DeepRob

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

Project 2—Updates

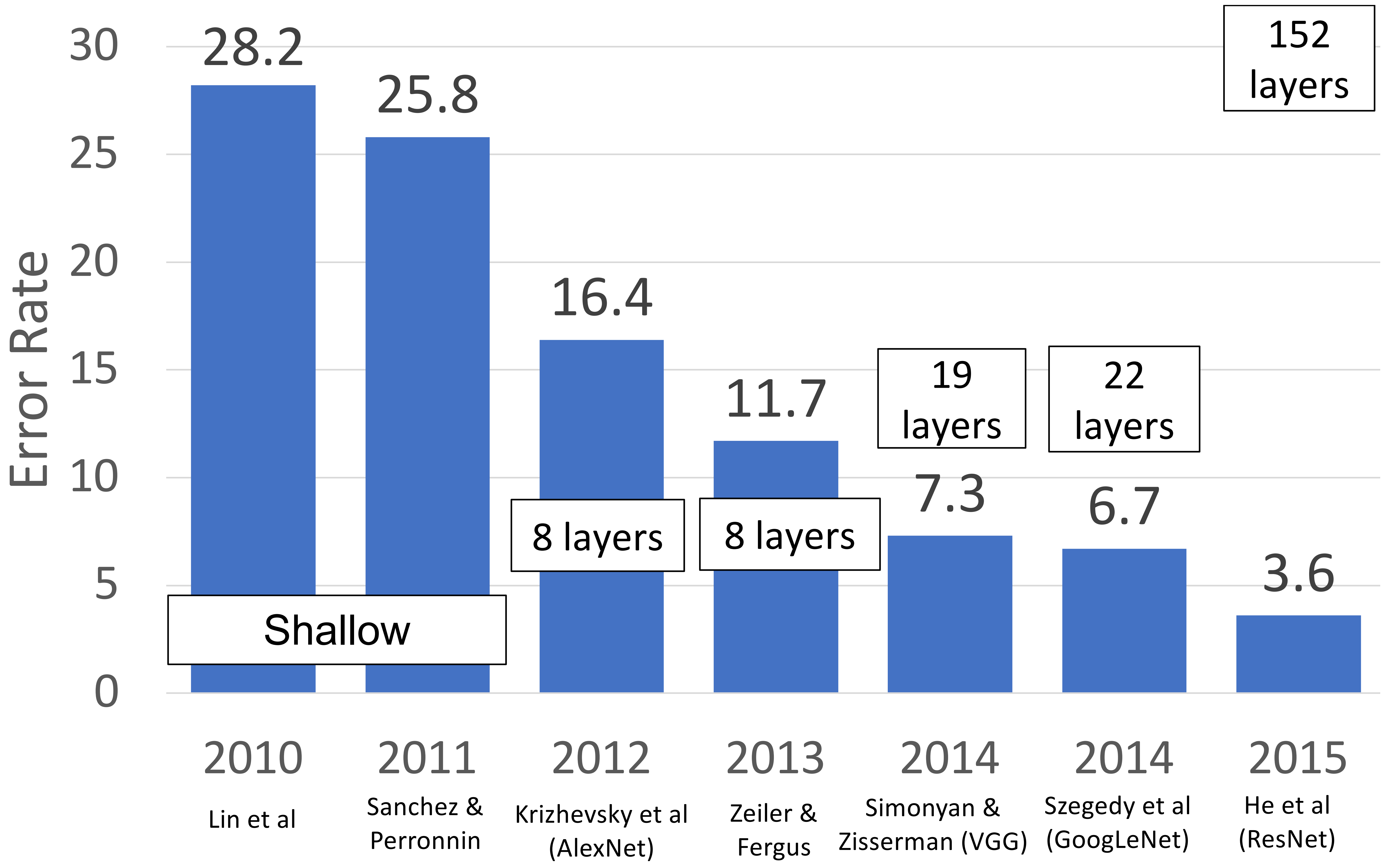
- Instructions available on the website
  - Here: deeprob.org/projects/project2/
- Starter code sent via email
- Implement two-layer neural network and generalize to FCN
- **Autograder will be available in next day or so**
- **Due Thursday, February 9th 11:59 PM EST**

Final Project Paper Selection Survey

- Published on gradescope
- To gauge your areas of interest
- Used for forming teams

- **Due Friday, February 3rd 11:59 PM EST**

Recap: CNN Architectures for ImageNet Classification

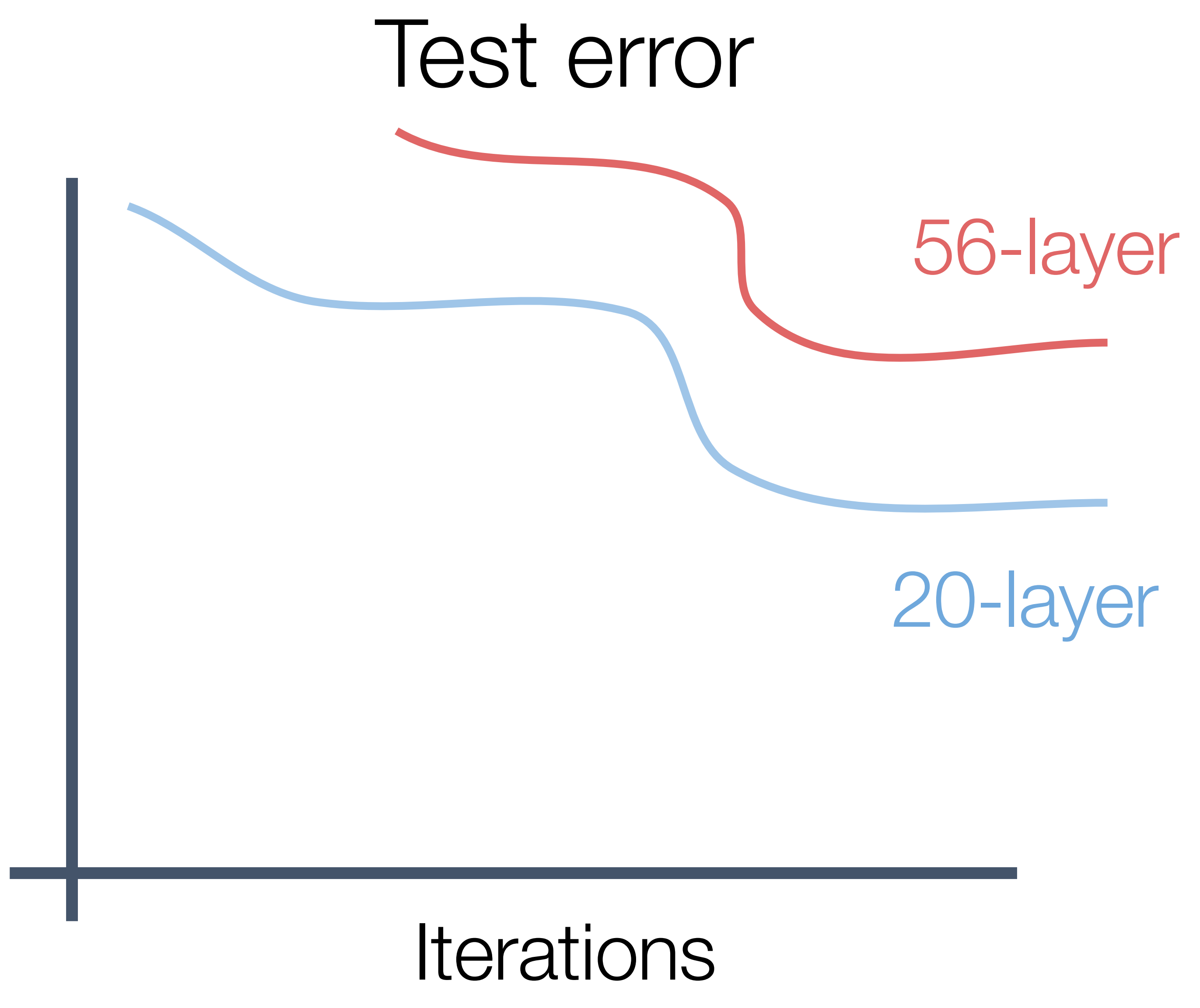


Residual Networks

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

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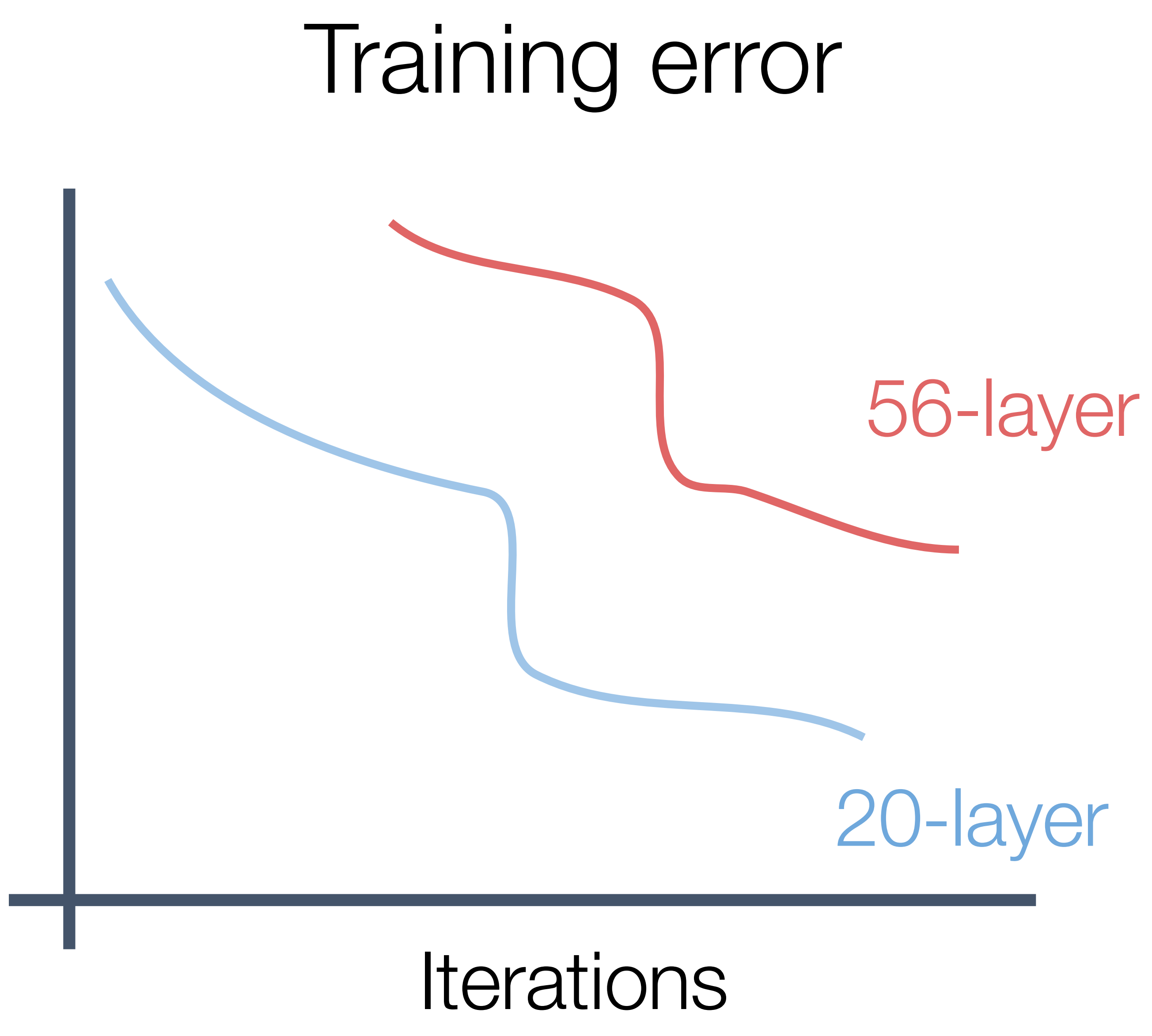

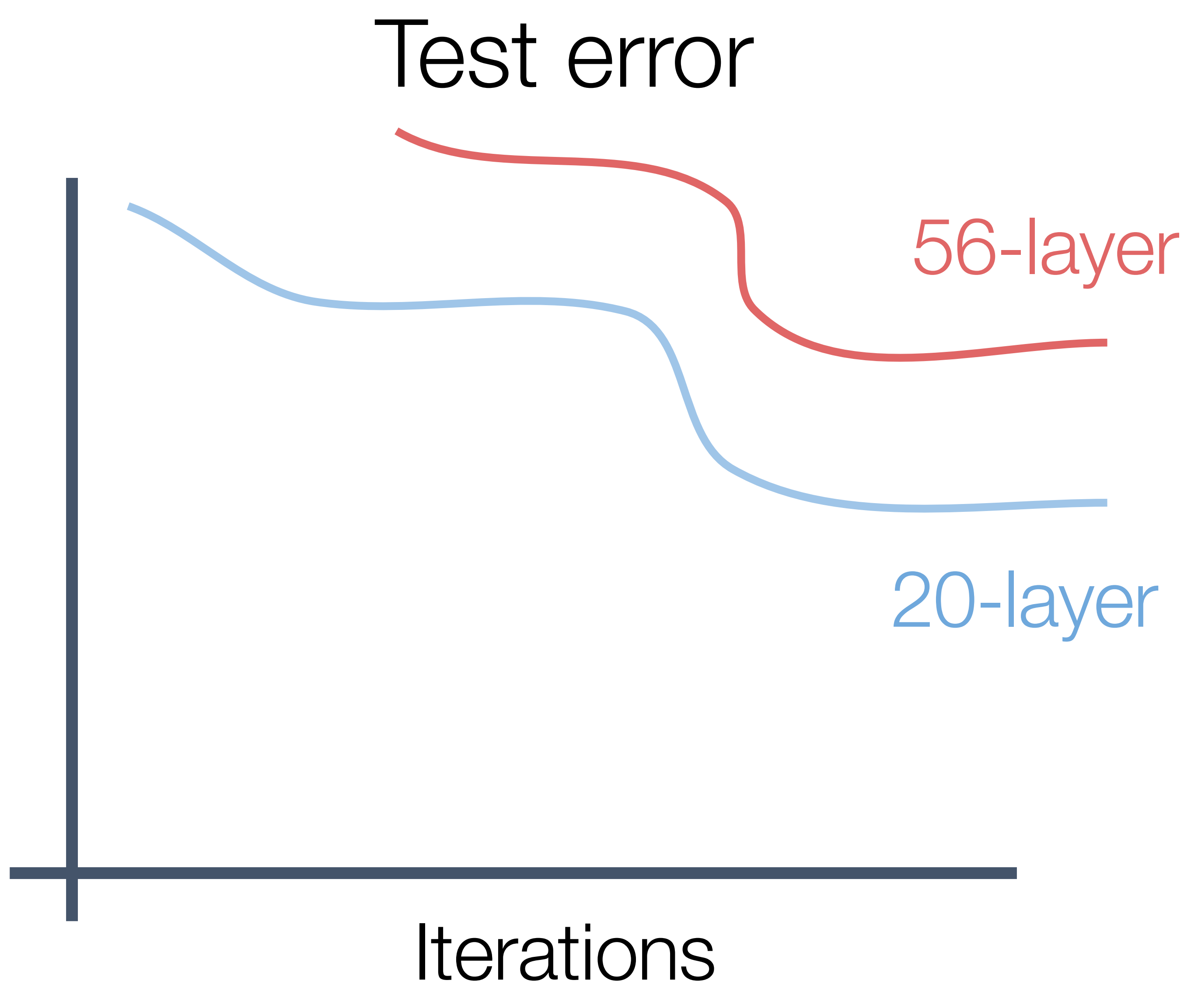

In fact the deep model seems to be **underfitting** since it also performs worse than the shallow model on the training set! It is actually **underfitting**

He et al, “Deep Residual Learning for Image Recognition”, CVPR 2016

Residual Networks

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

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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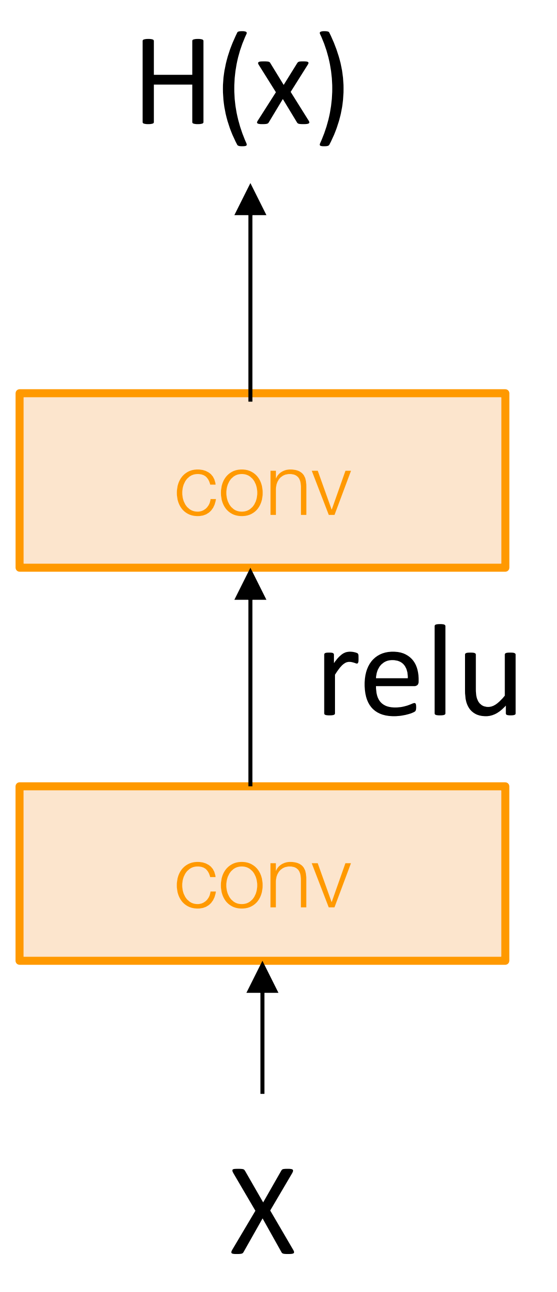
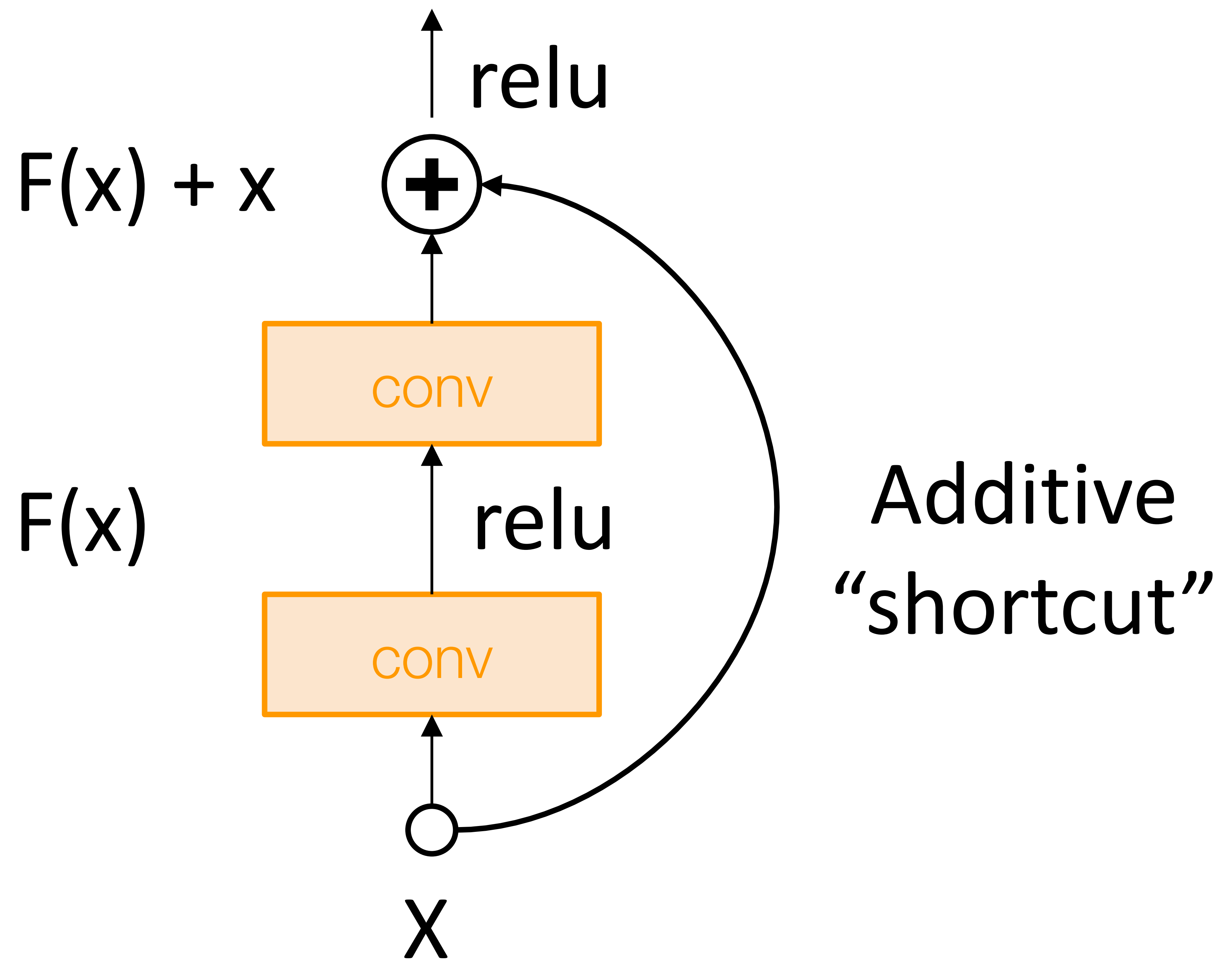


