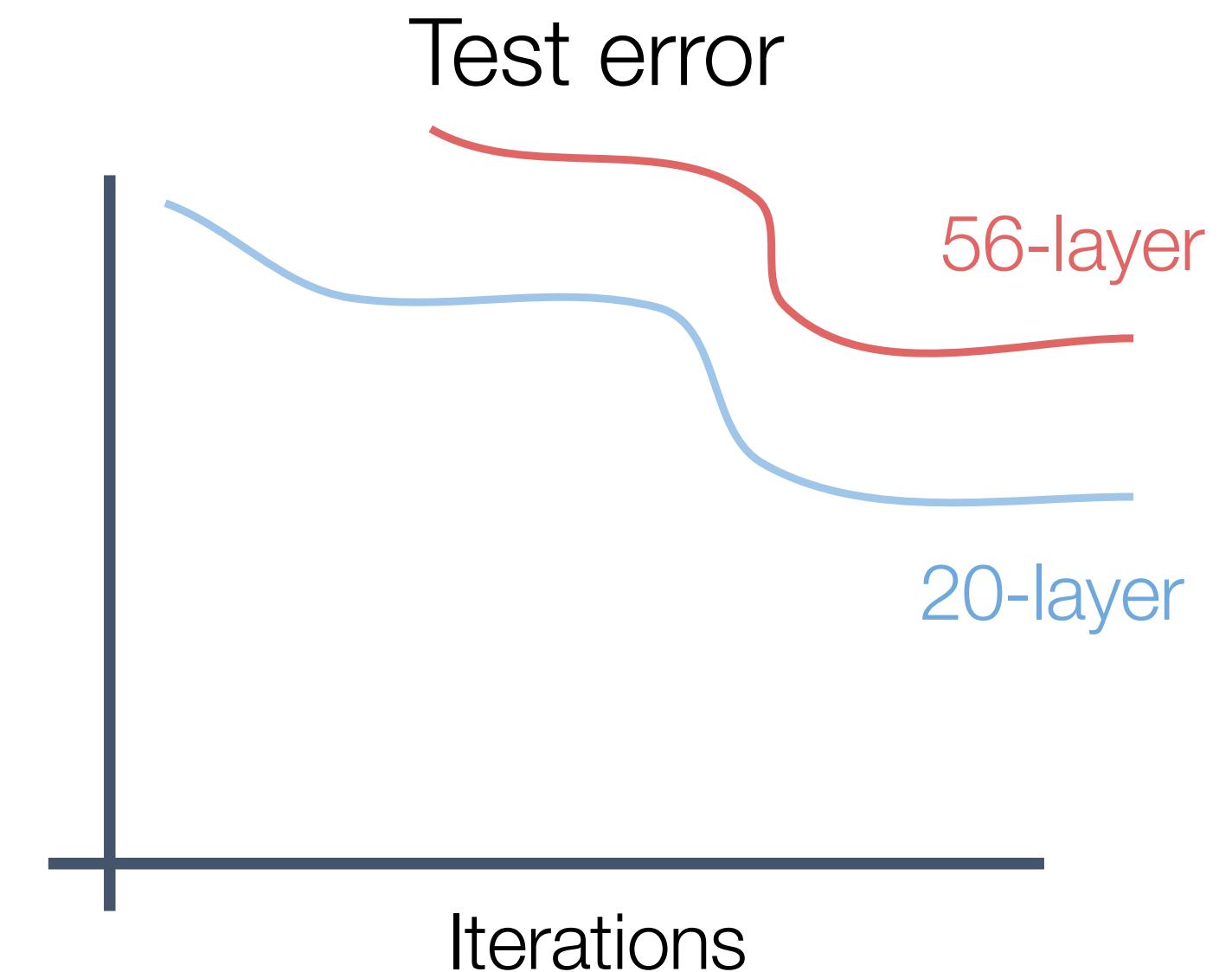


# Residual Networks

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

Deeper model does worse than shallow model!

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



# Residual Networks

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**



# Residual Networks

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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*





# Residual Networks

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

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





# Residual Networks

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

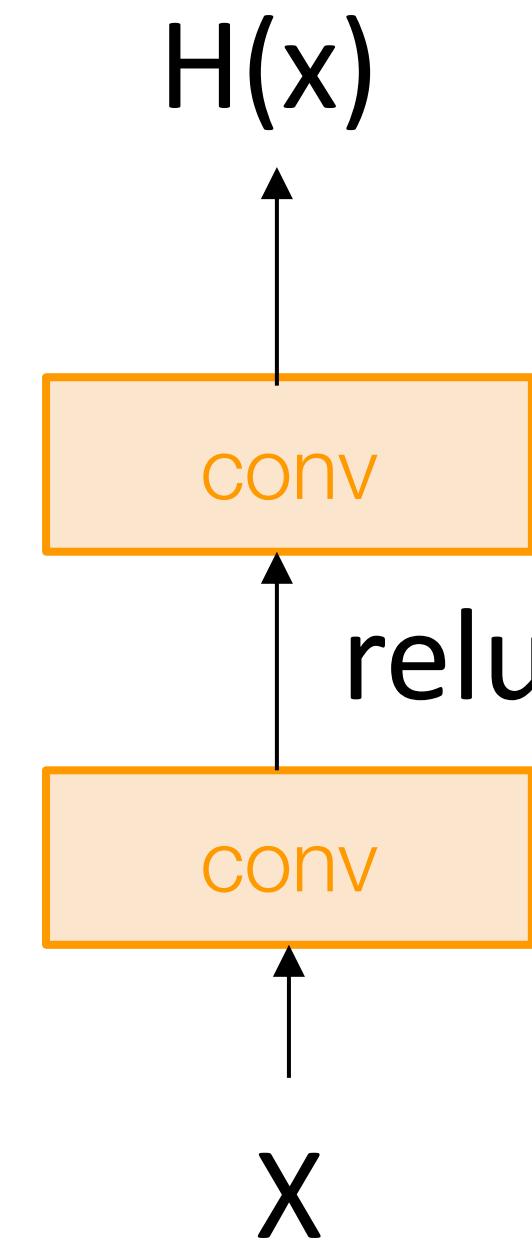
**Hypothesis:** This is an optimization problem. Deeper models are harder to optimize, and in particular don't learn identity functions to emulate shallow models

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

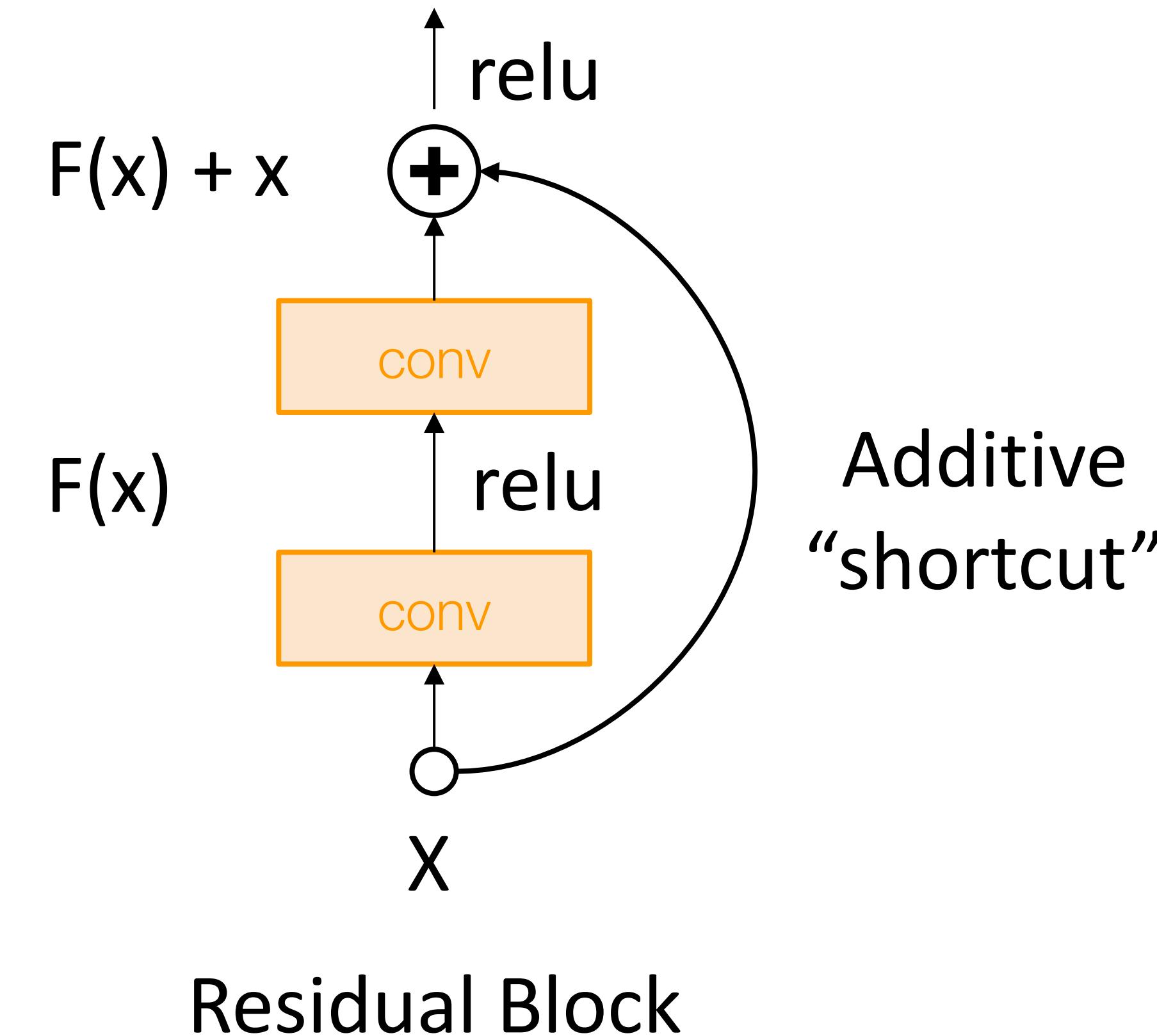


# Residual Networks

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



“Plain” block

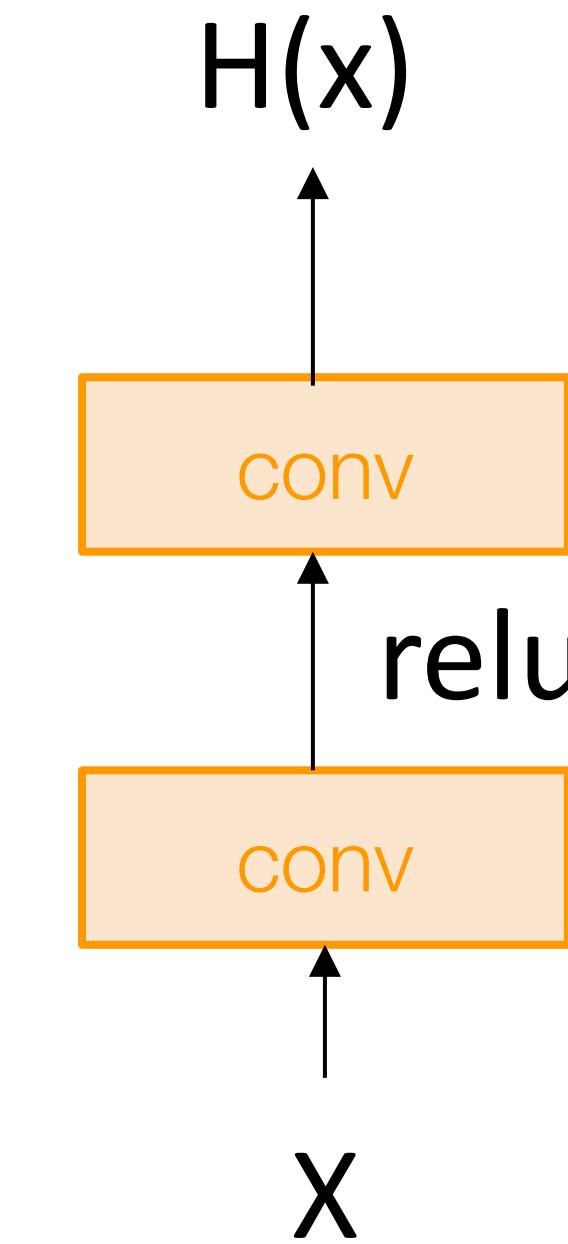


Residual Block



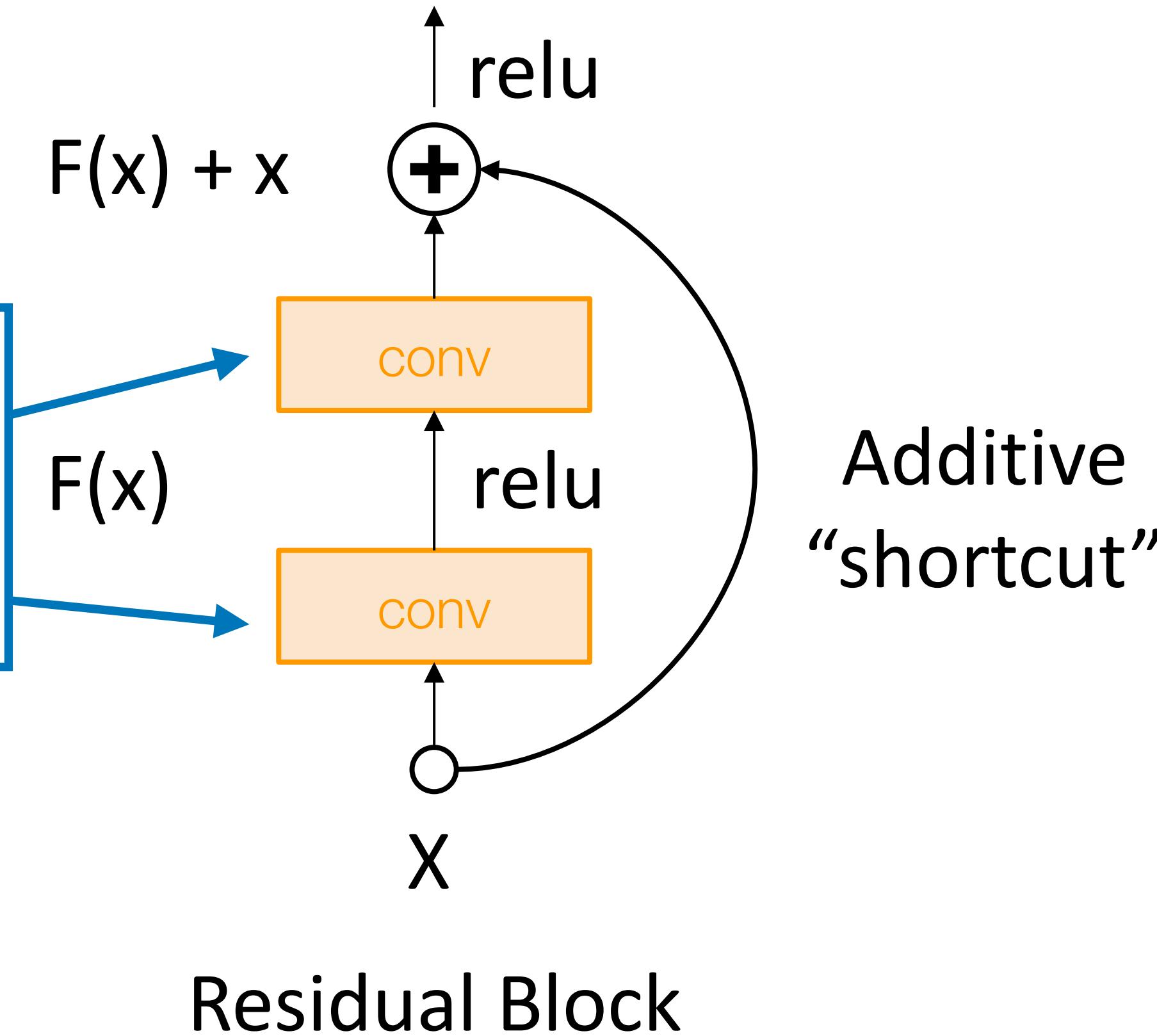
# Residual Networks

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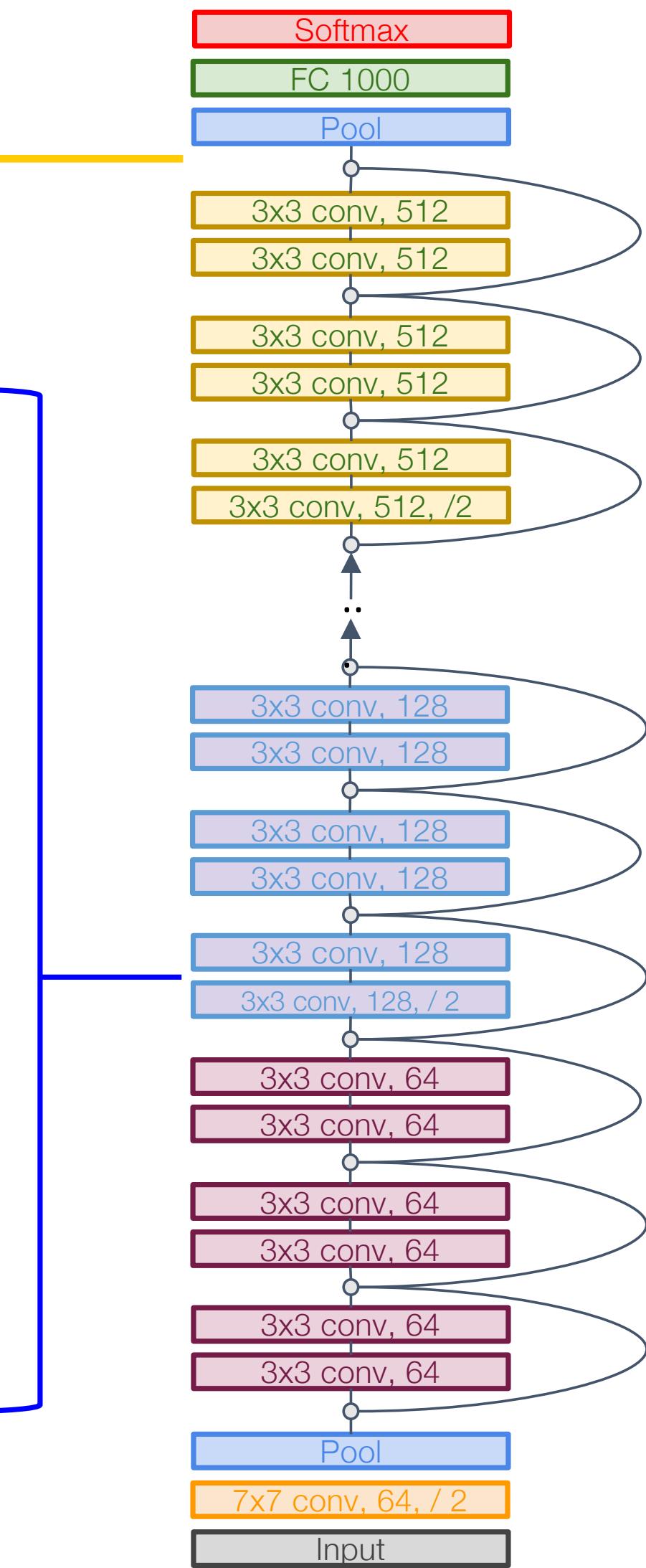
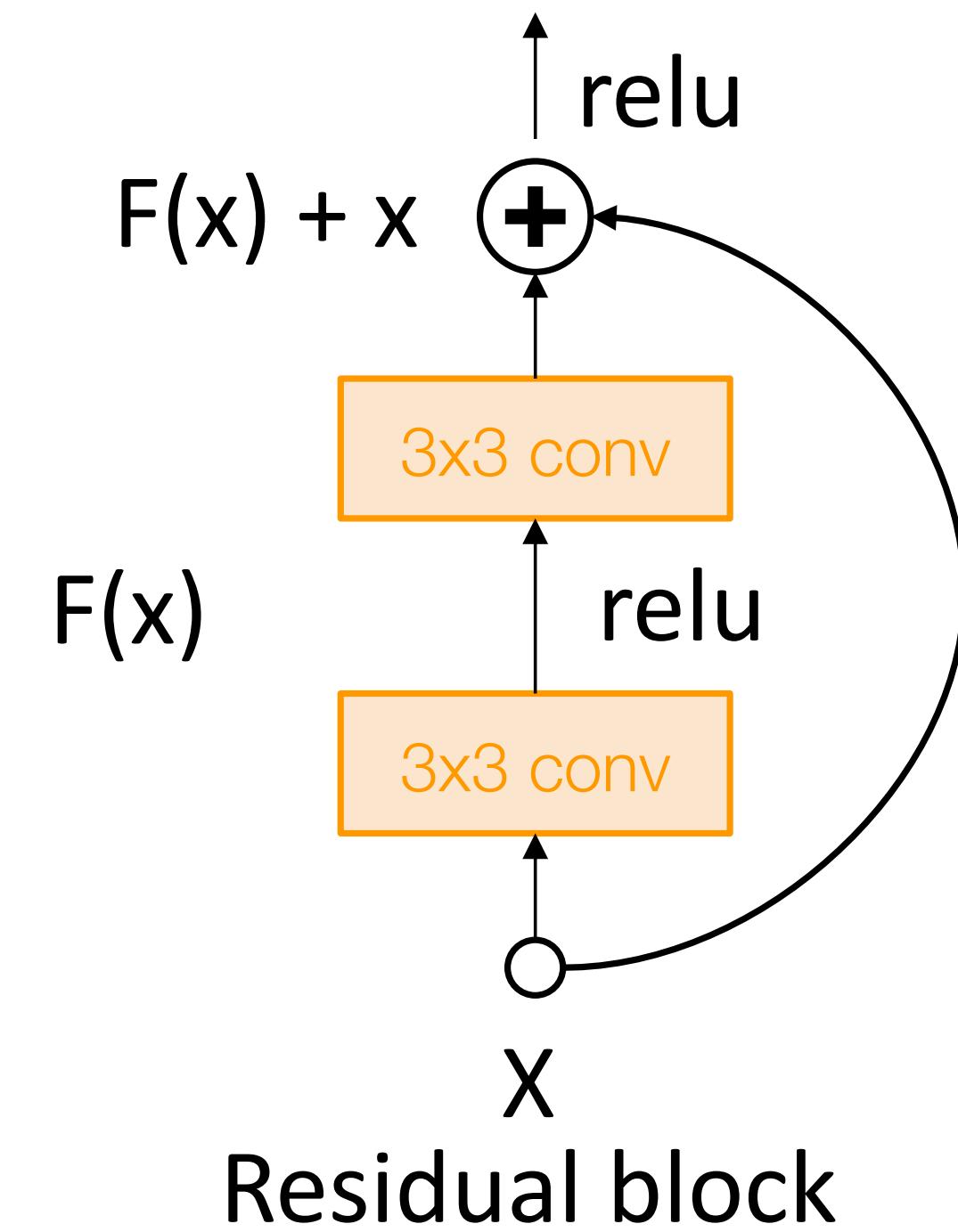
If you set these to 0, the whole block will compute the identity function!



Residual Block

# Residual Networks

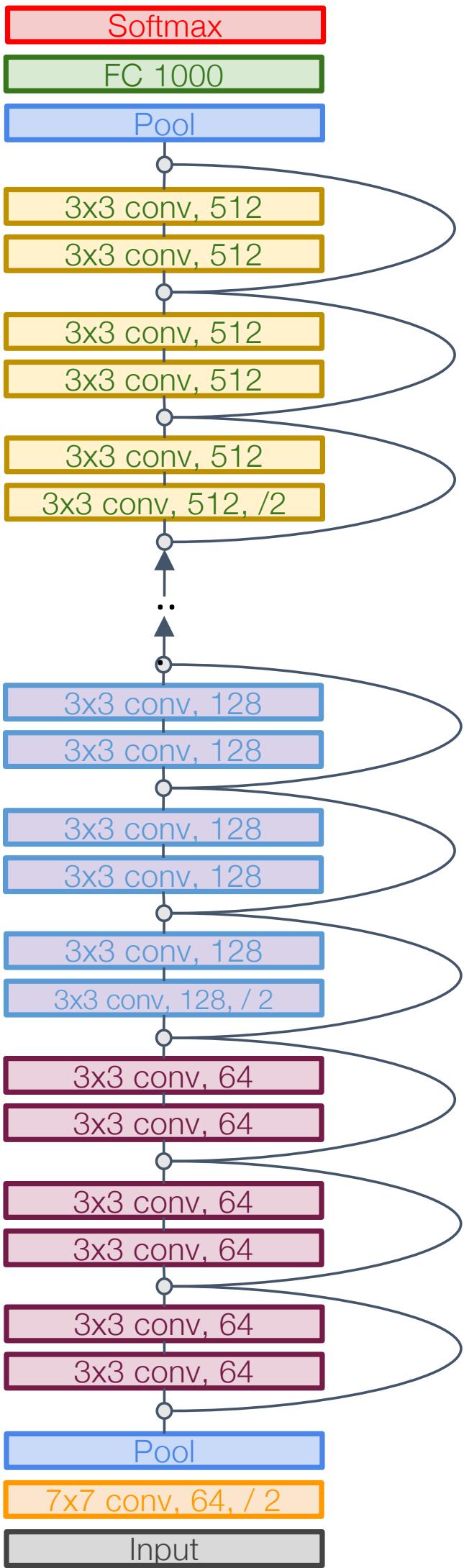
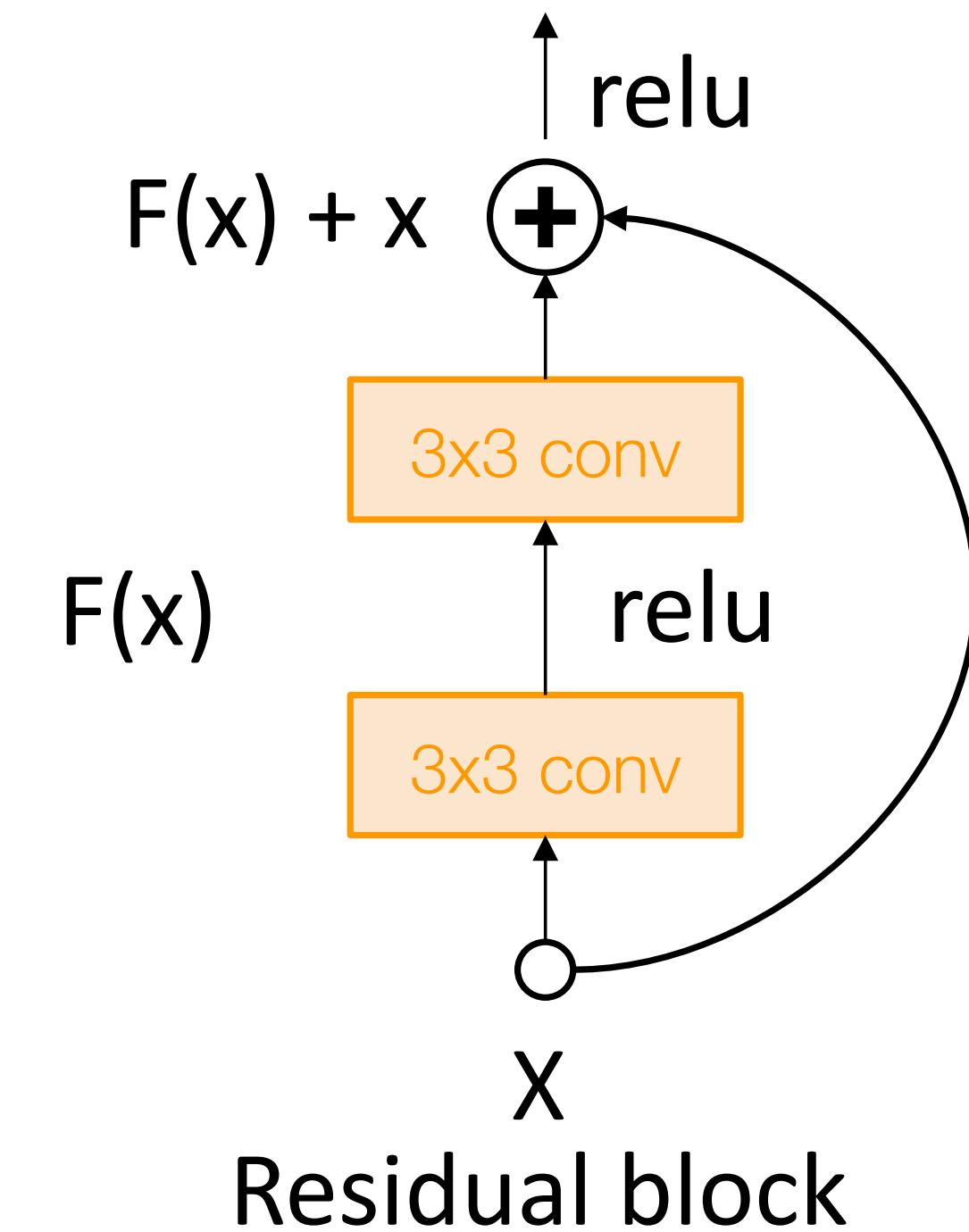
A residual network is a stack of many residual blocks



# Residual Networks

A residual network is a stack of many residual blocks

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

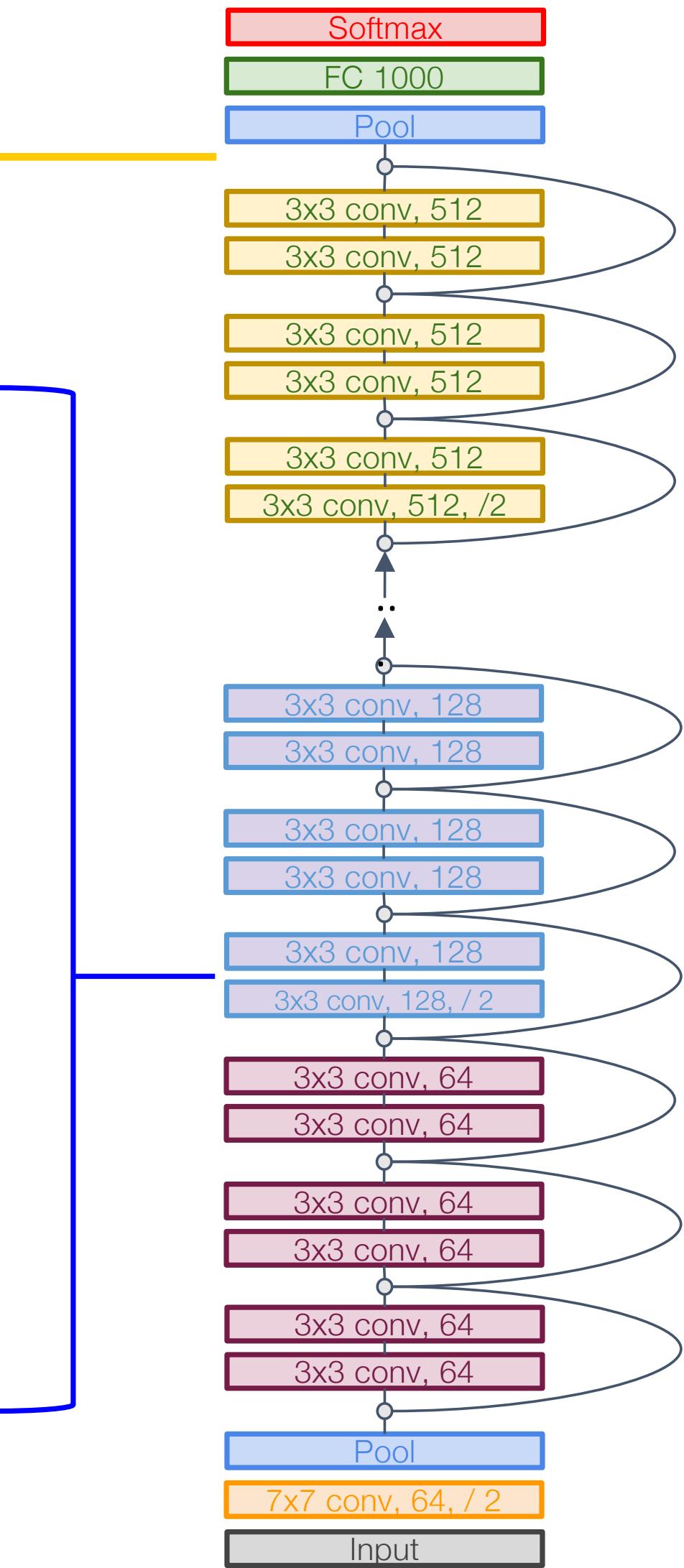
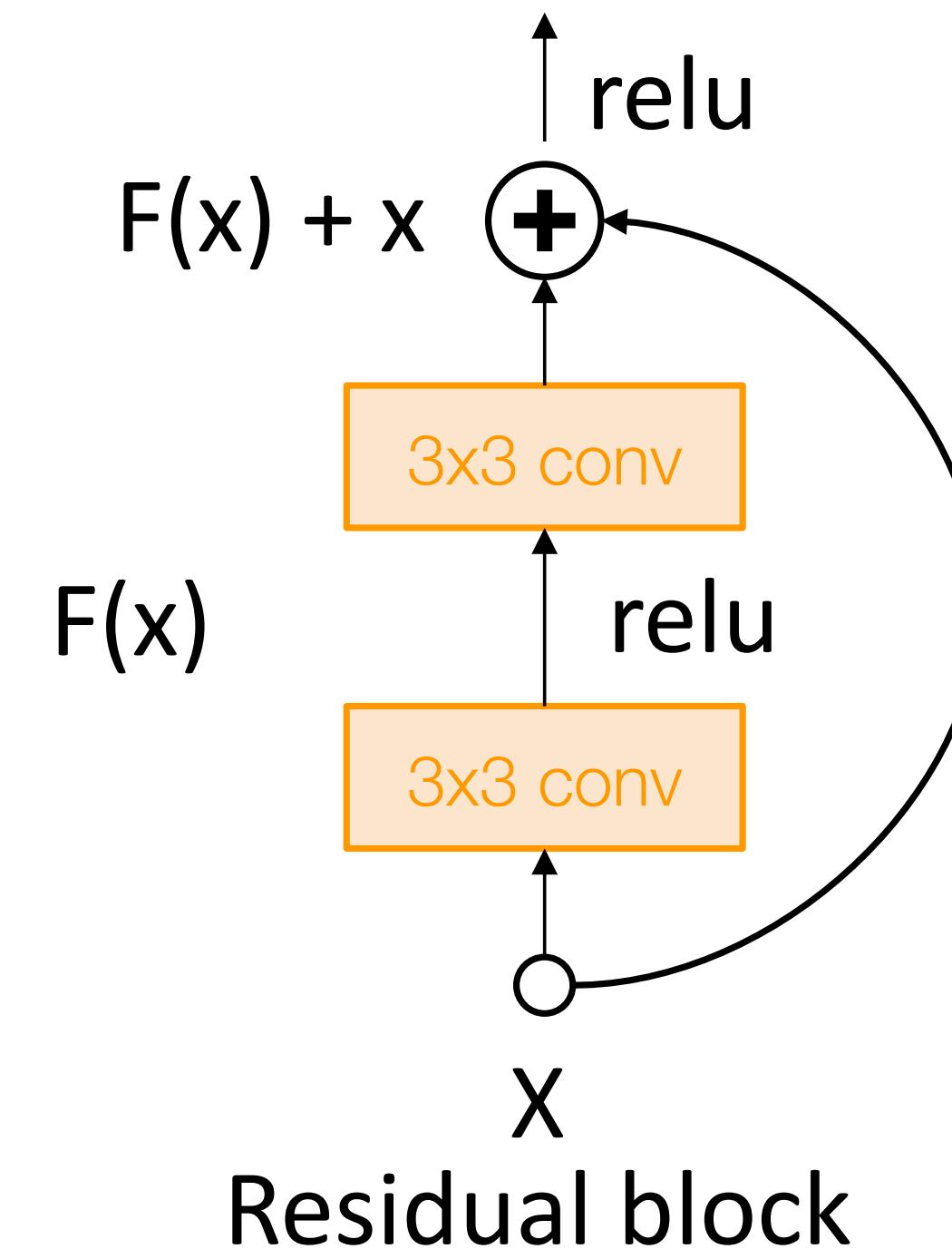