"Plain" block

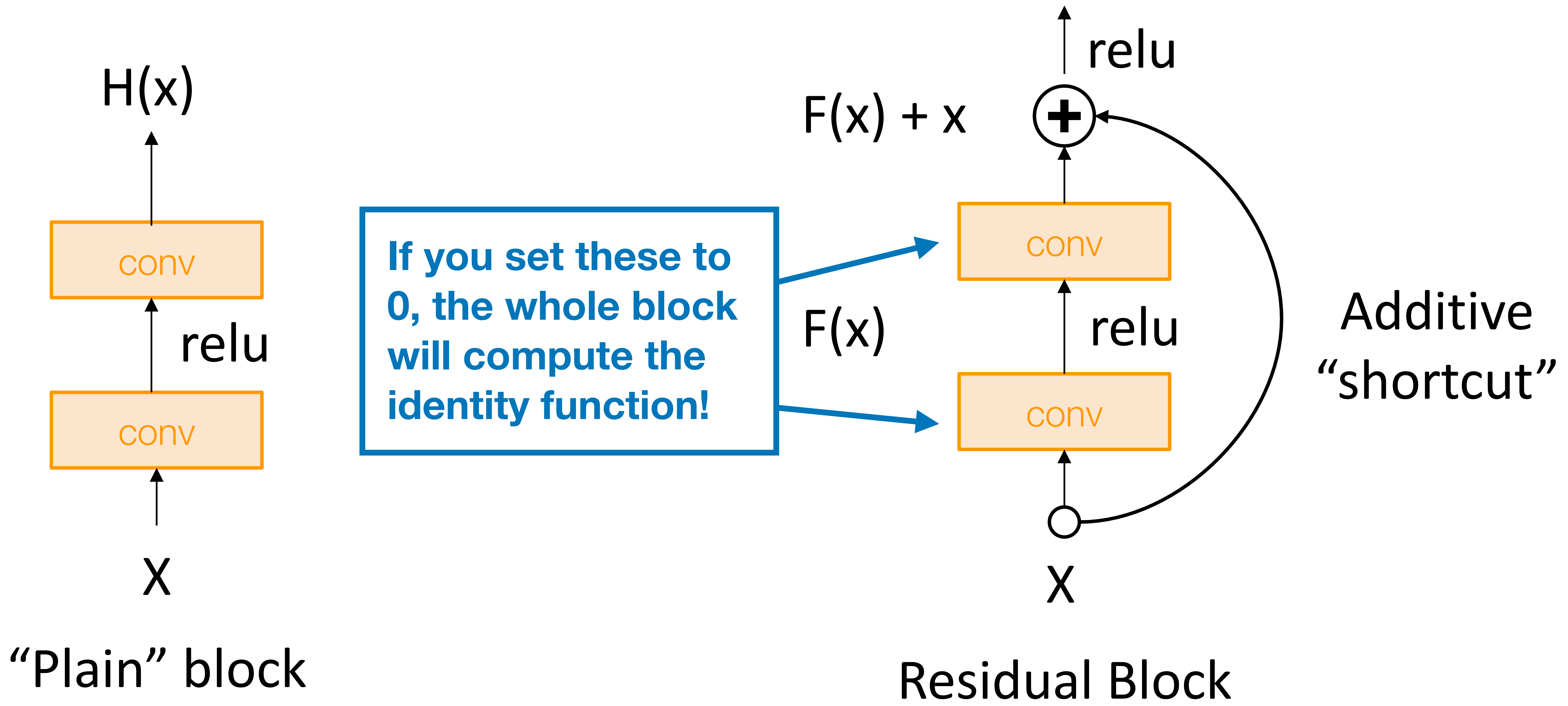


Residual Block

He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

Residual Networks

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



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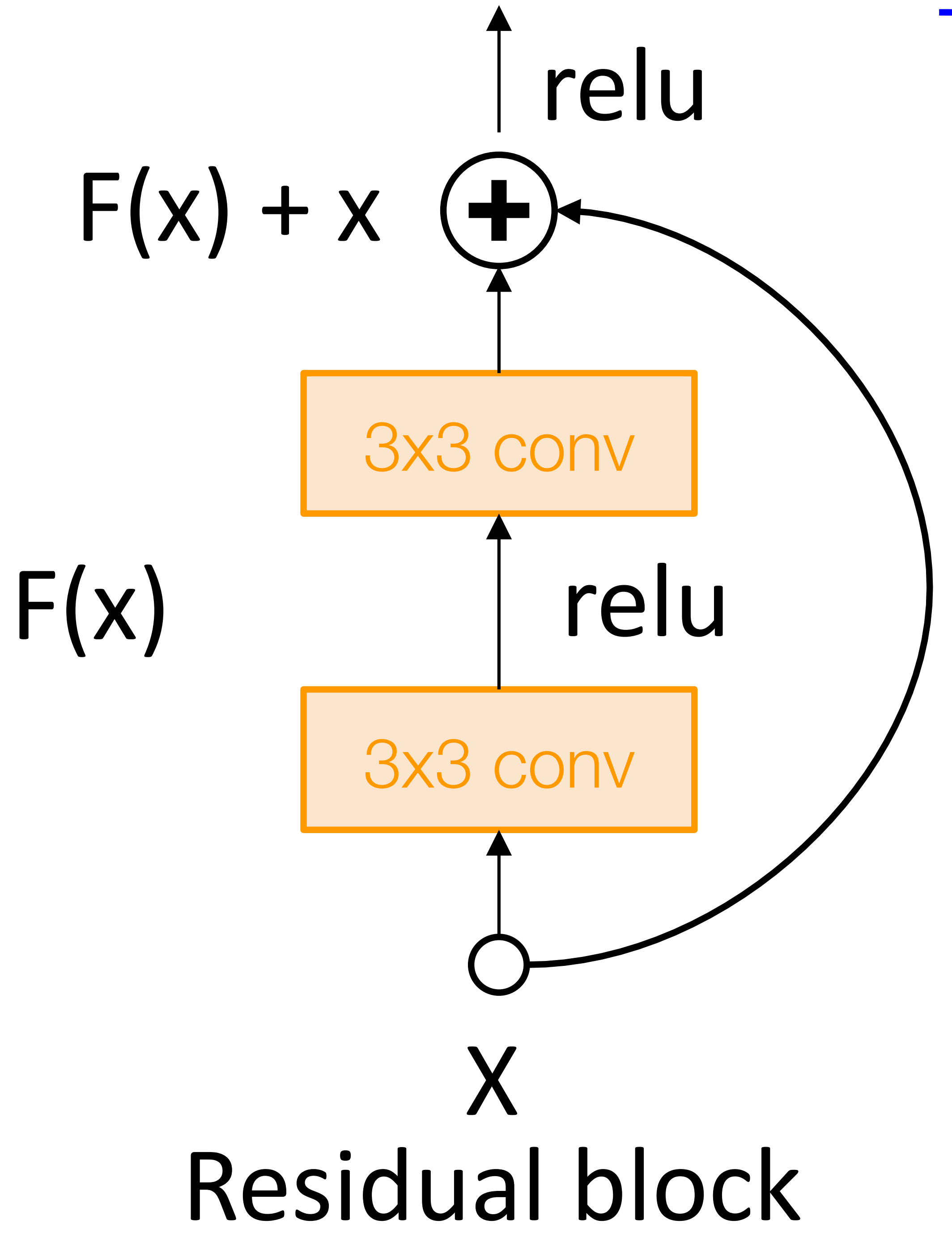
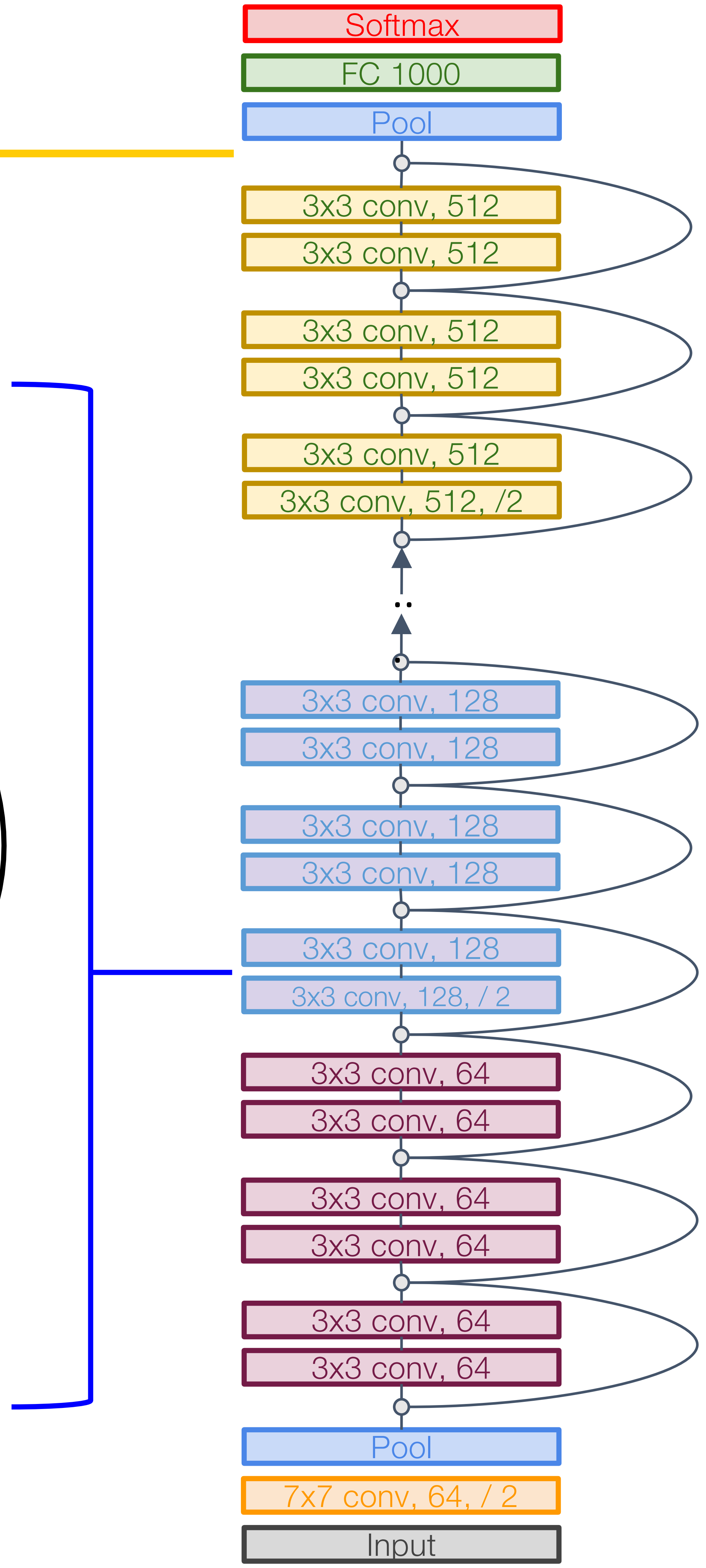
Residual Networks

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



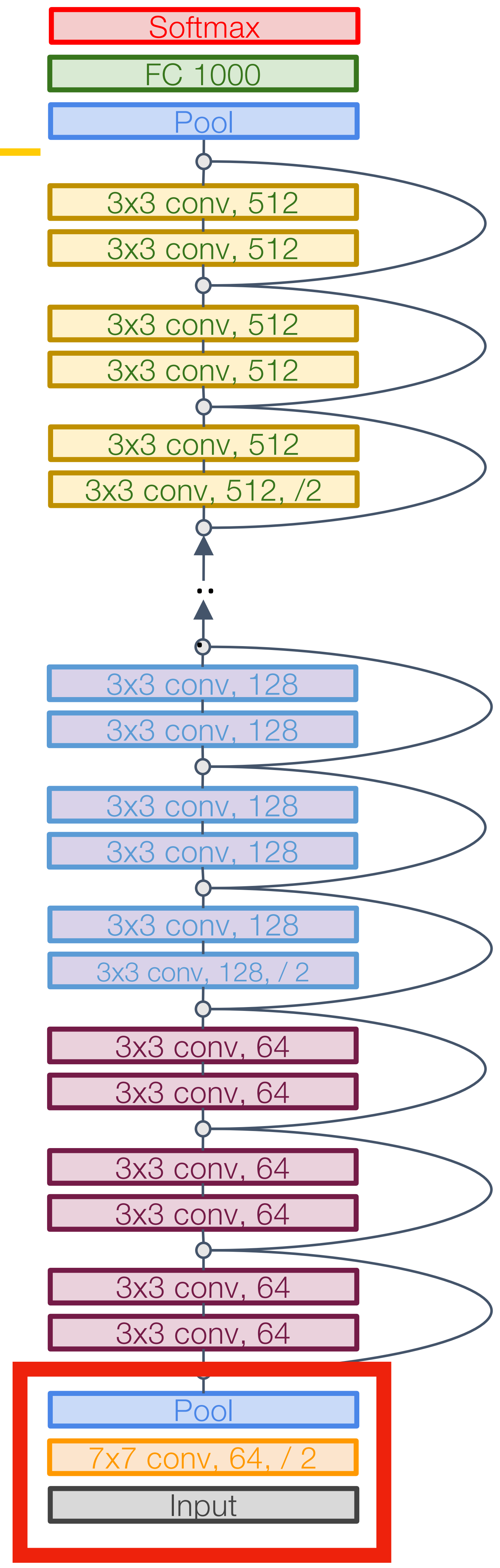


He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

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



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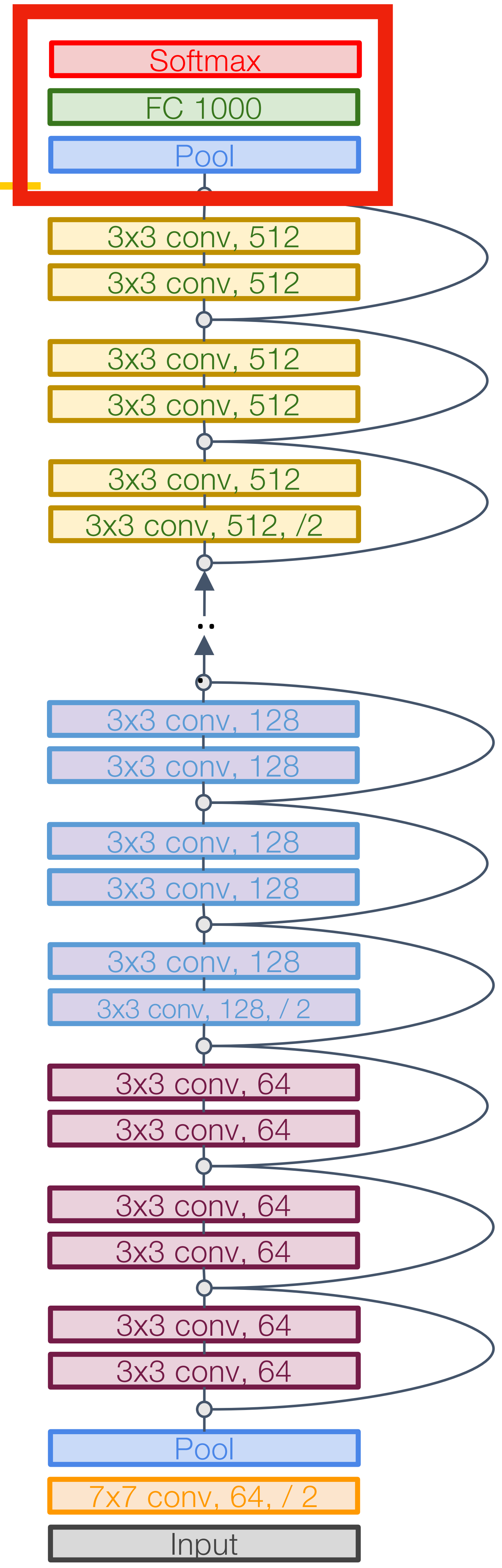
Residual Networks

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

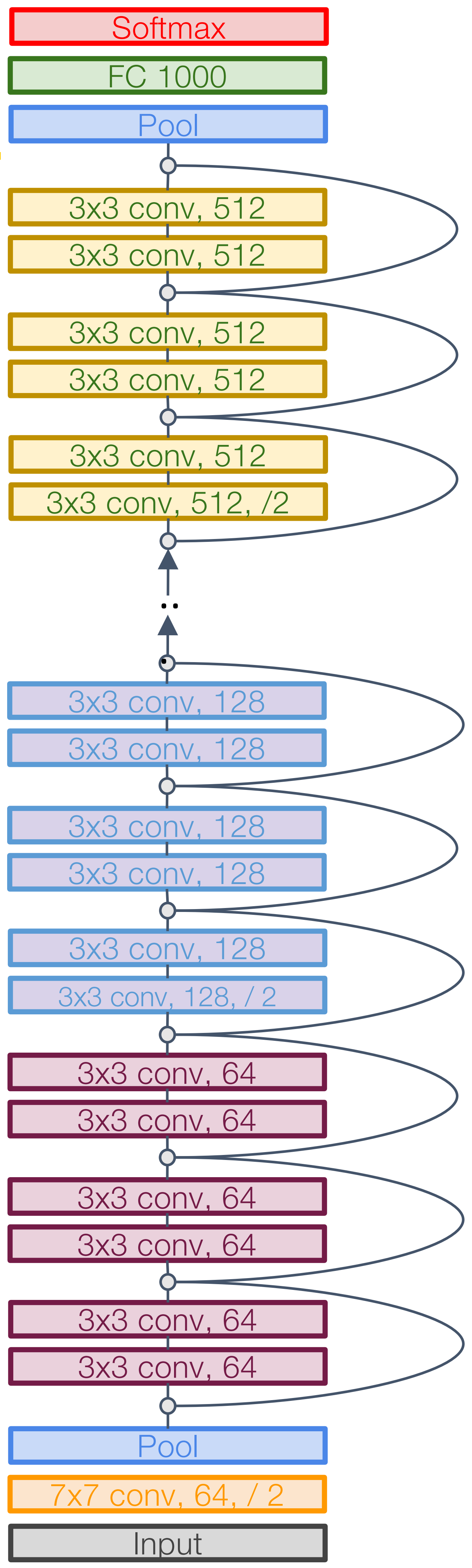


He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

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



He et al, "Deep Residual Learning for Image Recognition", CVPR 2016
Error rates are 224x224 single-crop testing, reported by torchvision

Residual Networks

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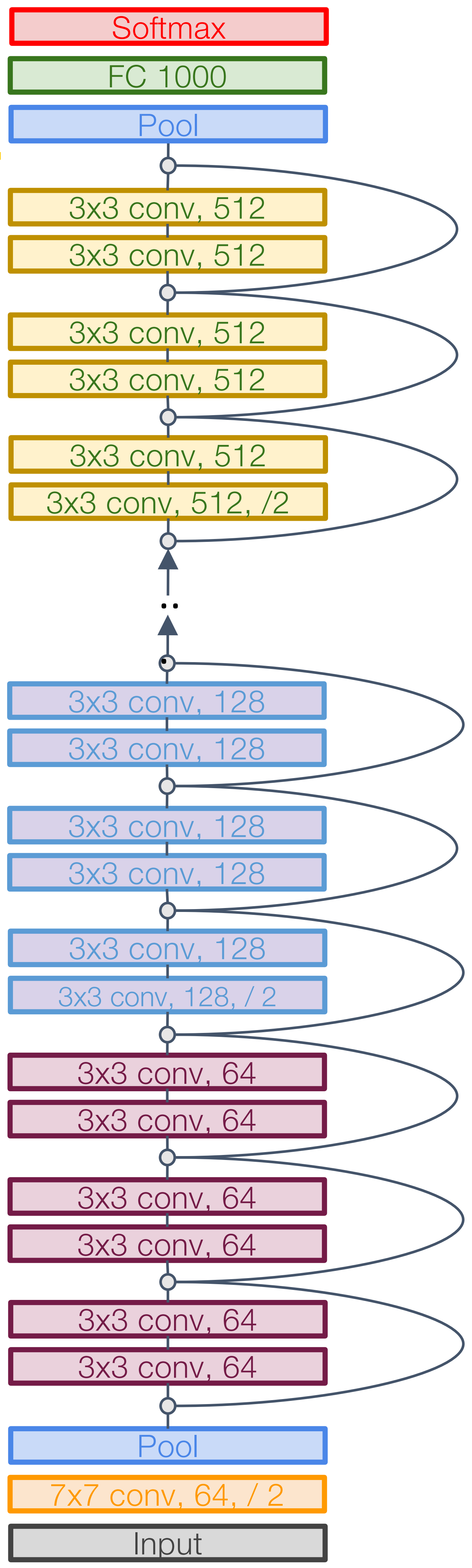
Stage 4 (C=512): 2 res. block = 4 conv
Linear

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



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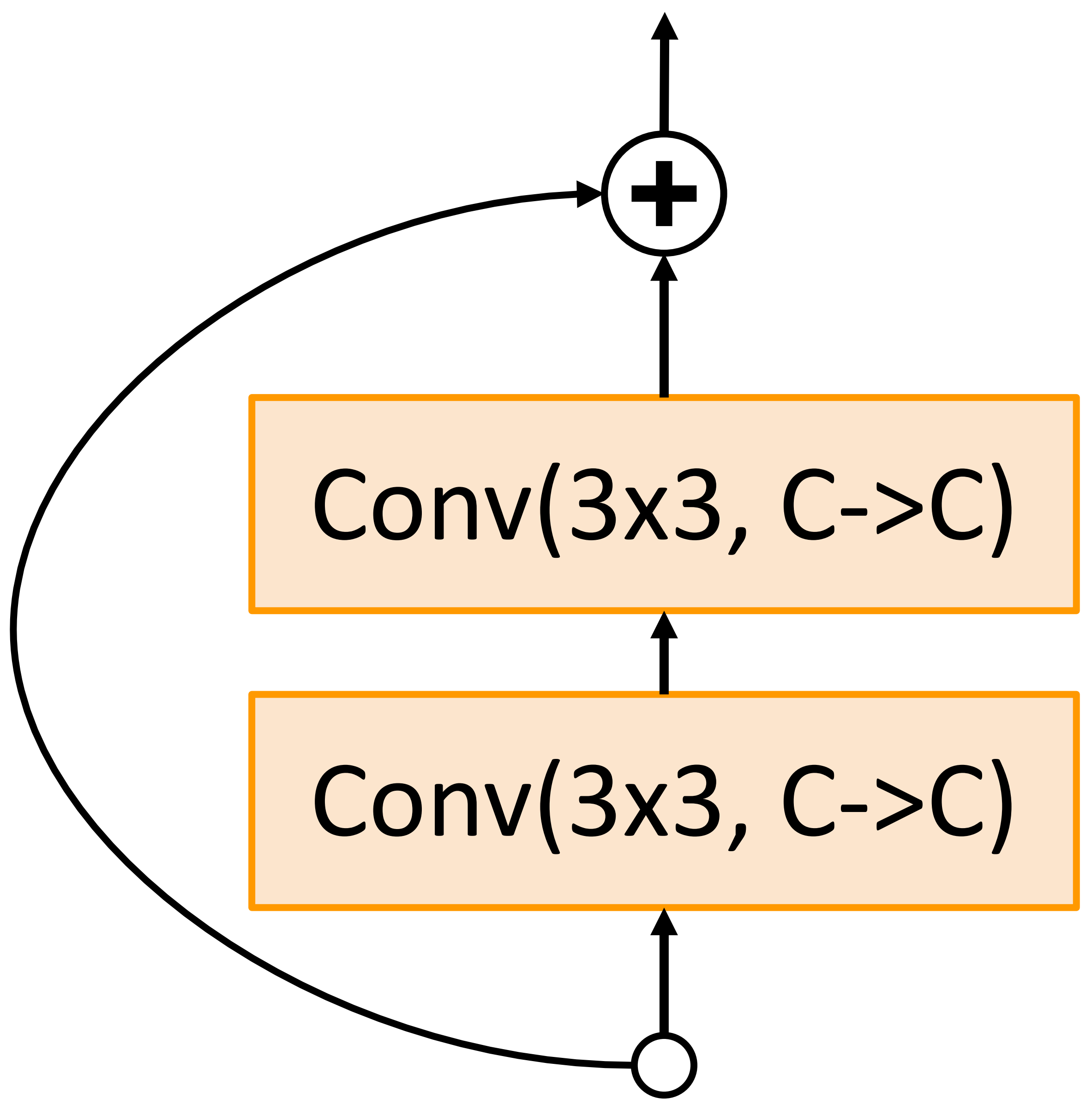
Residual Networks: Basic Block



FLOPs: $9HWC^2$

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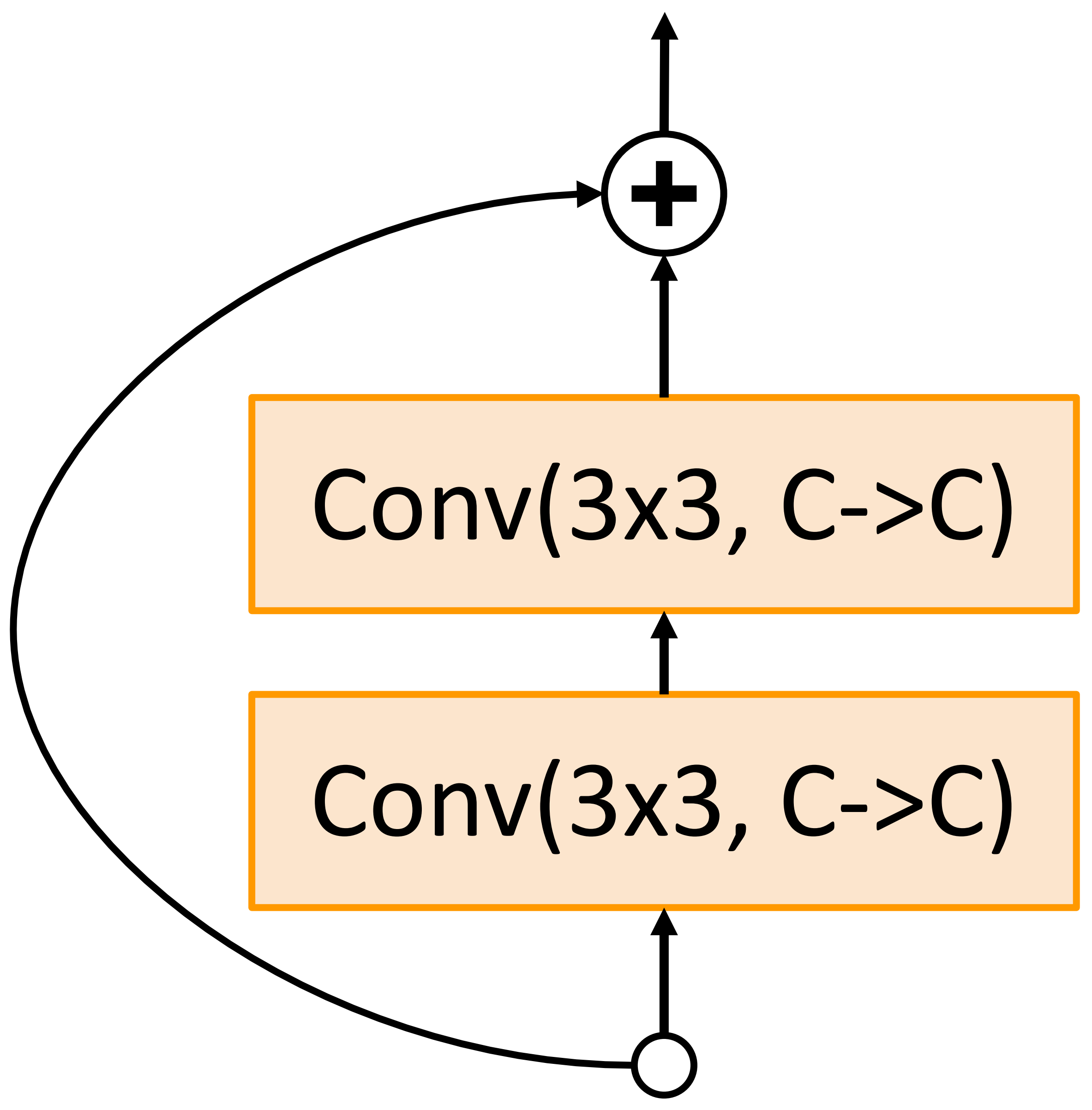
"Basic"
Residual block

Total FLOPs:
$18HWC^2$

He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

Residual Networks: Bottleneck Block



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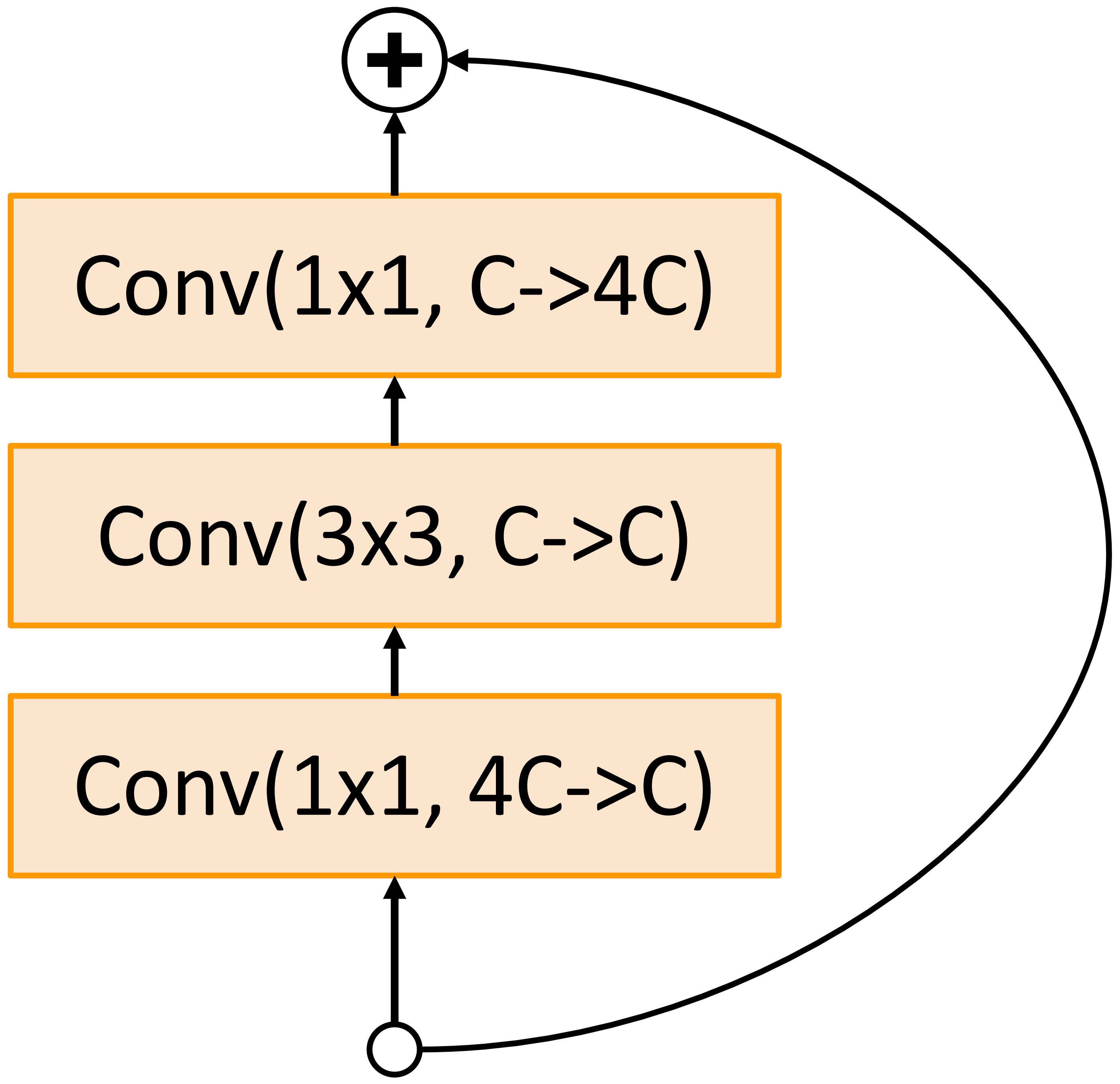
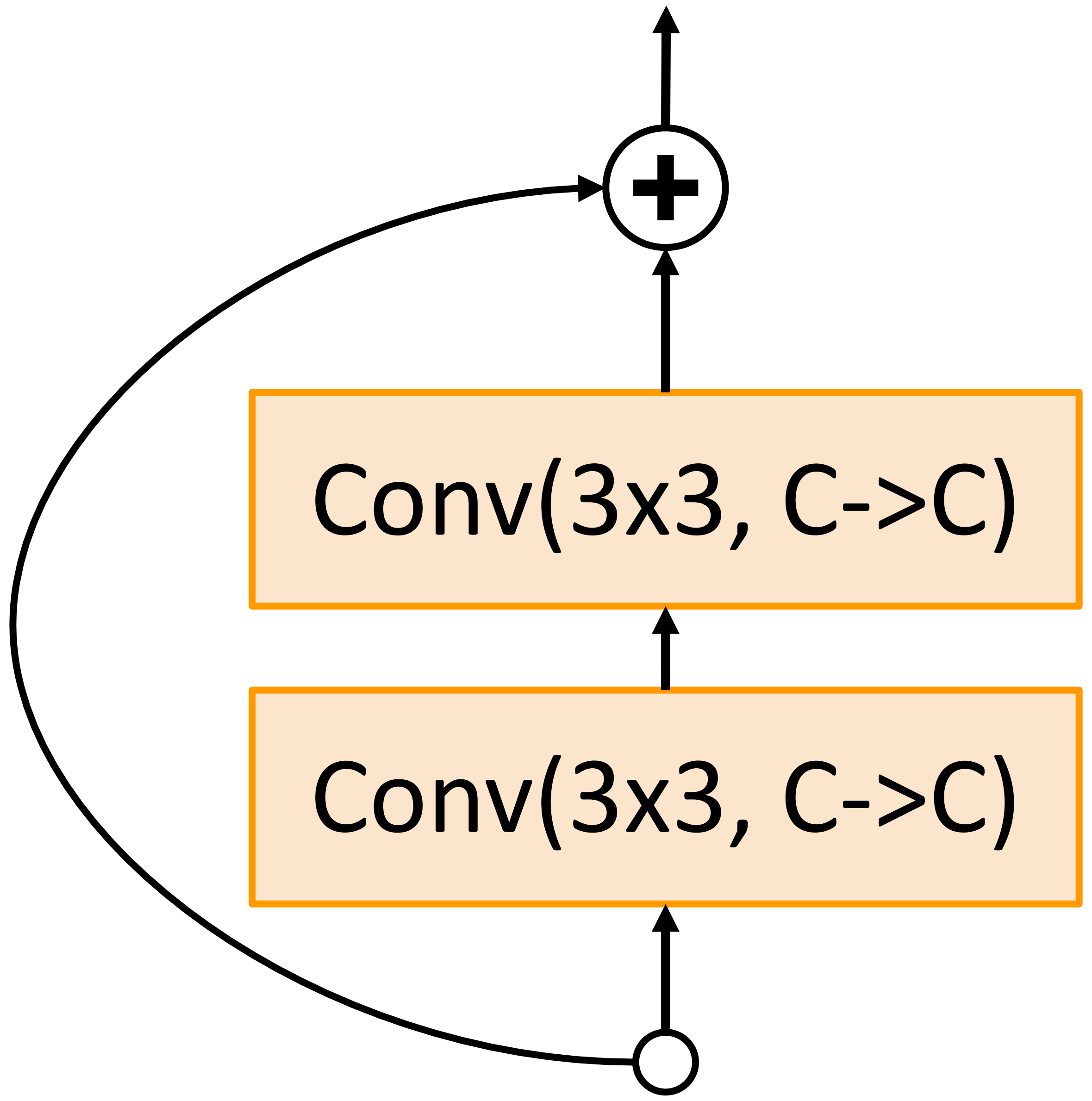


"Bottleneck"
Residual block

He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

Residual Networks: Bottleneck Block

More layers, less computational cost!



FLOPs: $9HWC^2$

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"Basic"
Residual block

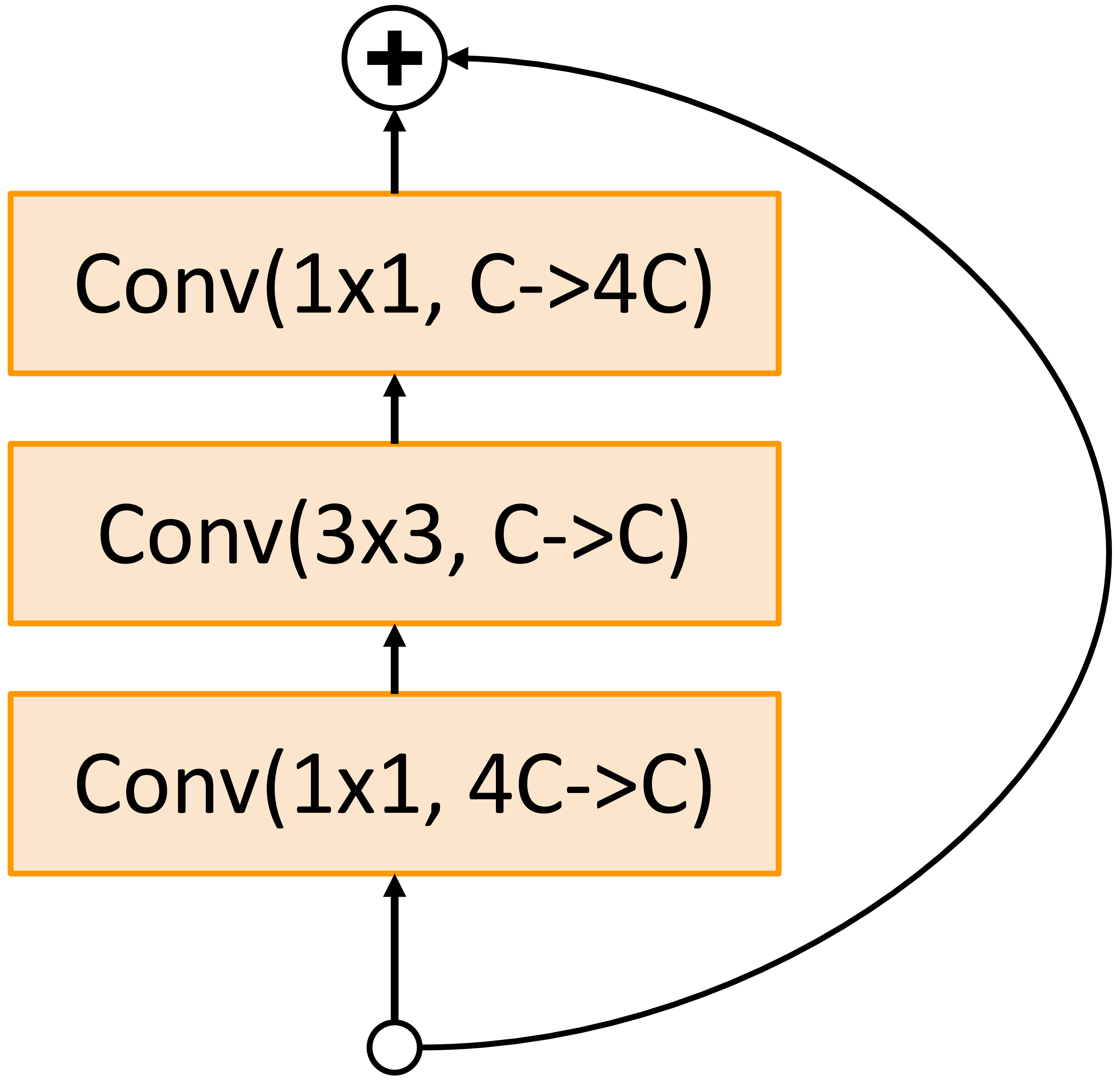
Total FLOPs:
$18HWC^2$

FLOPs: $4HWC^2$

FLOPs: $9HWC^2$

FLOPs: $4HWC^2$

Total FLOPs:
$17HWC^2$



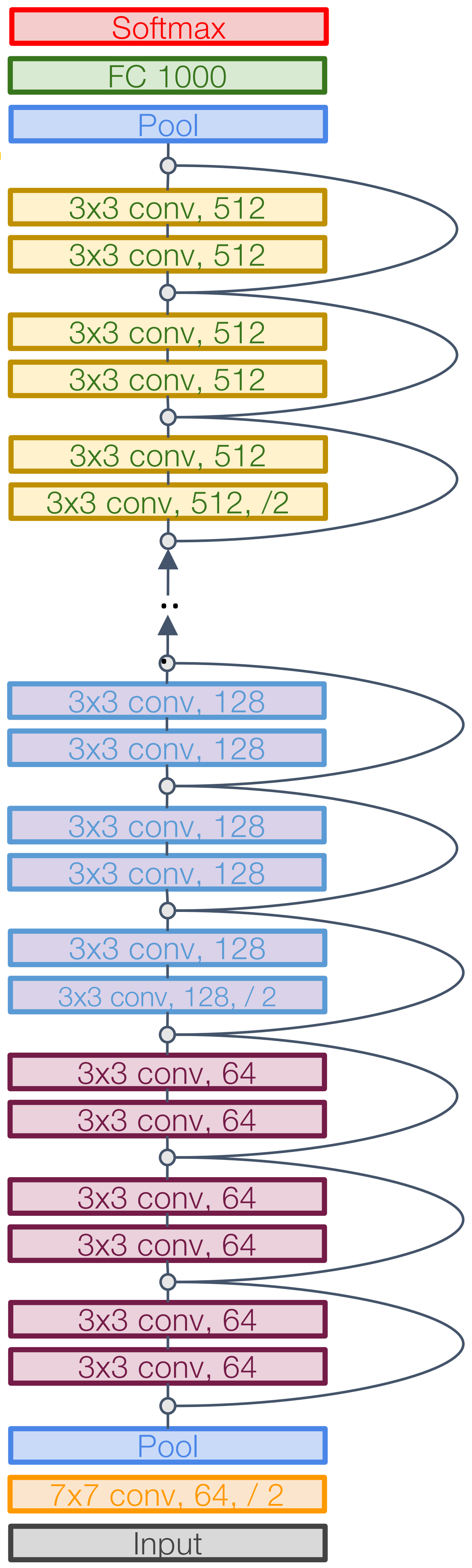
"Bottleneck"
Residual block

He et al, "Deep Residual Learning for Image Recognition", CVPR 2016

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**	**Blocks**	**Layers**	**Blocks**	**Layers**	**Blocks**	**Layers**	**Blocks**	**Layers**	**FC Layers**	**GFLOP**	**ImageNet**
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