# Residual Networks

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

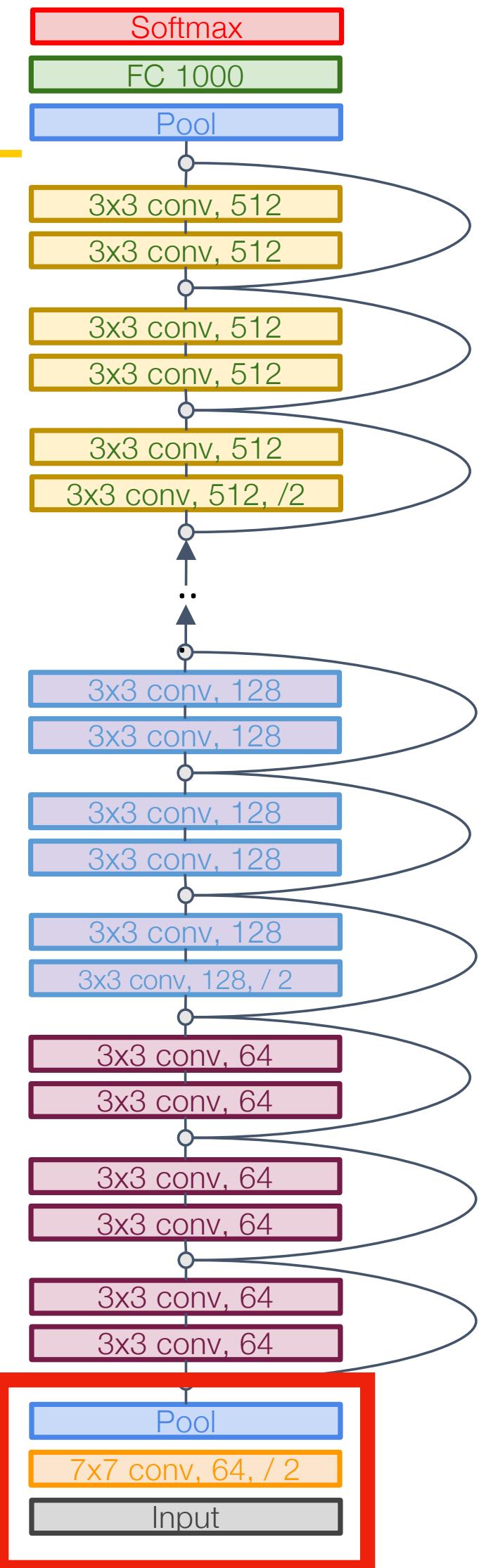




# Residual Networks

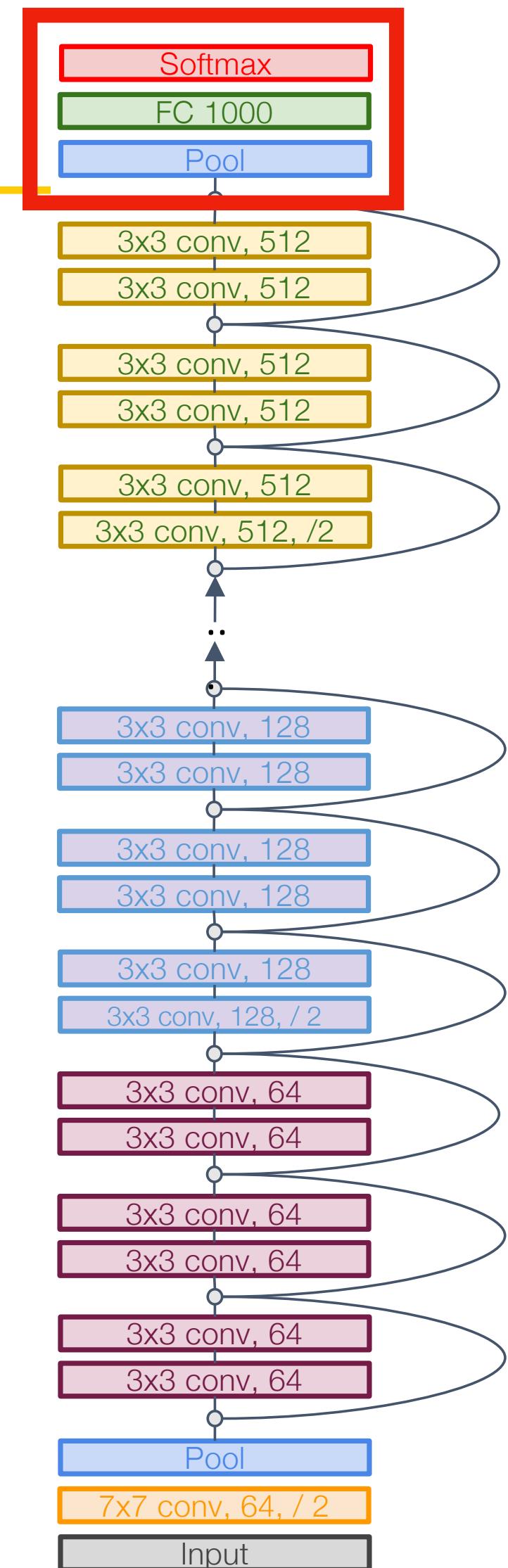
Uses the same aggressive **stem** as GoogleNet to downsample the input 4x before applying residual blocks:

	Input size		Layer				Output size				
Layer	C	H/W	Filters	Kernel	Stride	Pad	C	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



# Residual Networks

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





# Residual Networks

## ResNet-18:

Stem: 1 conv layer

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

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

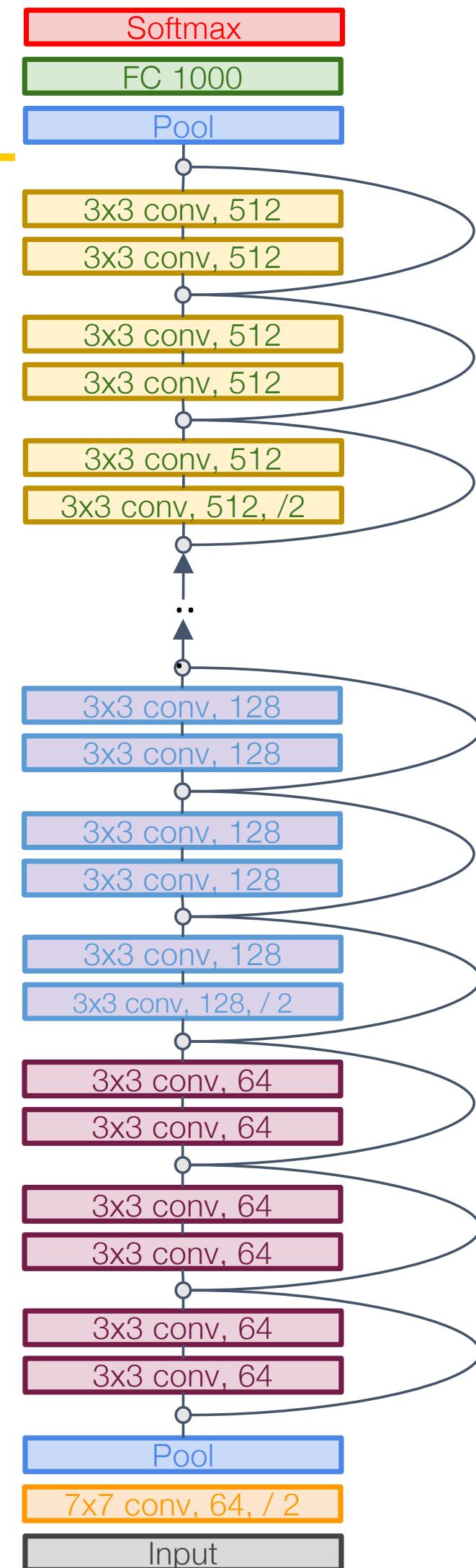
Stage 3 (C=256): 2 res. block = 4 conv

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

Linear

ImageNet top-5 error: 10.92

GFLOP: 1.8





# Residual Networks

# 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

# 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

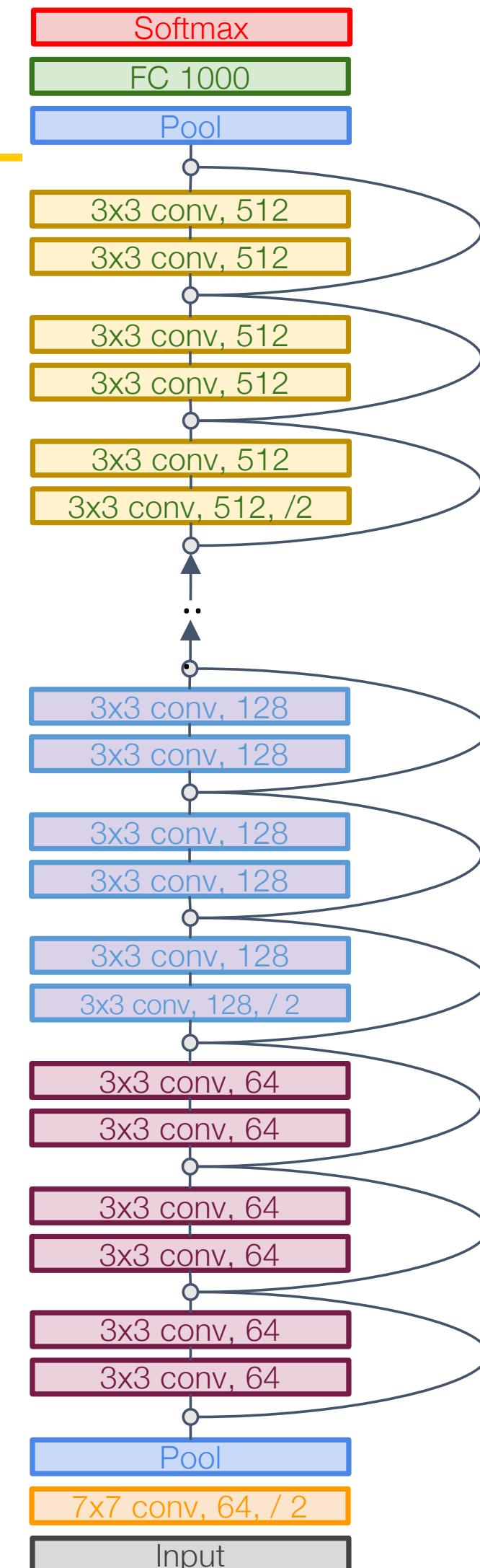
# ImageNet top-5 error: 8.58

# GFLOP: 3.6

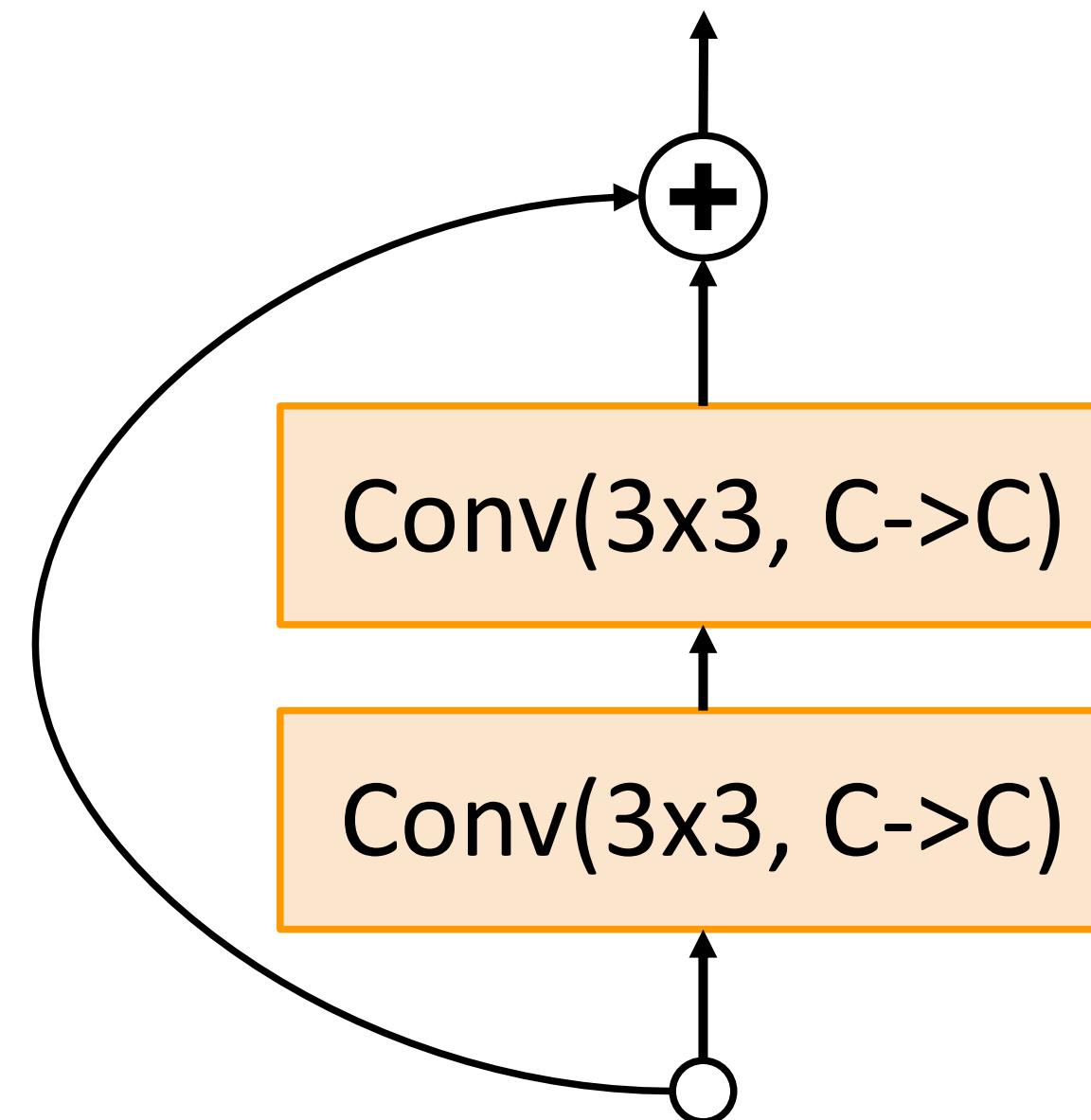
# VGG-16:

# ImageNet top-5 error: 9.62

# GFLOP: 13.6



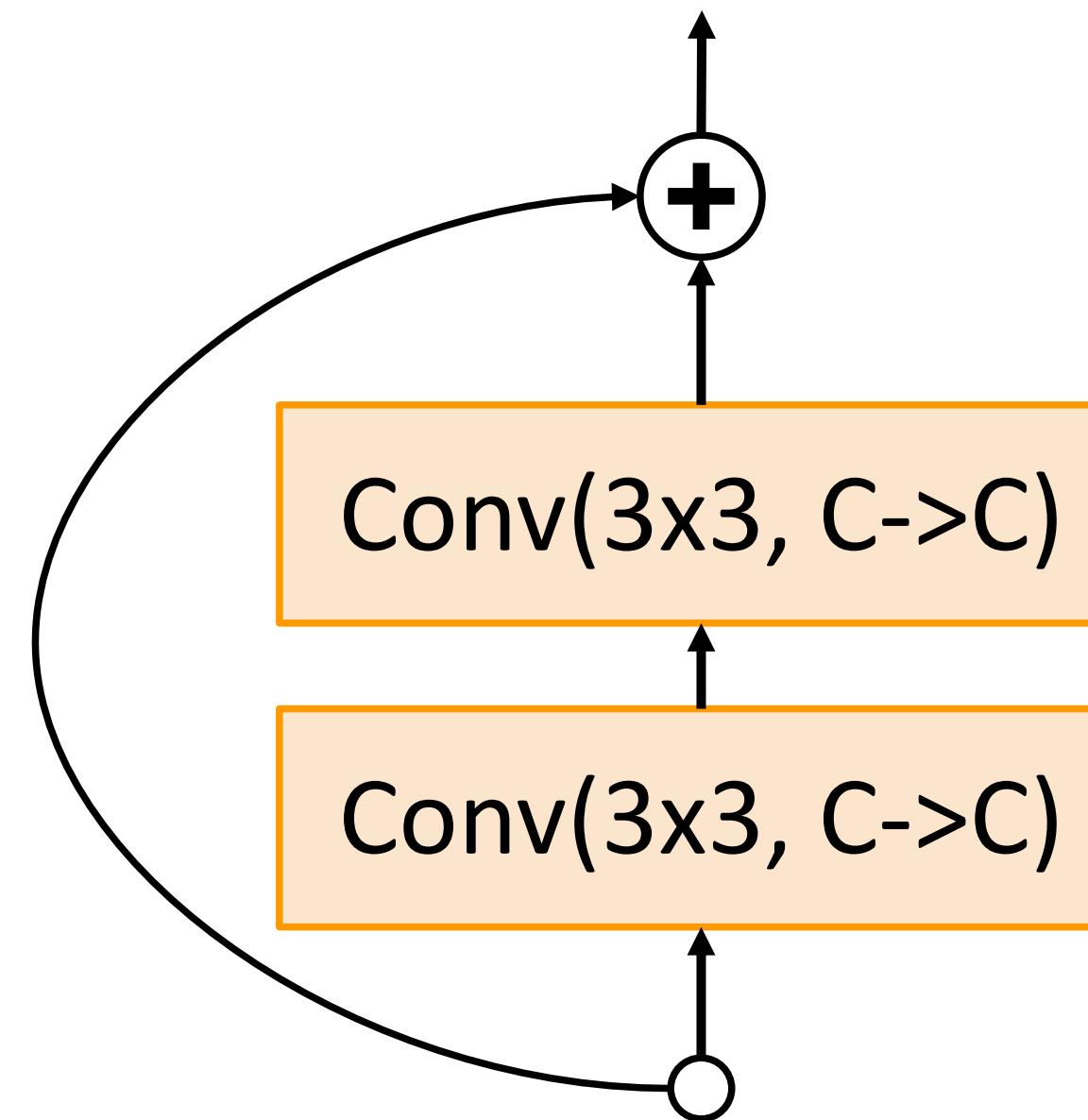
# Residual Networks: Basic Block



“Basic”  
Residual block



# Residual Networks: Basic Block



Conv( $3 \times 3$ ,  $C \rightarrow C$ )

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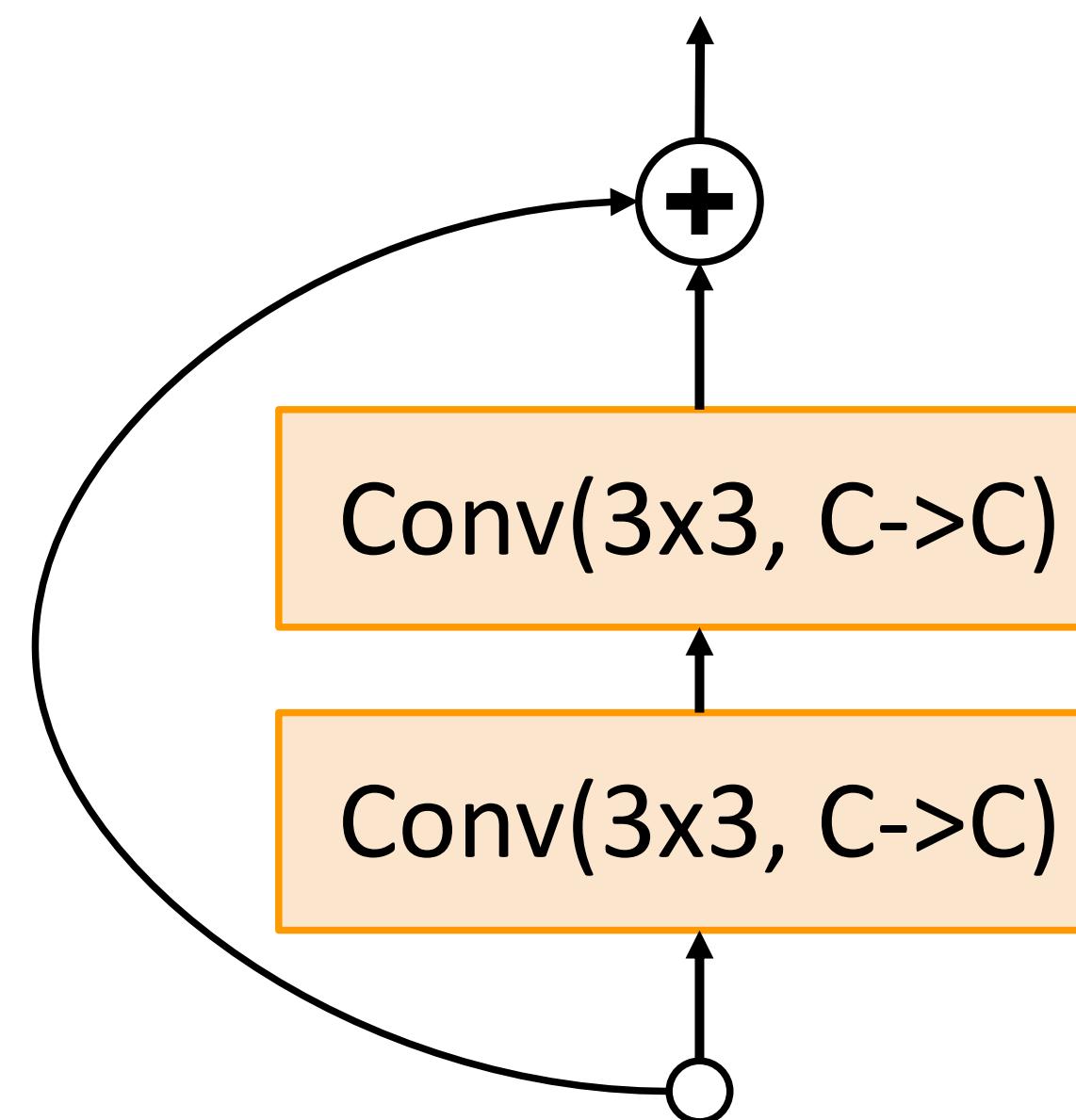
“Basic”  
Residual block

**FLOPs:**  $9HWC^2$

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**Total FLOPs:**  
 $18HWC^2$

# Residual Networks: Bottleneck Block



Conv(3x3, C->C)

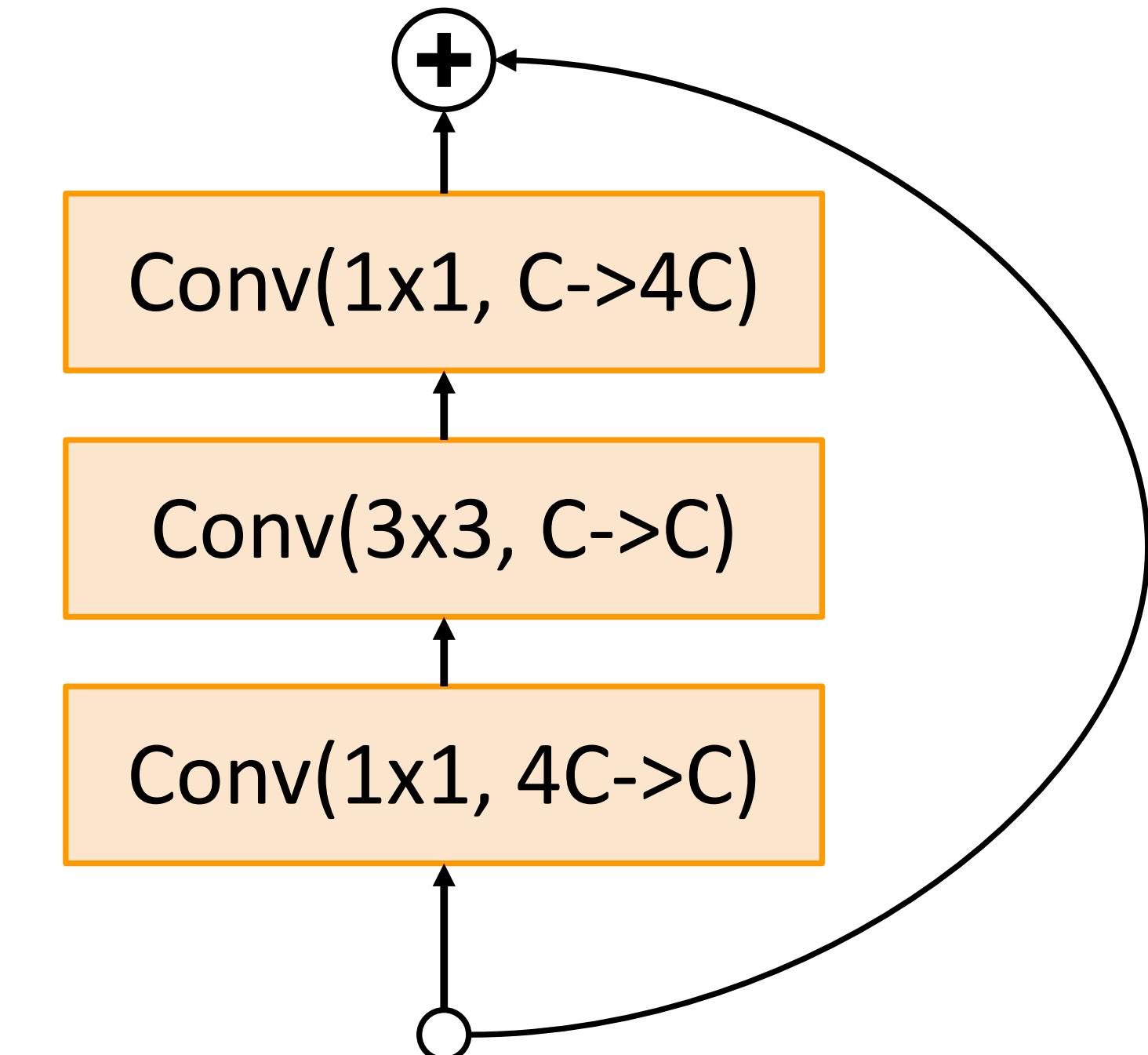
Conv(3x3, C->C)

“Basic”  
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**Total FLOPs:**  
 $18HWC^2$



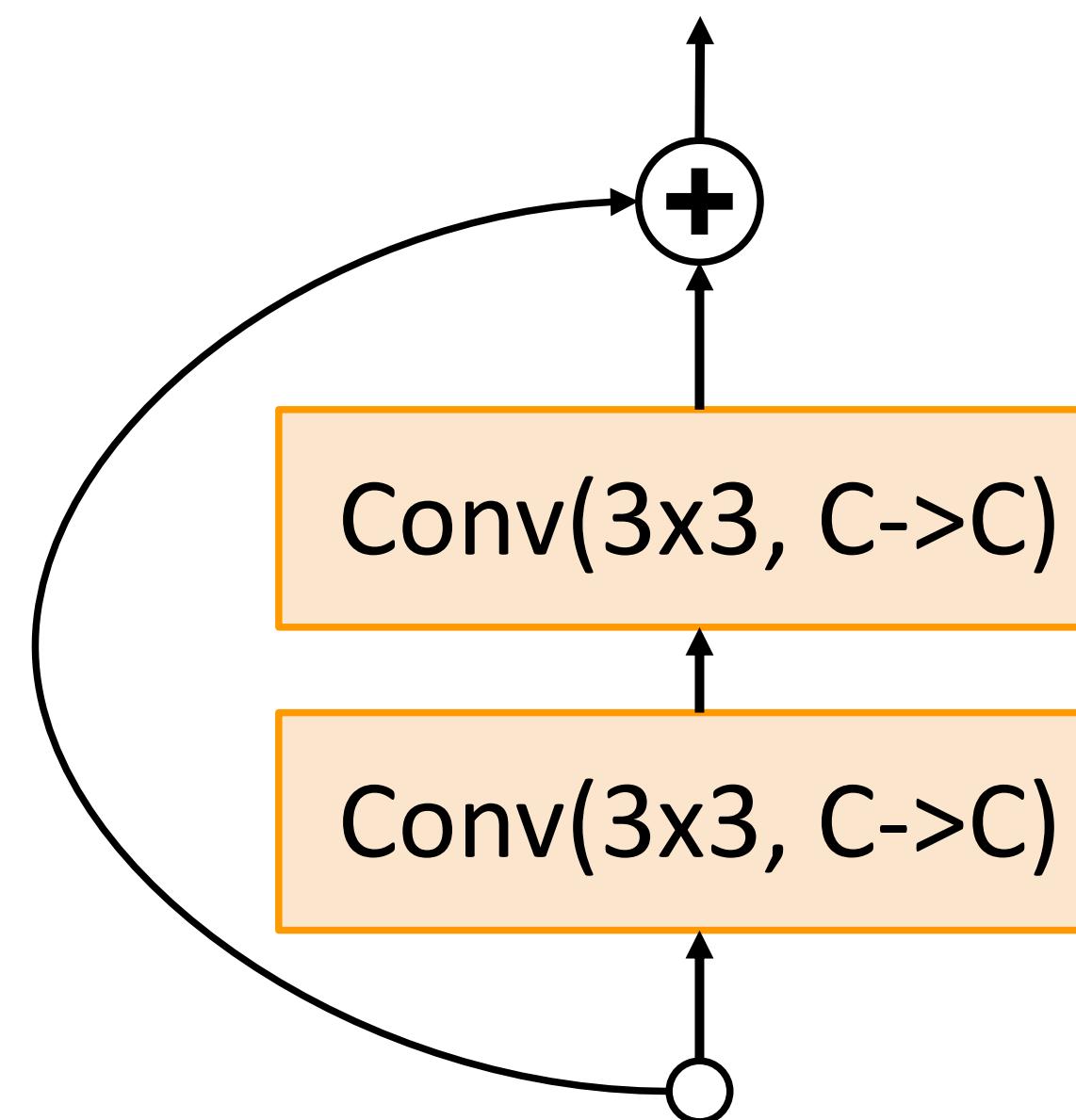
Conv(1x1, C->4C)

Conv(3x3, C->C)

Conv(1x1, 4C->C)

“Bottleneck”  
Residual block

# Residual Networks: Bottleneck Block



“Basic”  
Residual block

**More layers, less computational cost!**

**FLOPs:**  $9HWC^2$

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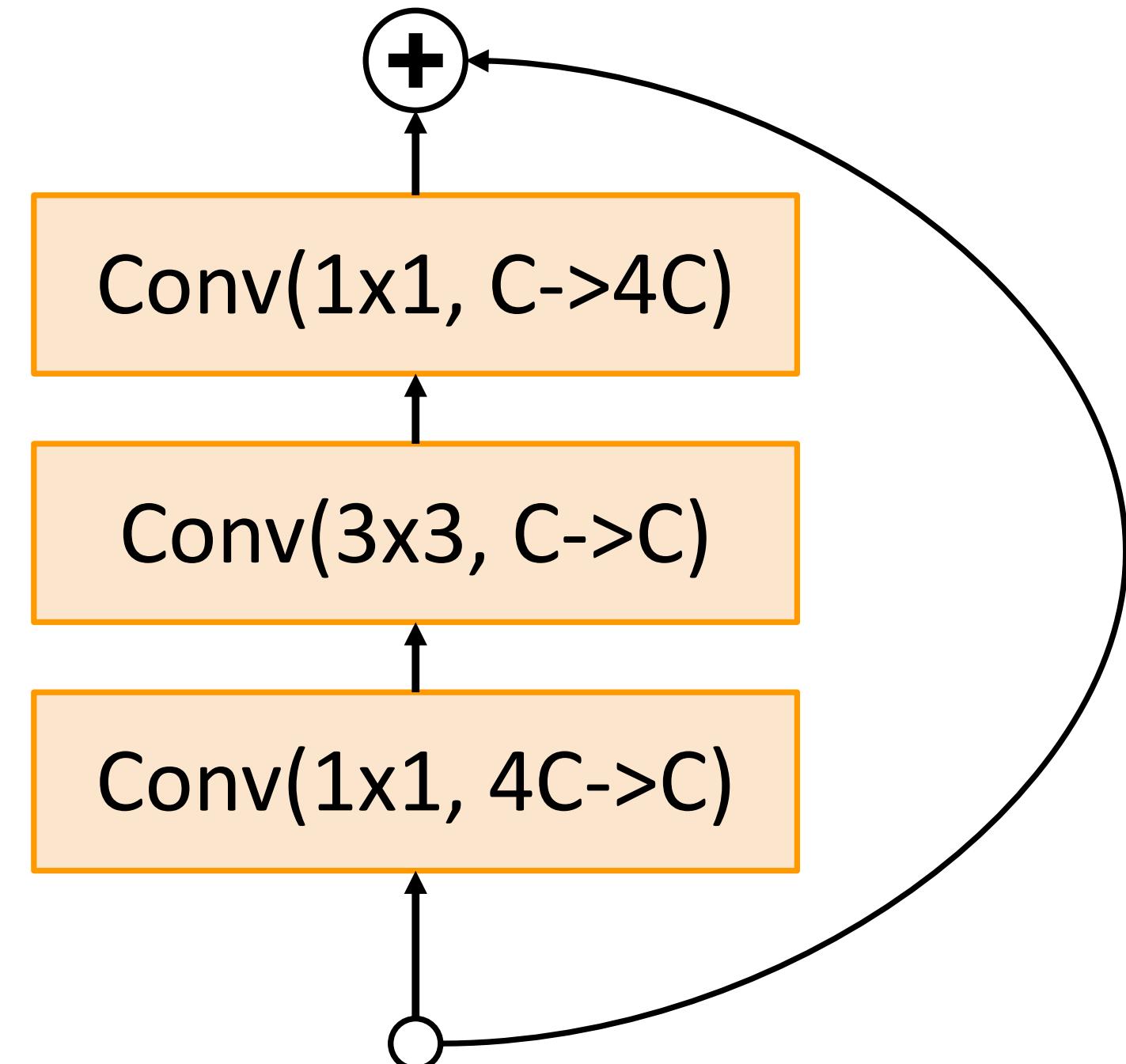
**Total FLOPs:**  
 $18HWC^2$

**FLOPs:**  $4HWC^2$

**FLOPs:**  $9HWC^2$

**FLOPs:**  $4HWC^2$

**Total FLOPs:**  
 $17HWC^2$

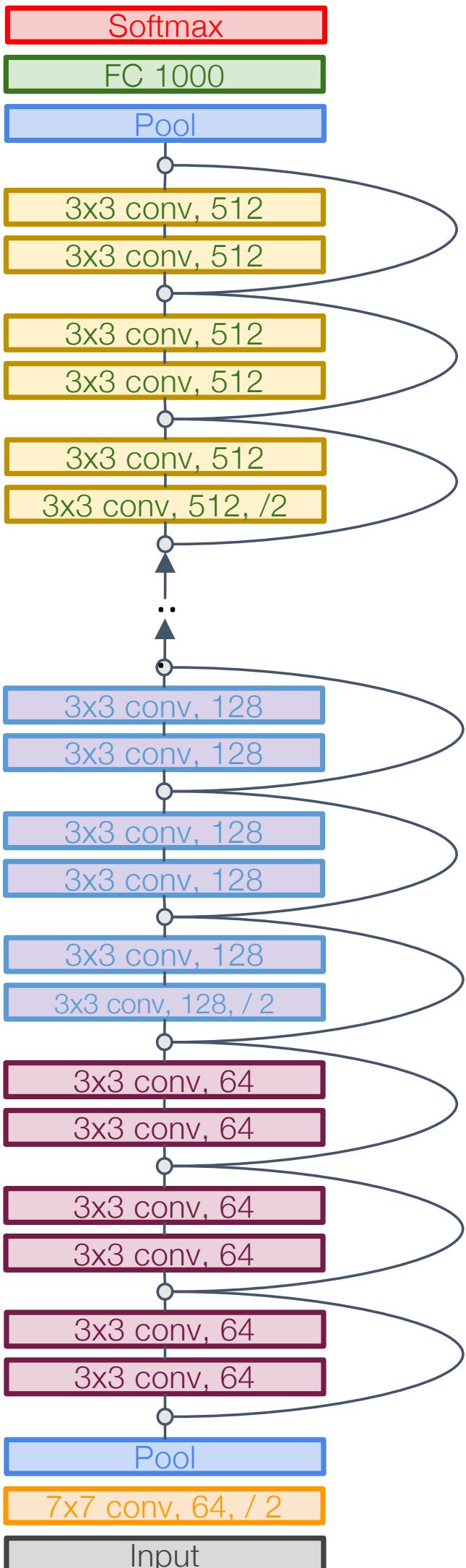


“Bottleneck”  
Residual block



# Residual Networks

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



# Residual Networks

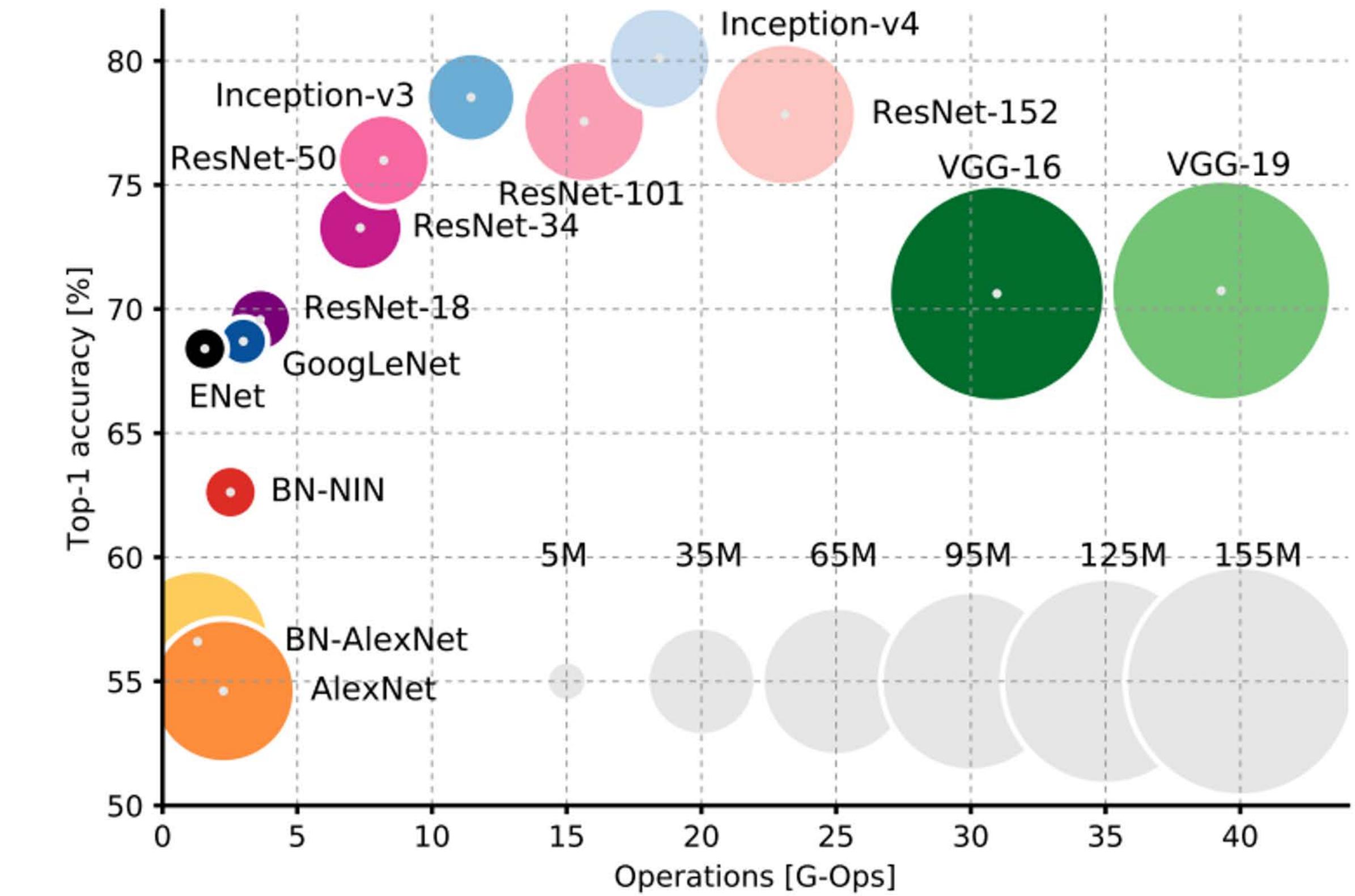
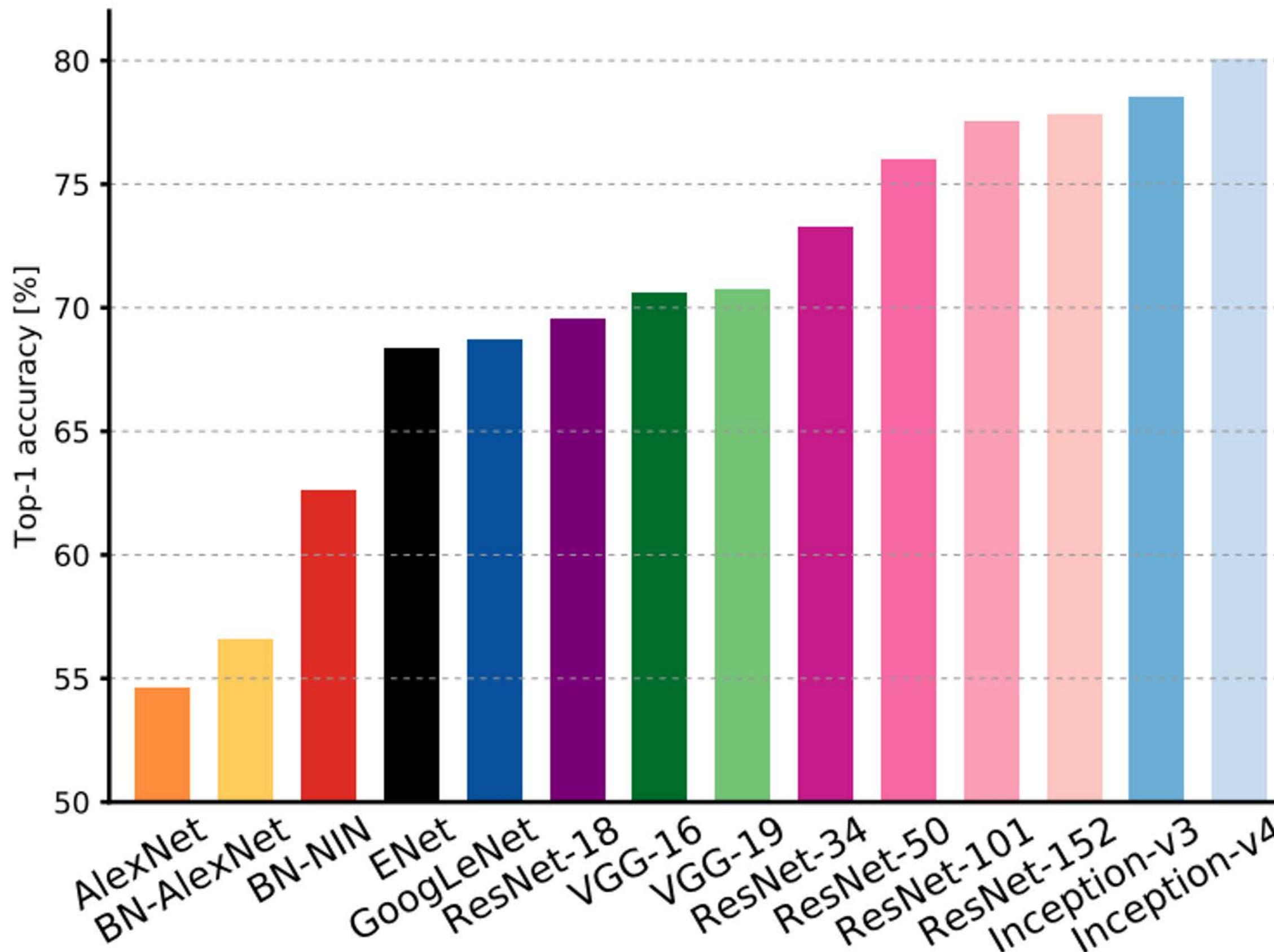
- Able to train very deep networks
- Deeper networks do better than shallow networks (as expected)
- Swept 1st place in all ILSVRC and COCO 2015 competitions
- Still widely used today

## 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

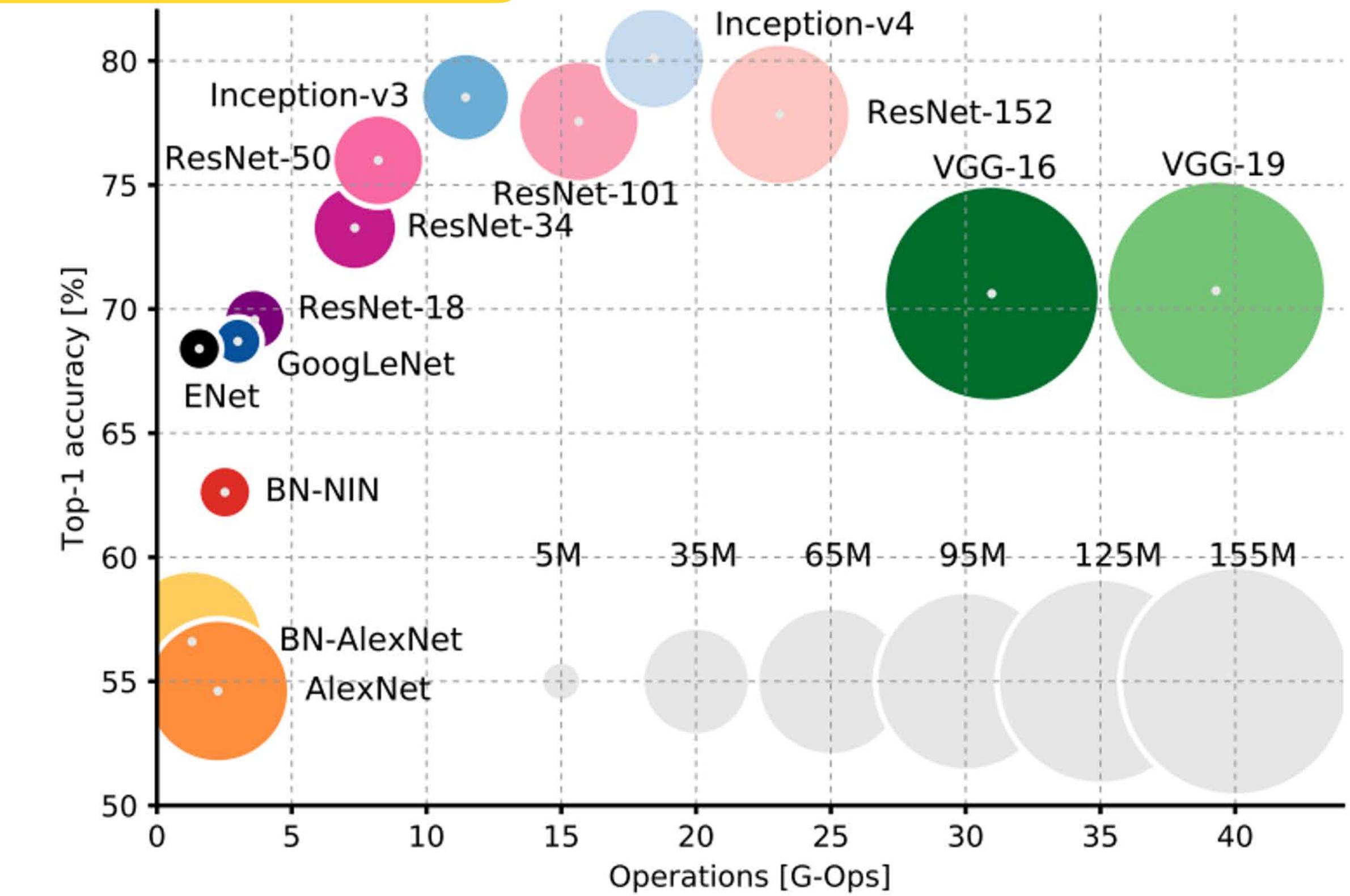
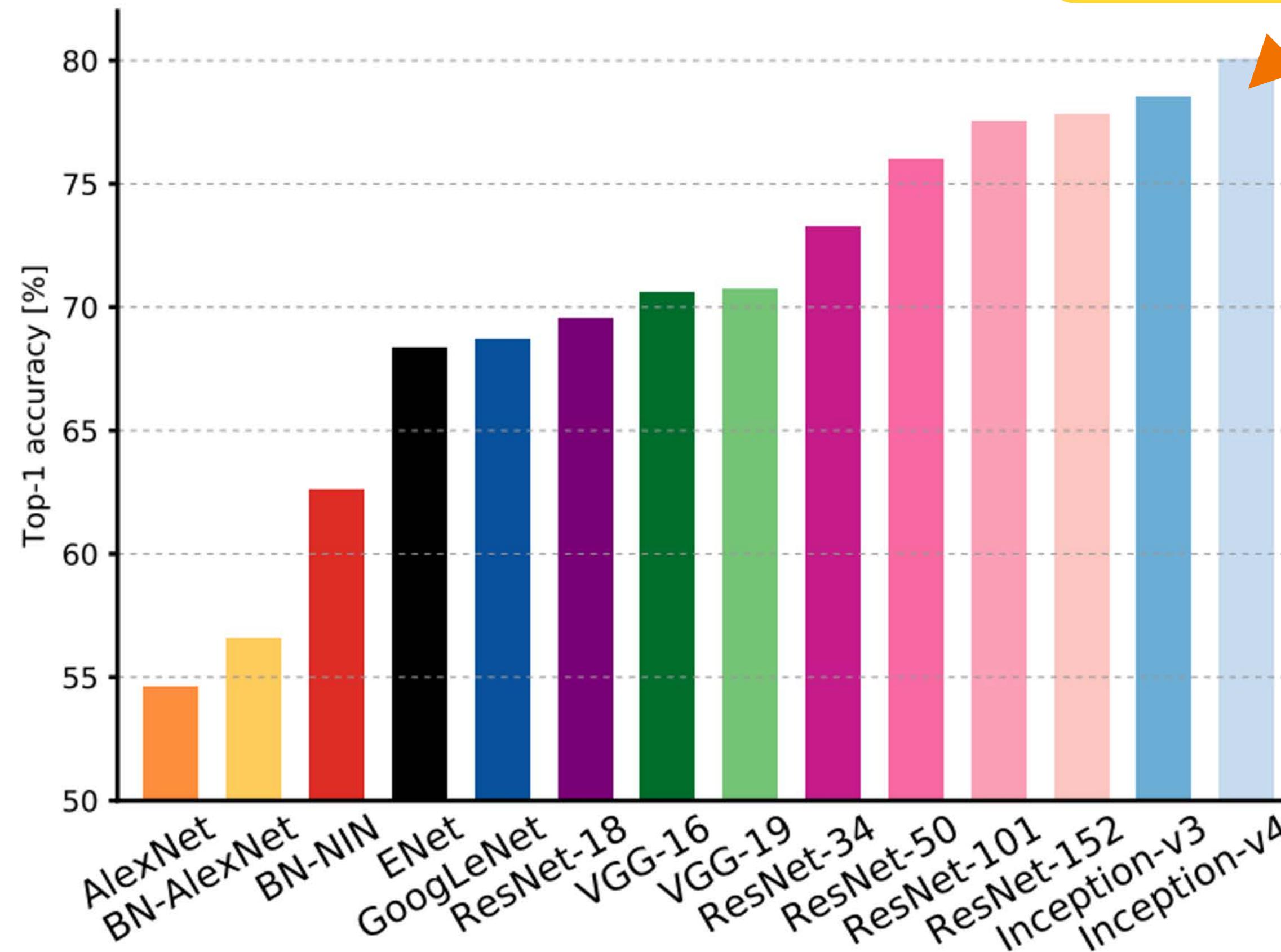


# Comparing Complexity



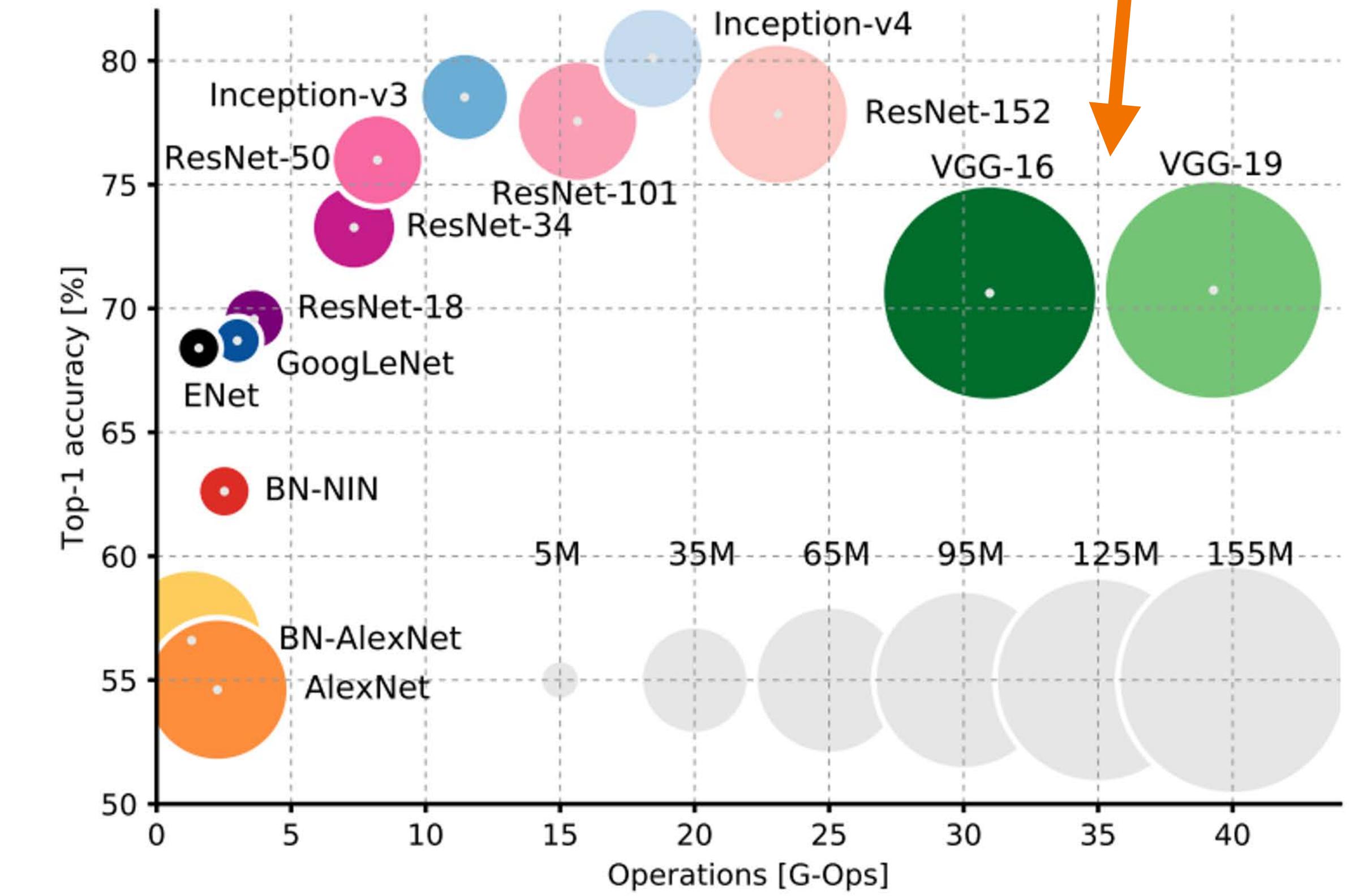
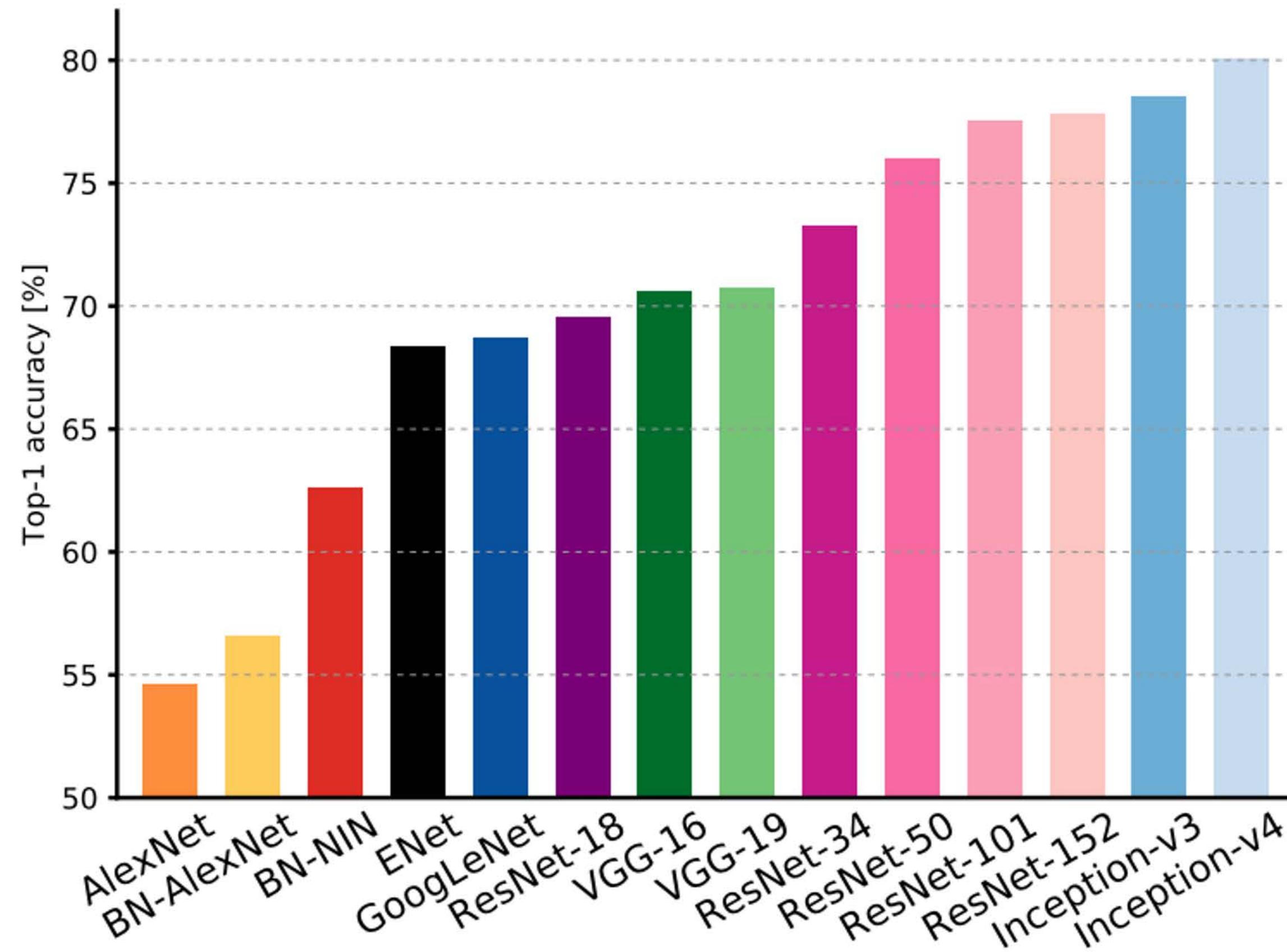
# Comparing Complexity

Inception-v4: ResNet + Inception!



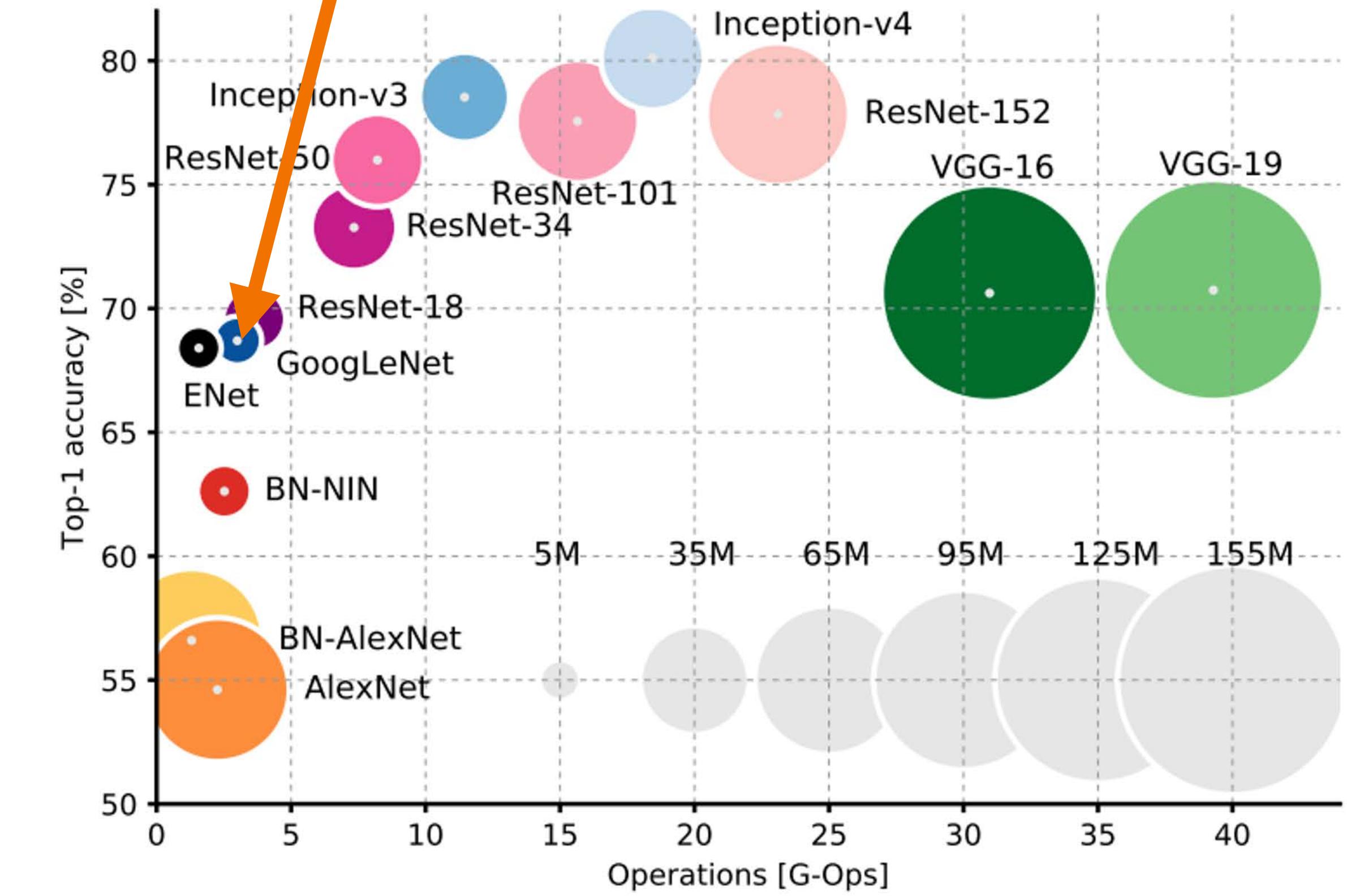
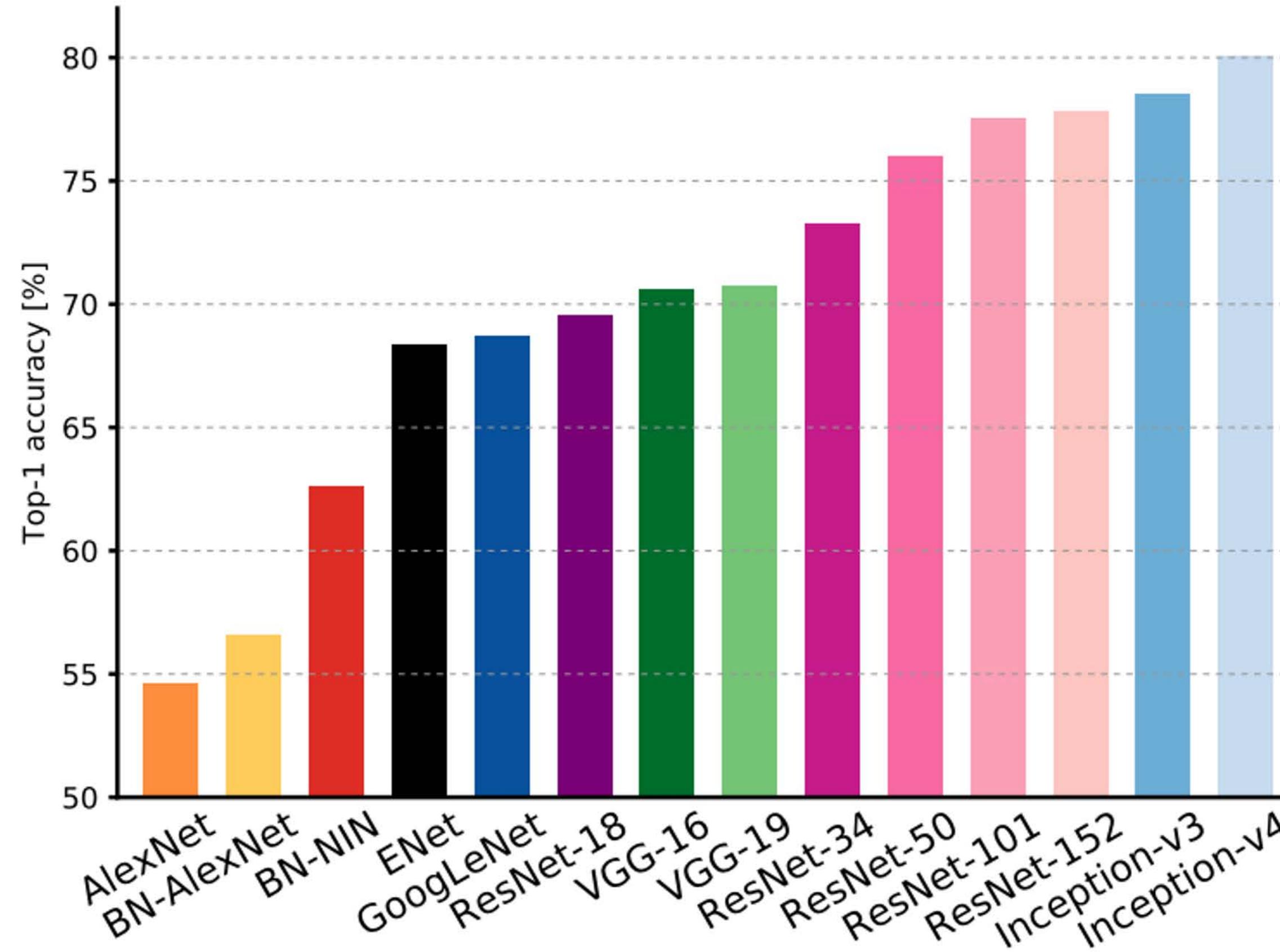
# Comparing Complexity

VGG:  
Highest memory,  
most operations

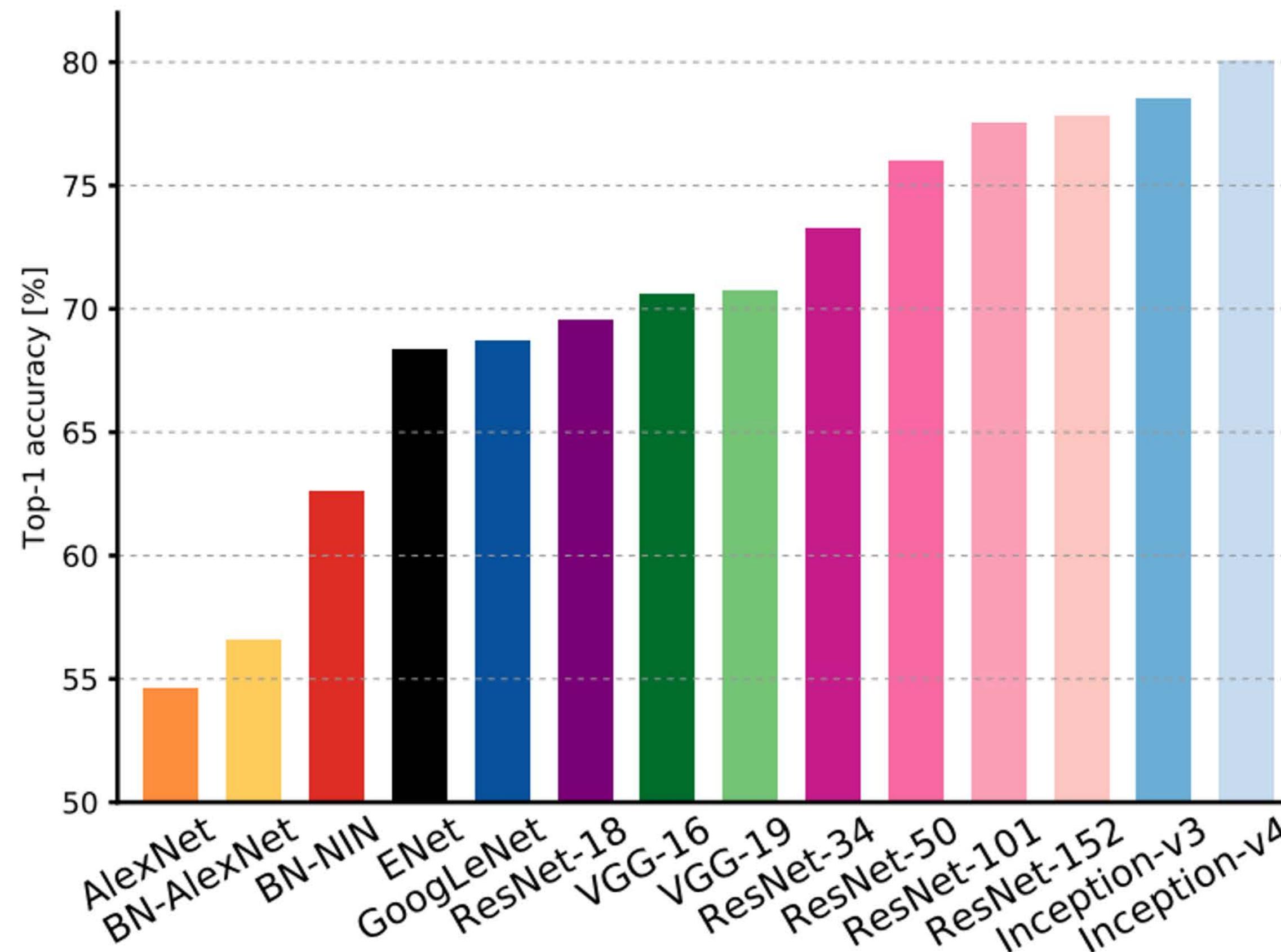


# Comparing Complexity

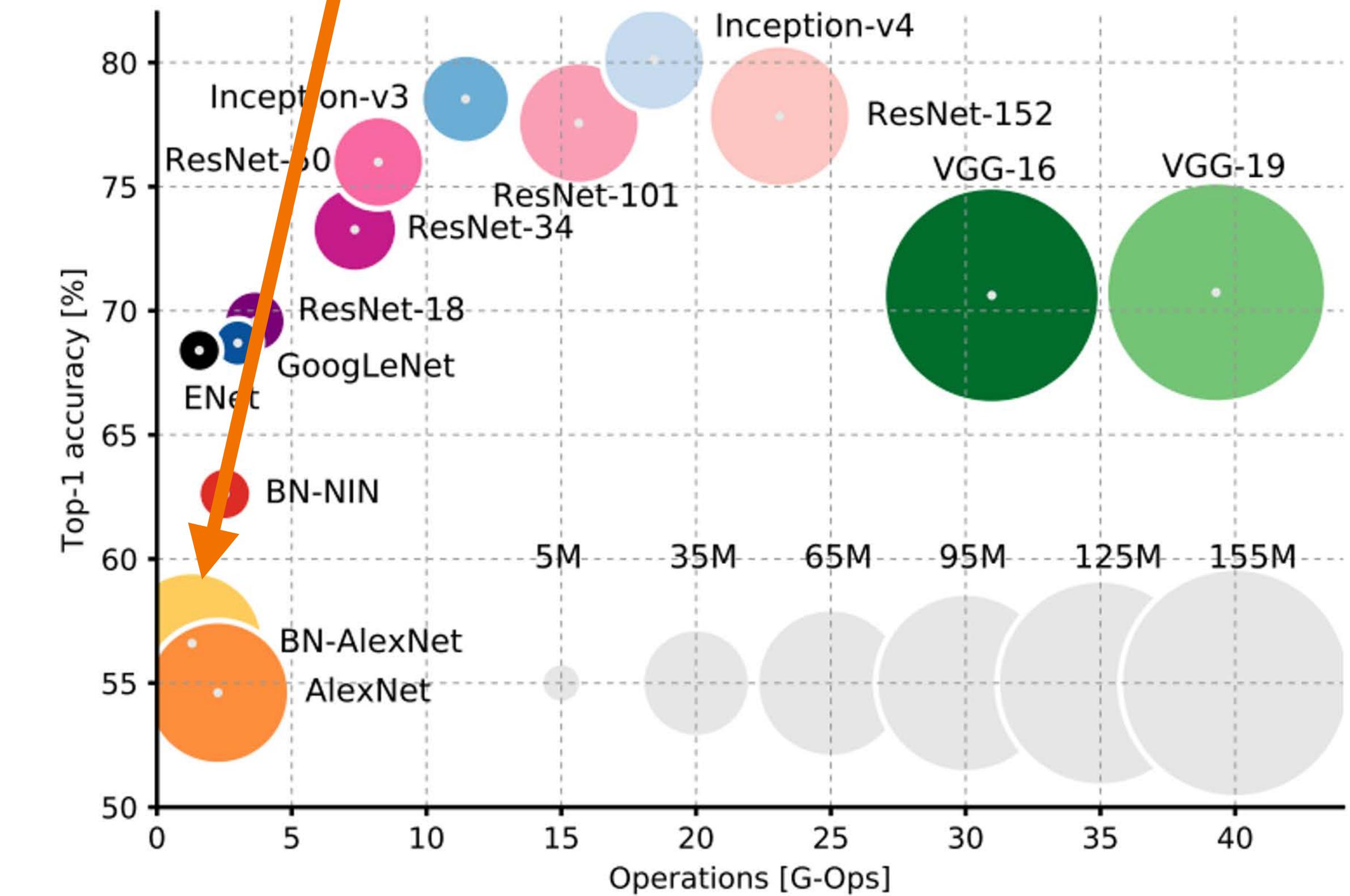
GoogLeNet:  
Very efficient!