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DR

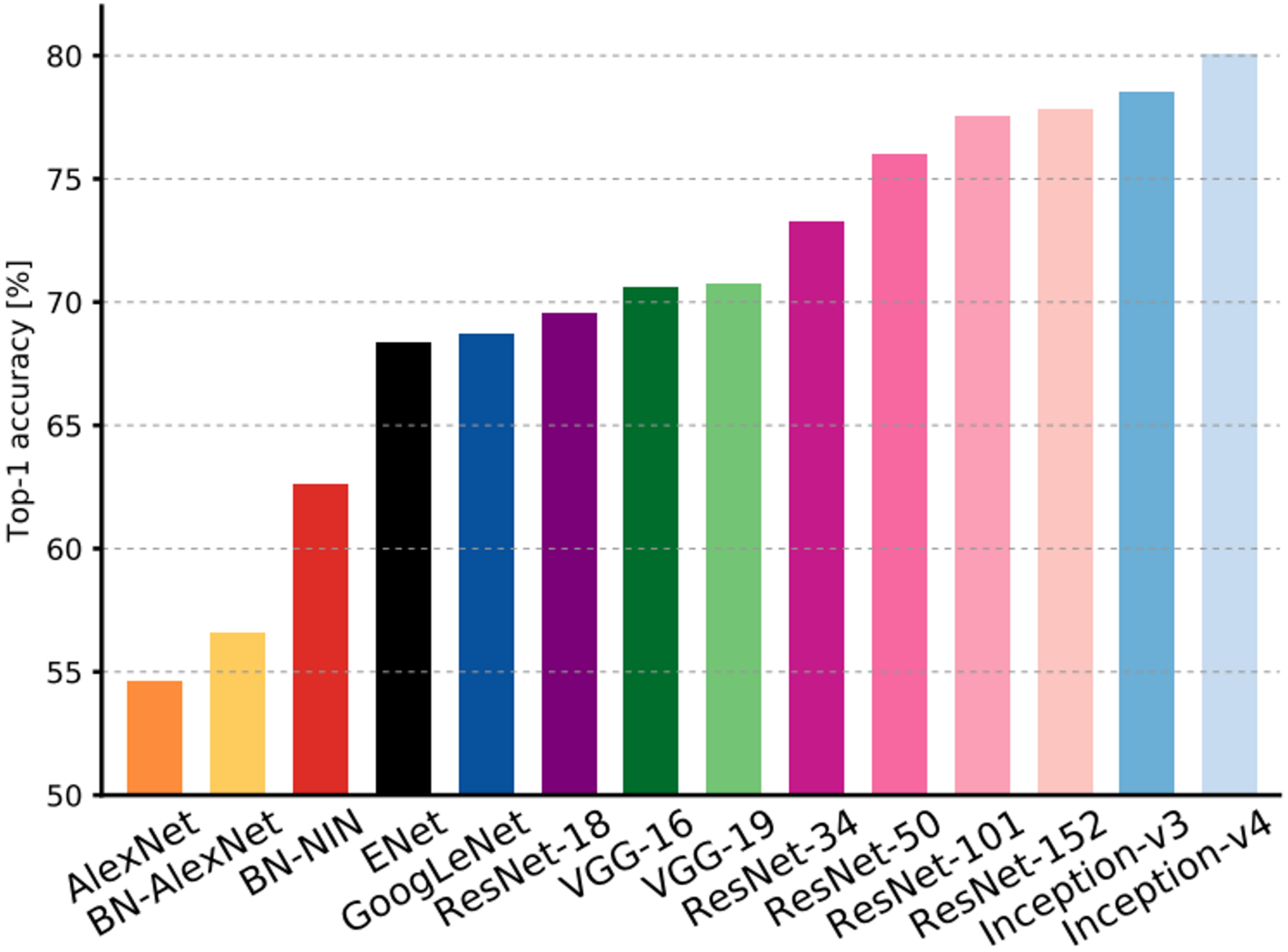
Residual Networks

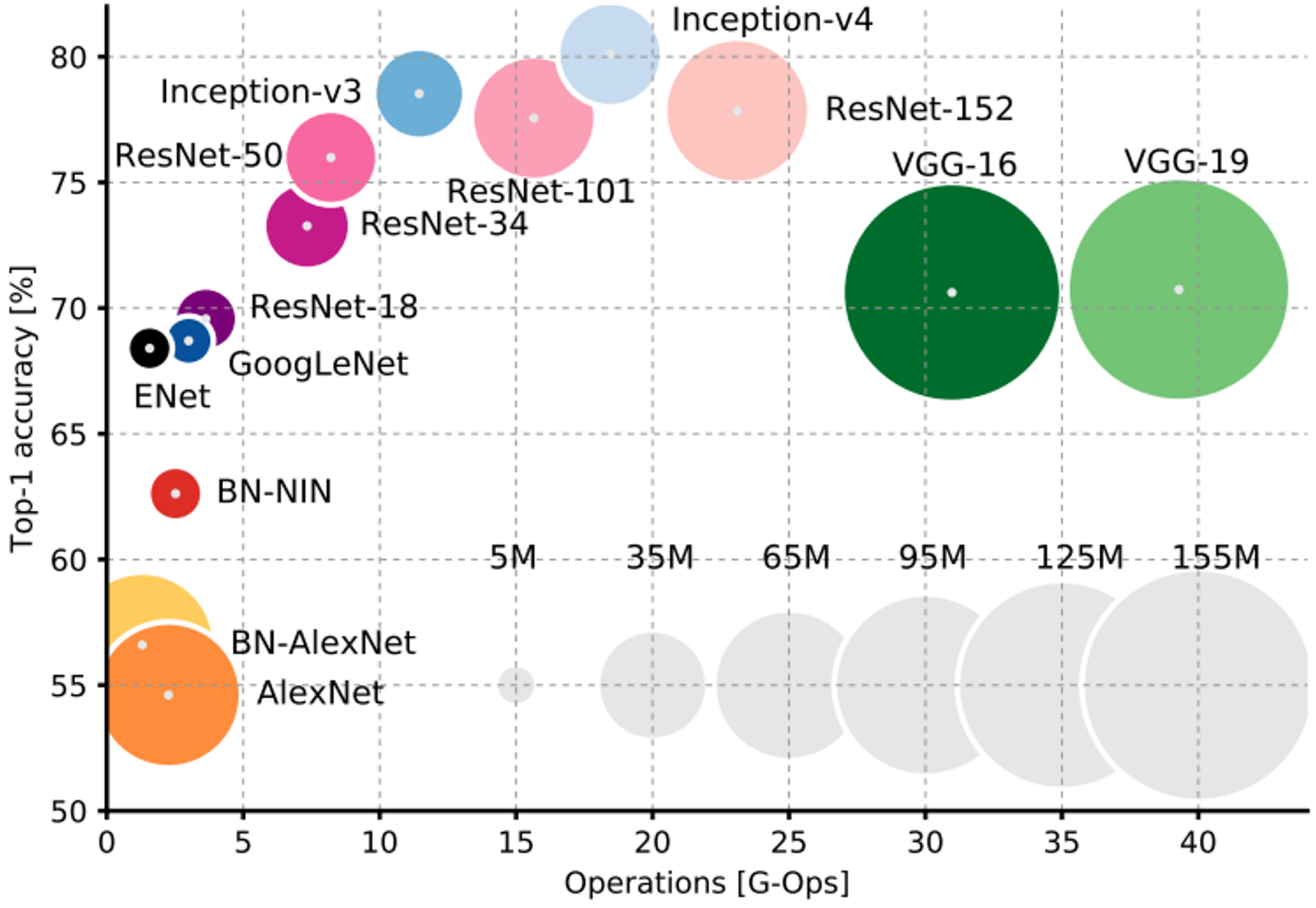
- Able to train very deep networks
- Deeper networks do better than shallow networks (as expected)
- Swept 1st place in all ILSVRC and COCO 2015 competitions
- Still widely used today

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

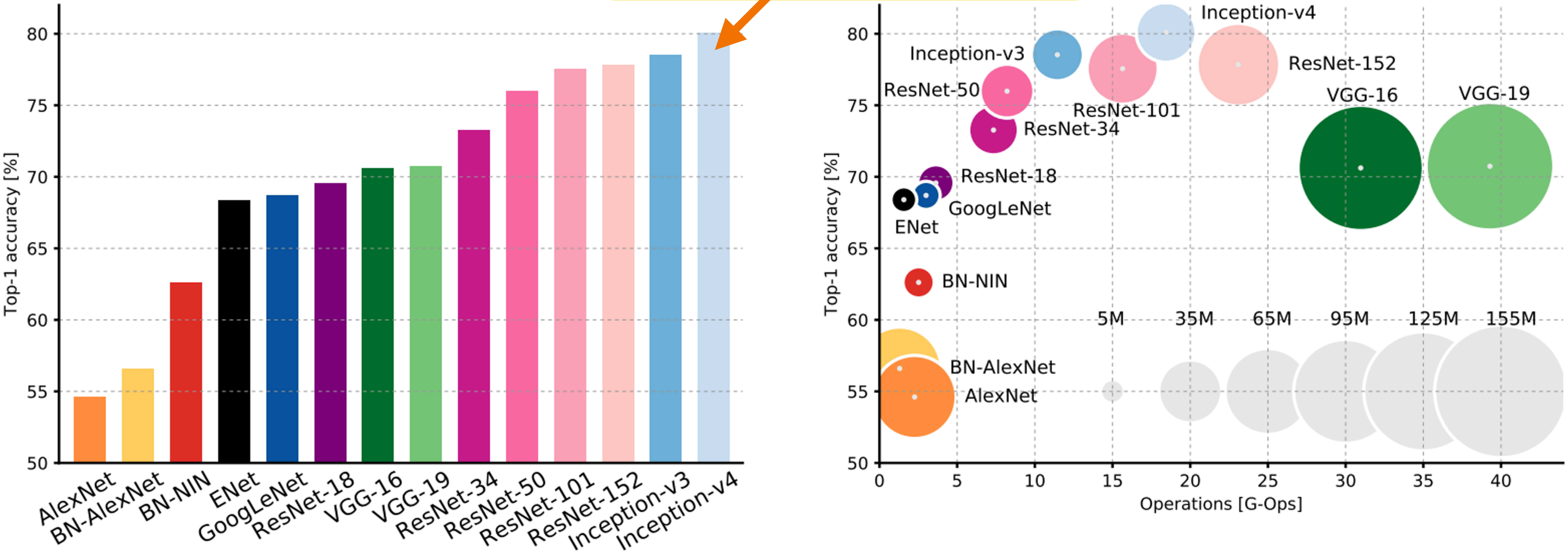




Canziani et al, “An analysis of deep neural network models for practical applications”, 2017

Comparing Complexity

Inception-v4: ResNet + Inception!



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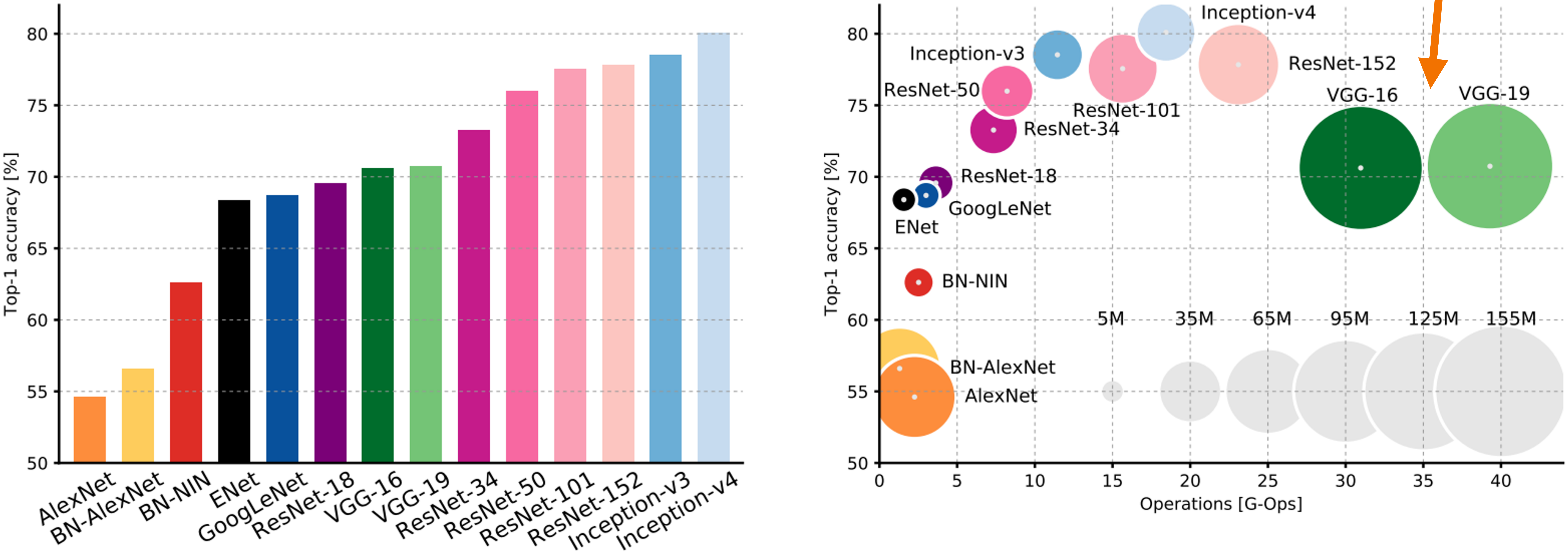
Comparing Complexity

**VGG:
Highest memory,
most operations**



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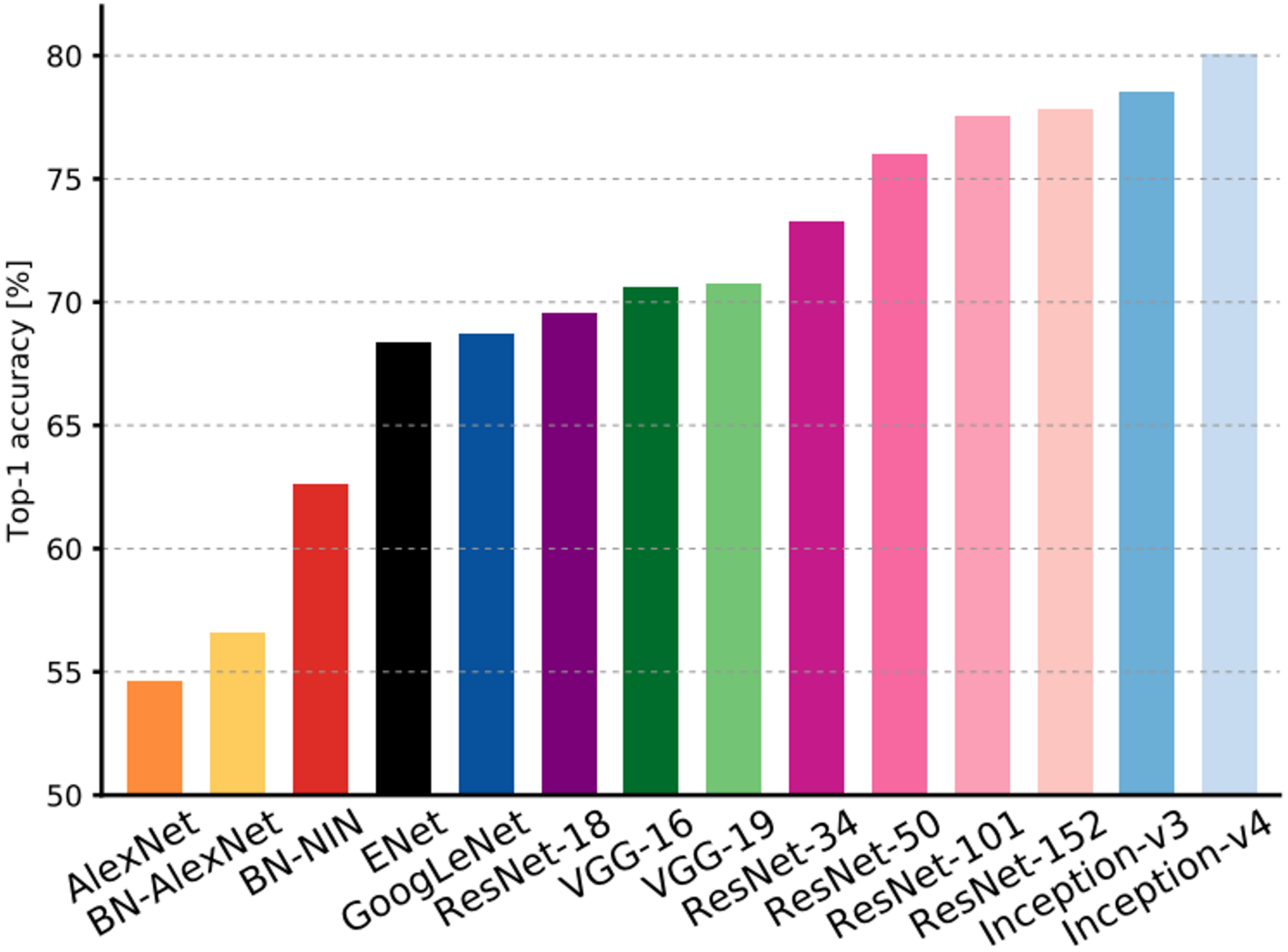
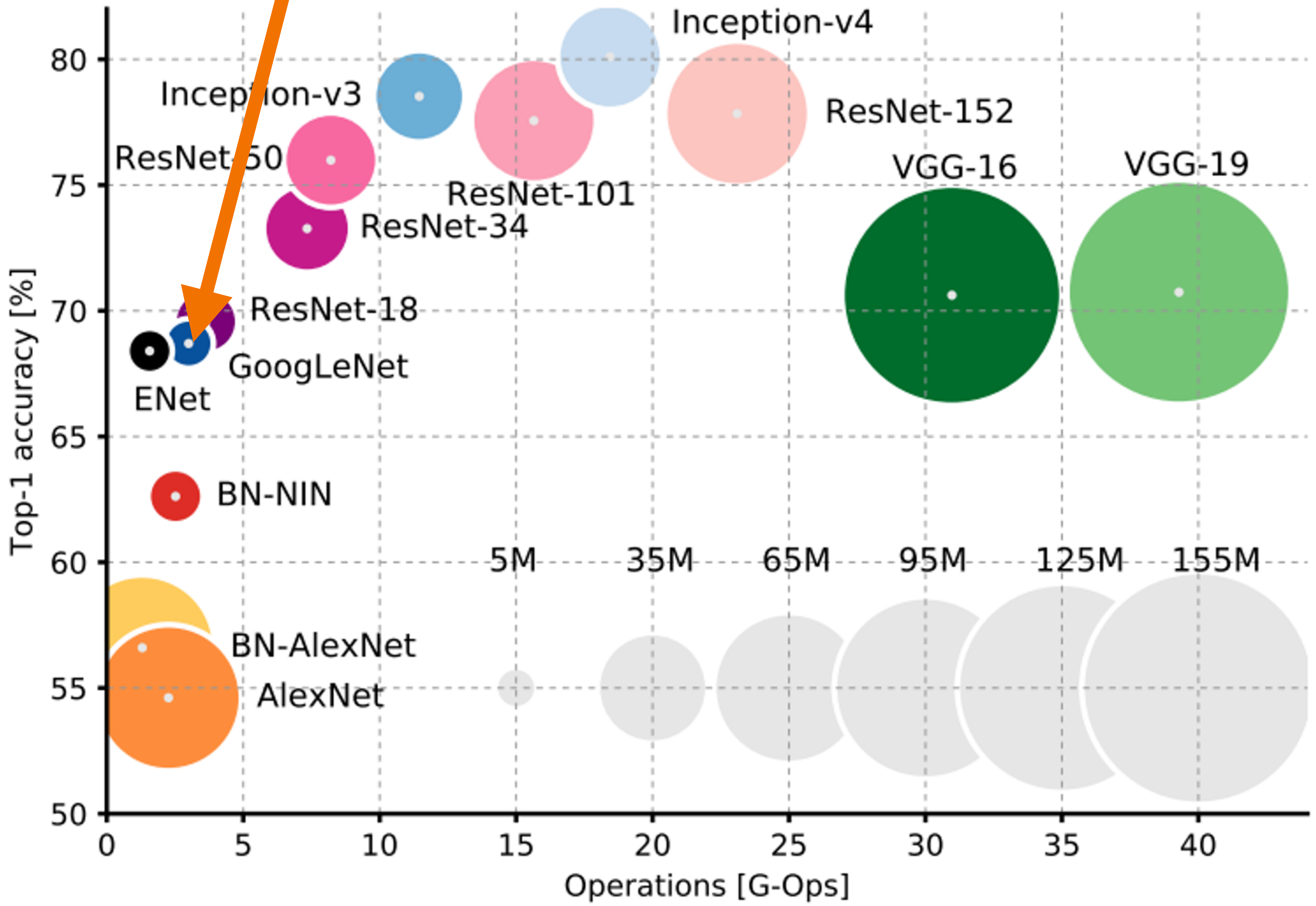


GoogLeNet: Very efficient!