# Comparing Complexity

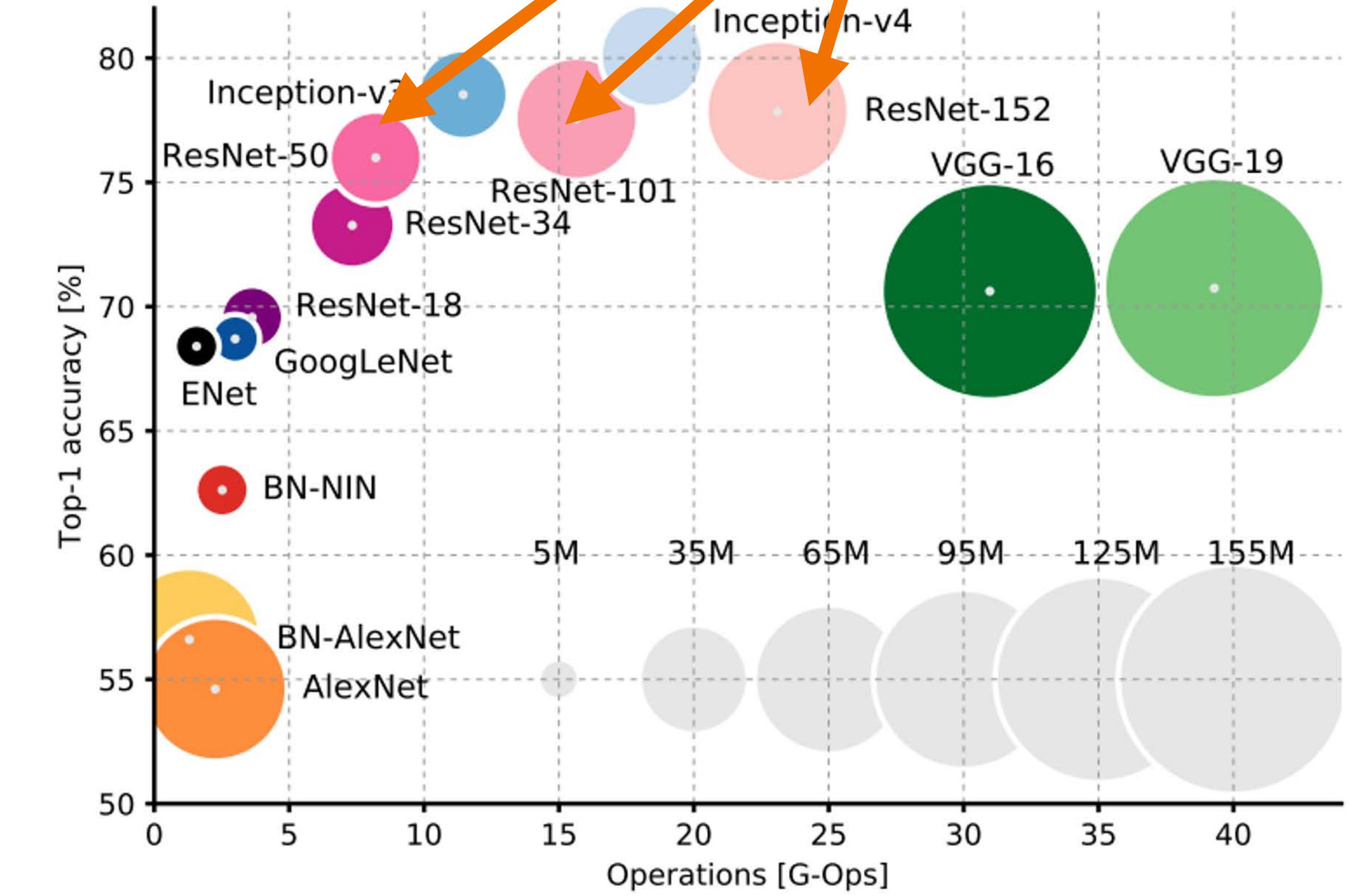
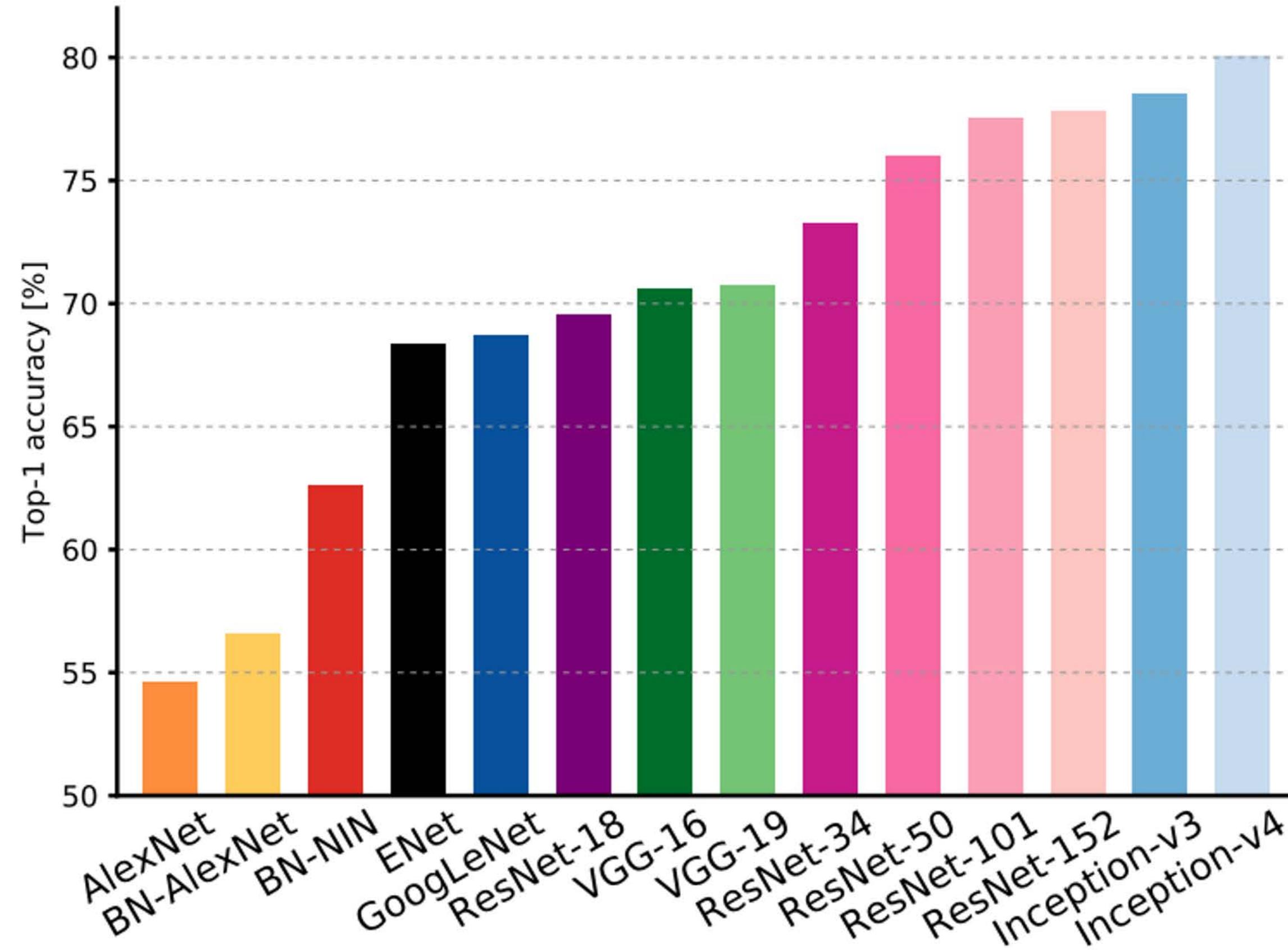


AlexNet: Low  
compute, lots of  
parameters



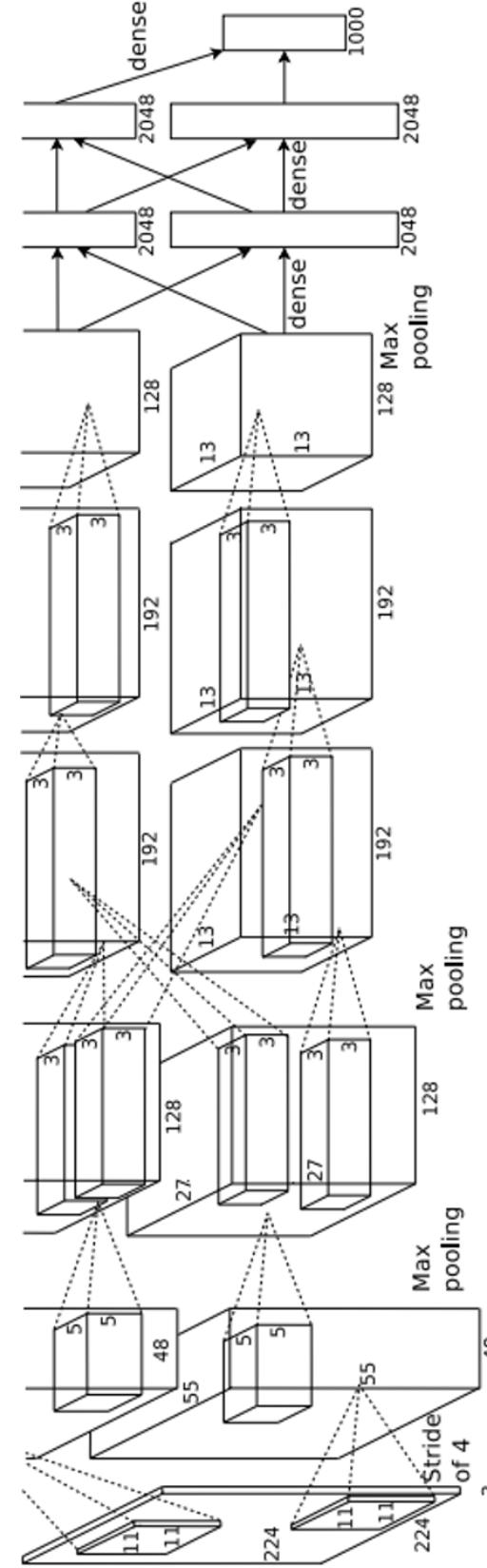
# Comparing Complexity

ResNet: Simple design,  
moderate efficiency, high  
accuracy

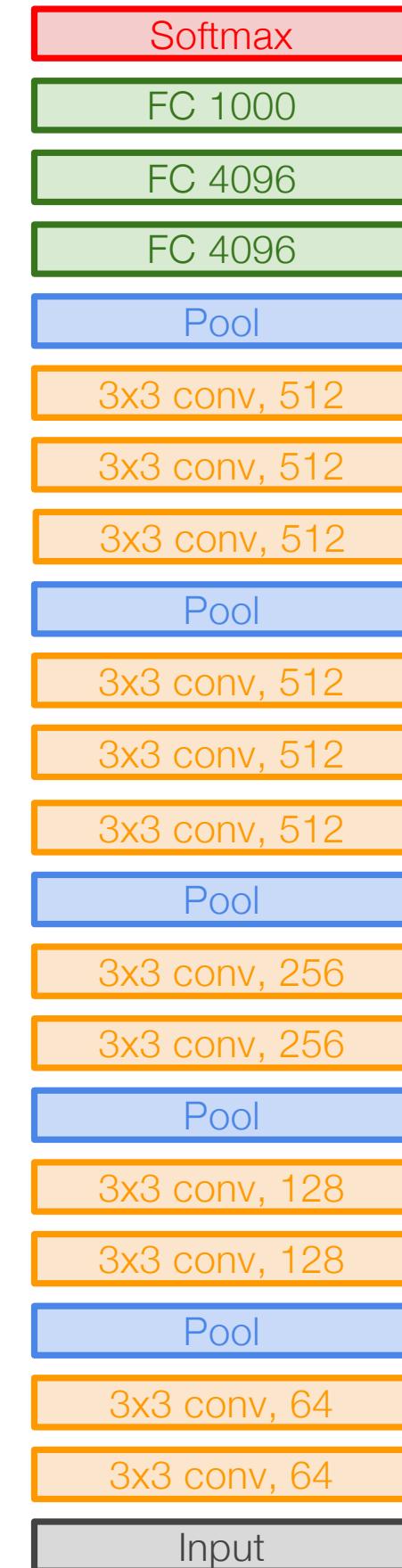




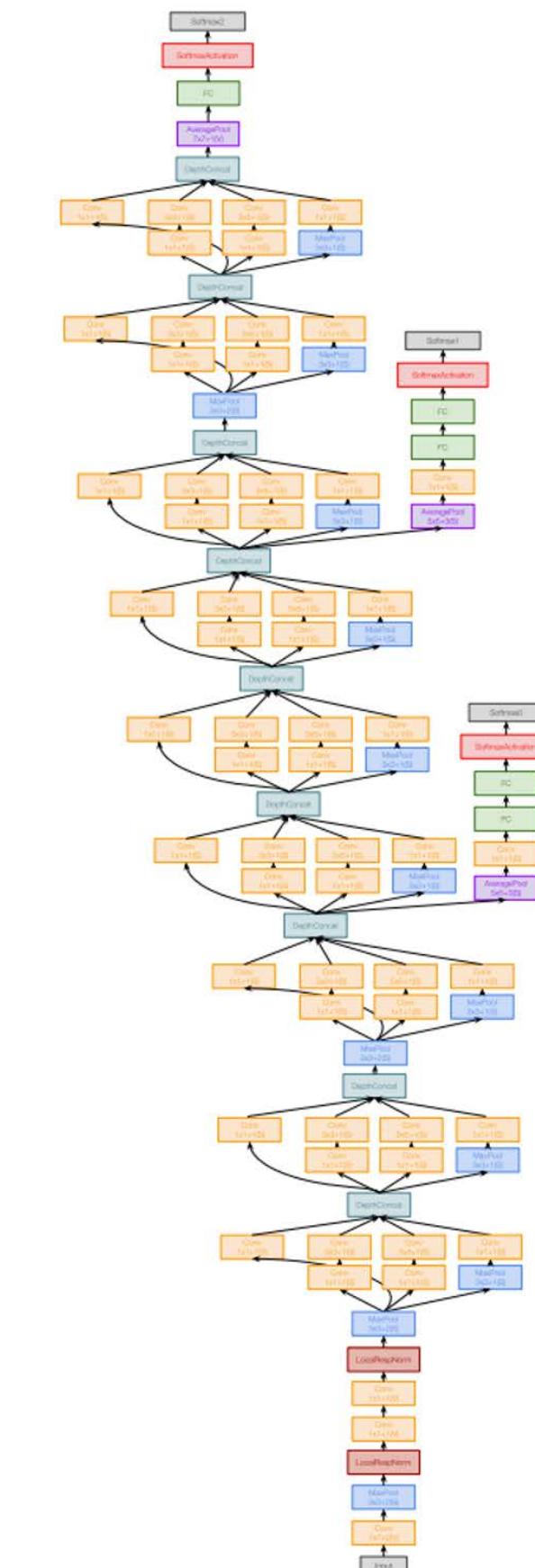
# Recap



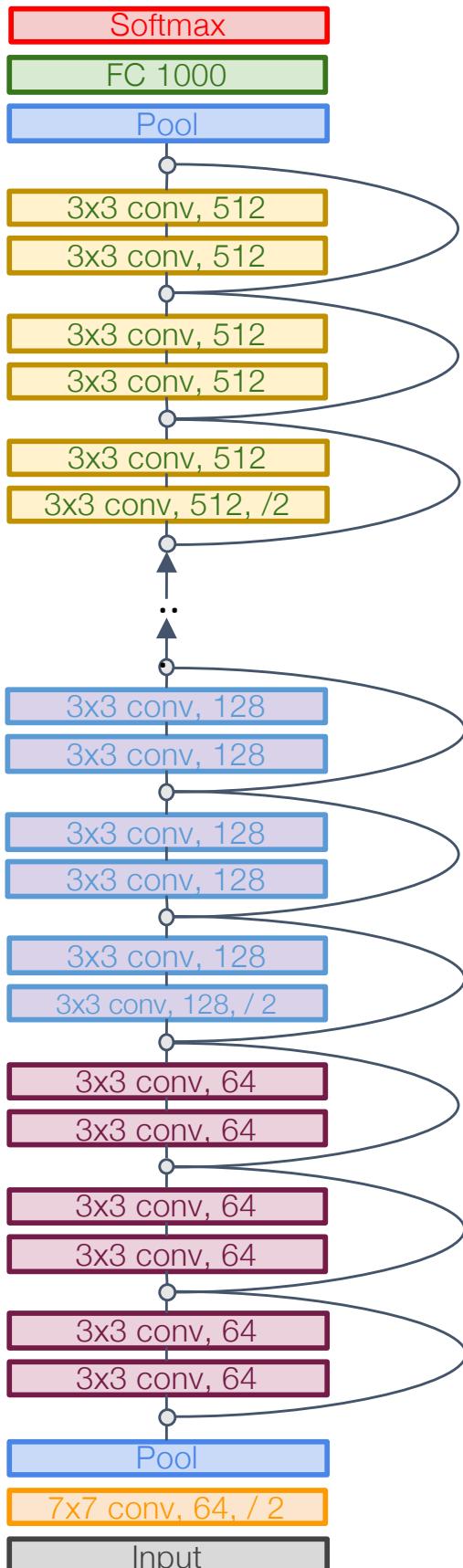
# AlexNet



VGG



# GoogLeNet



## ResNet



# Overview

## 1. One time setup:

- Activation functions, data preprocessing, weight initialization, regularization

Today

## 2. Training dynamics:

- Learning rate schedules; large-batch training; hyperparameter optimization

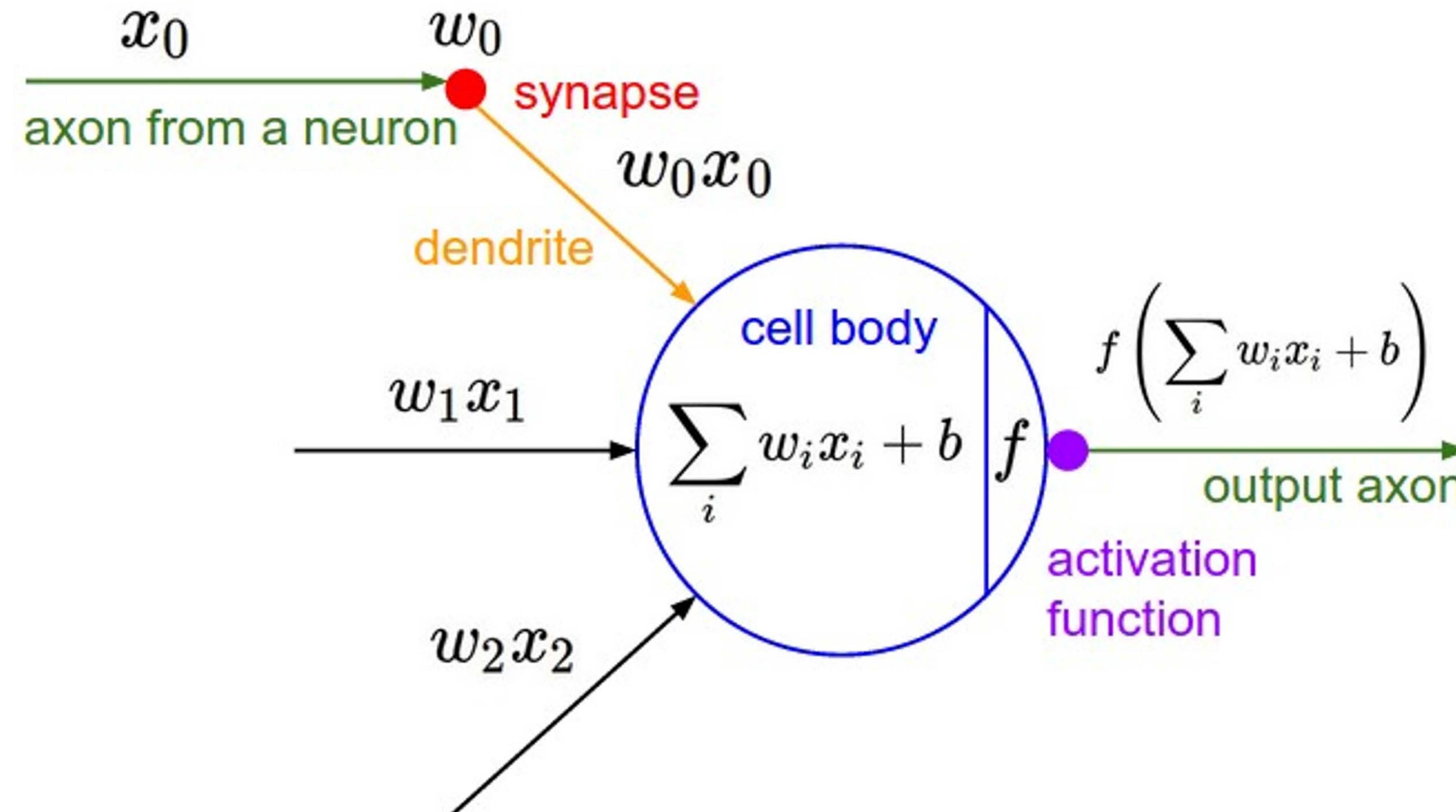
Next time

## 3. After training:

- Model ensembles, transfer learning



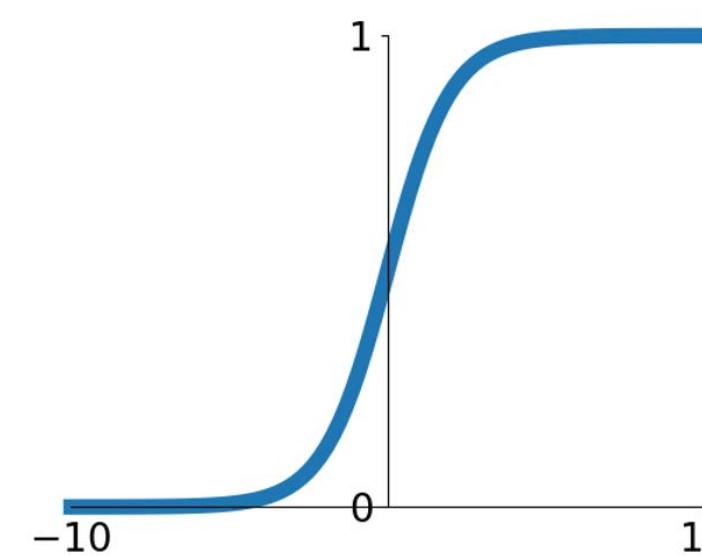
# Activation Functions



# Activation Functions

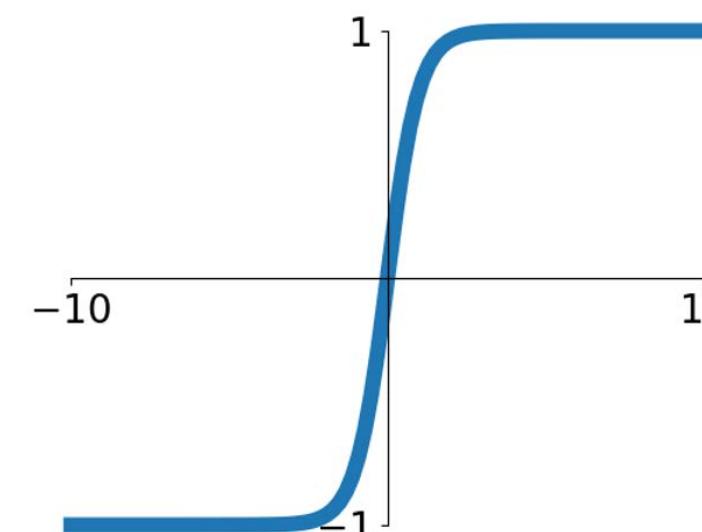
**Sigmoid**

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



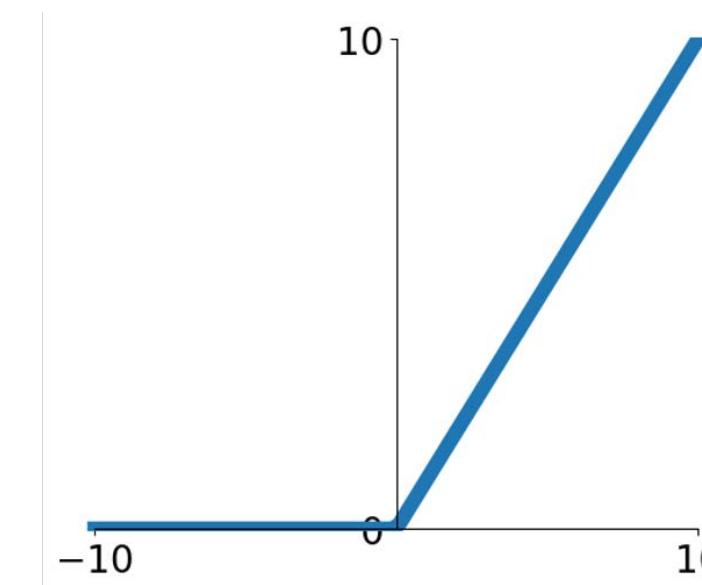
**tanh**

$$\tanh(x)$$



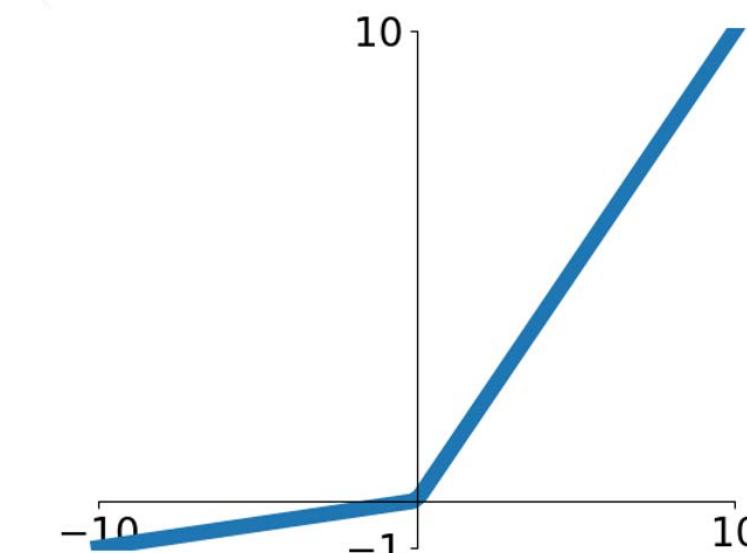
**ReLU**

$$\max(0, x)$$



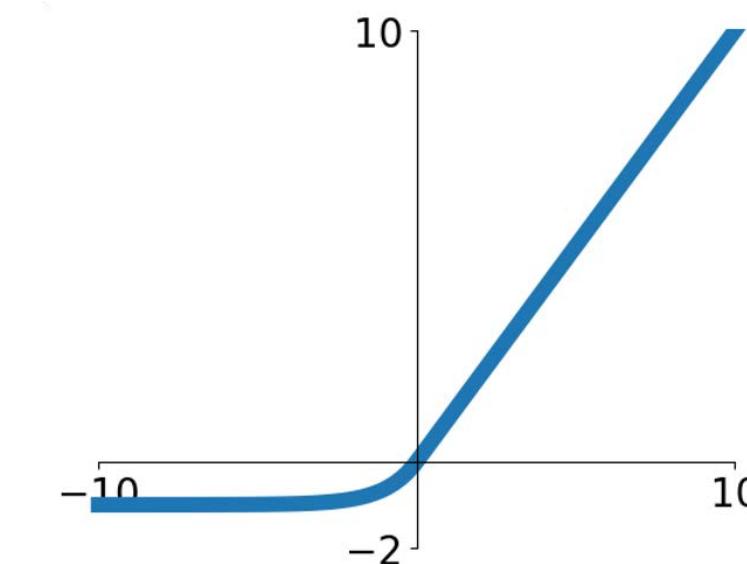
**Leaky ReLU**

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



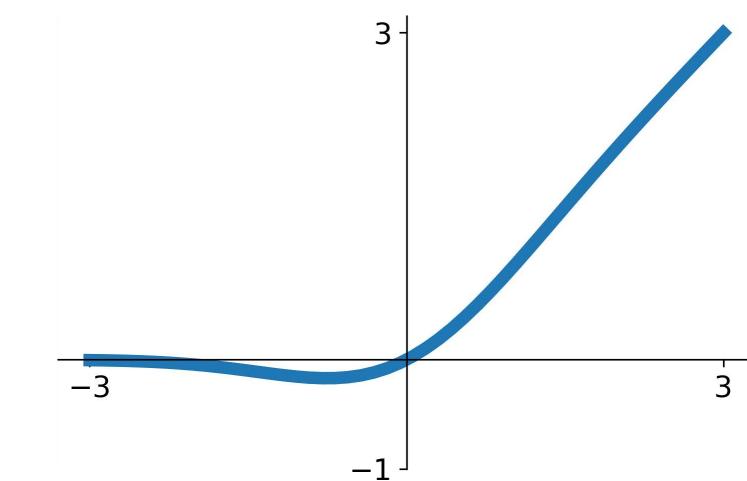
**ELU**

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



**GELU**

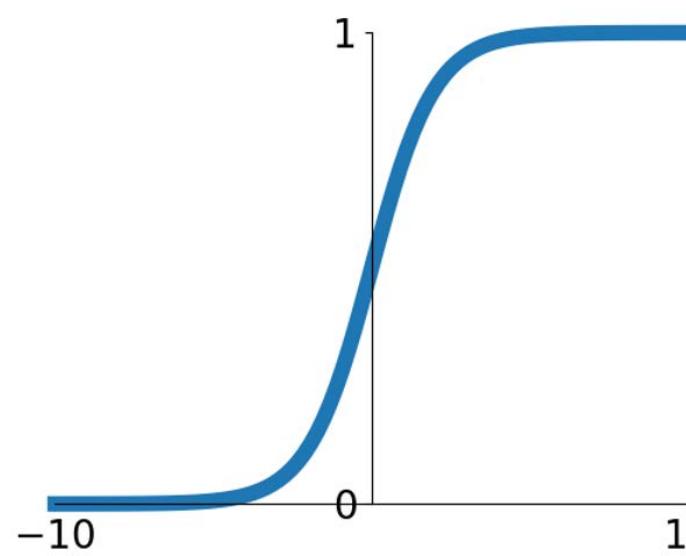
$$\approx x\alpha(1.702x)$$



# Activation Functions: Sigmoid

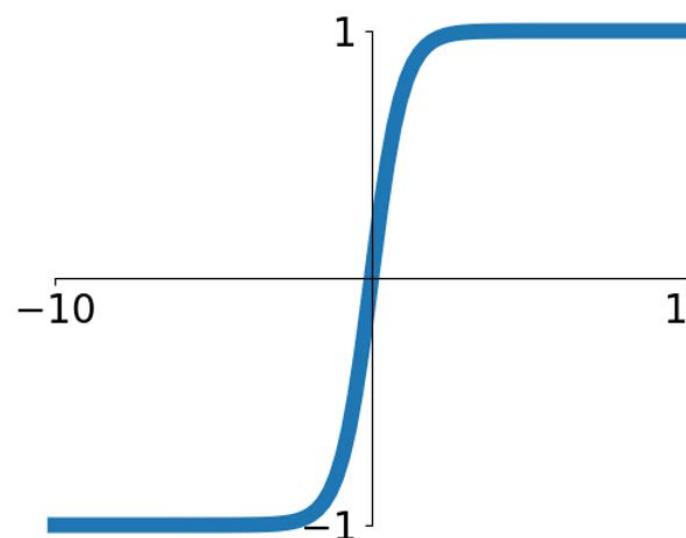
**Sigmoid**

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



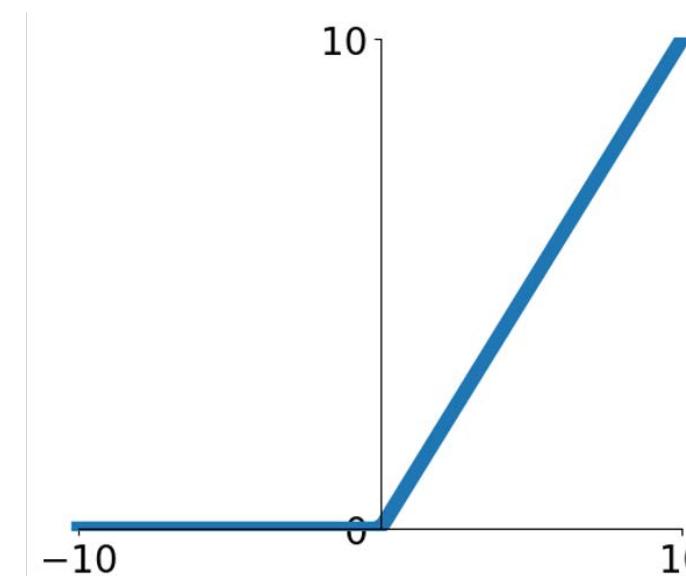
**tanh**

$$\tanh(x)$$



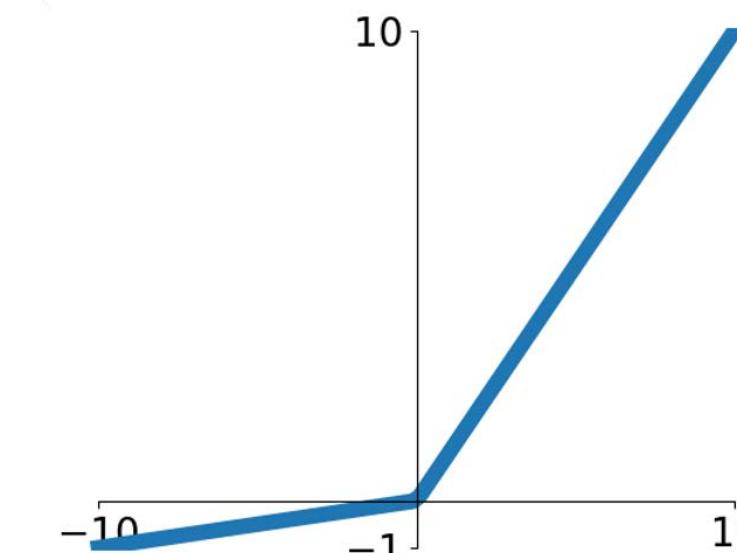
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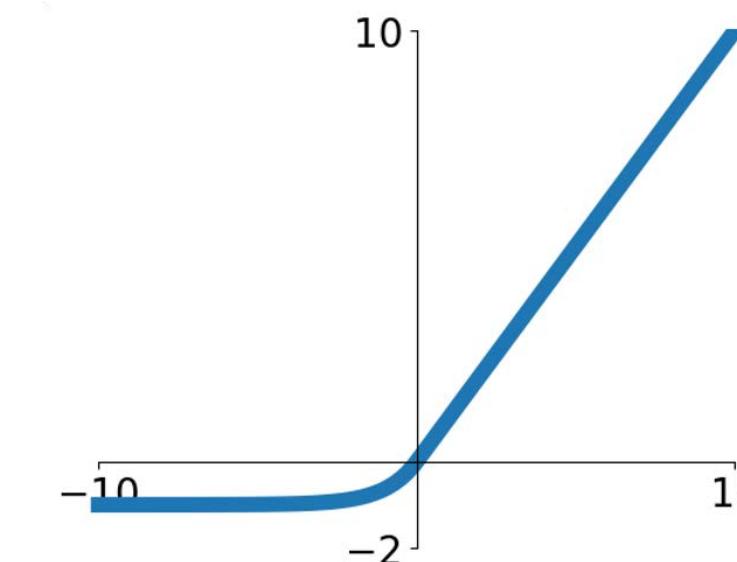
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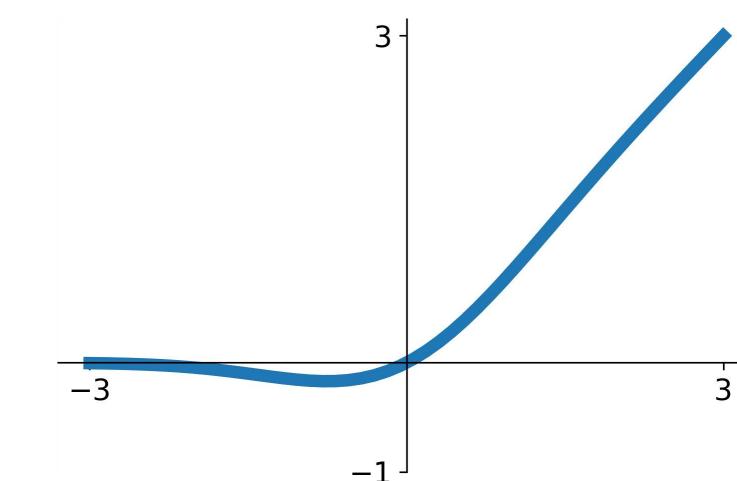
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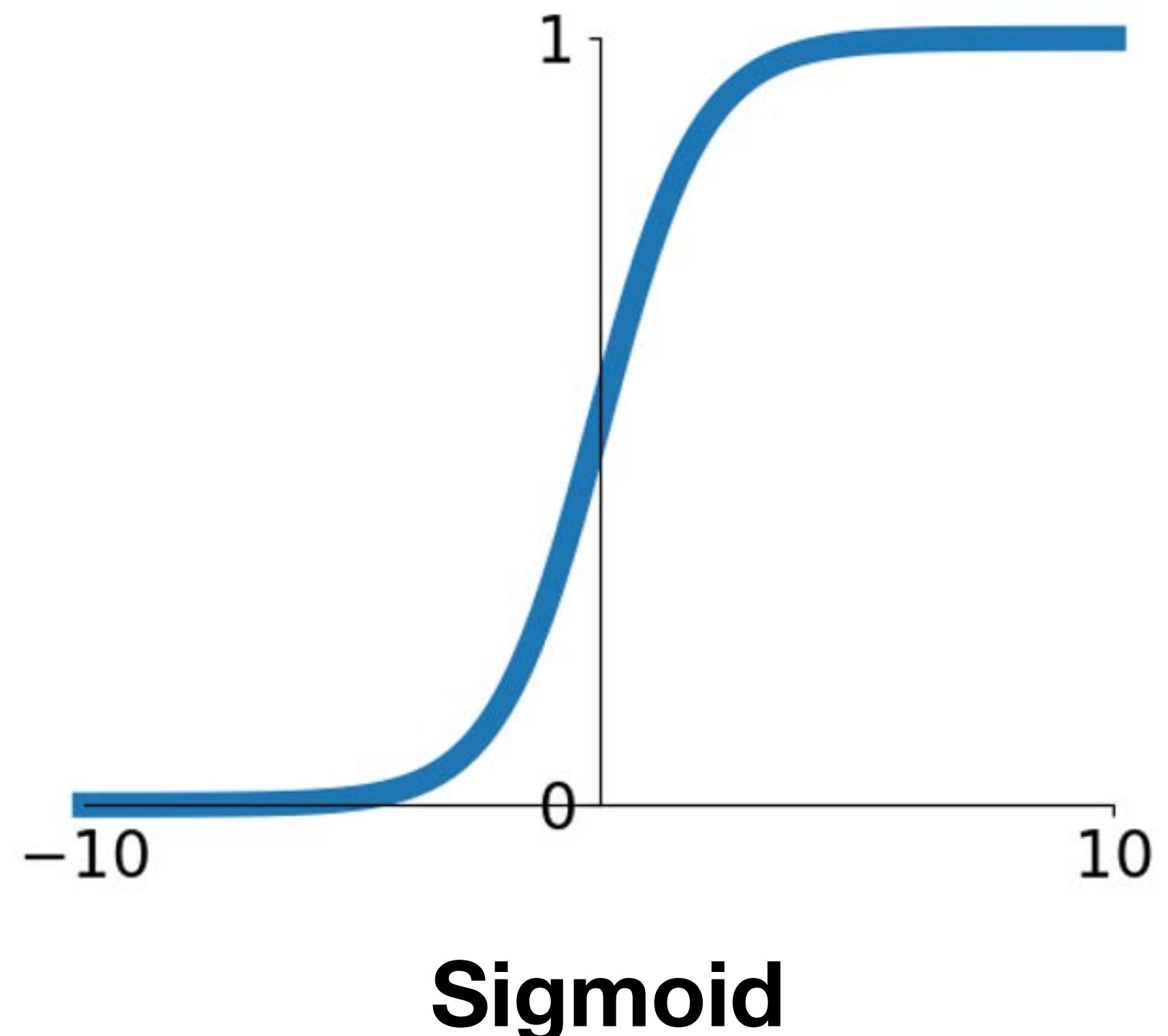


**GELU**

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



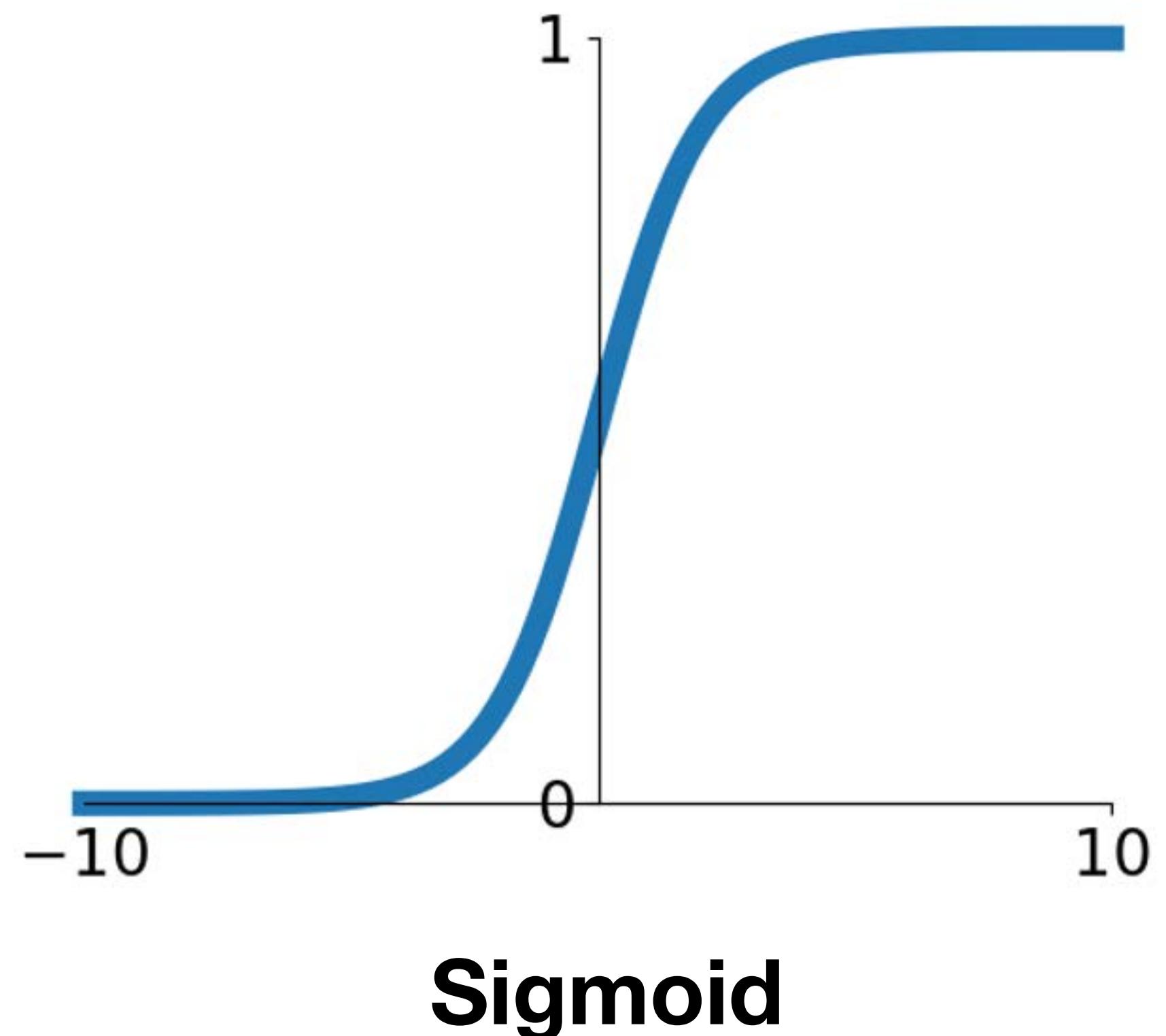
# Activation Functions: Sigmoid



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

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

# Activation Functions: Sigmoid



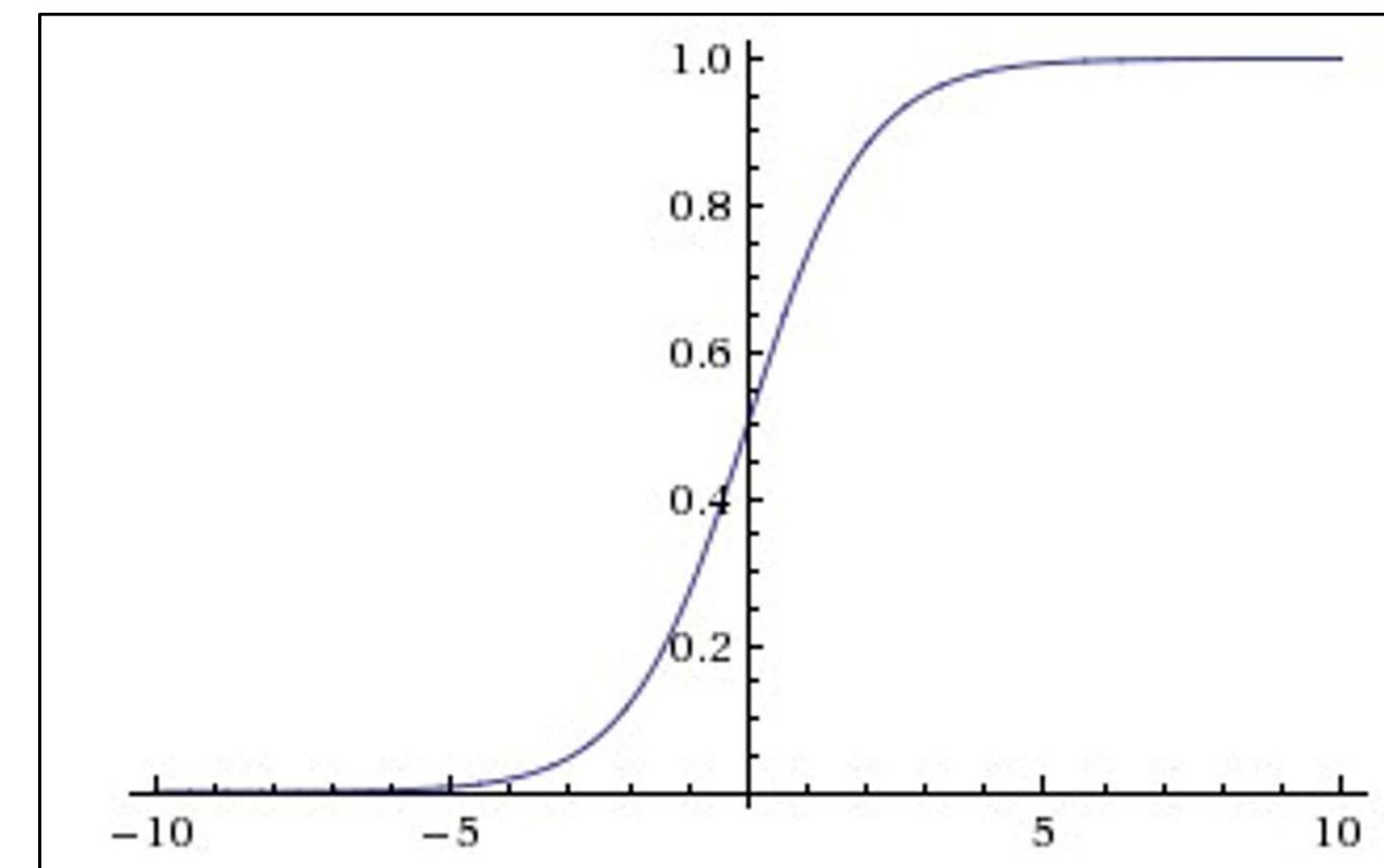
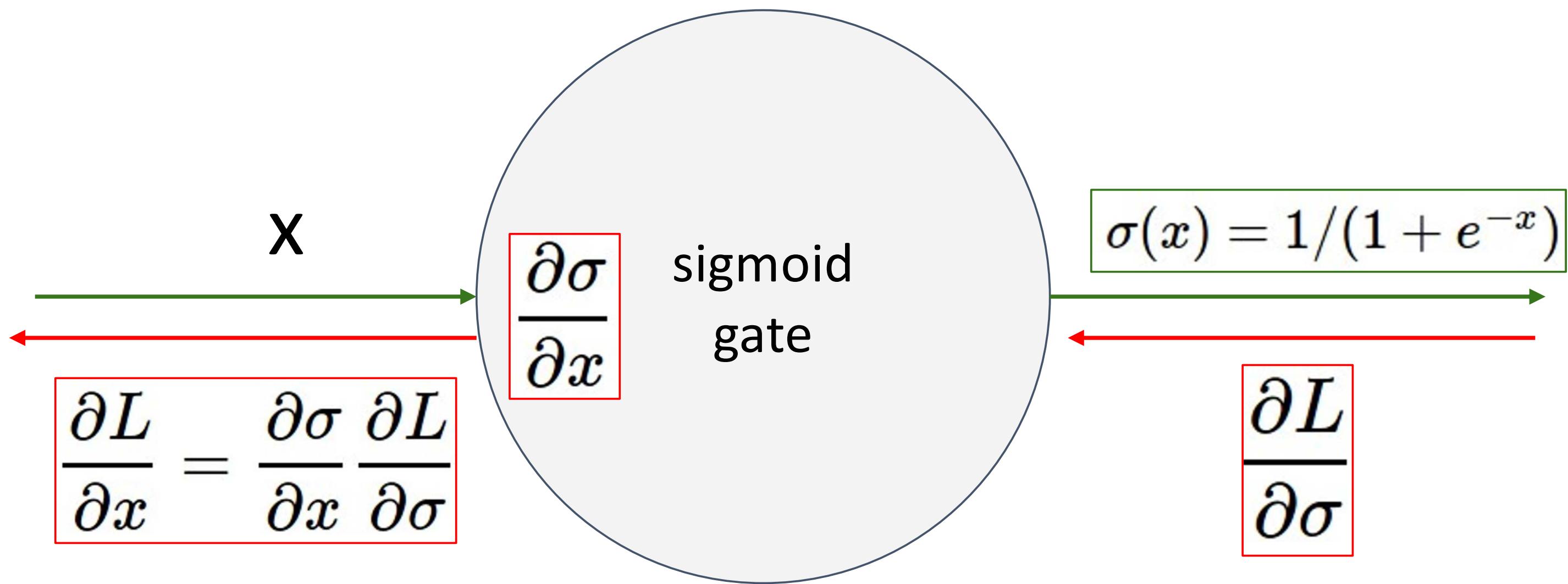
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3 problems:

1. Saturated neurons “kill” the gradients

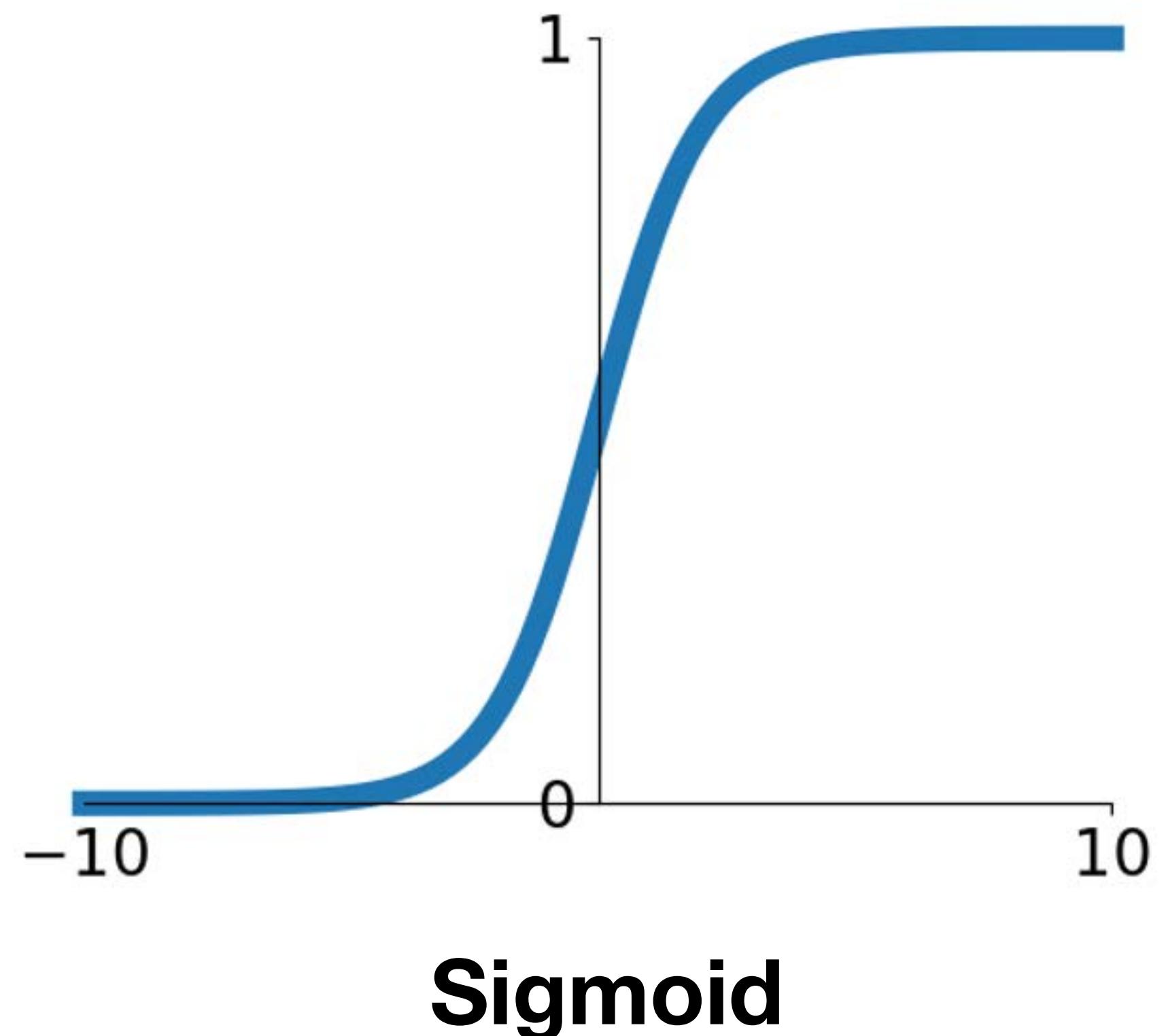
# Activation Functions: Sigmoid



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



# Activation Functions: Sigmoid



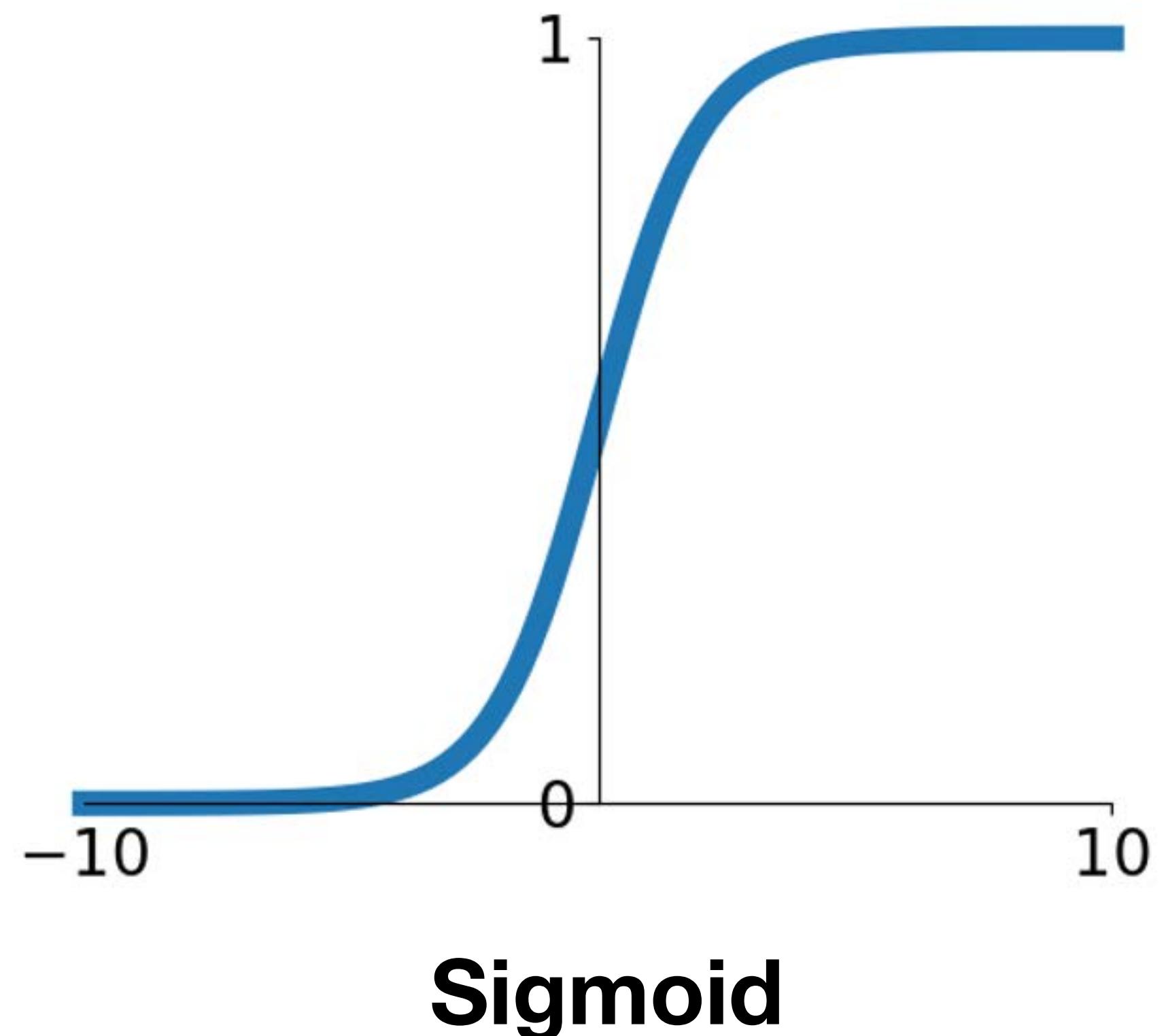
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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

3 problems:

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# Activation Functions: Sigmoid



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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

# Activation Functions: Sigmoid

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  $\ell$   
(before activation)

$w^{(\ell)}, b^{(\ell)}$  are the weights and bias of layer  $\ell$

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



# Activation Functions: Sigmoid

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Local gradient      Upstream gradient

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





# Activation Functions: Sigmoid

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

Local gradient      Upstream gradient

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

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



# Activation Functions: Sigmoid

Consider what happens when nonlinearity is always positive

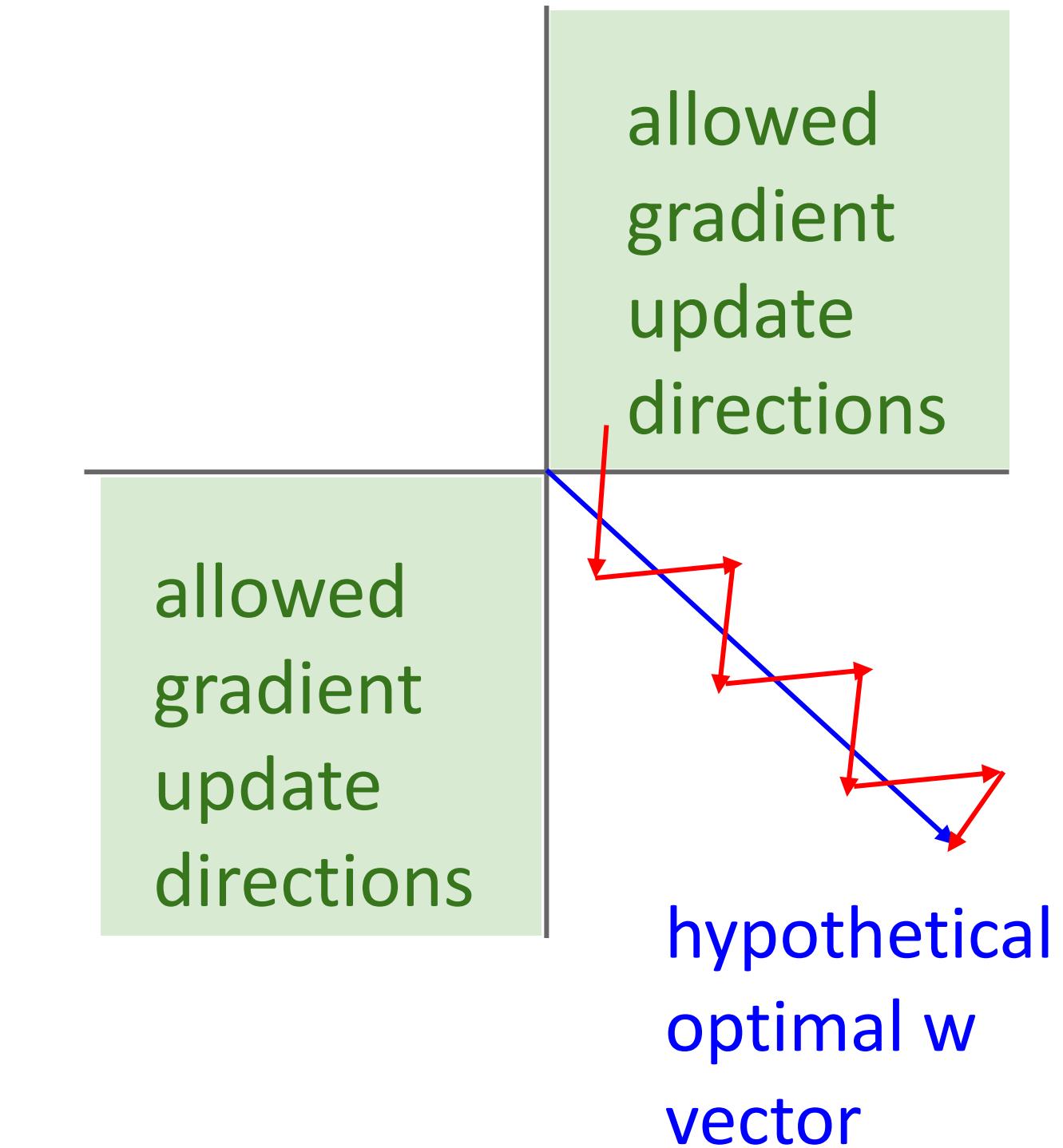
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Gradients on rows of  $w$  can only point in some directions; needs to “zigzag” to move in other directions

# Activation Functions: Sigmoid

Consider what happens when nonlinearity is always positive

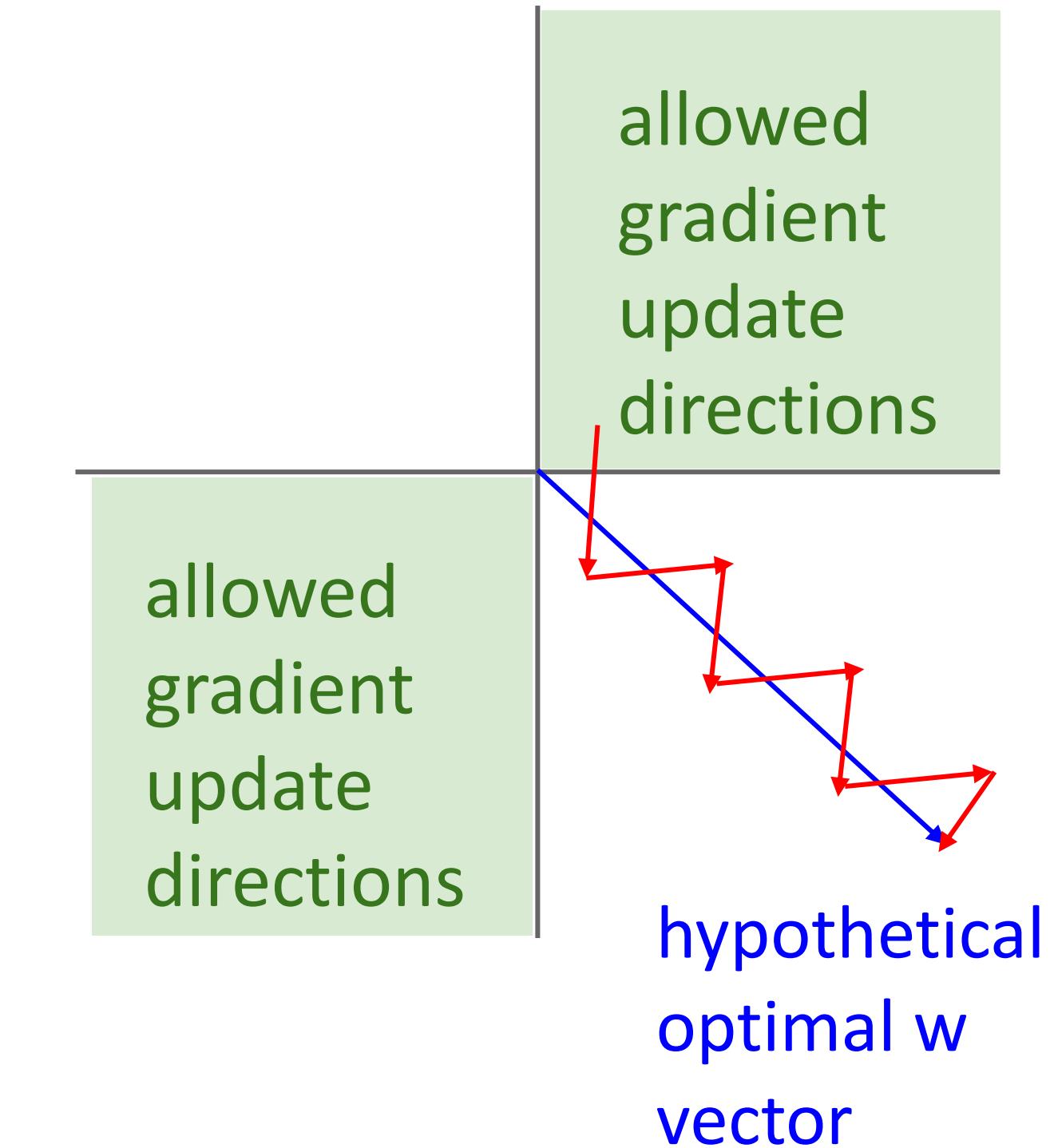
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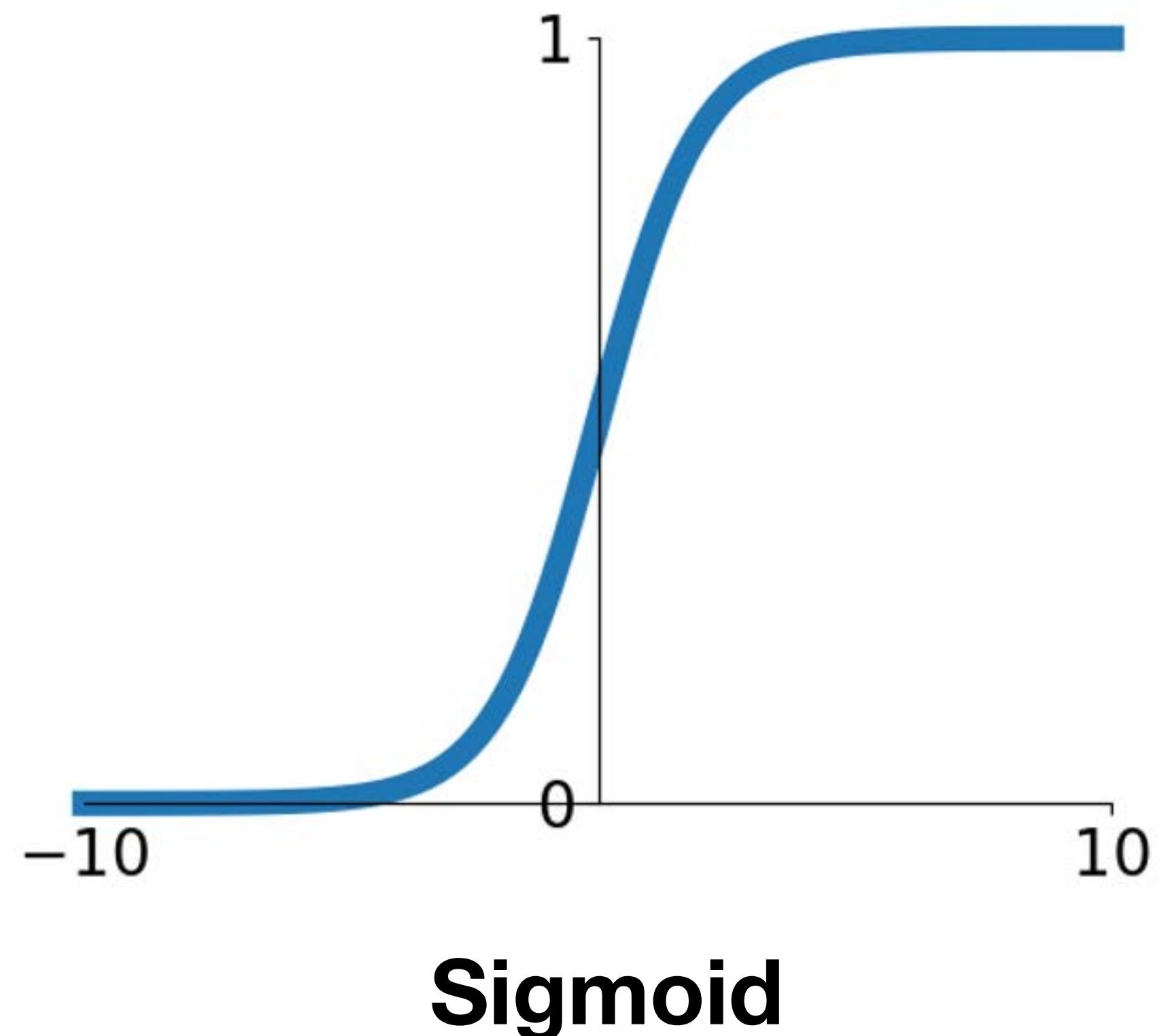
Gradients on all  $w_{i,j}^{(\ell)}$  have the same sign as upstream gradient  $\partial L / \partial h_i^{(\ell)}$



Not that bad in practice:

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

# Activation Functions: Sigmoid



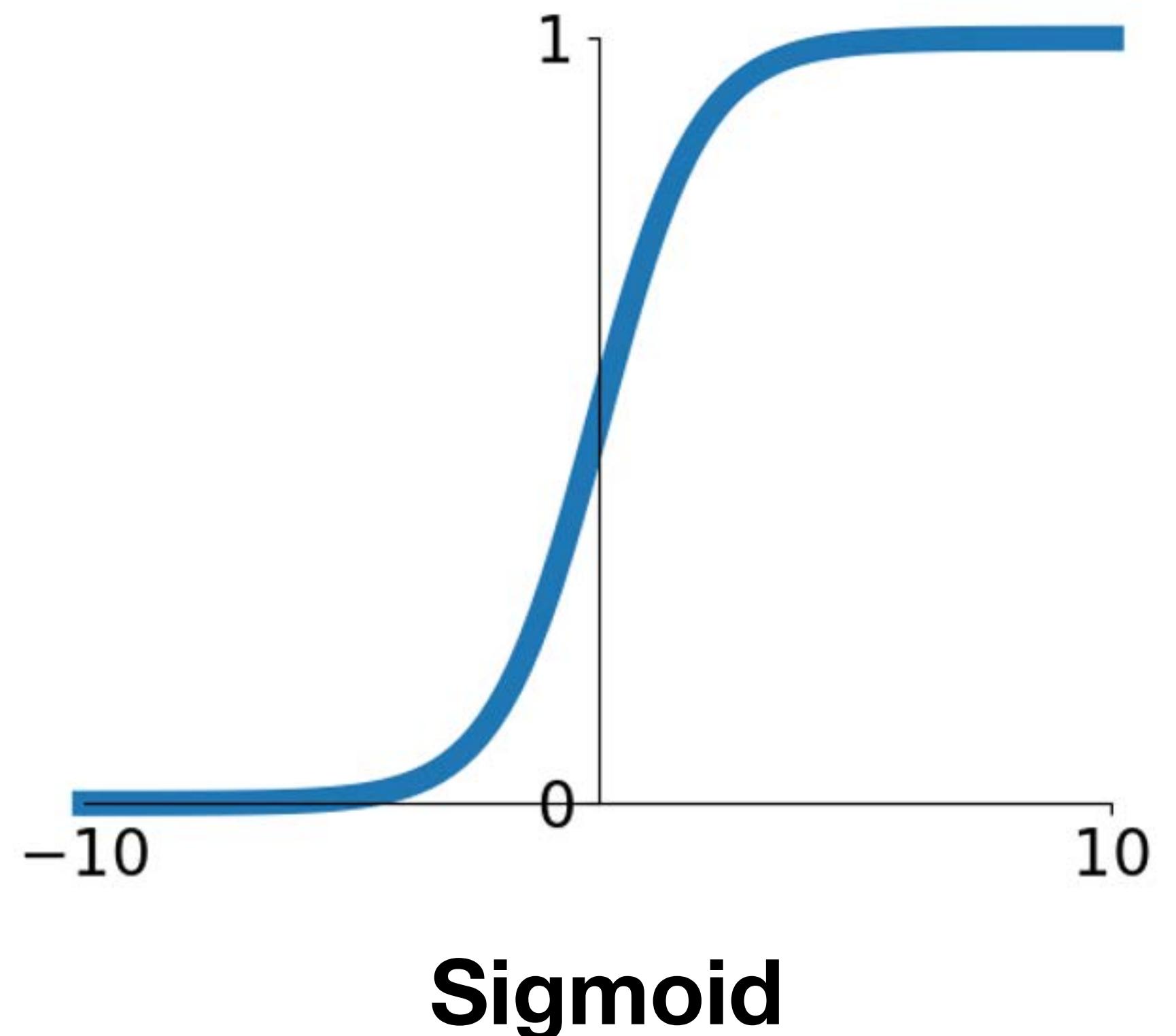
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- Squashes numbers to range [0, 1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