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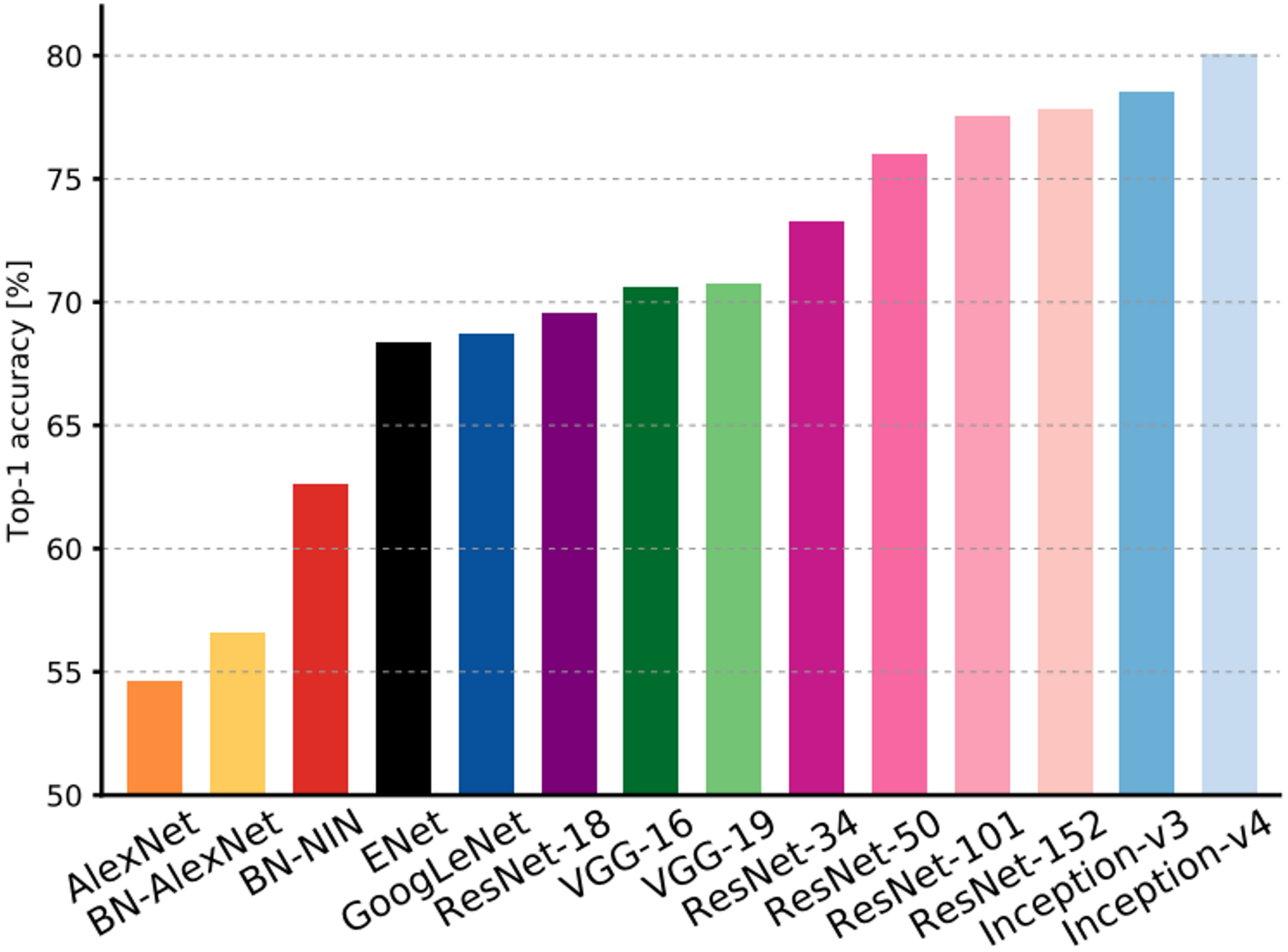
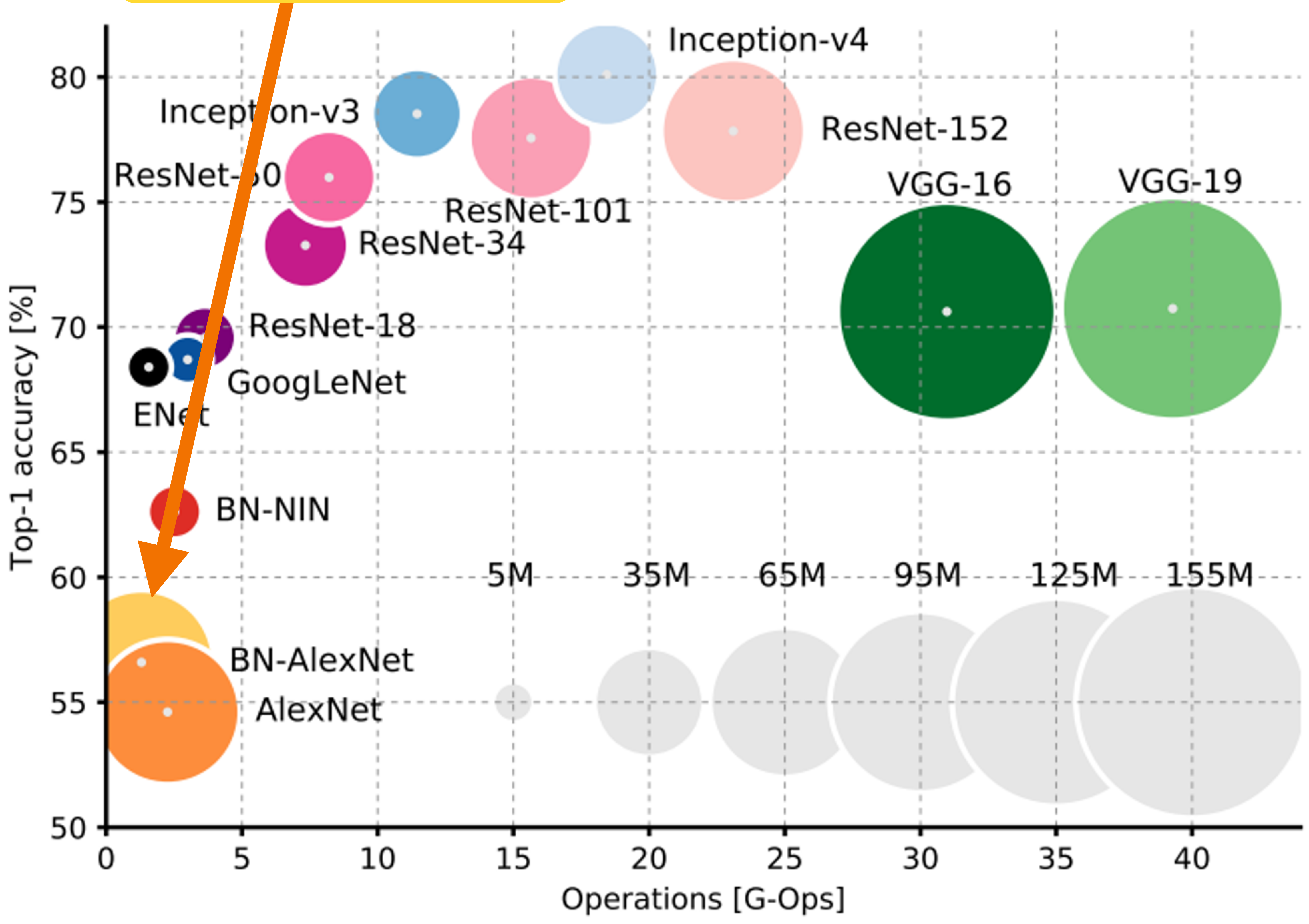


AlexNet: Low compute, lots of parameters



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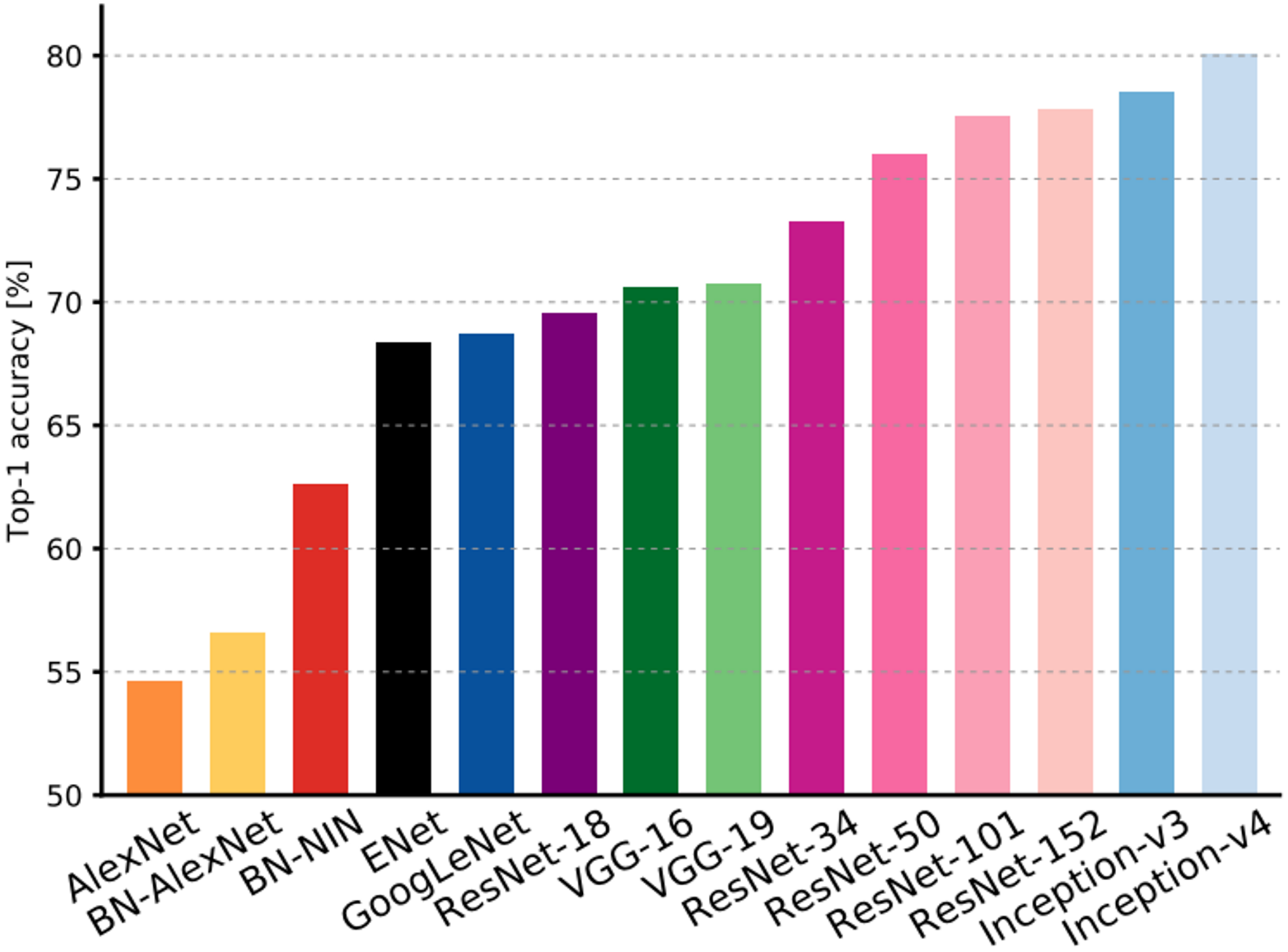
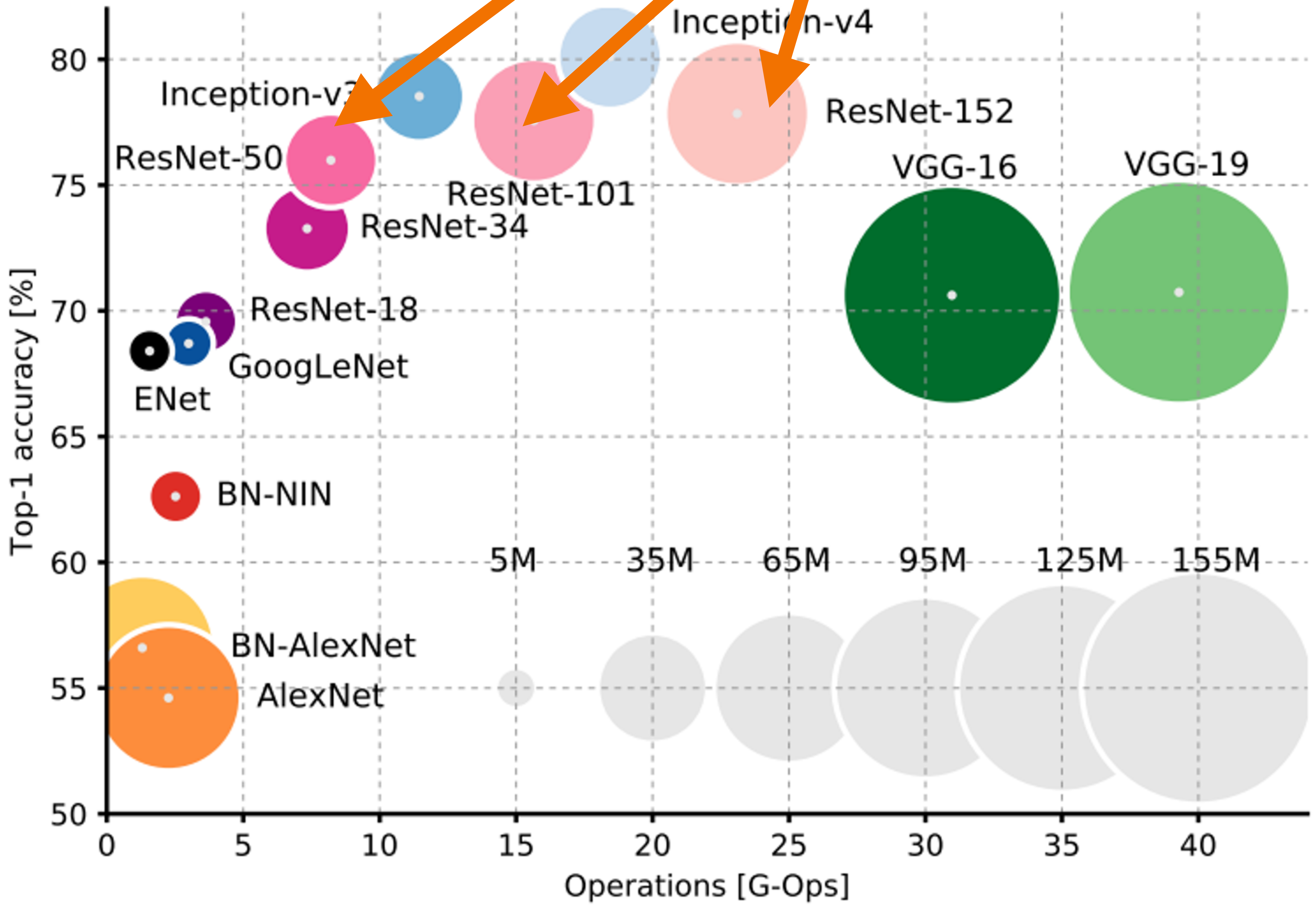
Comparing Complexity

ResNet: Simple design, moderate efficiency, high accuracy





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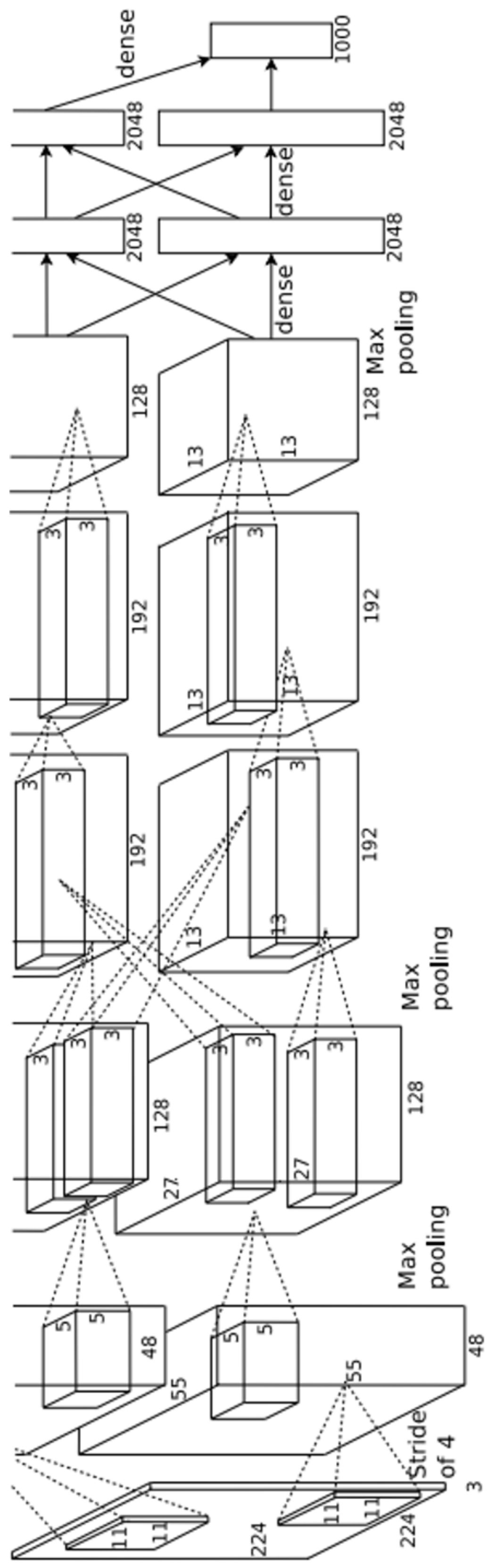
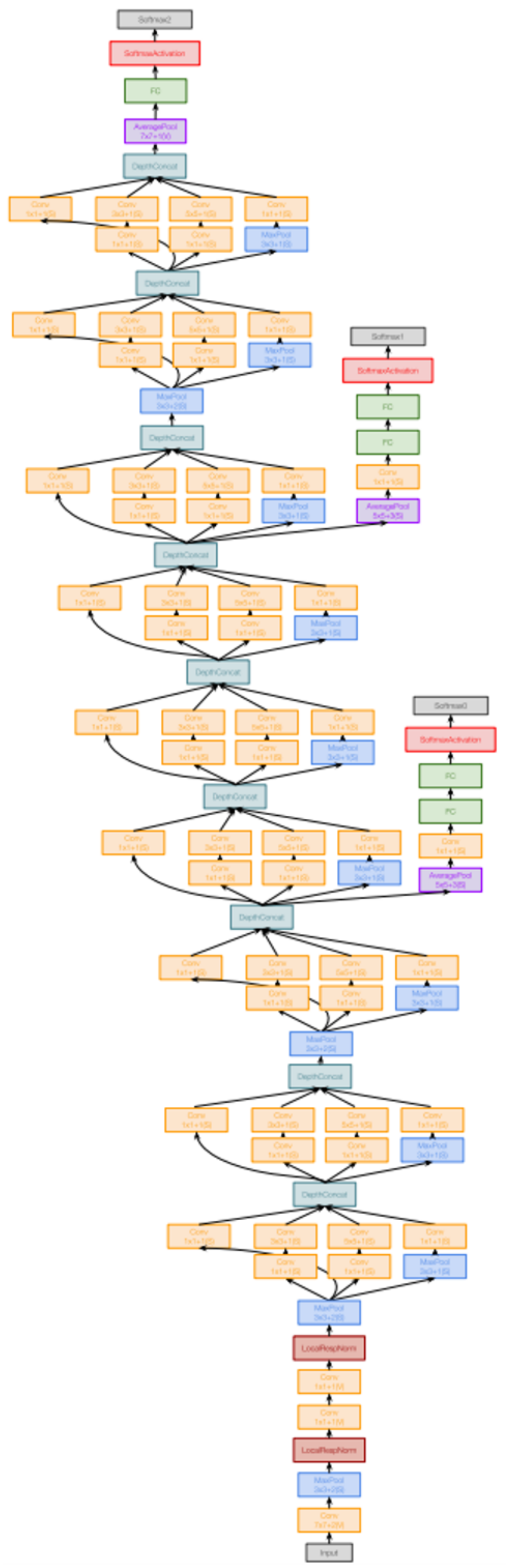
Recap