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

# Activation Functions: Sigmoid



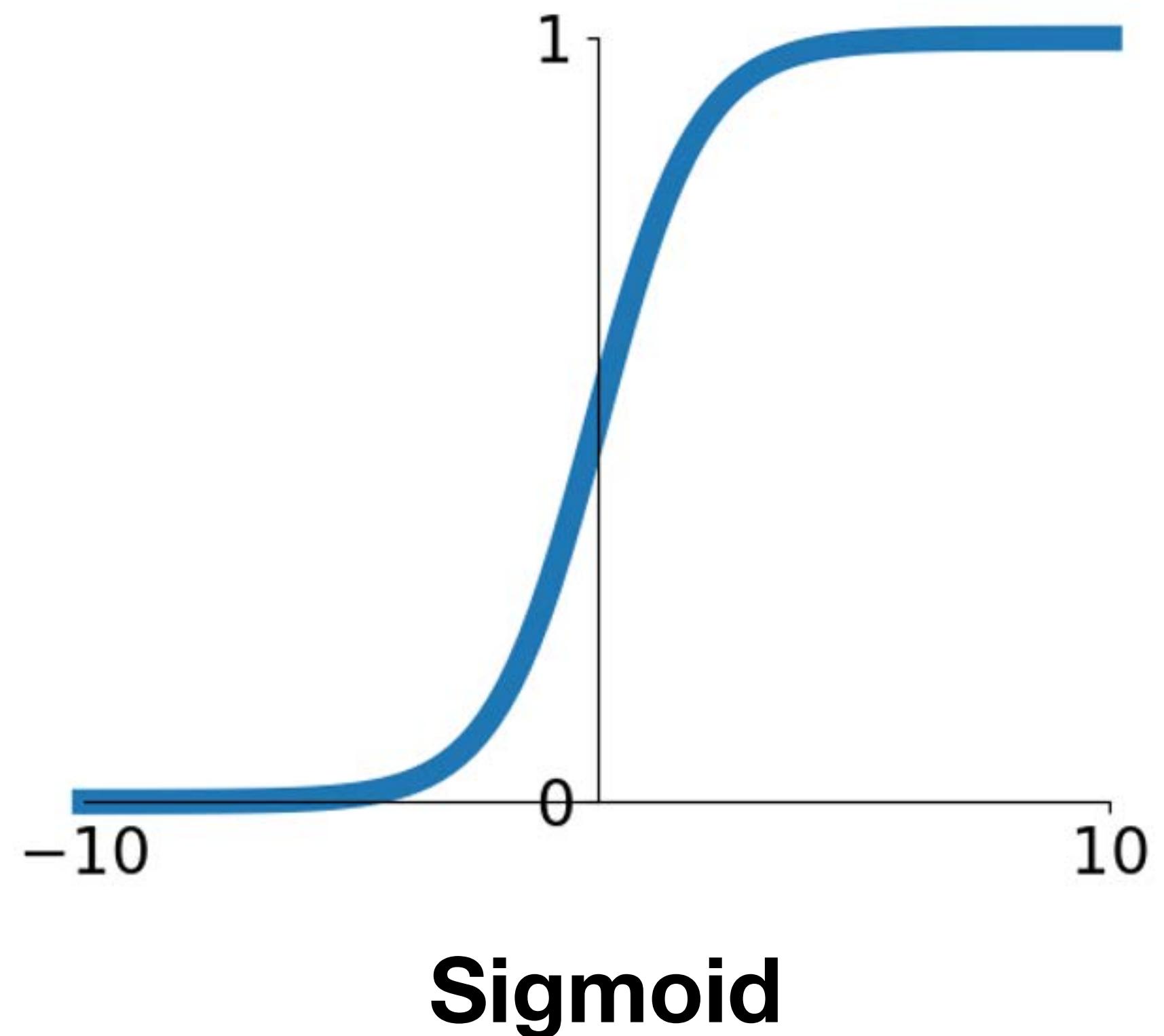
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3 problems:

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2. Sigmoid outputs are not zero-centered
3. `exp()` is a bit compute expensive

# Activation Functions: Sigmoid



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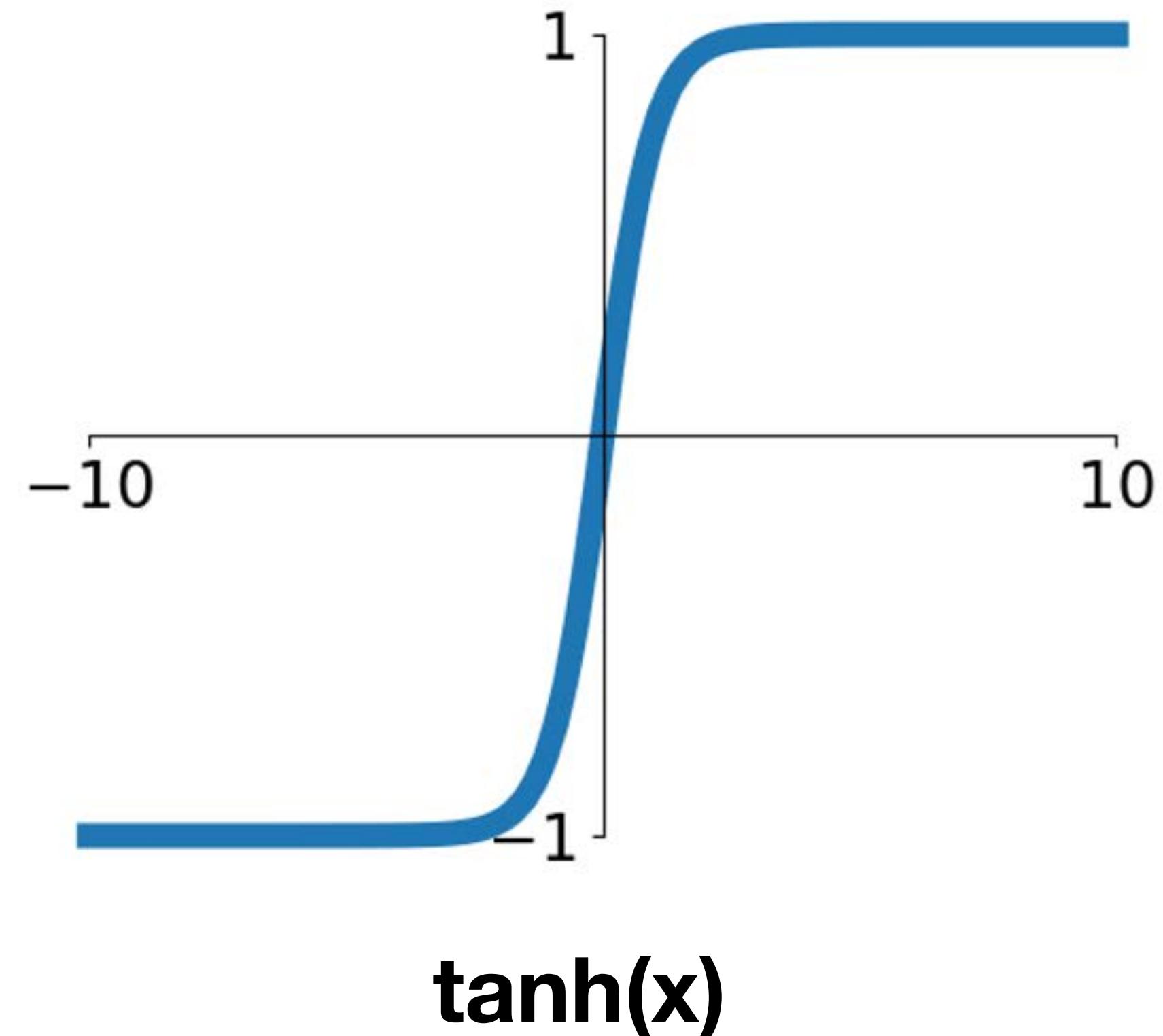
- Squashes numbers to range [0, 1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems: **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

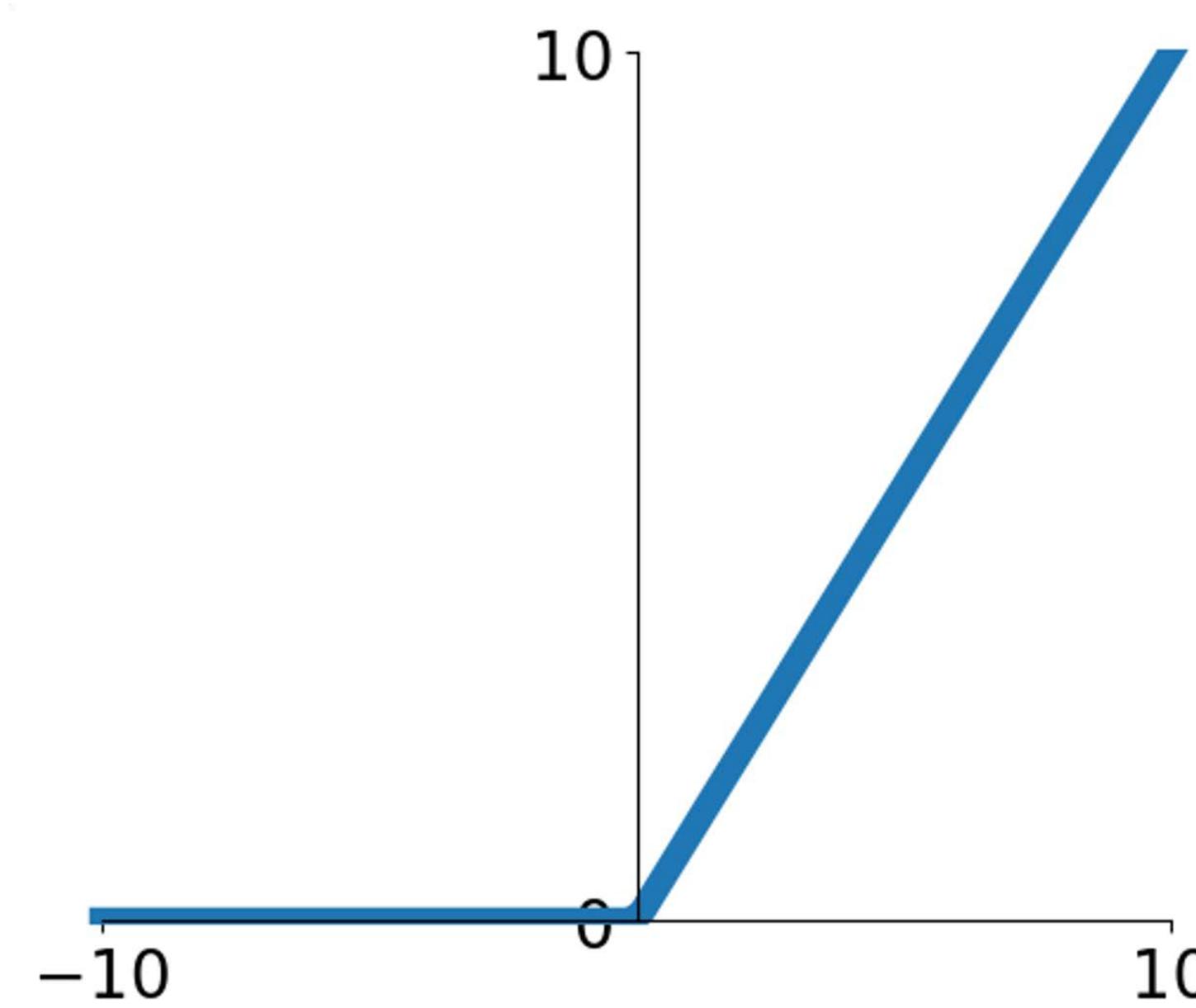
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- Squashes numbers to range  $[-1, 1]$
- Zero centered (nice)
- Still kills gradients when saturated :(

# Activation Functions: ReLU

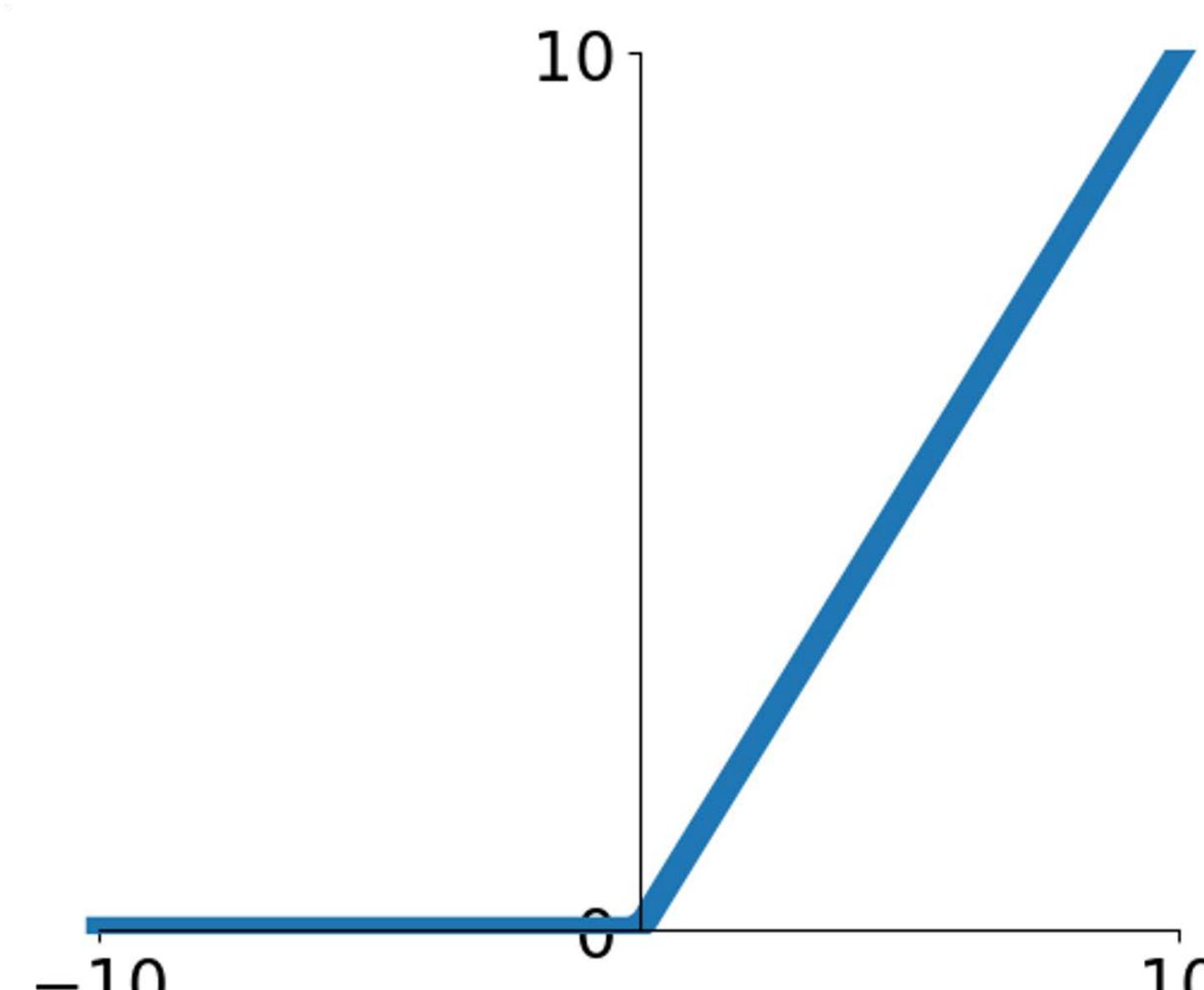
---



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

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

# Activation Functions: ReLU



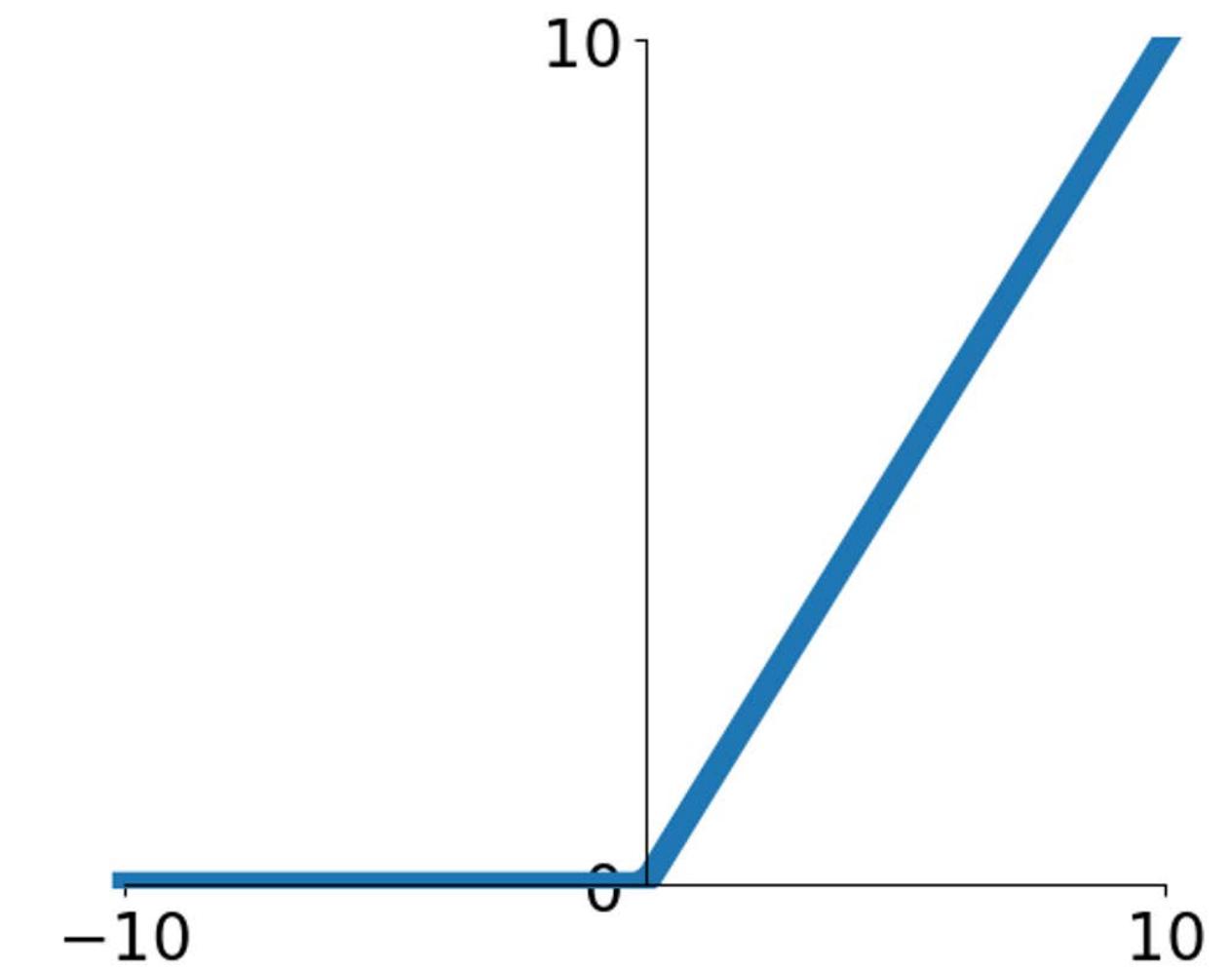
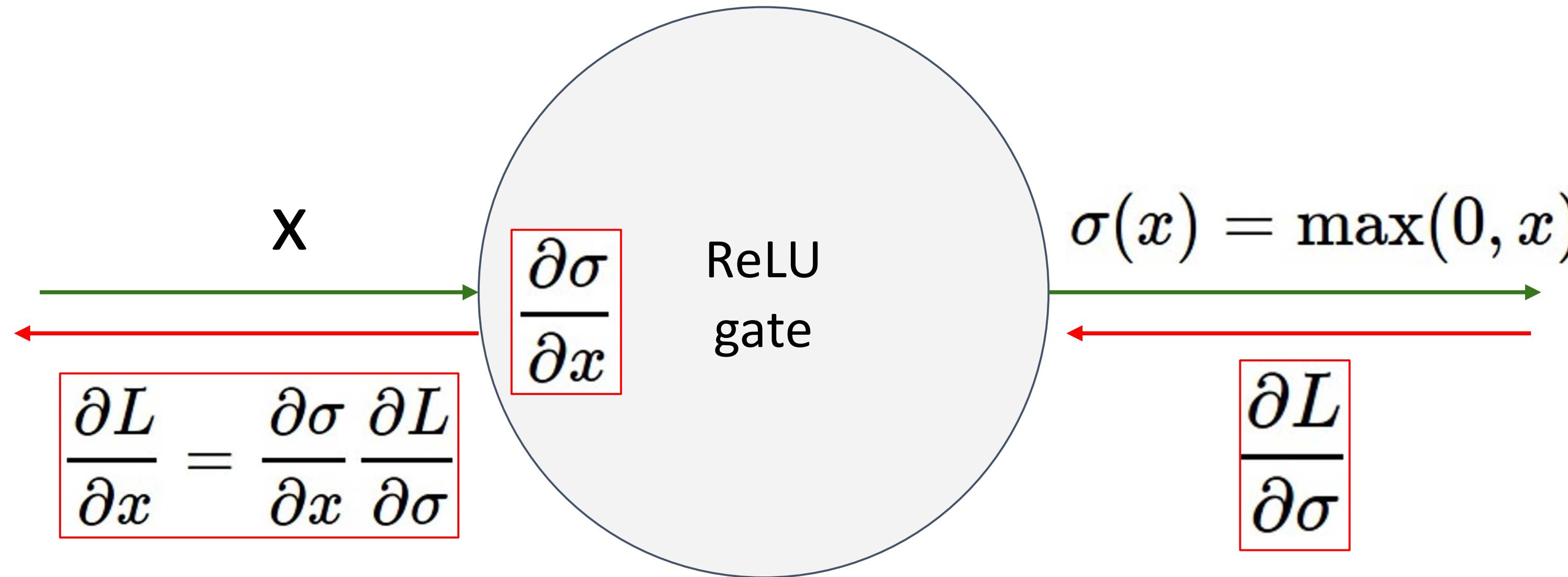
**ReLU**  
(Rectified Linear Unit)

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

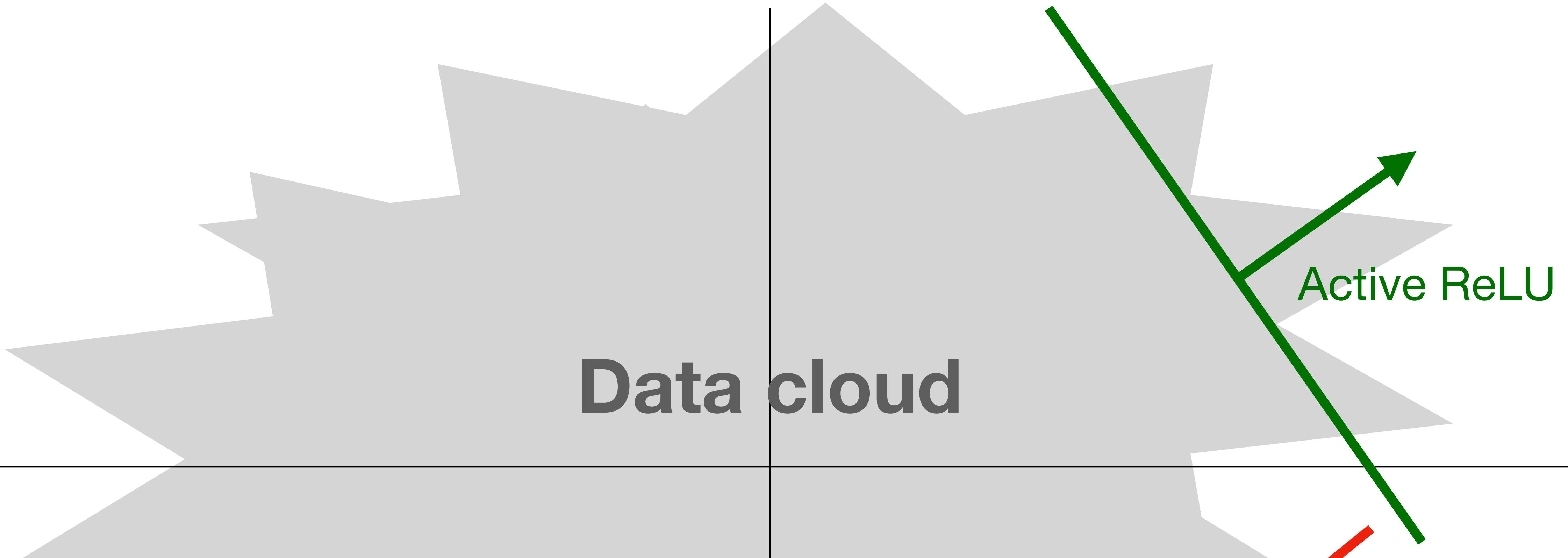
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid and tanh in practice (e.g. 6x)
- Not zero-centered output
- An annoyance:

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

# Activation Functions: ReLU



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





## Data cloud

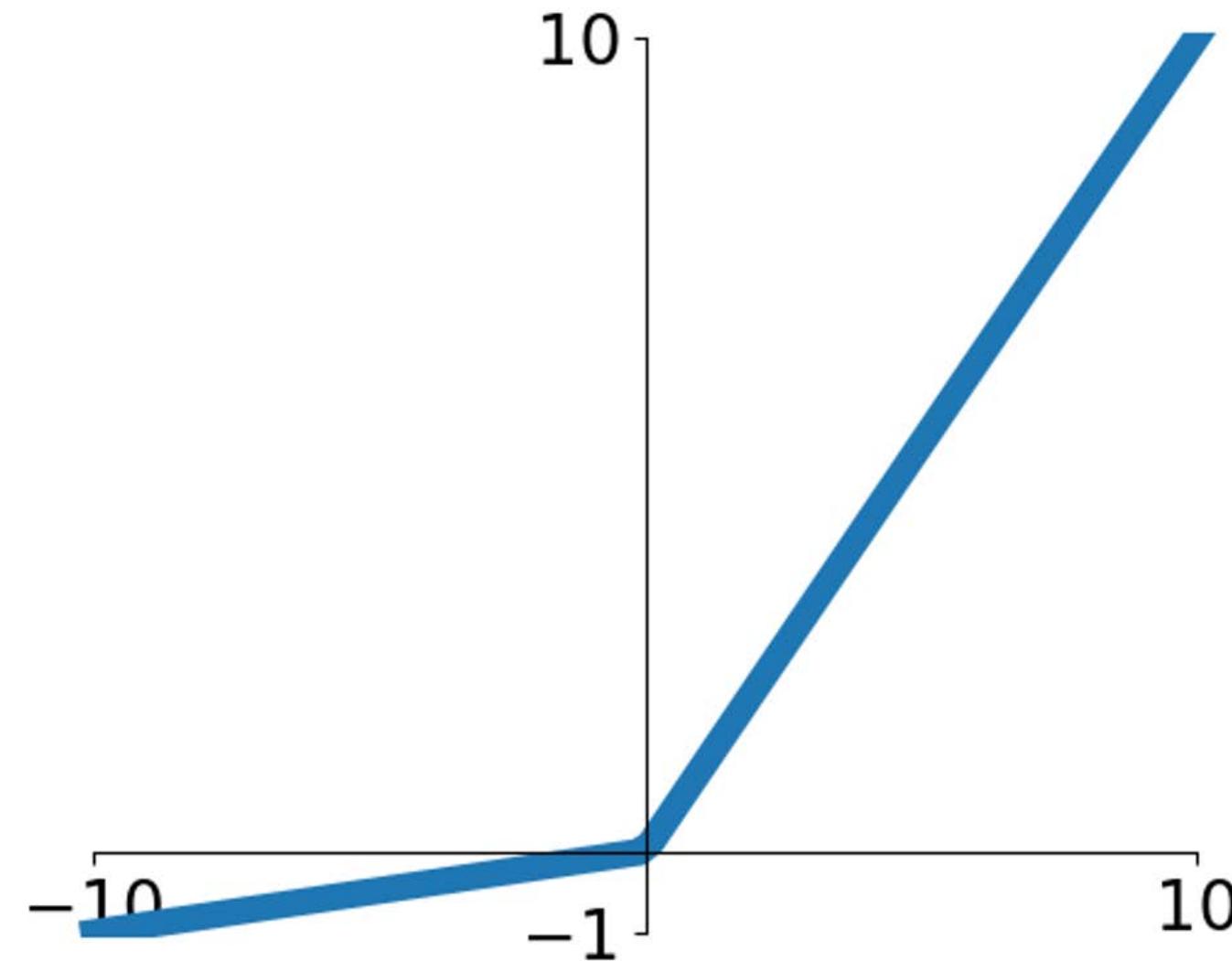
=> Sometimes initialize  
ReLU neurons with slightly  
positive biases (e.g. 0.01)

Active ReLU

Dead ReLU will never  
activate  
=> never update



# Activation Functions: Leaky ReLU



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

## Leaky ReLU

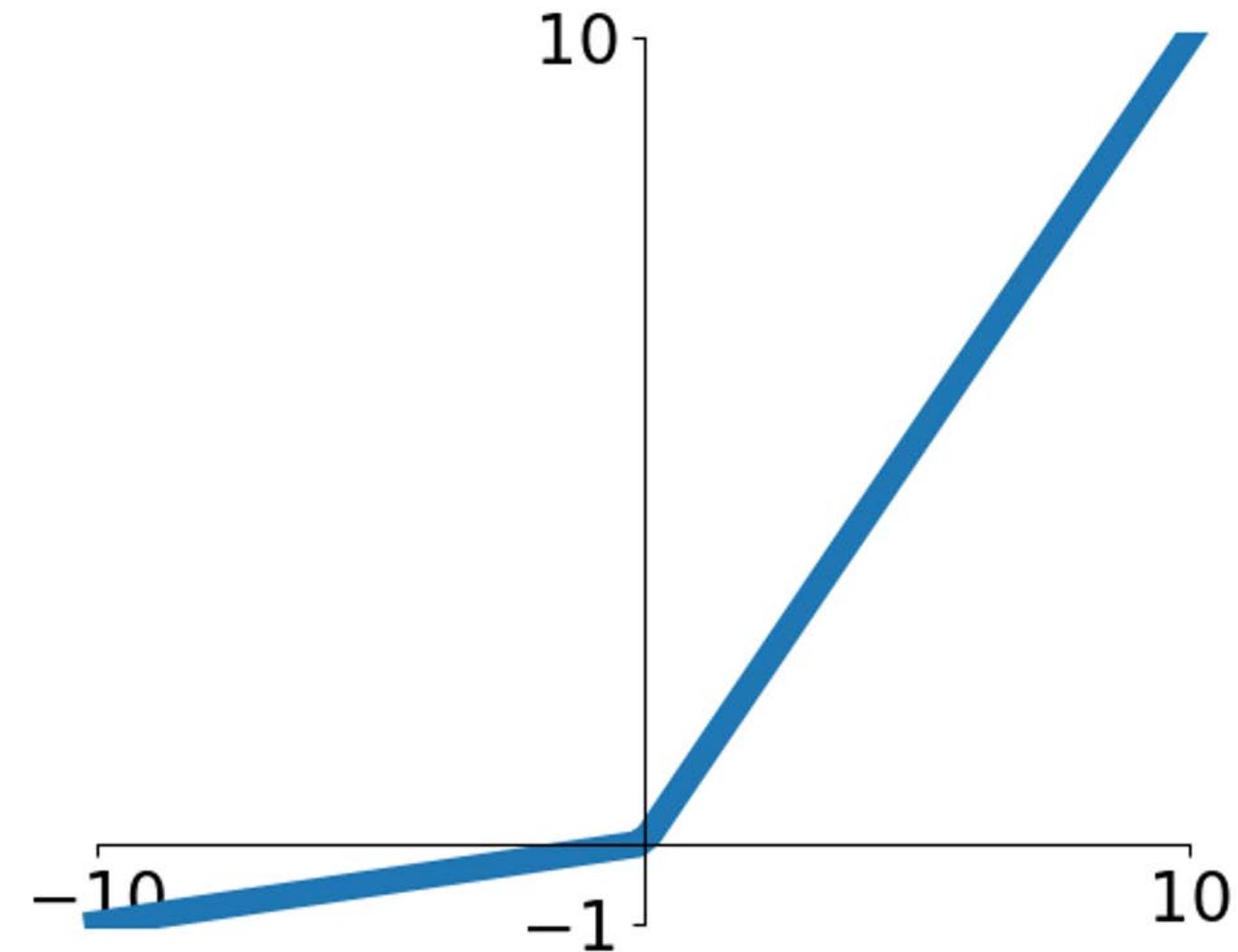
$$f(x) = \max(\alpha x, x)$$

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

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



# Activation Functions: Leaky ReLU



## Leaky ReLU

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

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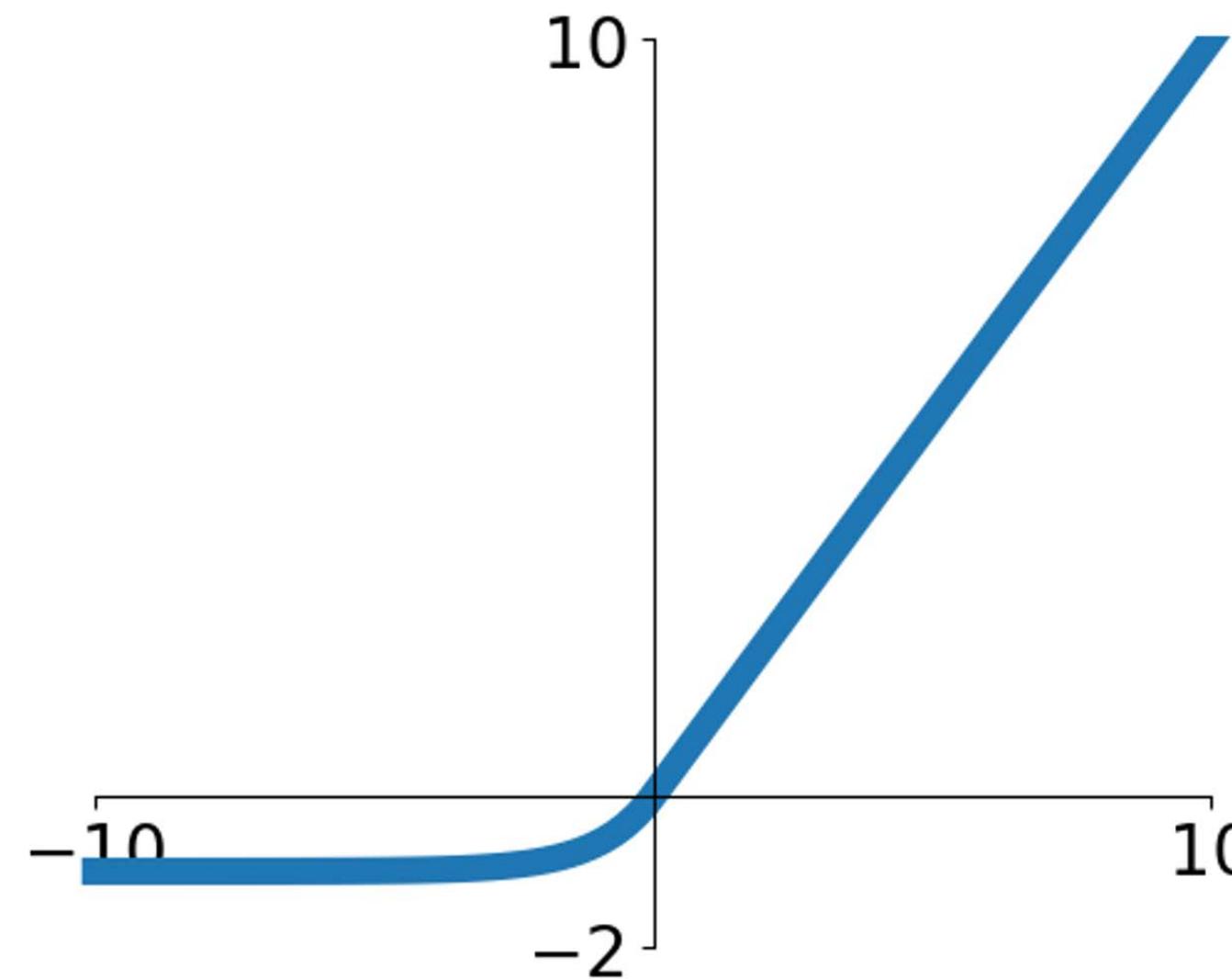
## Parametric ReLU (PReLU)