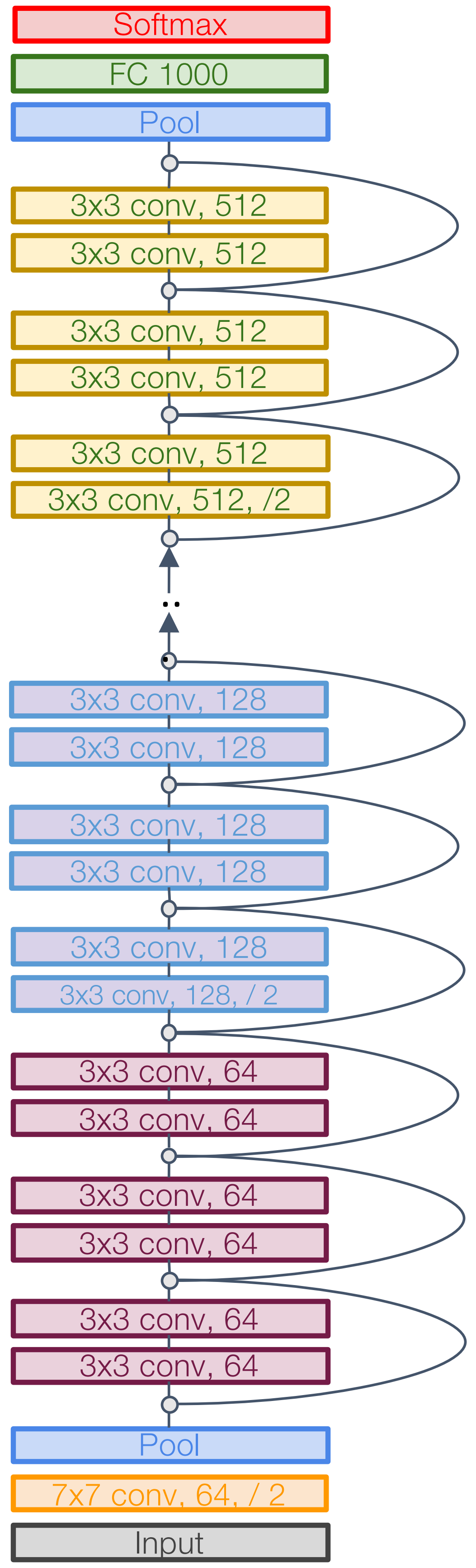


AlexNet

VGG



GoogLeNet

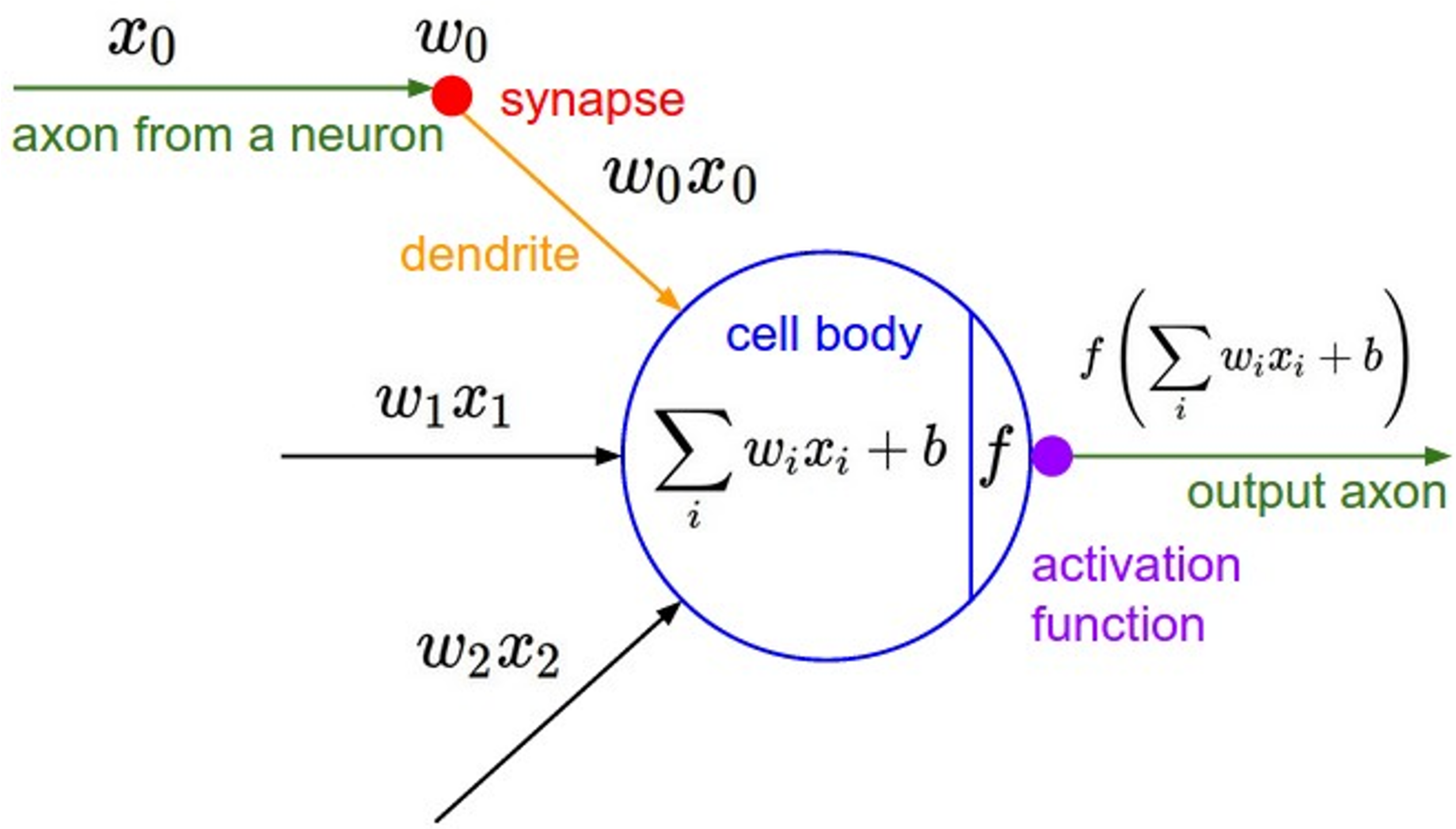


ResNet

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

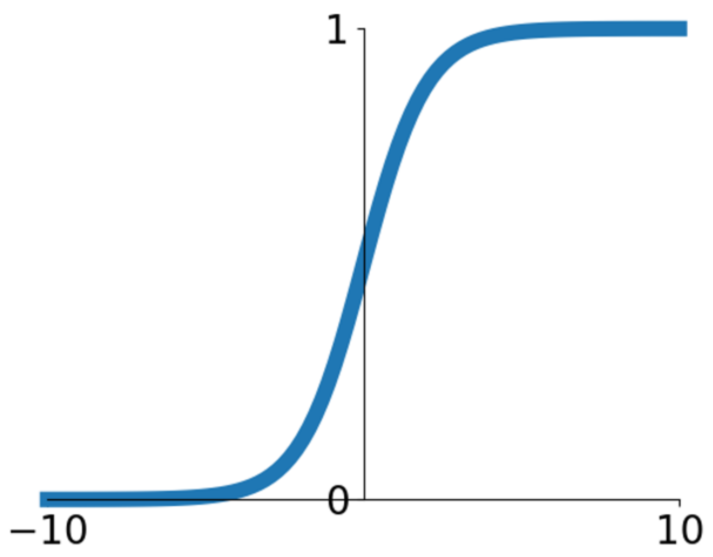
Activation Functions



Activation Functions

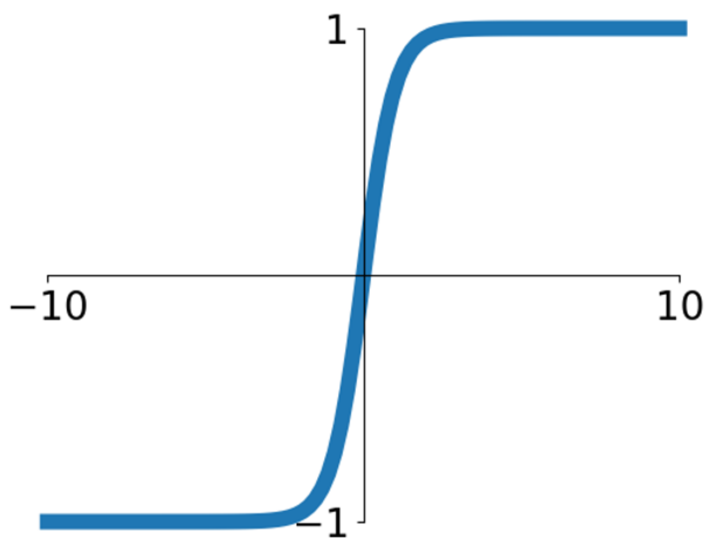
Sigmoid

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



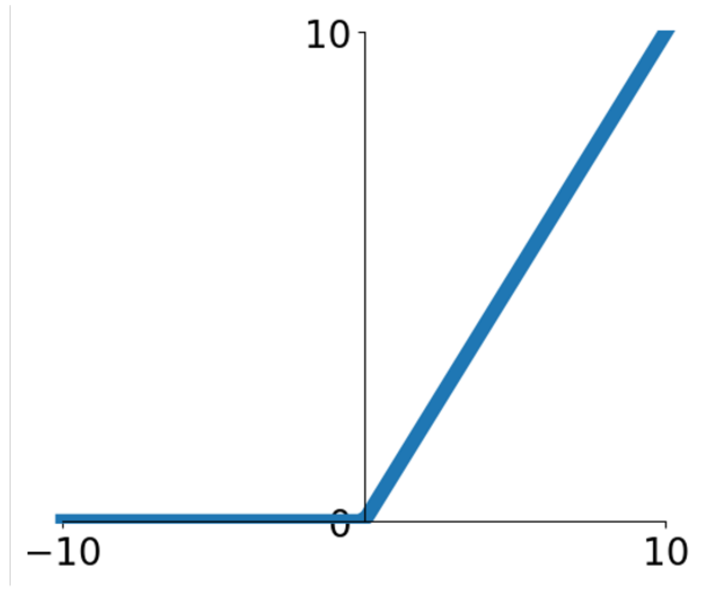
tanh

$$\tanh(x)$$



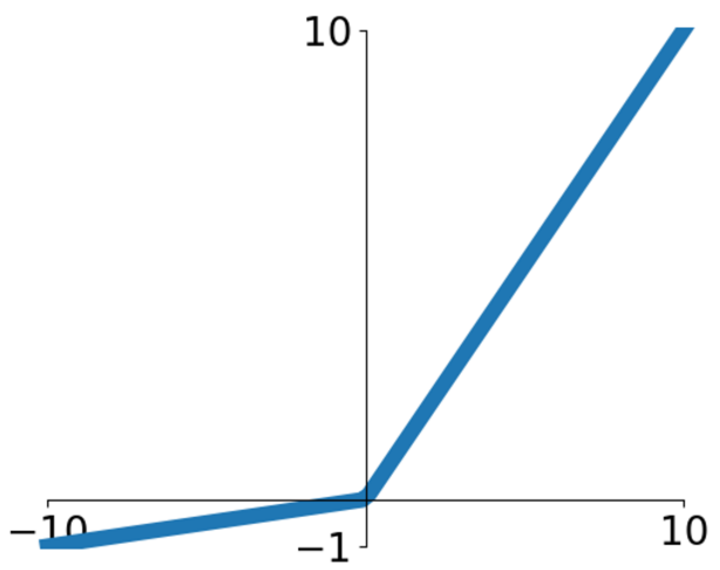
ReLU

$$\max(0,x)$$



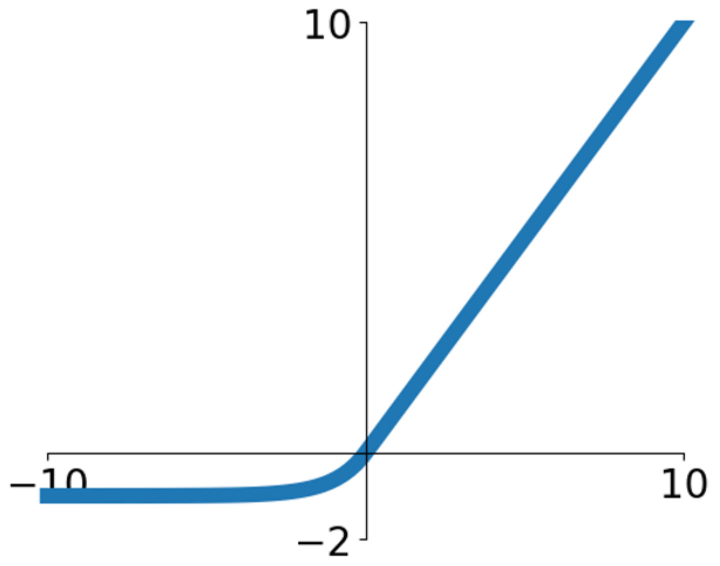
Leaky ReLU

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



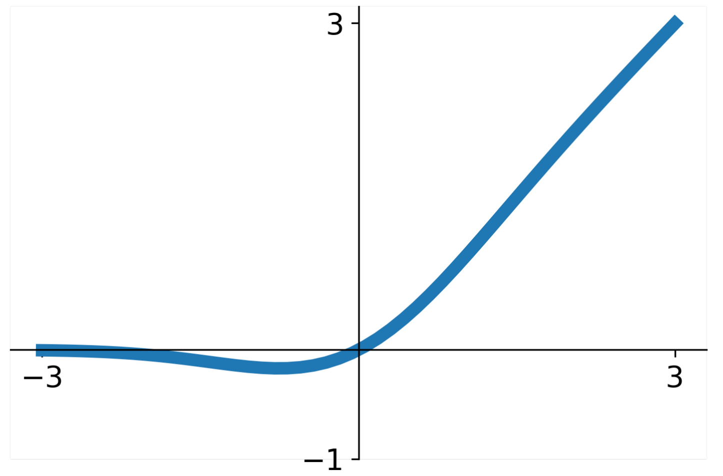
ELU

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



GELU

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



Activation Functions: Sigmoid

Sigmoid

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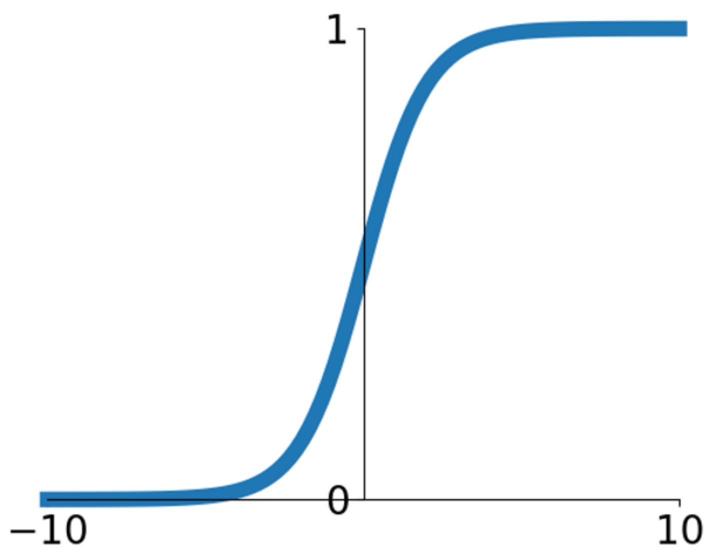
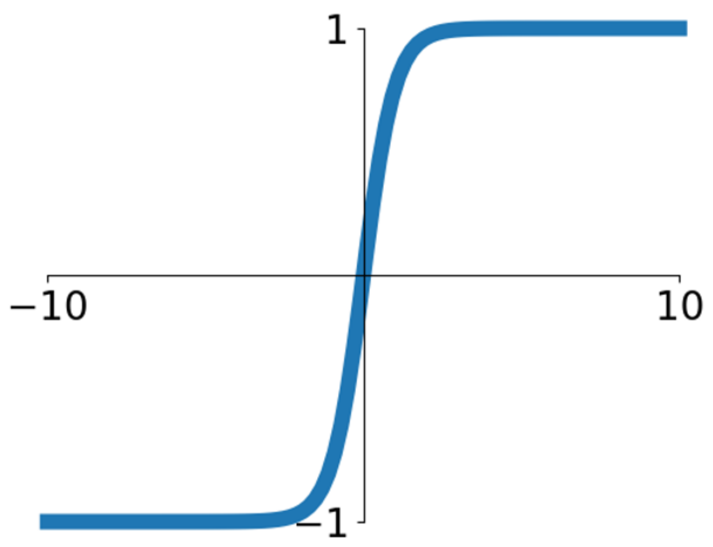


tanh

$$\tanh(x)$$



ReLU

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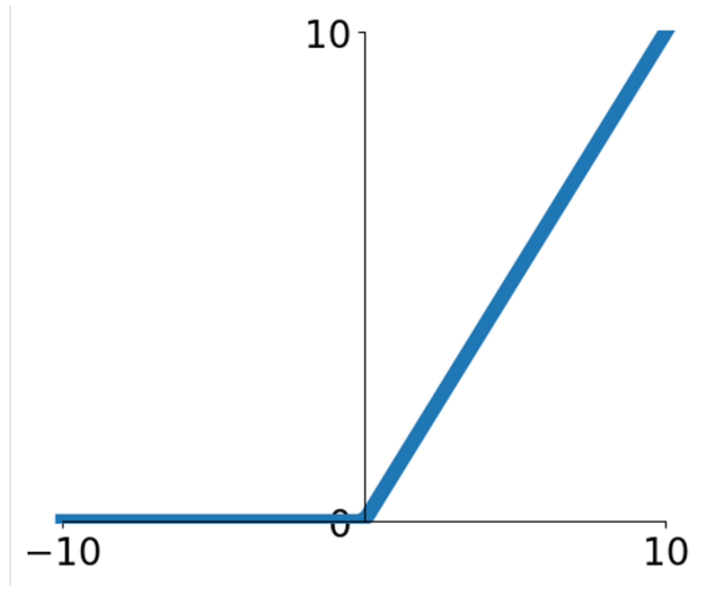

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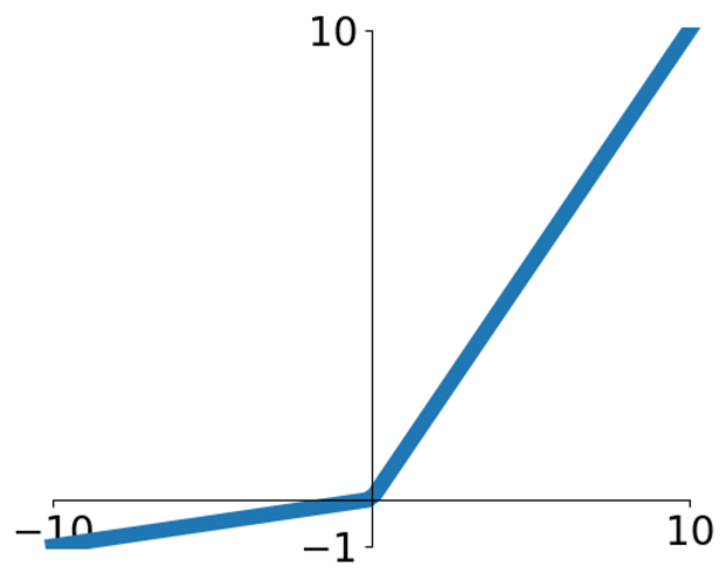

ELU

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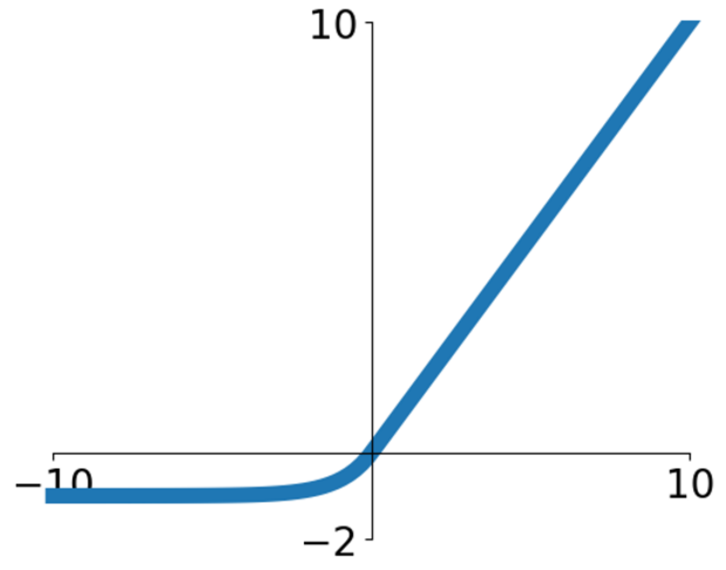
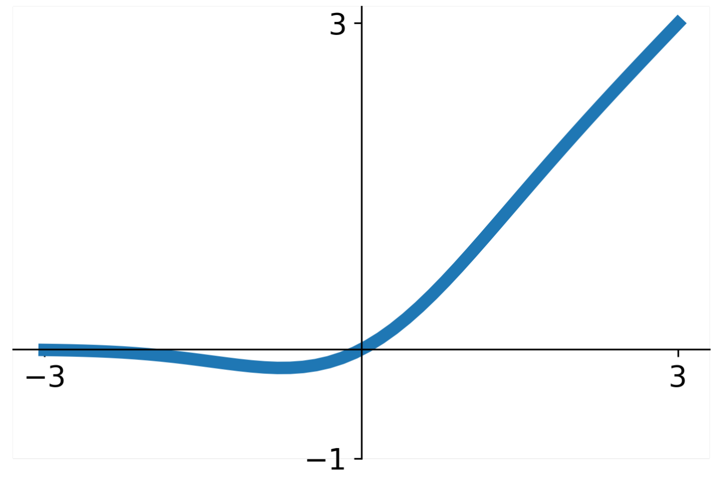
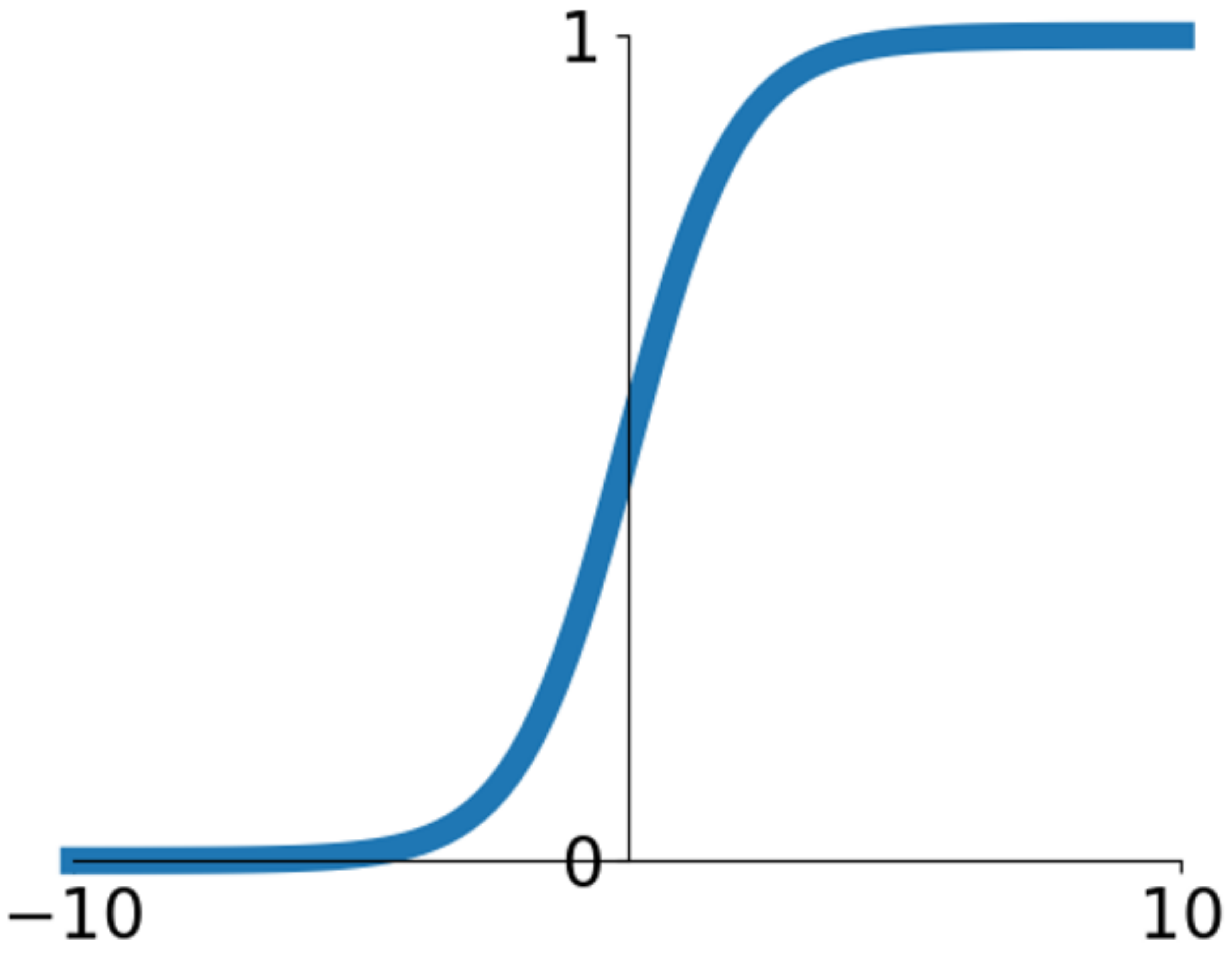