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

$\alpha$  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)

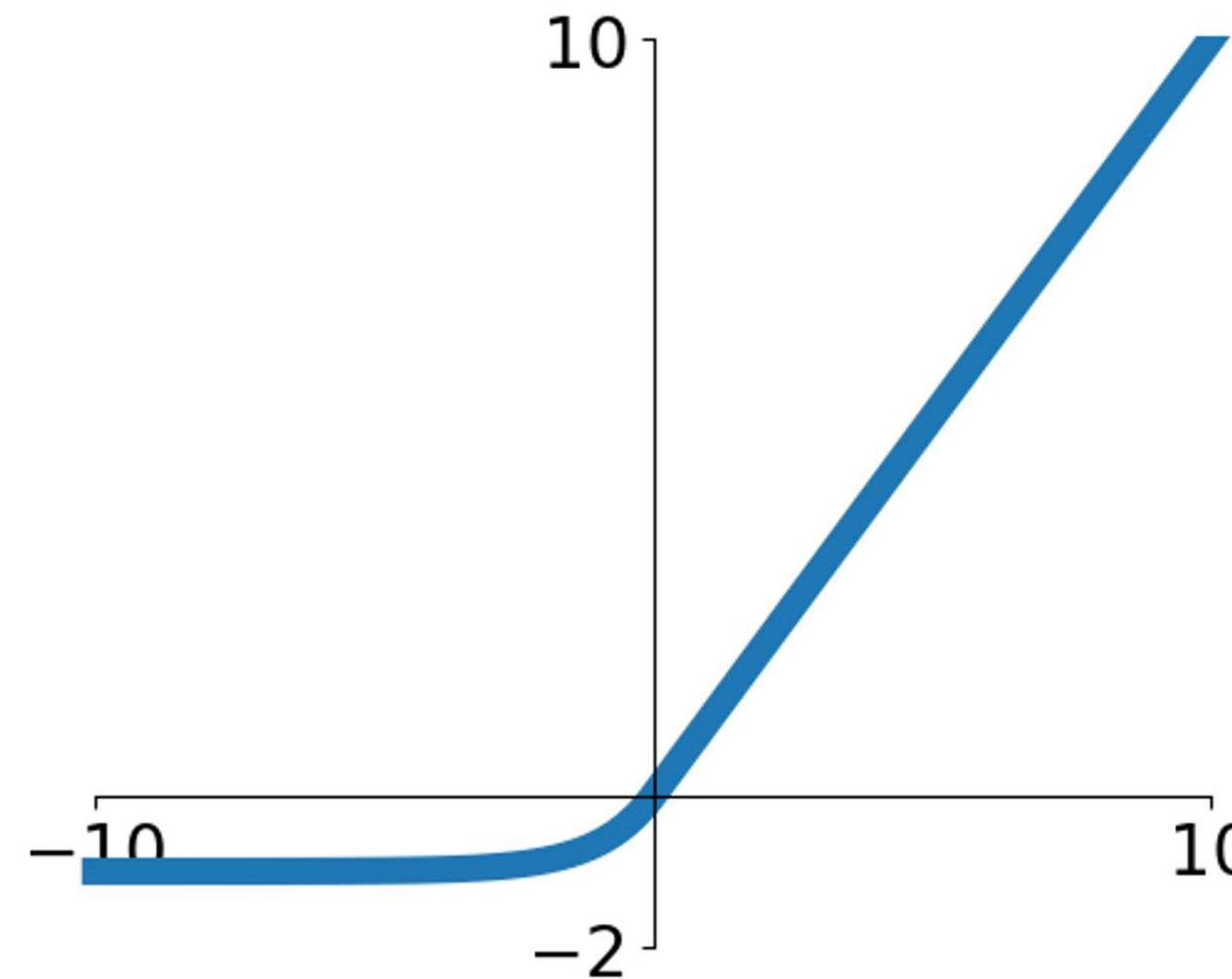


- All benefits of ReLU
- Closer to zero means outputs
- Negative saturation regime compared with Leaky ReLU adds some robustness to noise

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

(Default  $\alpha = 1$ )

# Activation Functions: Exponential Linear Unit (ELU)



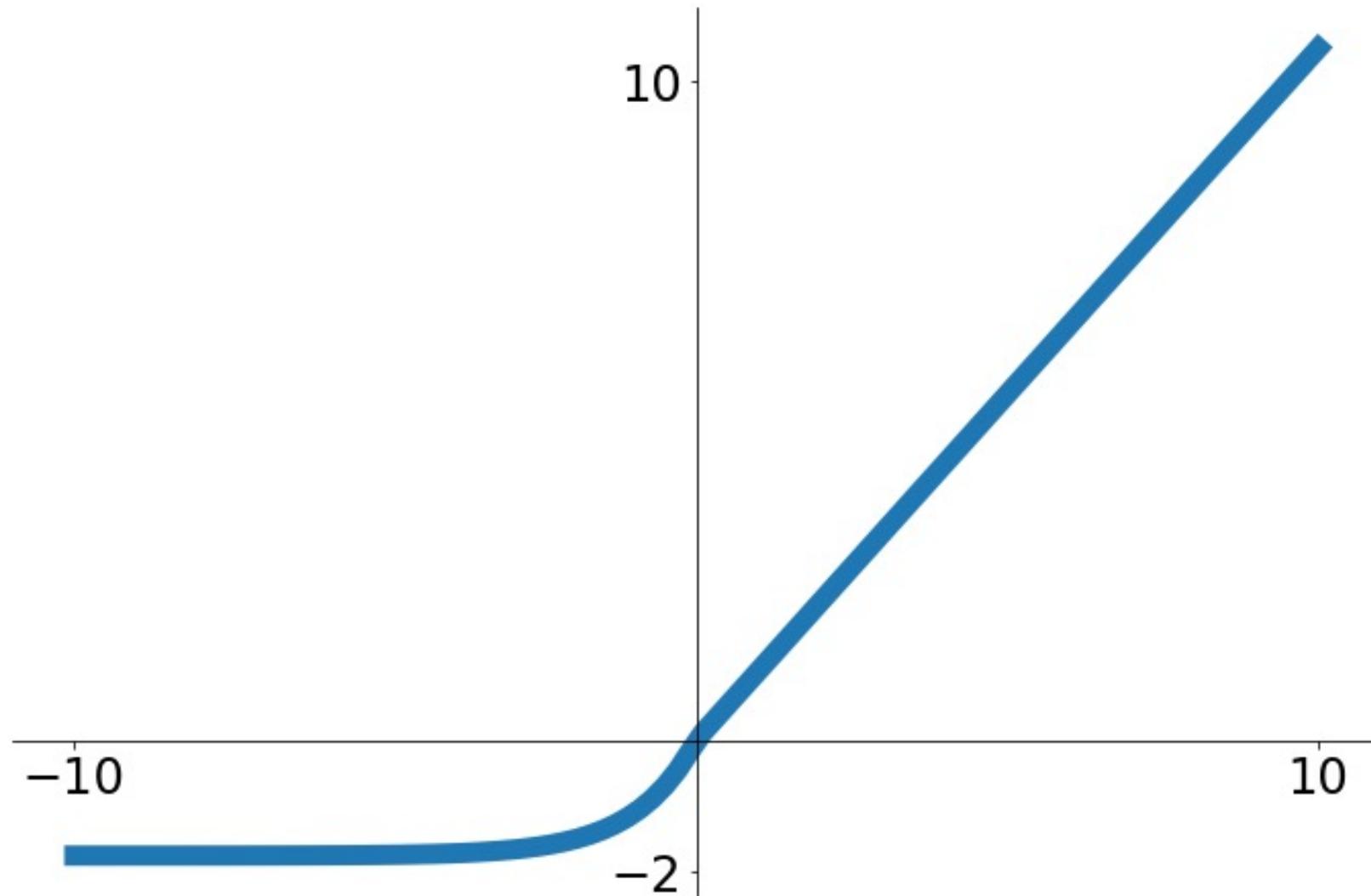
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(Default  $\alpha = 1$ )

- 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

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

$$\alpha = 1.6732632423543772848170429916717$$

$$\lambda = 1.0507009873554804934193349852946$$



# Activation Functions: Scale Exponential Linear Unit (SELU)

•  $0 \leq \mu \leq 1$  and  $0 \leq \omega \leq 0.1$ :  
 $g$  is increasing in  $\mu$  and increasing in  $\omega$ . We set  $\mu = 1$  and  $\omega = 0.1$ .  
 $g(1, 0.1, 3, 1.25, \lambda_{01}, \alpha_{01}) = -0.0180173$ . (43)

Therefore the maximal value of  $g$  is  $-0.0180173$ .  $\square$

**A3.3 Proof of Theorem 3**

First we recall Theorem 8. We consider  $\lambda = \lambda_{01}$ ,  $\alpha = \alpha_{01}$  and the two domains  $\Omega_1 = \{(\mu, \nu, \tau) \mid -0.1 \leq \mu \leq 0.1, -0.1 \leq \nu \leq 0.1, 0.05 \leq \tau \leq 0.8\}$  and  $\Omega_2 = \{(\mu, \nu, \tau) \mid -0.1 \leq \mu \leq 0.1, -0.1 \leq \nu \leq 0.1, 0.05 \leq \nu \leq 0.24, 0.9 \leq \tau \leq 1.25\}$ .  
The mapping of the variance  $\tilde{\nu}(\mu, \omega, \nu, \tau, \lambda, \alpha)$  given in Eq. (5) increases in both  $\Omega_1$  and  $\Omega_2$ . All fixed points  $(\mu, \nu)$  of mapping Eq. (5) and Eq. (4) ensure for  $0.8 < \tau < \nu$  that  $\nu > 0.16$  and for  $0.9 \leq \tau < \nu$  that  $\nu > 0.24$ . Consequently, the variance mapping Eq. (5) and Eq. (4) ensures a lower bound on the variance  $\nu$ .

*Proof.* The mean value theorem states that there exists a  $t \in [0, 1]$  for which

$$\tilde{\xi}(\mu, \omega, \nu, \tau, \lambda_{01}, \alpha_{01}) - \tilde{\xi}(\mu, \omega, \nu_{\min}, \tau, \lambda_{01}, \alpha_{01}) = \frac{\partial}{\partial \nu} \tilde{\xi}(\mu, \omega, \nu + t(\nu_{\min} - \nu), \tau, \lambda_{01}, \alpha_{01}) (\nu - \nu_{\min}). \quad (45)$$

Therefore we are interested to bound the derivative of the  $\xi$ -mapping Eq. (13) with respect to  $\nu$ :

$$\frac{\partial}{\partial \nu} \tilde{\xi}(\mu, \omega, \nu, \tau, \lambda_{01}, \alpha_{01}) = \frac{1}{2} \lambda^2 \tau e^{-\frac{\mu^2 \tau^2}{2}} \left( \alpha^2 \left( e^{\left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right)^2} \operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) \right) - 2e^{\left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right)^2} \operatorname{erfc} \left( \frac{\mu \omega + 2\nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) \right) - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2. \quad (47)$$

The sub-term Eq. (46) enters the derivative Eq. (47) with a negative sign! According to Lemma 18, the minimal value of sub-term Eq. (46) is obtained by the largest largest  $\nu$ , by the smallest  $\tau$ , and the largest  $\mu = \mu \omega = 0.01$ . Also the positive term  $\operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2$  is multiplied by  $\tau$ , which is minimized by using the smallest  $\tau$ . Therefore we can use the smallest  $\tau$  in whole formula Eq. (47) as lower bound.

First we consider the domain  $0.05 \leq \nu \leq 0.16$  and  $0.8 \leq \tau \leq 1.25$ . The factor consisting of the exponential in front of the brackets has its smallest value for  $e^{-\frac{\mu^2 \tau^2}{2}} \approx 0.8$ . In order to obtain the maximal decreasing we inserted the smallest argument via  $\operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) \approx 0.00008$  in order to obtain the maximal negative contribution. Thus, applying Lemma 18, we obtain the lower bound on the derivative:

$$1.2 \lambda^2 \tau e^{-\frac{\mu^2 \tau^2}{2}} \left( \alpha^2 \left( - \left( e^{\left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right)^2} \operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) \right) - 2e^{\left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right)^2} \operatorname{erfc} \left( \frac{\mu \omega + 2\nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) \right) \right) - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2. \quad (48)$$

18

19

20

In the following, we denote two Jacobians: (1) the Jacobian  $J$  of the and (2) the Jacobian  $H$  of the mapping  $g : (\mu, \nu) \mapsto (\hat{\mu}, \hat{\nu})$  because the and many properties of the system can already be seen on  $J$ :

$$\begin{aligned} J_{11} &= \begin{pmatrix} \frac{\partial}{\partial \mu} \tilde{\mu} \\ \frac{\partial}{\partial \nu} \tilde{\mu} \end{pmatrix} \\ J_{21} &= \begin{pmatrix} \frac{\partial}{\partial \mu} \tilde{\nu} \\ \frac{\partial}{\partial \nu} \tilde{\nu} \end{pmatrix} \end{aligned} \quad (52)$$

$$\begin{aligned} H_{11} &= \begin{pmatrix} \frac{\partial}{\partial \mu} \hat{\mu} \\ \frac{\partial}{\partial \nu} \hat{\mu} \end{pmatrix} \\ H_{21} &= \begin{pmatrix} \frac{\partial}{\partial \mu} \hat{\nu} \\ \frac{\partial}{\partial \nu} \hat{\nu} \end{pmatrix} \end{aligned} \quad (53)$$

The Jacobian  $J$  is:

$$\begin{aligned} \frac{\partial}{\partial \mu} \tilde{\mu}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2 & \\ \frac{\partial}{\partial \nu} \tilde{\mu}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} - (\alpha - 1) \sqrt{\frac{2}{\pi \nu \tau}} e^{-\frac{\mu^2 \omega^2}{2 \nu \tau}} & \\ \frac{\partial}{\partial \nu} \tilde{\xi}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) + & \\ + \frac{2 \nu \tau}{2 \sqrt{2} \sqrt{\nu \tau}} + \mu \omega \left( 2 - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) \right) + \sqrt{\frac{2}{\pi} \sqrt{\nu \tau} e^{-\frac{\mu^2 \omega^2}{2 \nu \tau}}} & \\ \frac{\partial}{\partial \nu} \tilde{\xi}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) + & \\ \omega + 2 \nu \tau - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2 & \end{aligned} \quad (54)$$

$$\begin{aligned} \frac{\partial}{\partial \mu} \tilde{\nu}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \frac{4 - 0.9 + 0.01}{2 \sqrt{2} \cdot 0.9} - & \\ \operatorname{erfc} \left( \frac{-0.01}{\sqrt{2} \cdot 0.9} \right) + 2 & \end{aligned} \quad (55)$$

$$\begin{aligned} \frac{\partial}{\partial \nu} \tilde{\nu}(\mu, \omega, \nu, \tau, \lambda, \alpha) &= \\ \operatorname{erfc} \left( \frac{\mu \omega + \nu \tau}{\sqrt{2} \sqrt{\nu \tau}} \right) + & \\ \omega + 2 \nu \tau - \operatorname{erfc} \left( \frac{\mu \omega}{\sqrt{2} \sqrt{\nu \tau}} \right) + 2 & \end{aligned} \quad (56)$$

largest singular value of the Jacobian. If the largest singular value is smaller than 1, then the spectral norm of the Jacobian is smaller than 1. Then the of the mean and variance to the mean and variance in the next layer is

lar value is smaller than 1 by evaluating the function  $S(\mu, \omega, \nu, \tau, \lambda, \alpha)$  can Value Theorem to prove the derivative of the function  $S$  between the evaluated point and the gradient of  $S$  with respect to  $(\mu, \omega, \nu, \tau, \lambda, \alpha)$ . If all times the deltas (differences between grid points and evaluated points) have proofed that the function is below 1.

2 matrix

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \quad (58)$$

$$(a_{22})^2 + (a_{21} - a_{11})^2 + \sqrt{(a_{11} - a_{22})^2 + (a_{12} + a_{21})^2} \quad (59)$$

$$(a_{22})^2 + (a_{21} - a_{11})^2 - \sqrt{(a_{11} - a_{22})^2 + (a_{12} + a_{21})^2}. \quad (60)$$

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

$$\alpha = 1.6732632423543772848170429916717$$

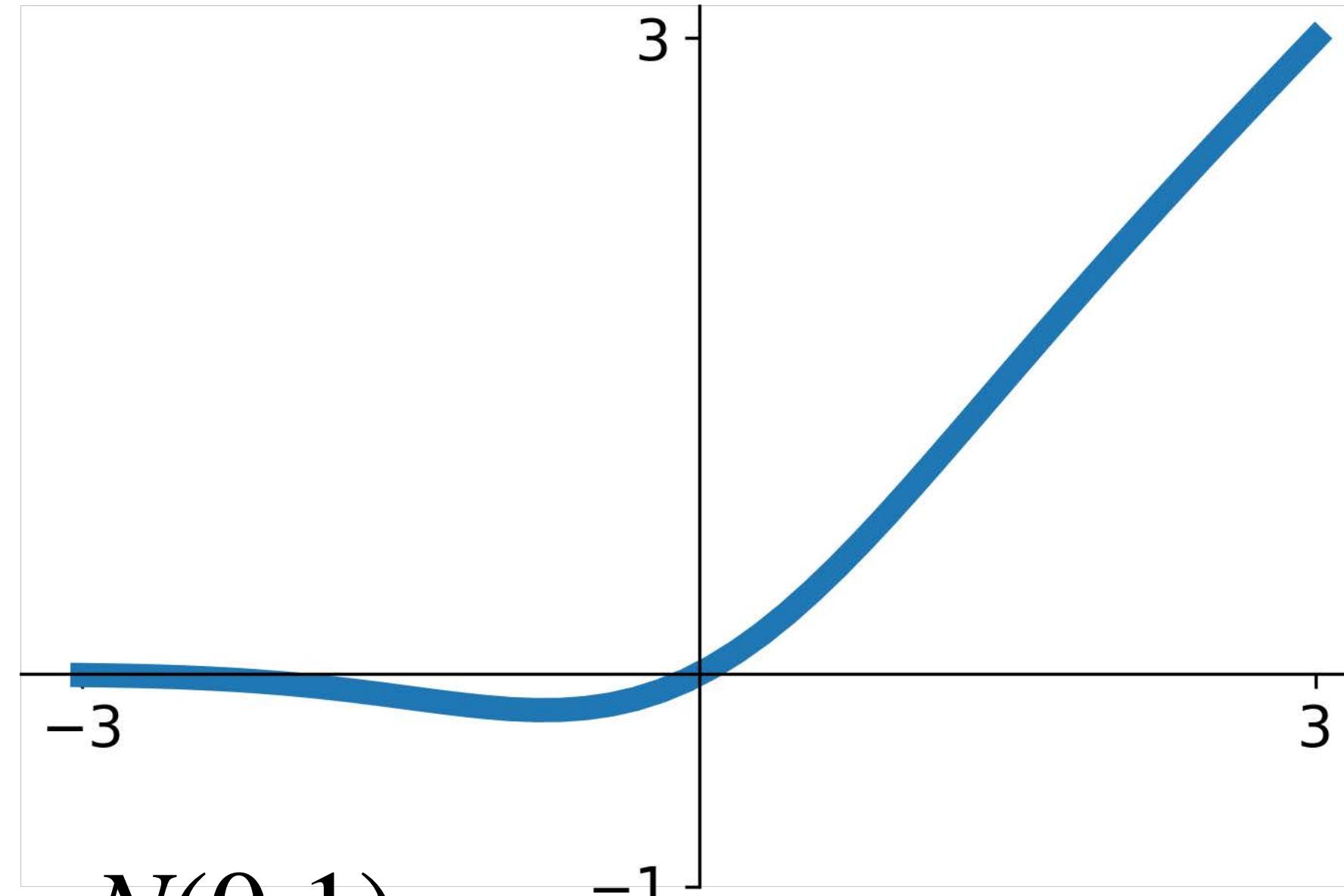
$$\lambda = 1.0507009873554804934193349852946$$



- 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...

# Activation Functions: Gaussian Error Linear Unit (GELU)



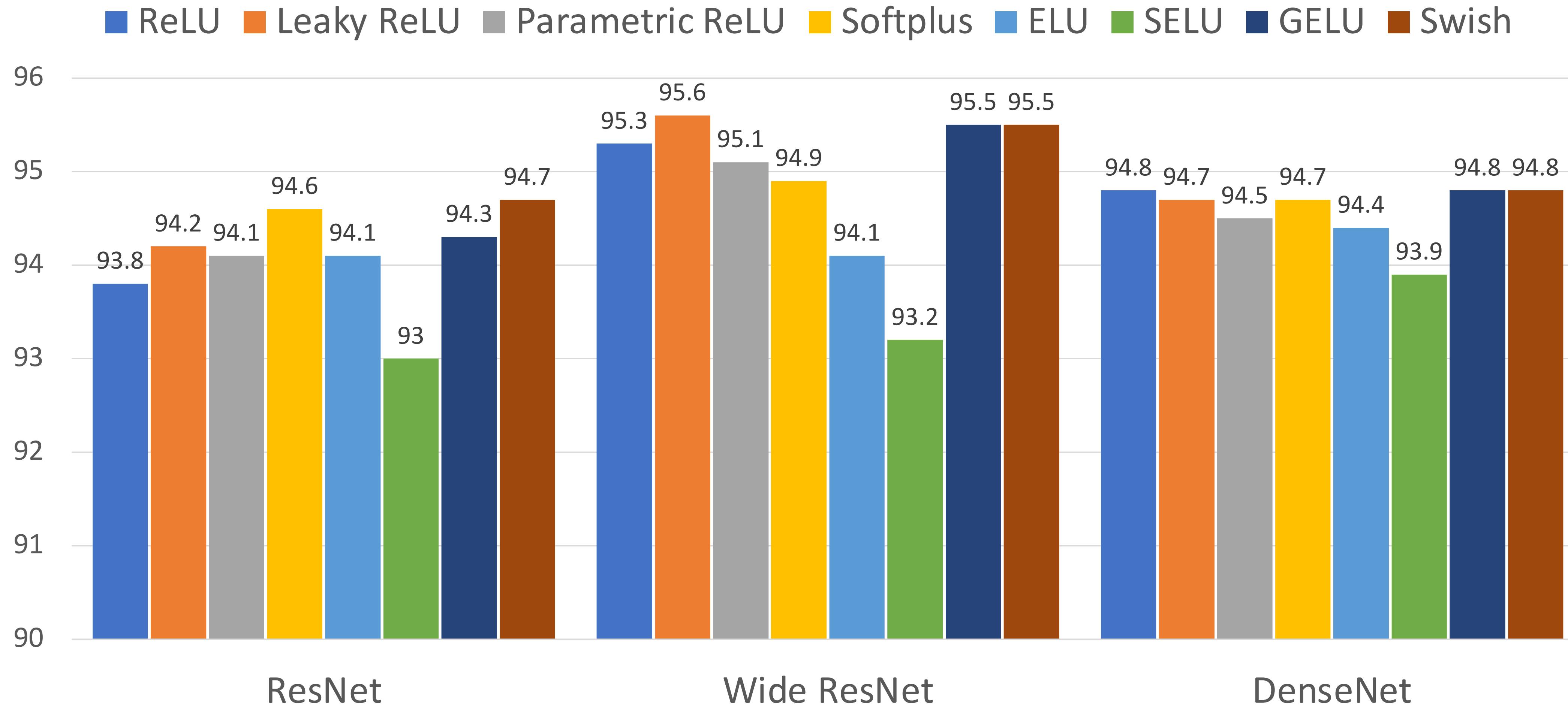
$X \sim N(0, 1)$

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

- **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 (data-dependent 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