GELU

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



Activation Functions: Sigmoid

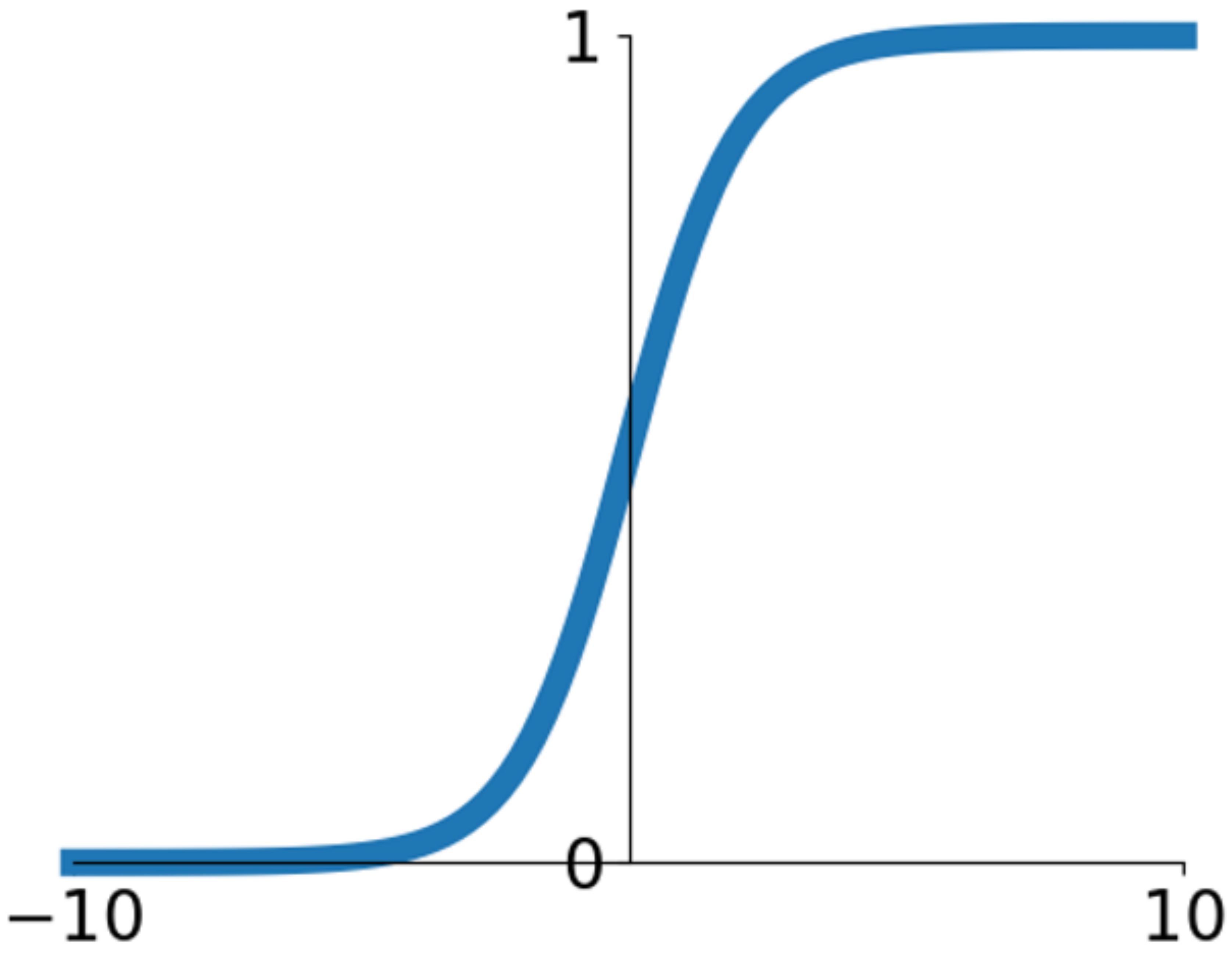


Sigmoid

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

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

Activation Functions: Sigmoid



Sigmoid

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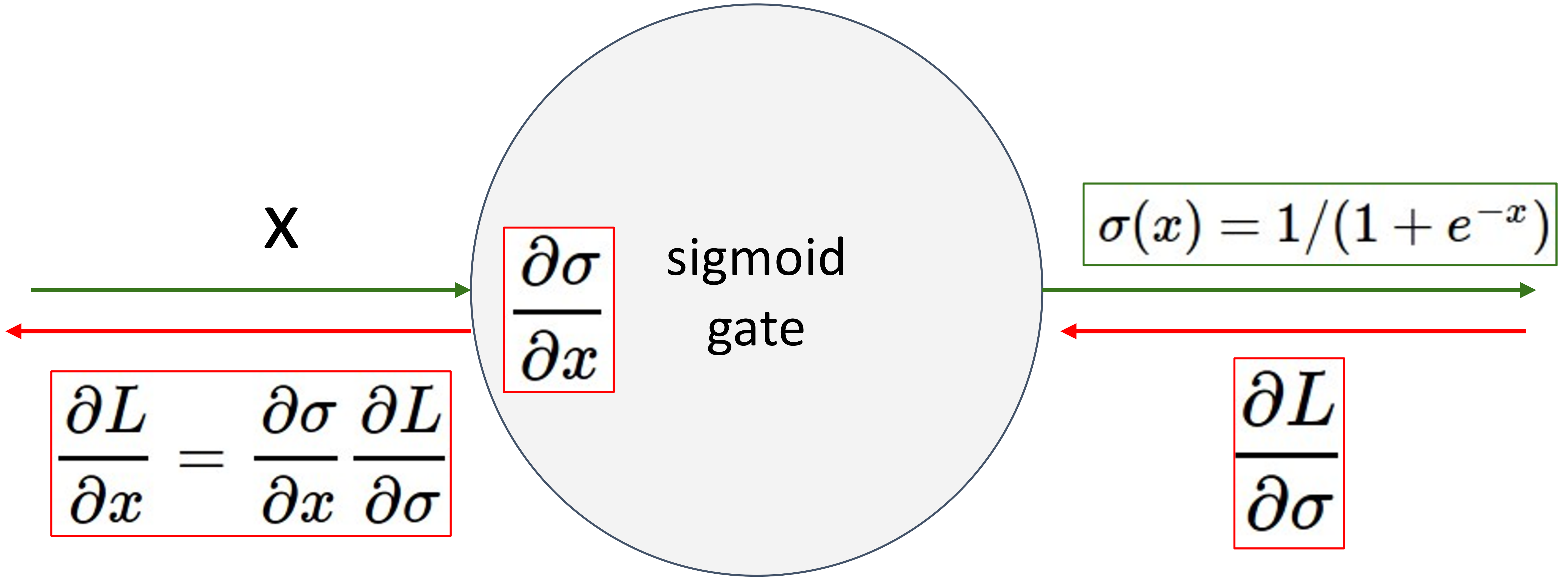
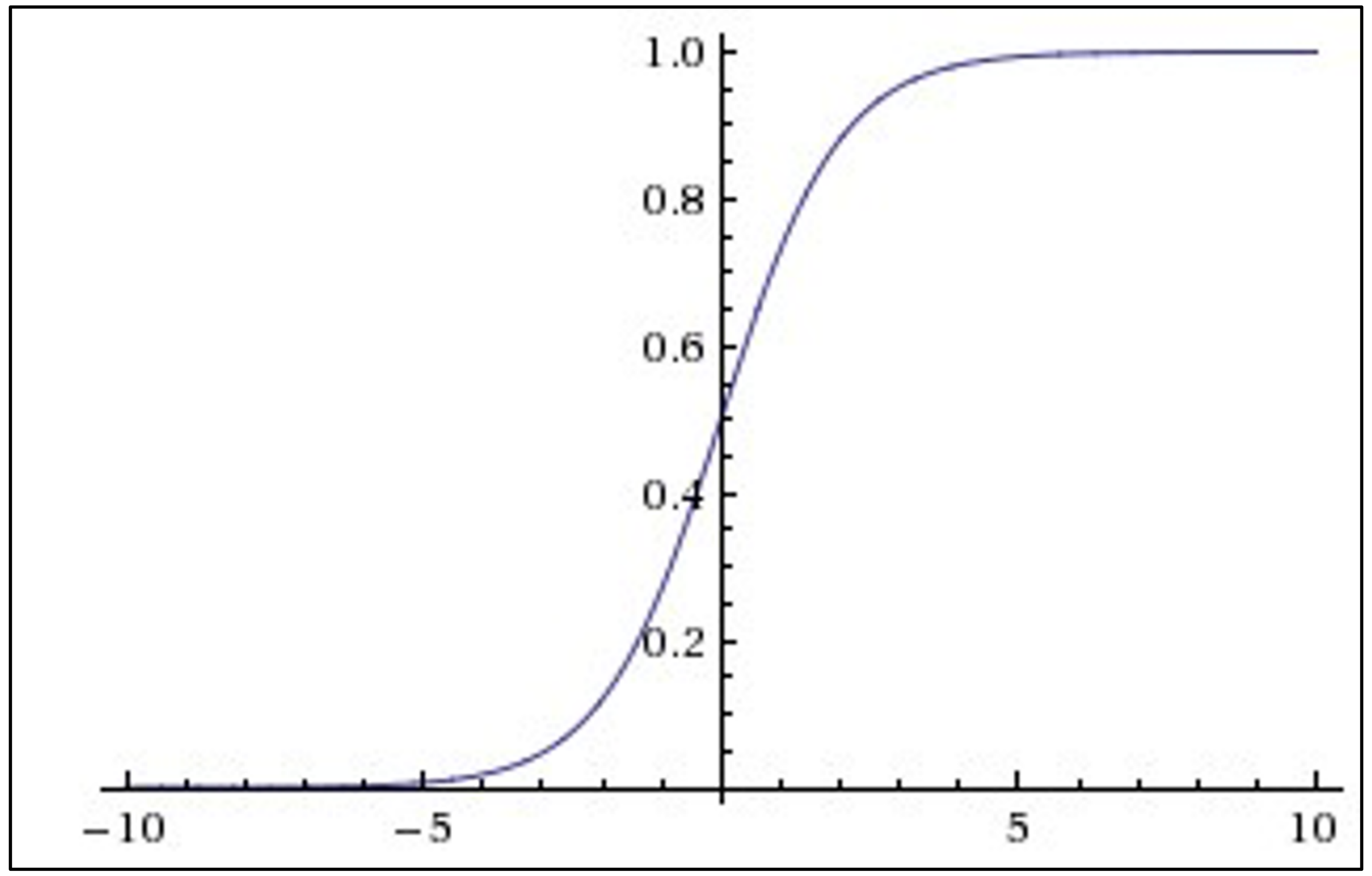
3 problems:

1. Saturated neurons "kill" the gradients

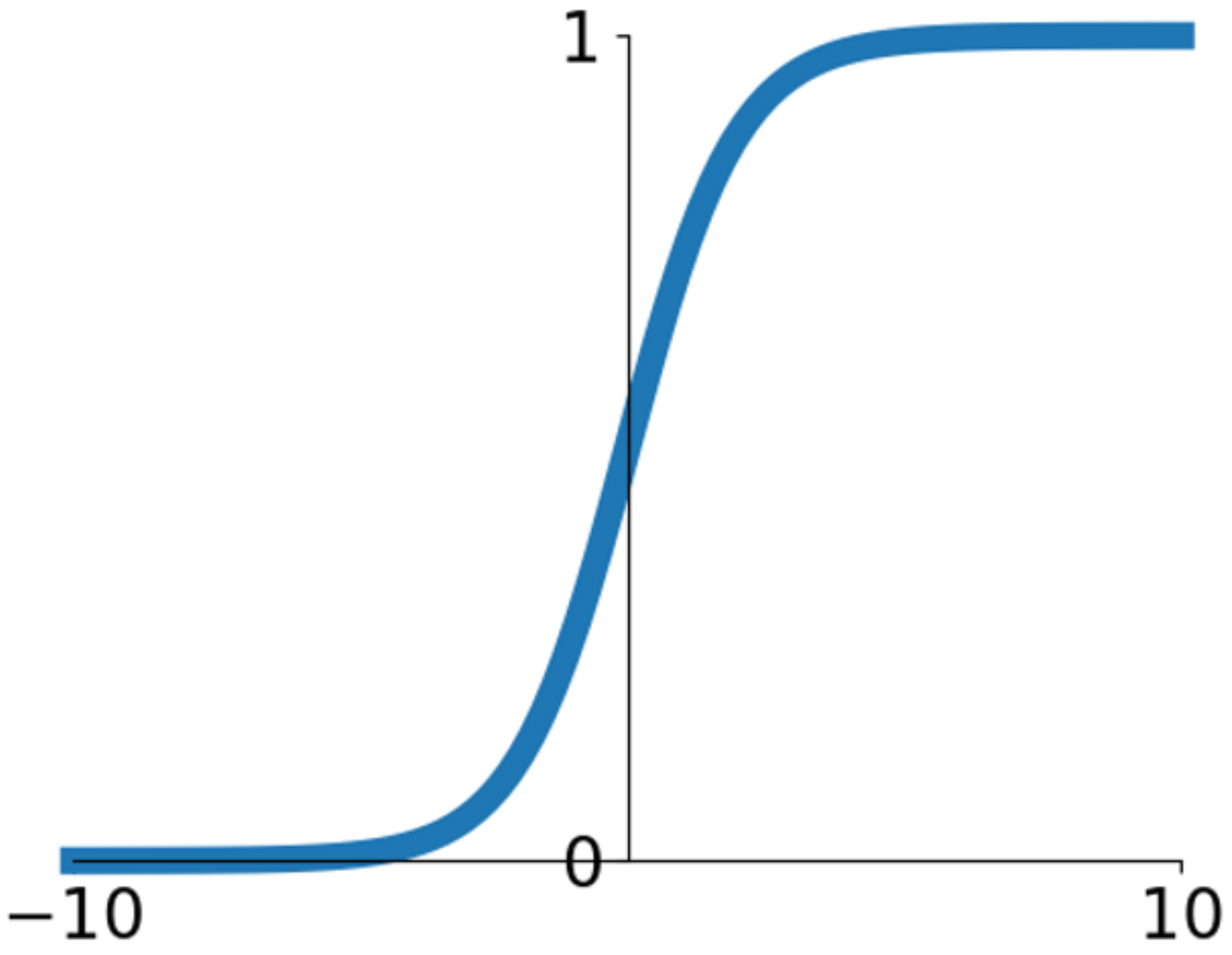
Activation Functions: Sigmoid





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

Activation Functions: Sigmoid



Sigmoid

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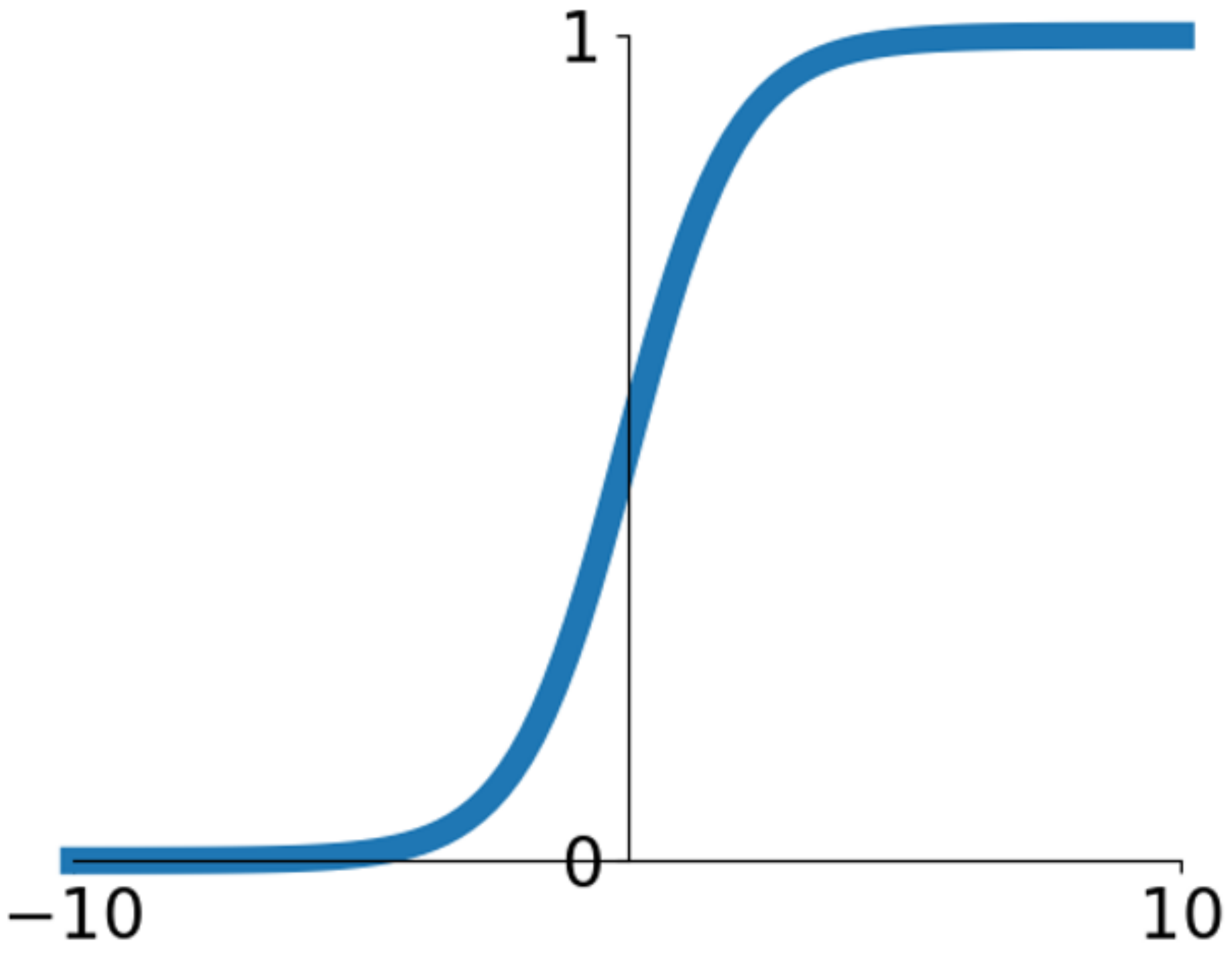
- Squashes numbers to range [0, 1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

1. Saturated neurons “kill” the gradients

Activation Functions: Sigmoid



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3 problems:

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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 ith 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 $w^{(\ell)}$?