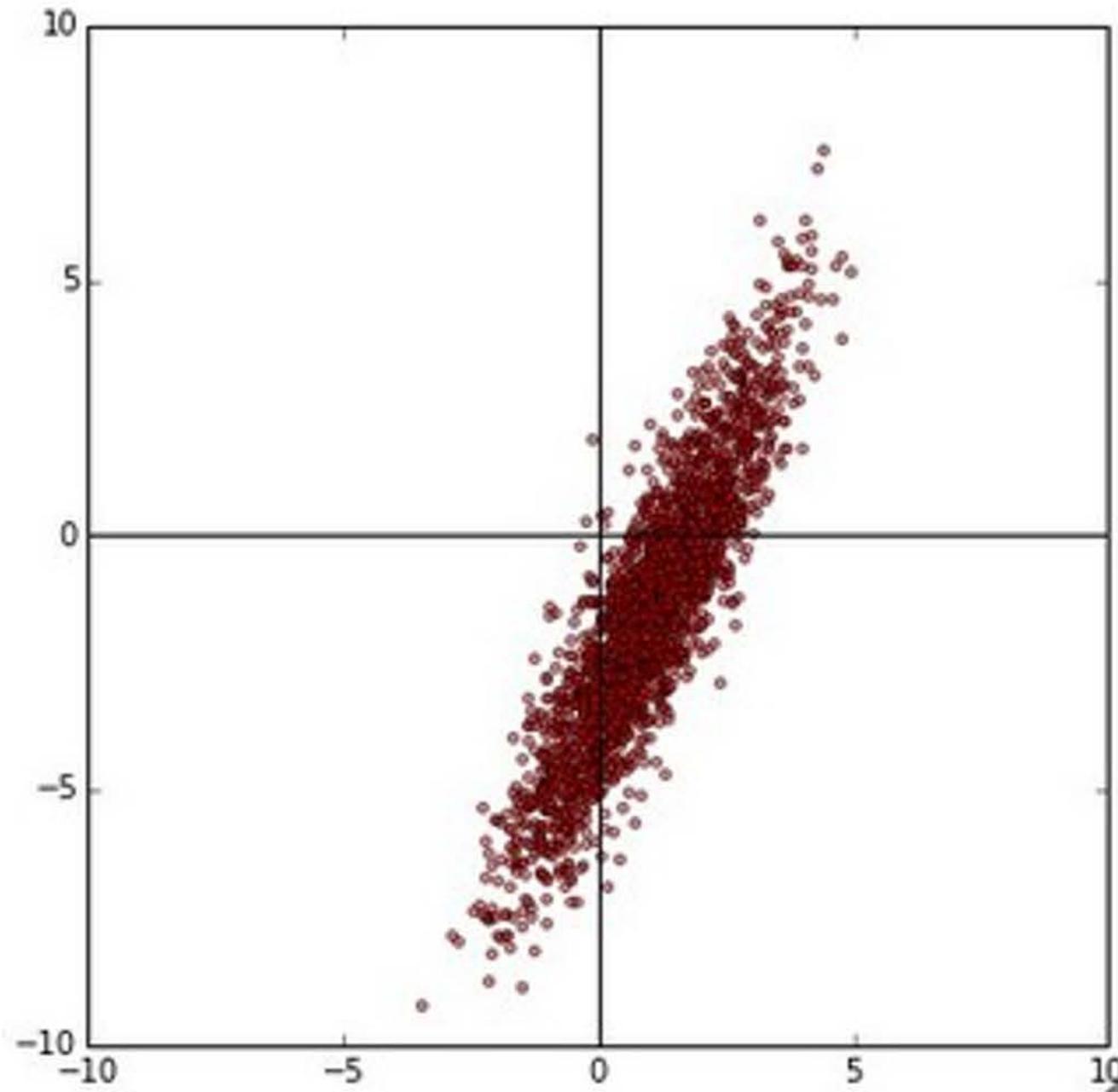


# Data preprocessing

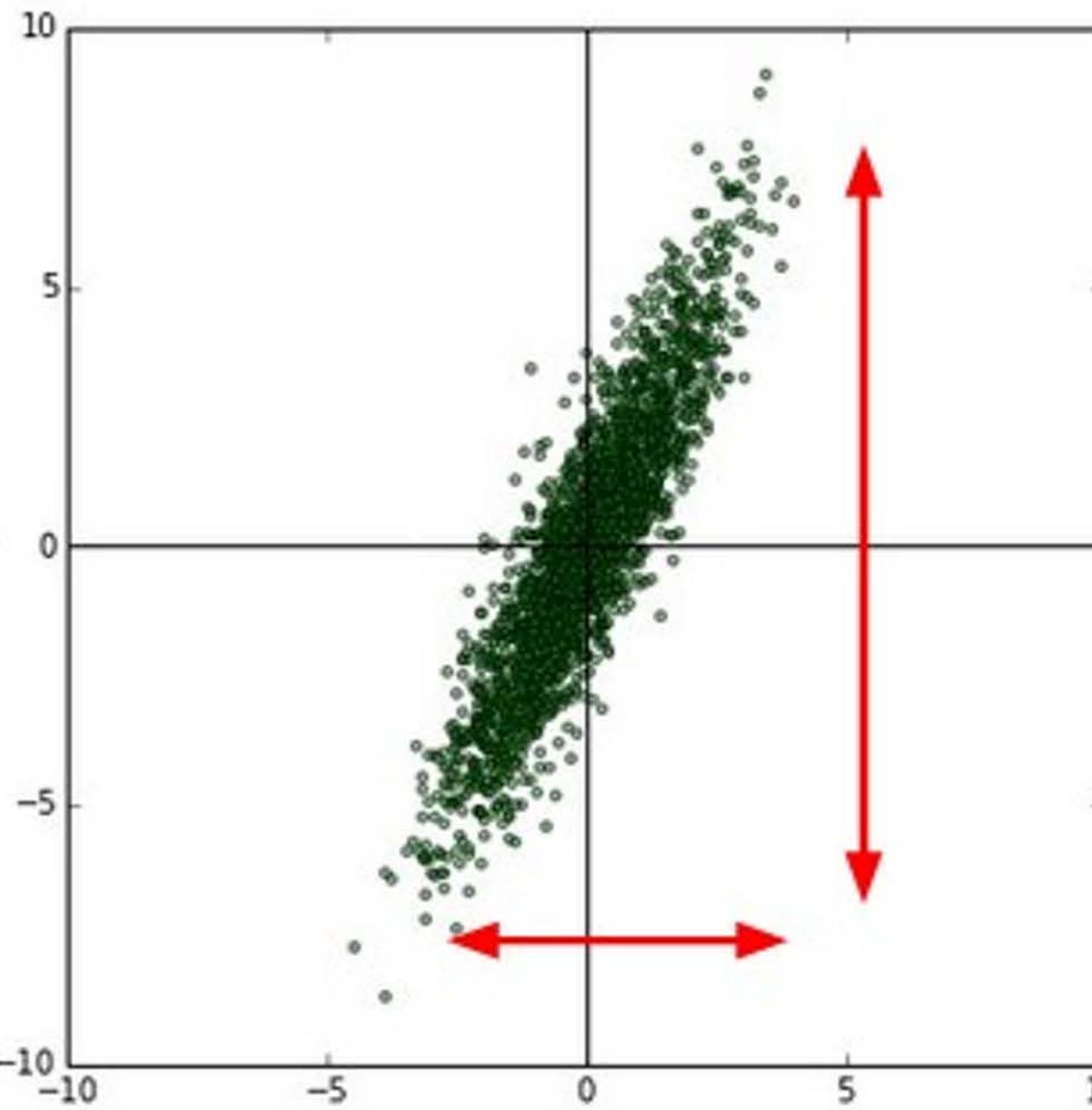


# Data preprocessing

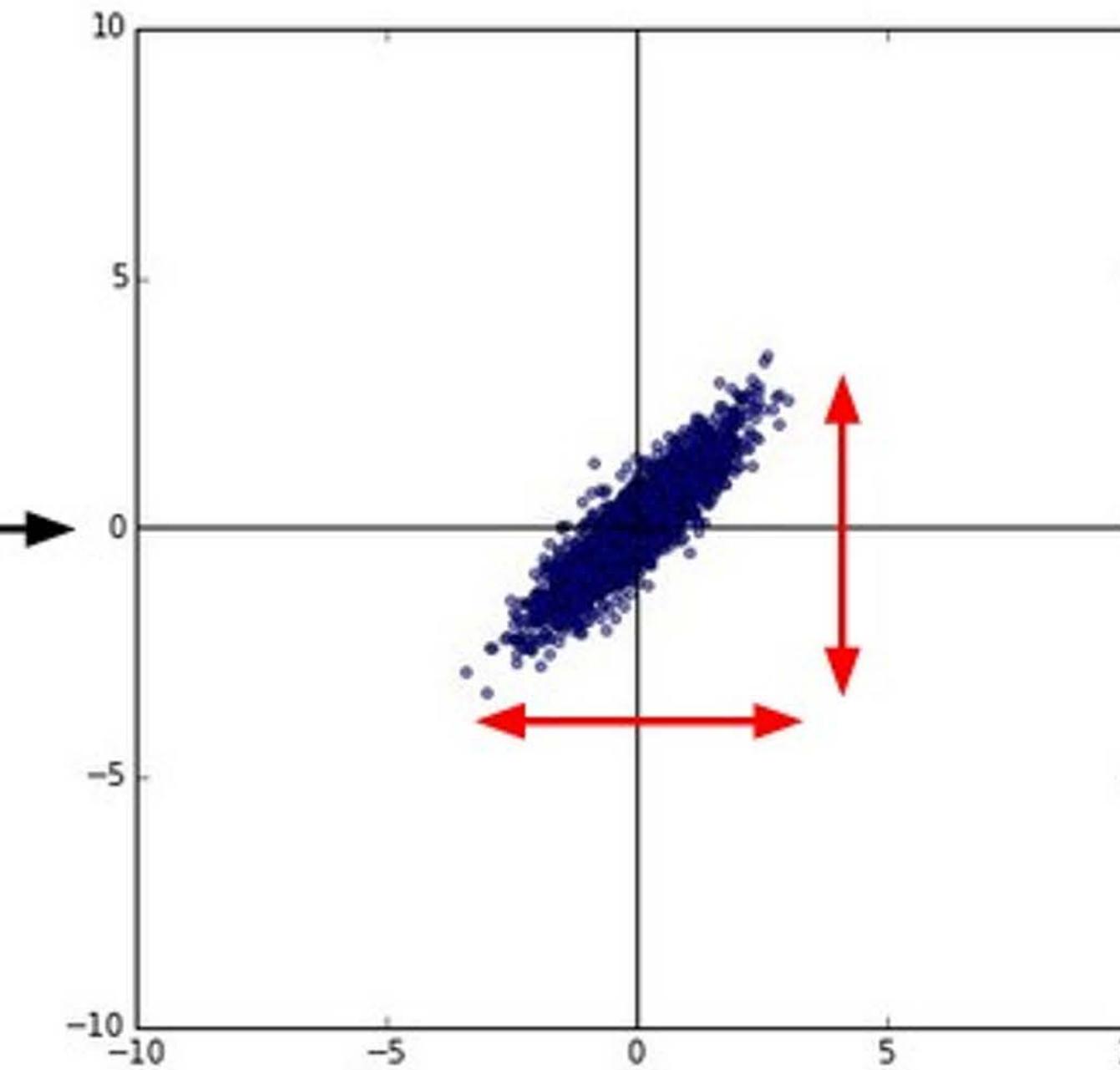
original data



zero-centered data



normalized data



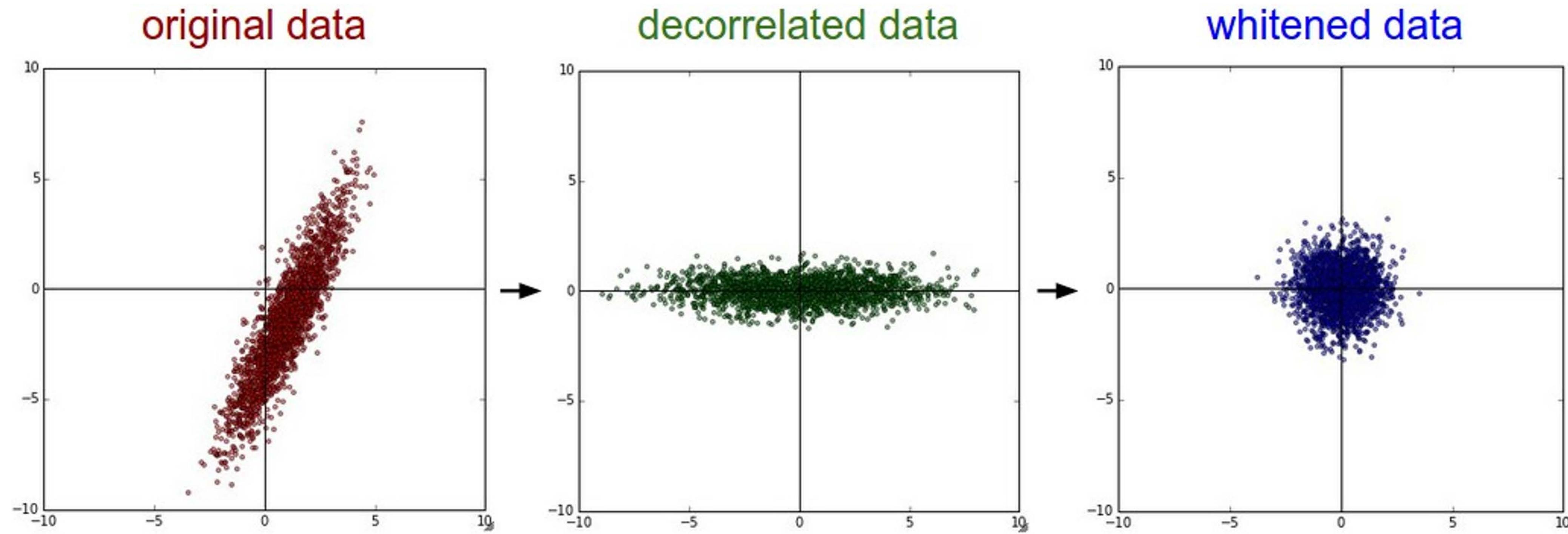
```
X -= np.mean(X, axis = 0)
```

```
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

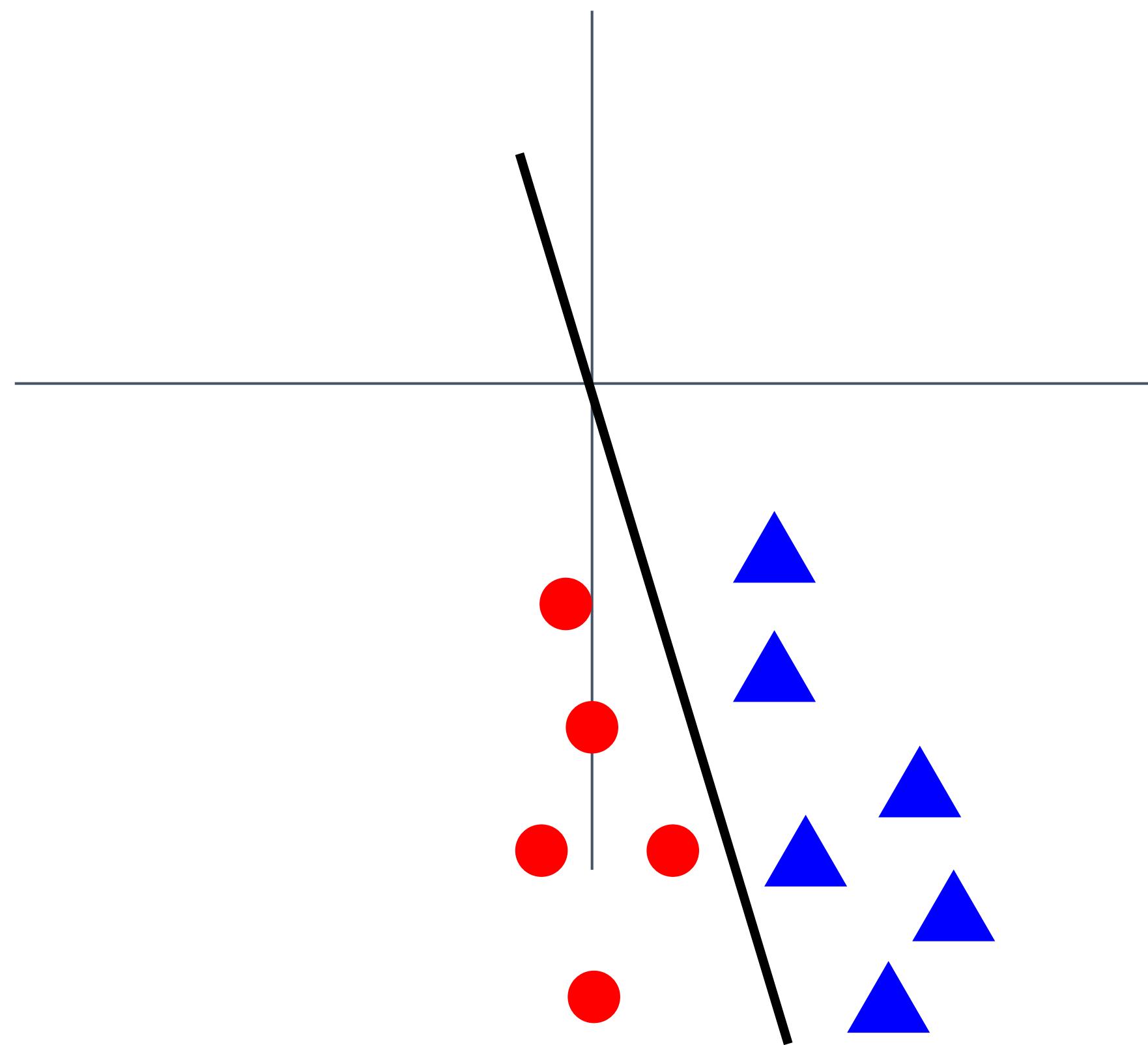


(Data has diagonal covariance matrix)

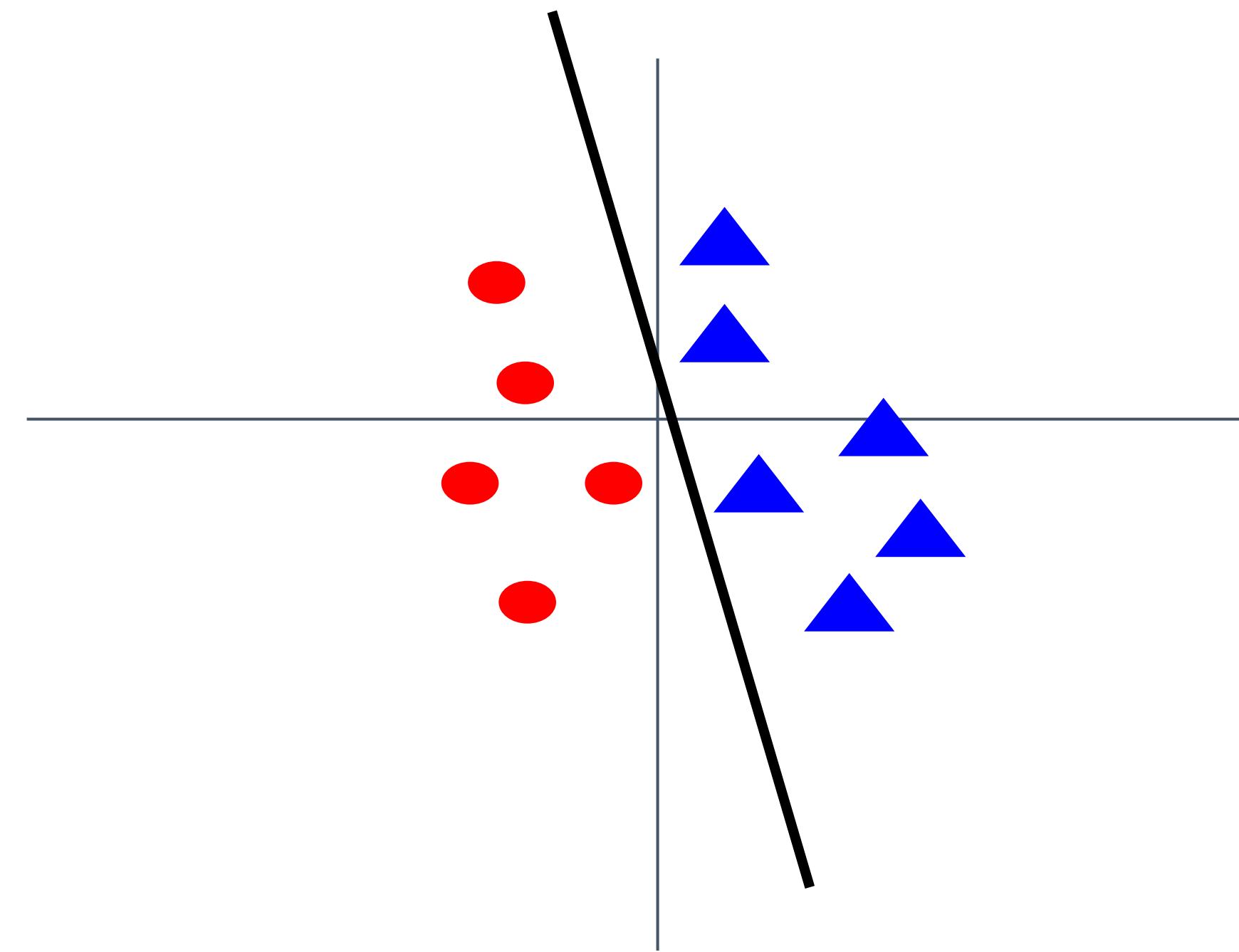
(Covariance matrix is the identity matrix)

# 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

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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)

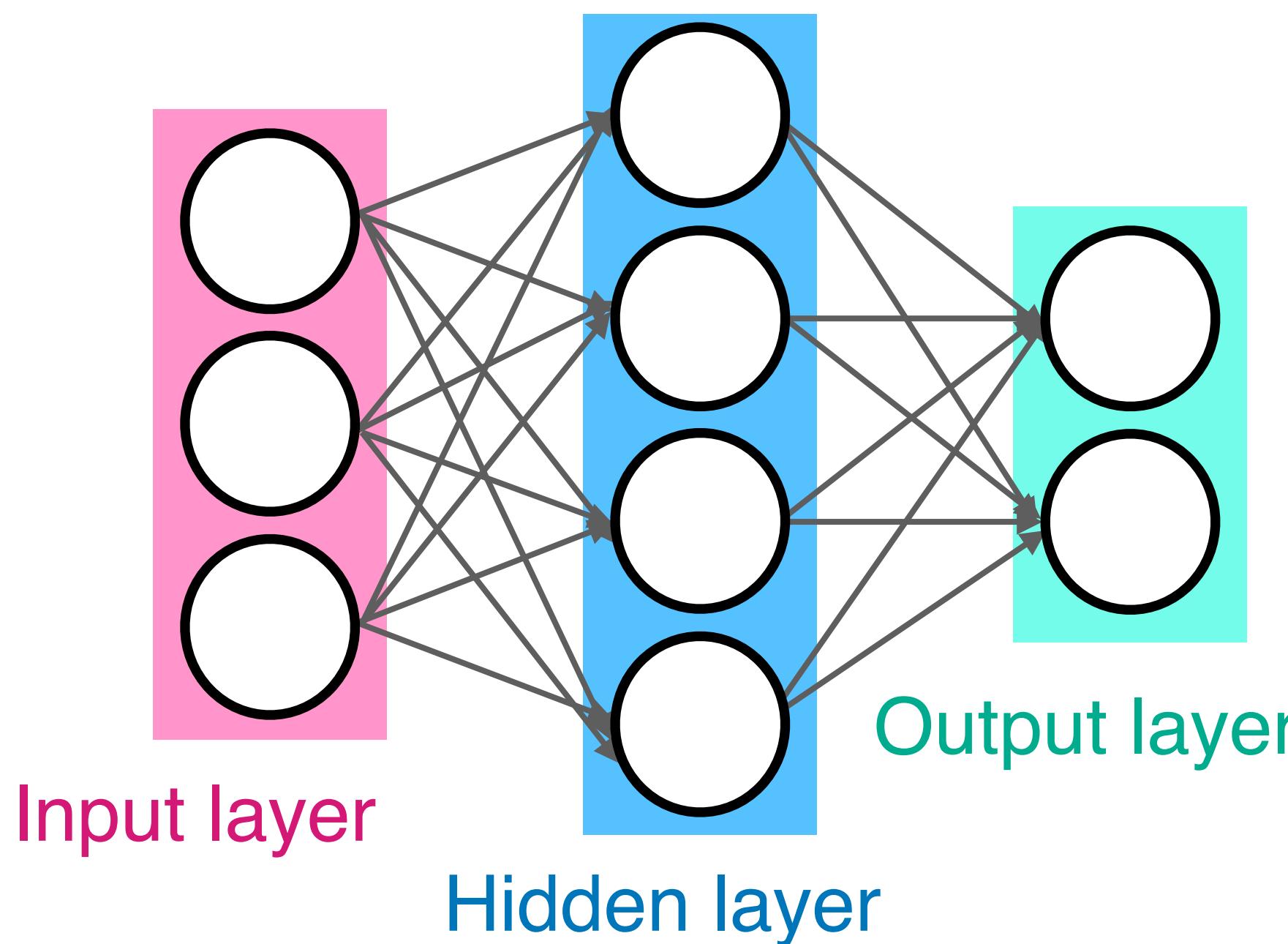
Not common to do  
PCA or whitening



# Weight initialization



# Weight initialization



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

**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      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)
```

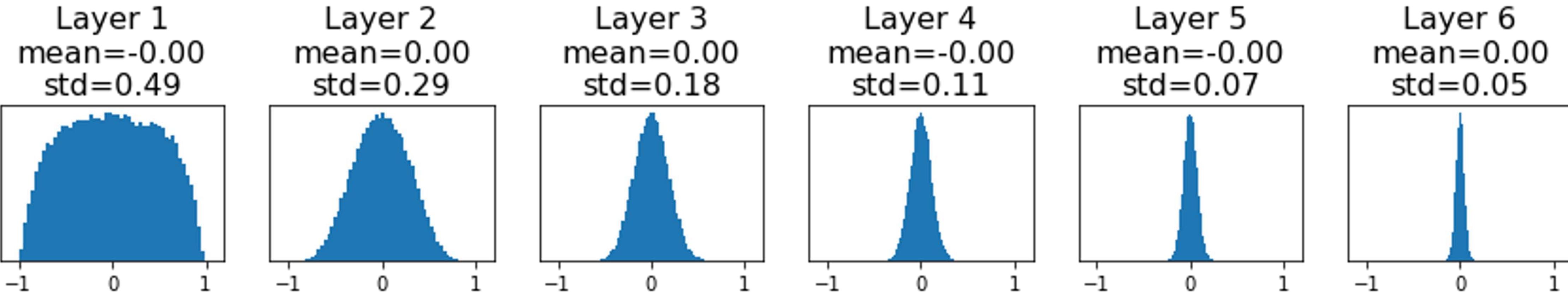


# Weight initialization: Activation statistics

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```

All activations tend to zero for deeper network layers

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



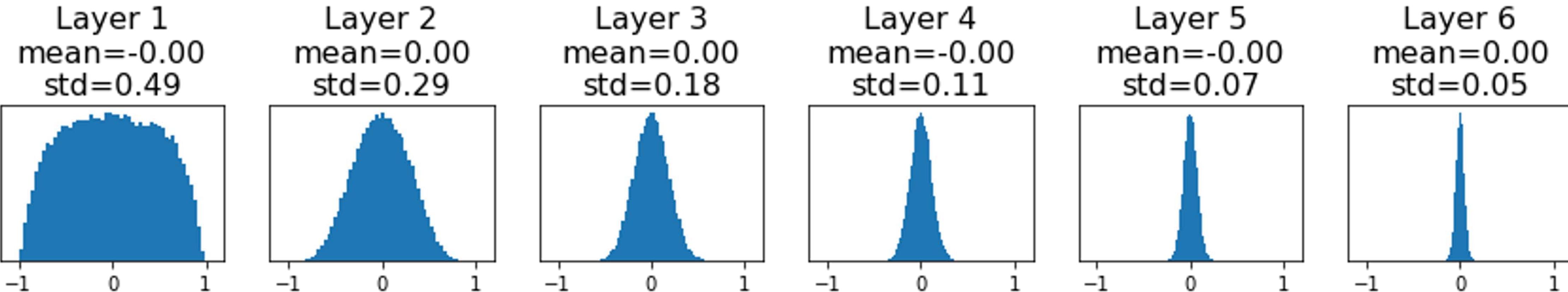
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    hs.append(x)
```

All activations tend to zero for deeper network layers

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

**A:** All zero, no learning :(

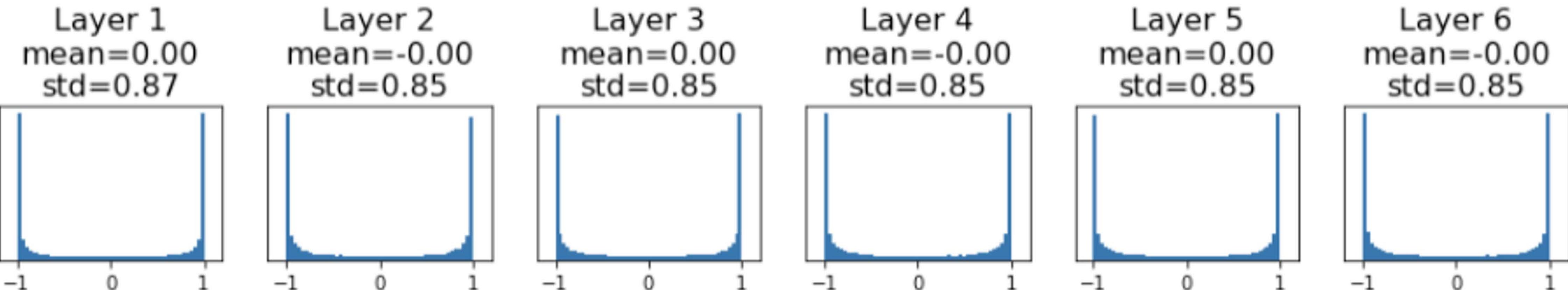


# Weight initialization: Activation statistics

```
dims = [4096] * 7    Increase std of initial weights  
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)
```

All activations saturate

Q: What do the gradients look like?



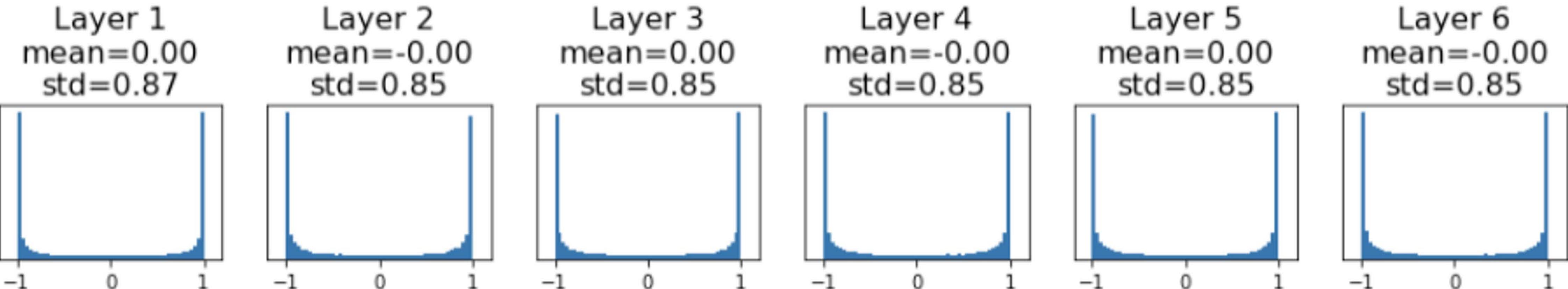
# Weight initialization: Activation statistics

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

All activations saturate

**Q:** What do the gradients look like?

**A:** Local gradients all zero, no learning :(





# Weight initialization: Xavier Initialization

```
dims = [4096] * 7          "Xavier" initialization:  
hs = []                      std = 1/sqrt(Din)  
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)
```

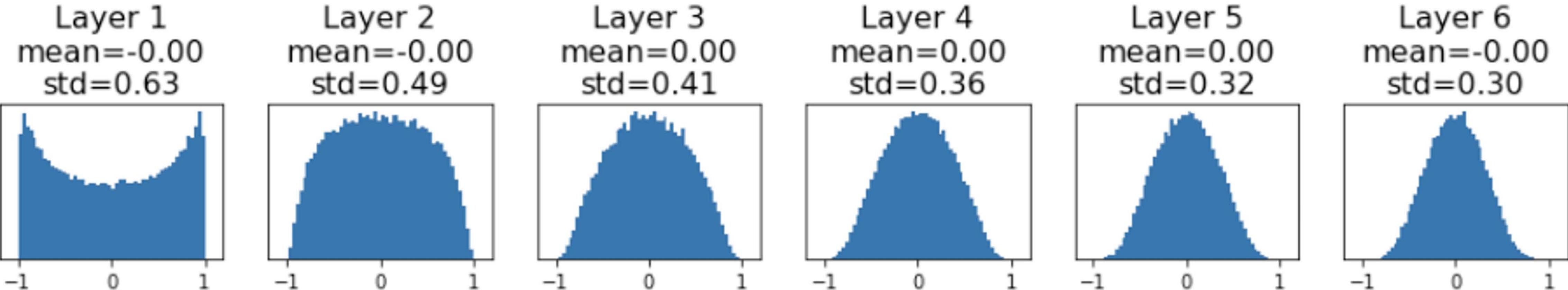
“Just right”: Activations are nicely scaled for all layers!



# Weight initialization: Xavier Initialization

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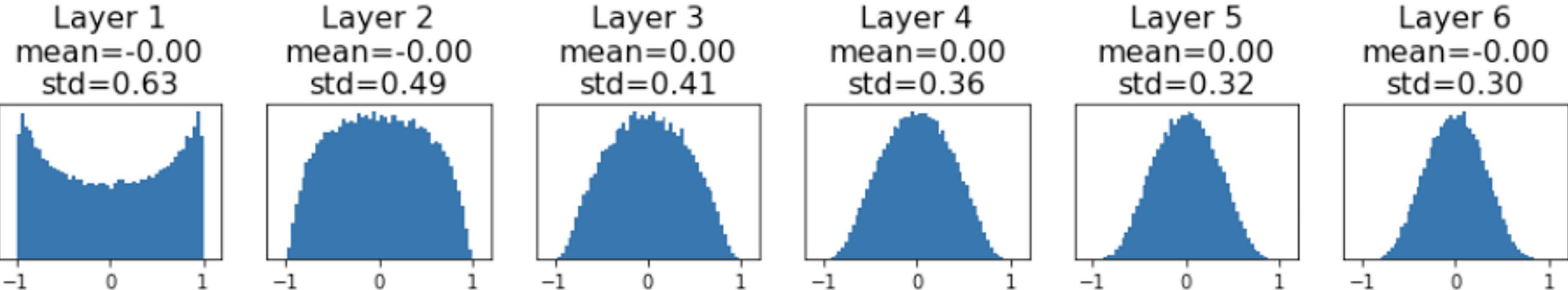


# Weight initialization: Xavier Initialization

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

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

For conv layers, Din is kernel\_size<sup>2</sup> 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

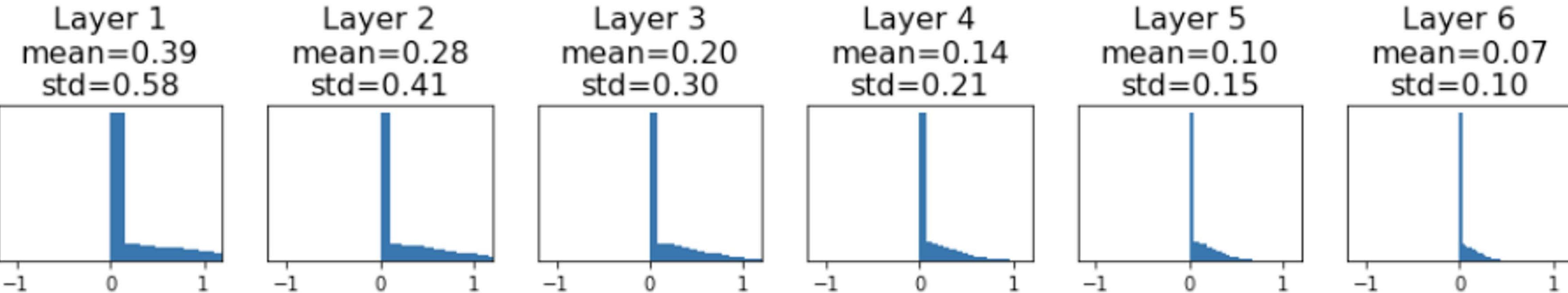


# Weight initialization: What about ReLU?

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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 :(



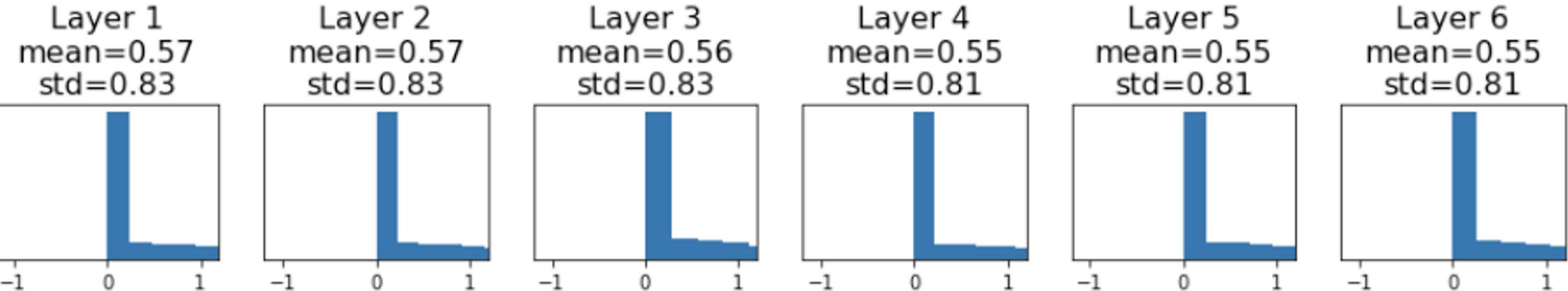
# Weight initialization: Kaiming / MSRA initialization

```

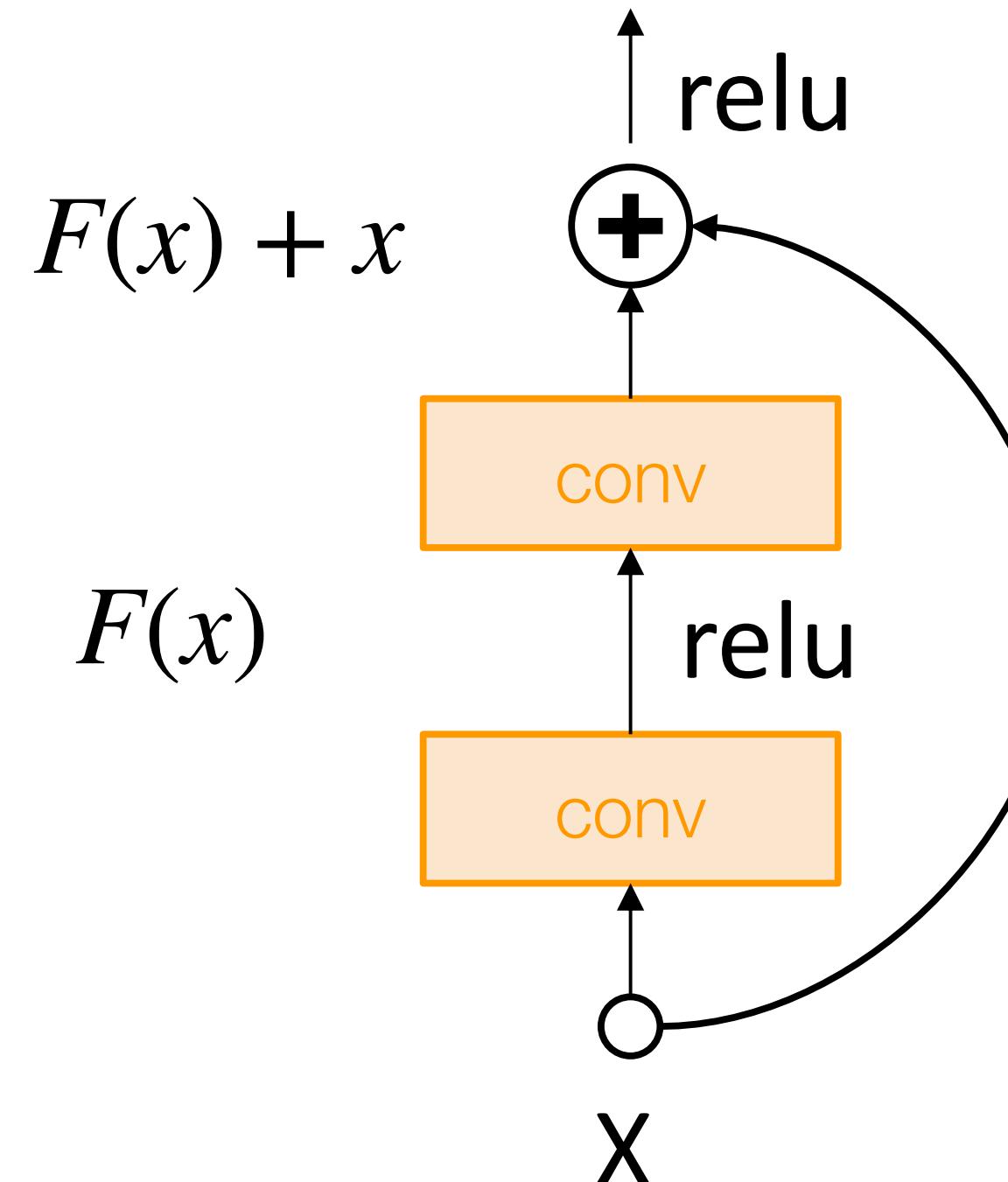
dims = [4096] * 7 ReLU correction: std = sqrt(2 / Din)
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)

```

“Just right” - activations nicely scaled for all layers



# Weight initialization: Residual Networks

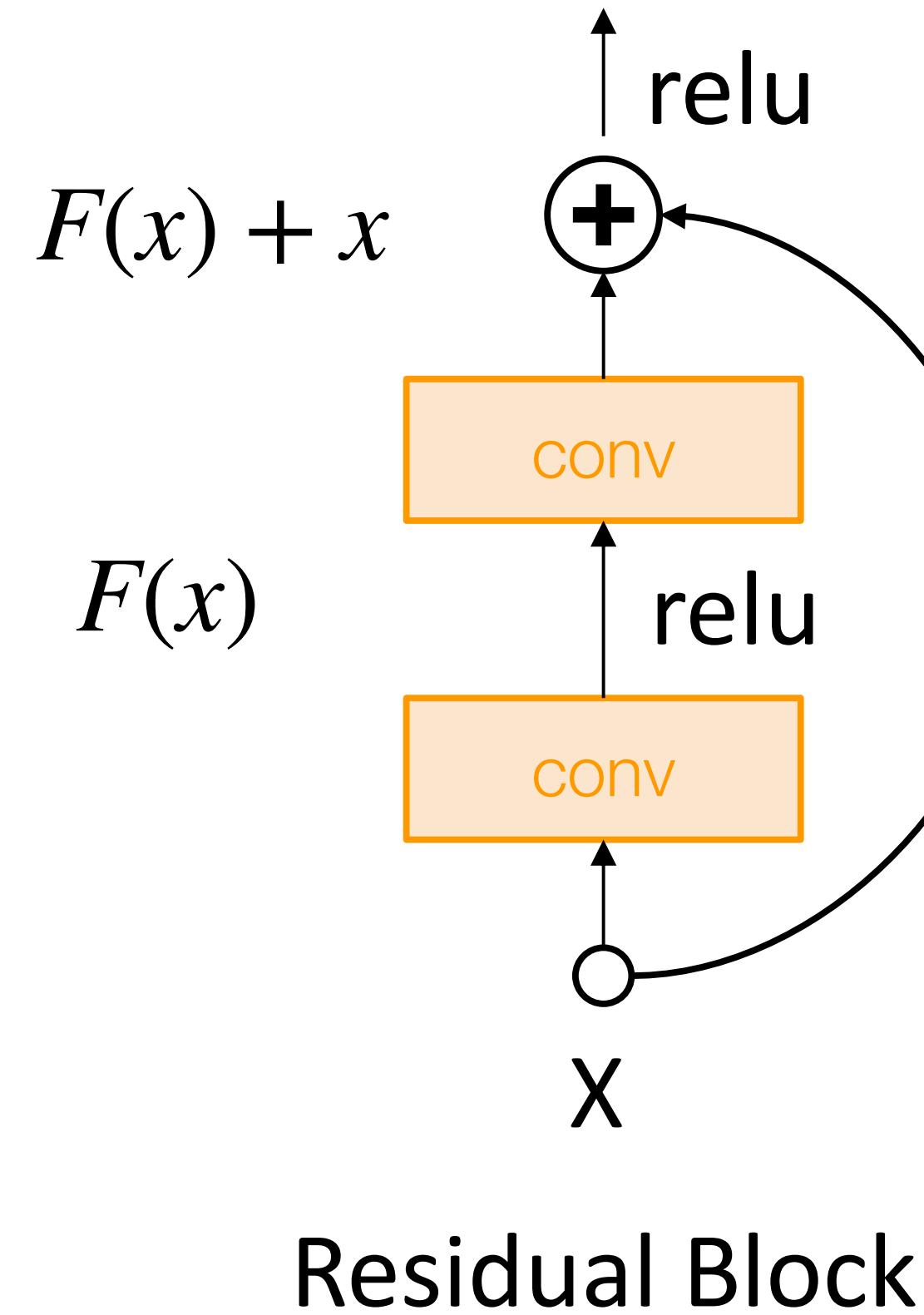


Residual Block

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



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

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

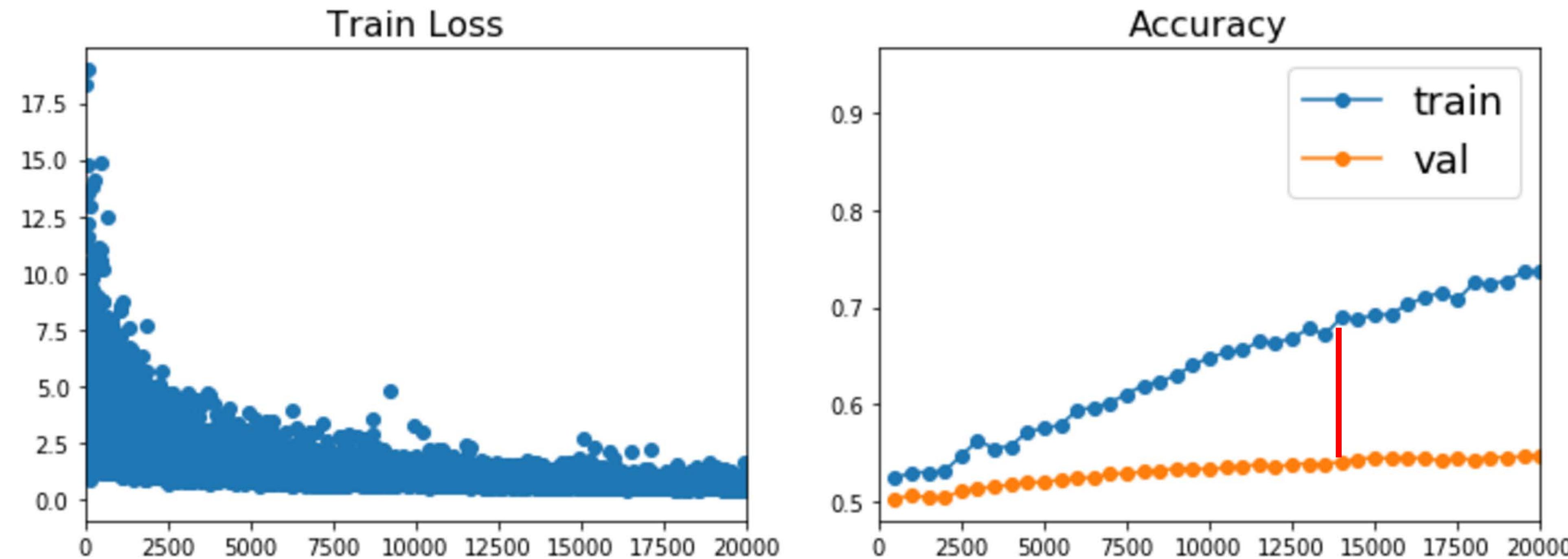
**Solution:** Initialize first conv with MSRA,  
initialize second conv to zero. Then  
 $Var(F(x) + x) = Var(x)$

# 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

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



## Regularization

# Summary

## 1. One time setup:

- Activation functions, data preprocessing, weight initialization, regularization

Today

## 2. Training dynamics:

- Learning rate schedules; large-batch training; hyperparameter optimization

Next time

## 3. After training:

- Model ensembles, transfer learning





# Next Time: Training Neural Networks II





# Reminder: Form your final project teams

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- Read the individual brainstorming documents from other students in the google-folder.
- Talk to your fellow classmates.
  - Discuss your project idea with them.
  - Start working toward more concrete project as a team.
    - Adapt/Modify/Narrow down your ideas a team.
    - *Talk to Karthik during his OH to see the feasibility.*
  - Pick a few lecture topics from the list (provided [here](#)).
  - Pick 3 papers to read.
    - To reimplement as your project.
    - To help your project.
- Form a team of 2-3 students by **10/07 EOD using the [google-sheet](#).**
  - You **do not have to** finalize your project by this date.
  - You should finalize your group.





# Visit RPM Lab!





# DeepRob

Lecture 9  
Training Neural Networks I  
University of Minnesota