Activation Functions: Sigmoid

Consider what happens when nonlinearity is always positive

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

Local gradient · Upstream gradient

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

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Local gradient | Upstream gradient

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

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

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

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

Activation Functions: Sigmoid

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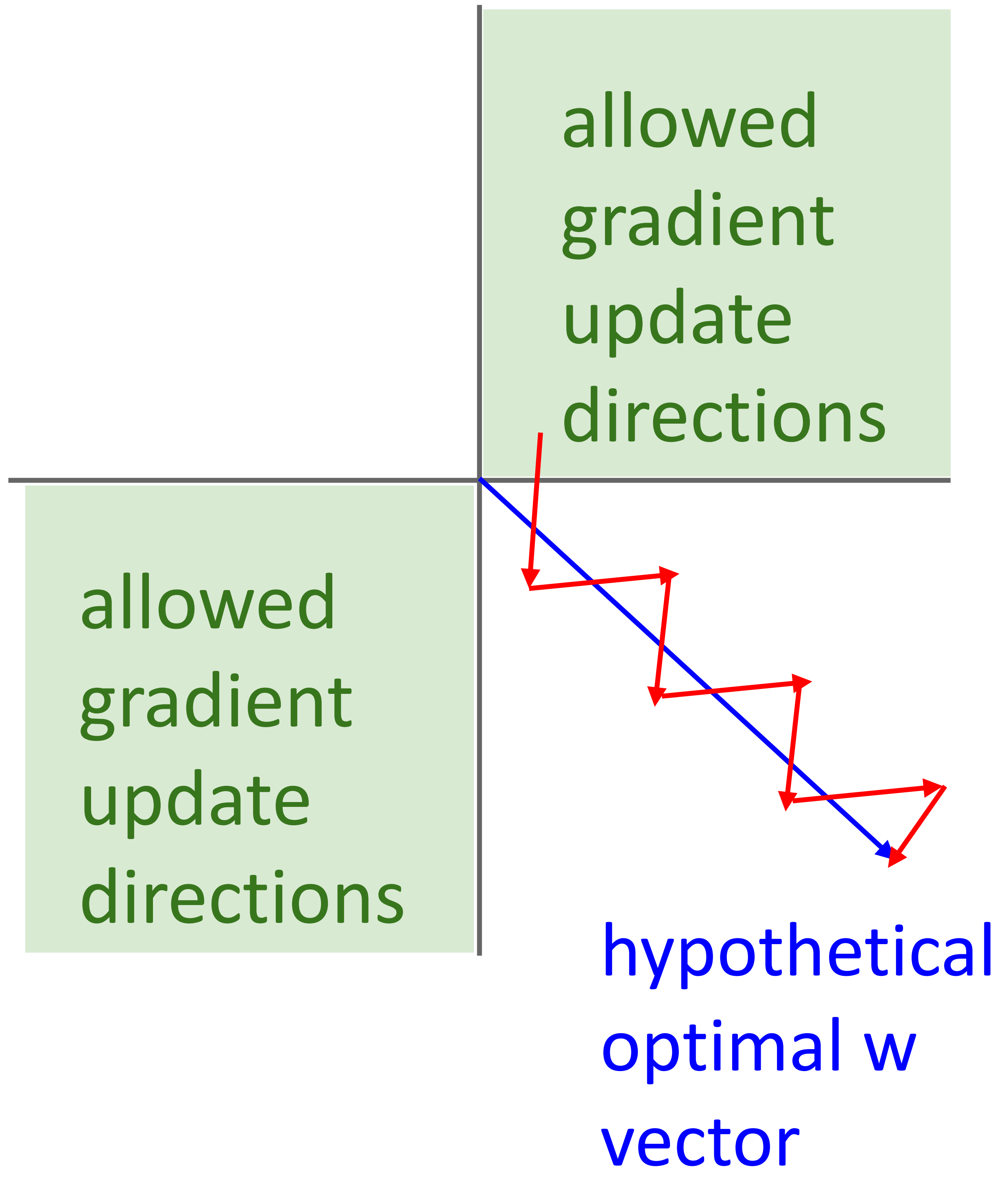

Gradients on rows of w can only point in some directions; needs to "zigzag" to move in other directions

Activation Functions: Sigmoid

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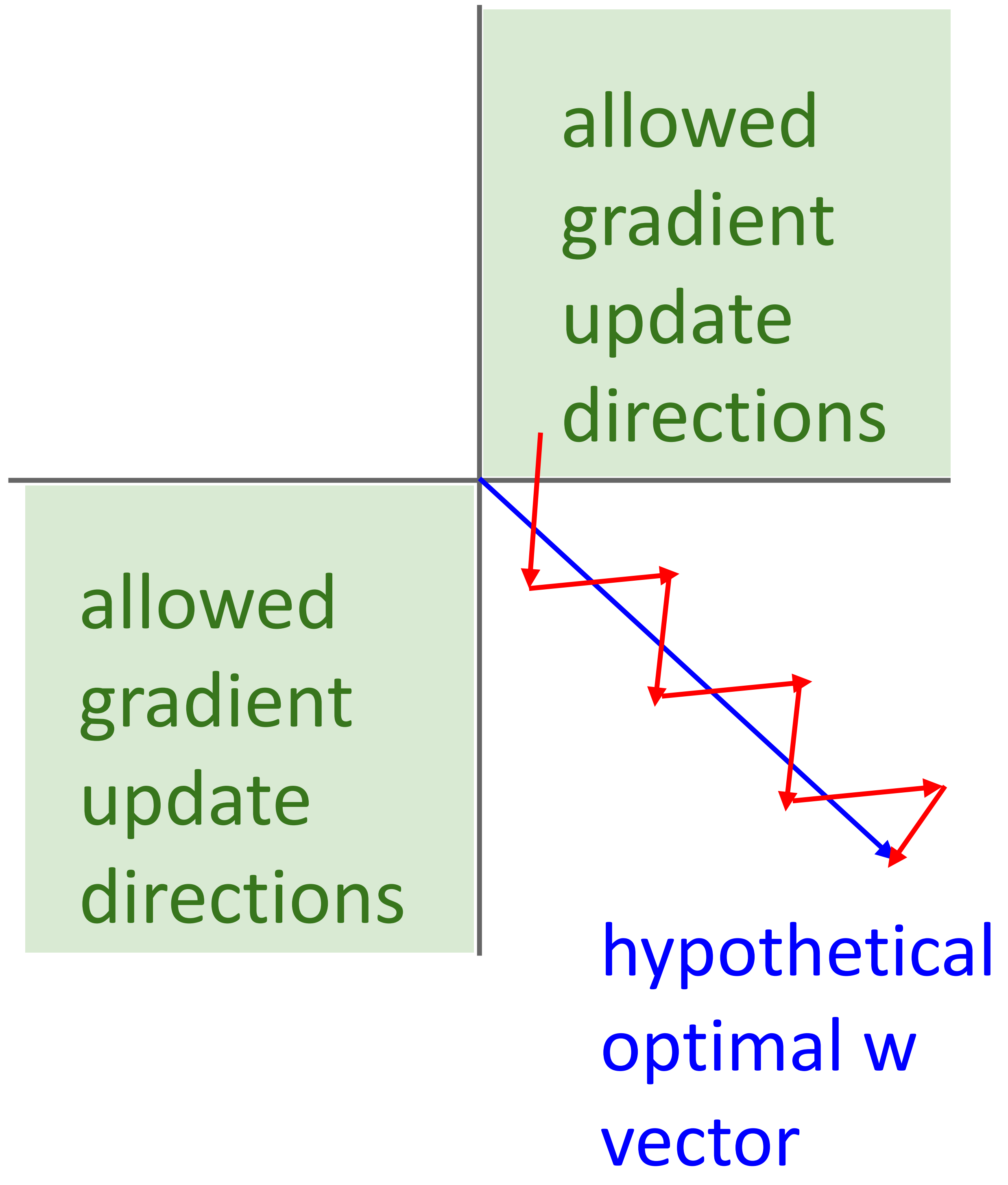
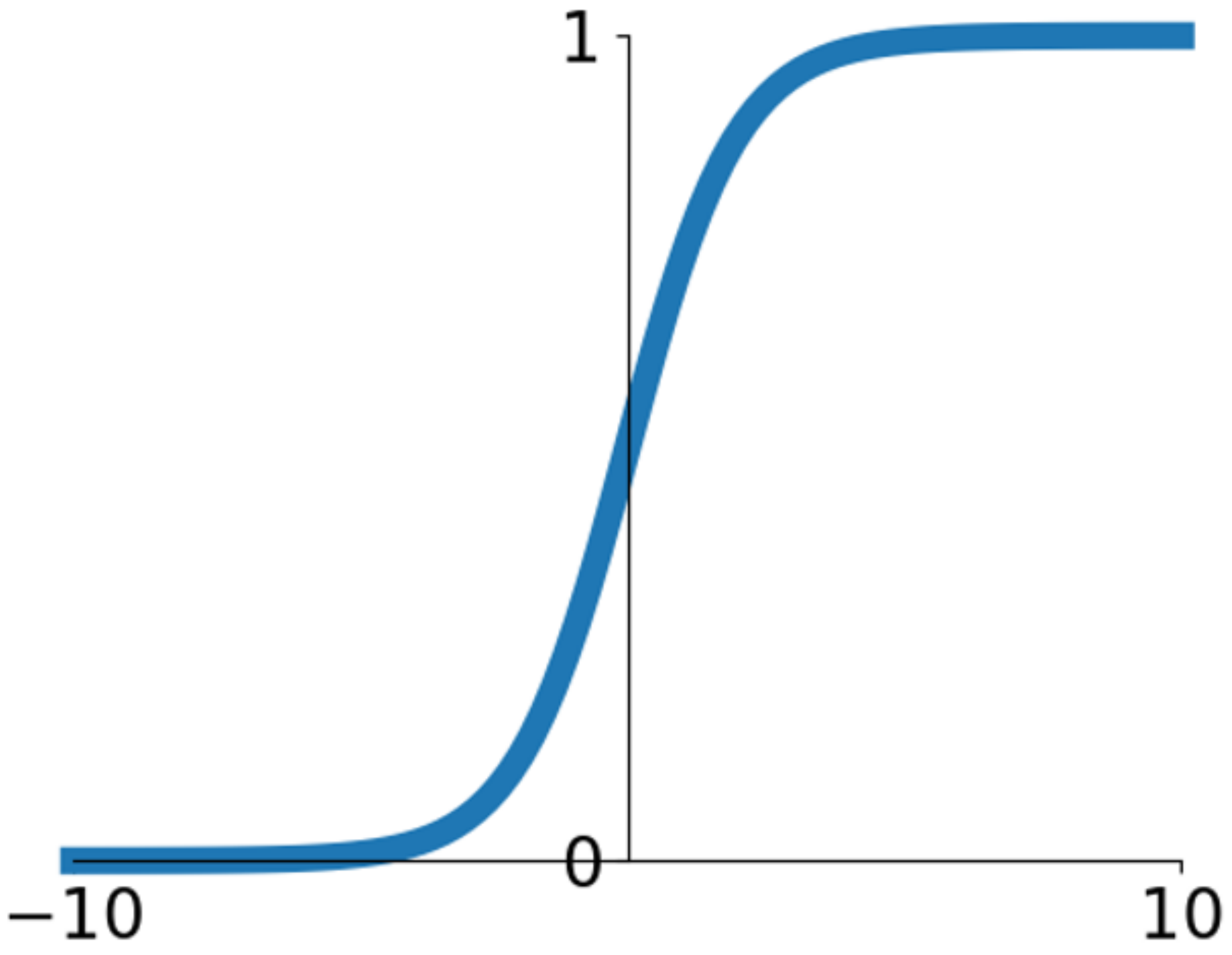


Not that bad in practice:
- Only true for a single example, mini batches help
- BatchNorm can also avoid this

Activation Functions: Sigmoid



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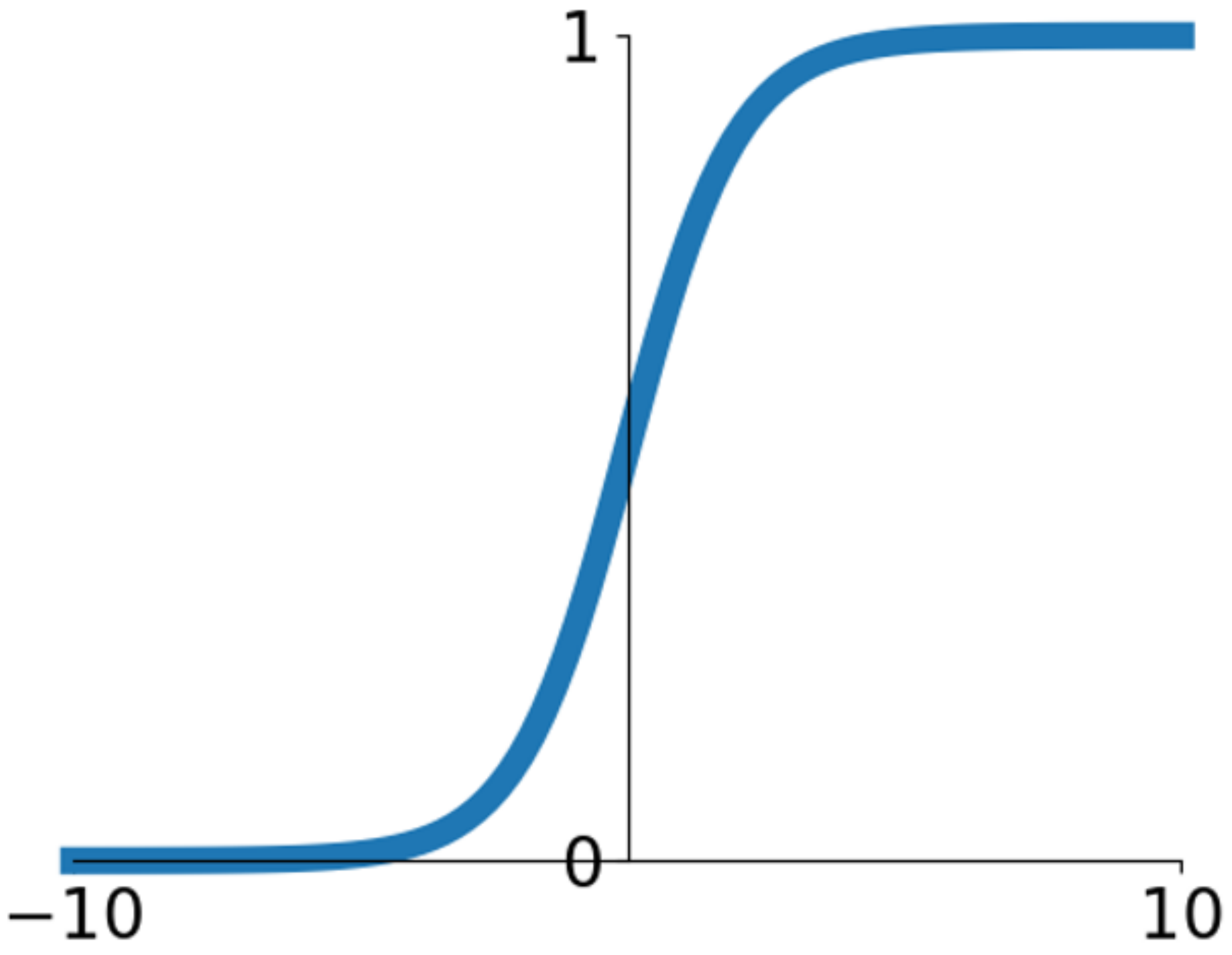
2. Sigmoid outputs are not zero-centered

Activation Functions: Sigmoid



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3 problems:

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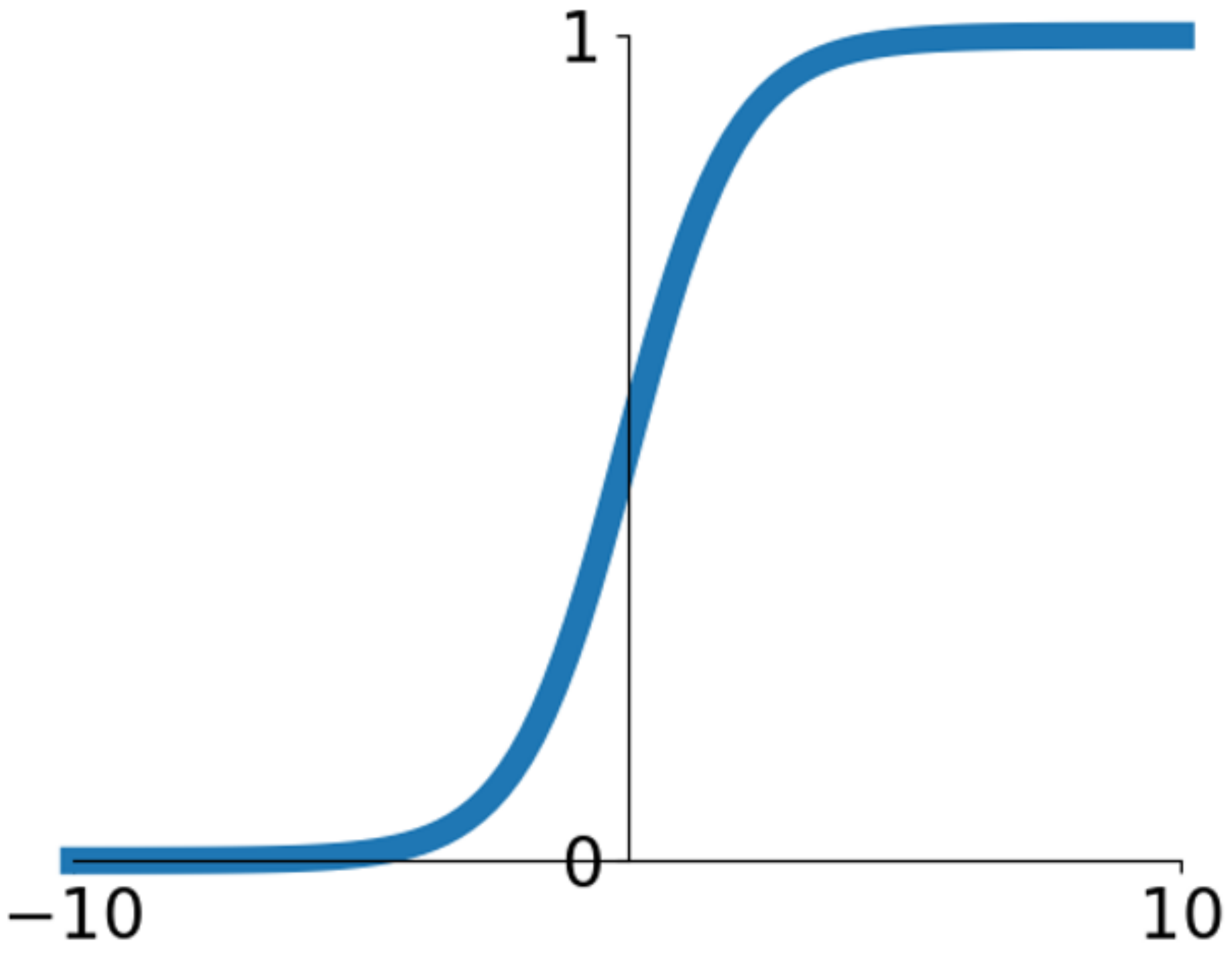
3. exp() is a bit compute expensive

Activation Functions: Sigmoid



Sigmoid

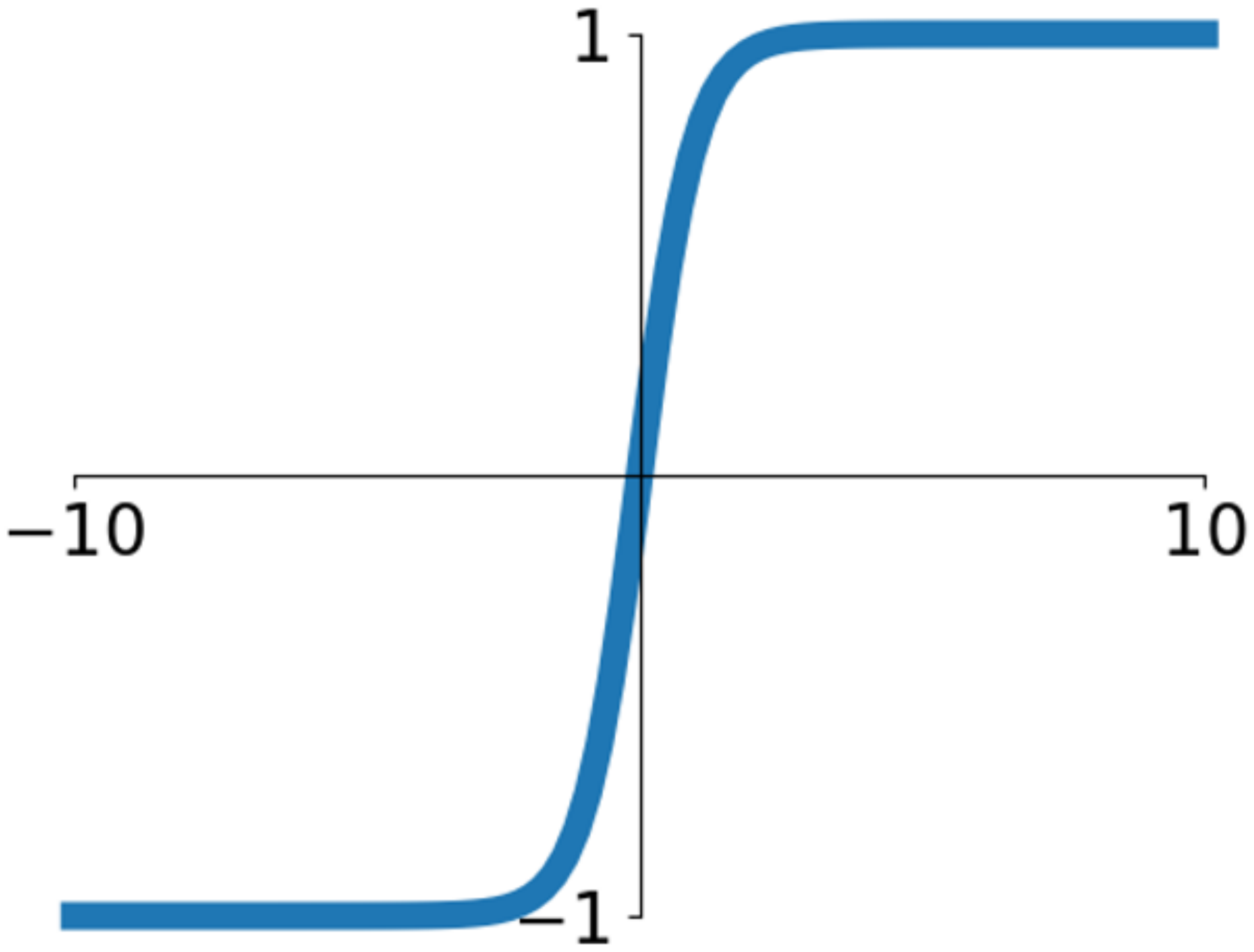
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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

3 problems: **Worst problem in practice**

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

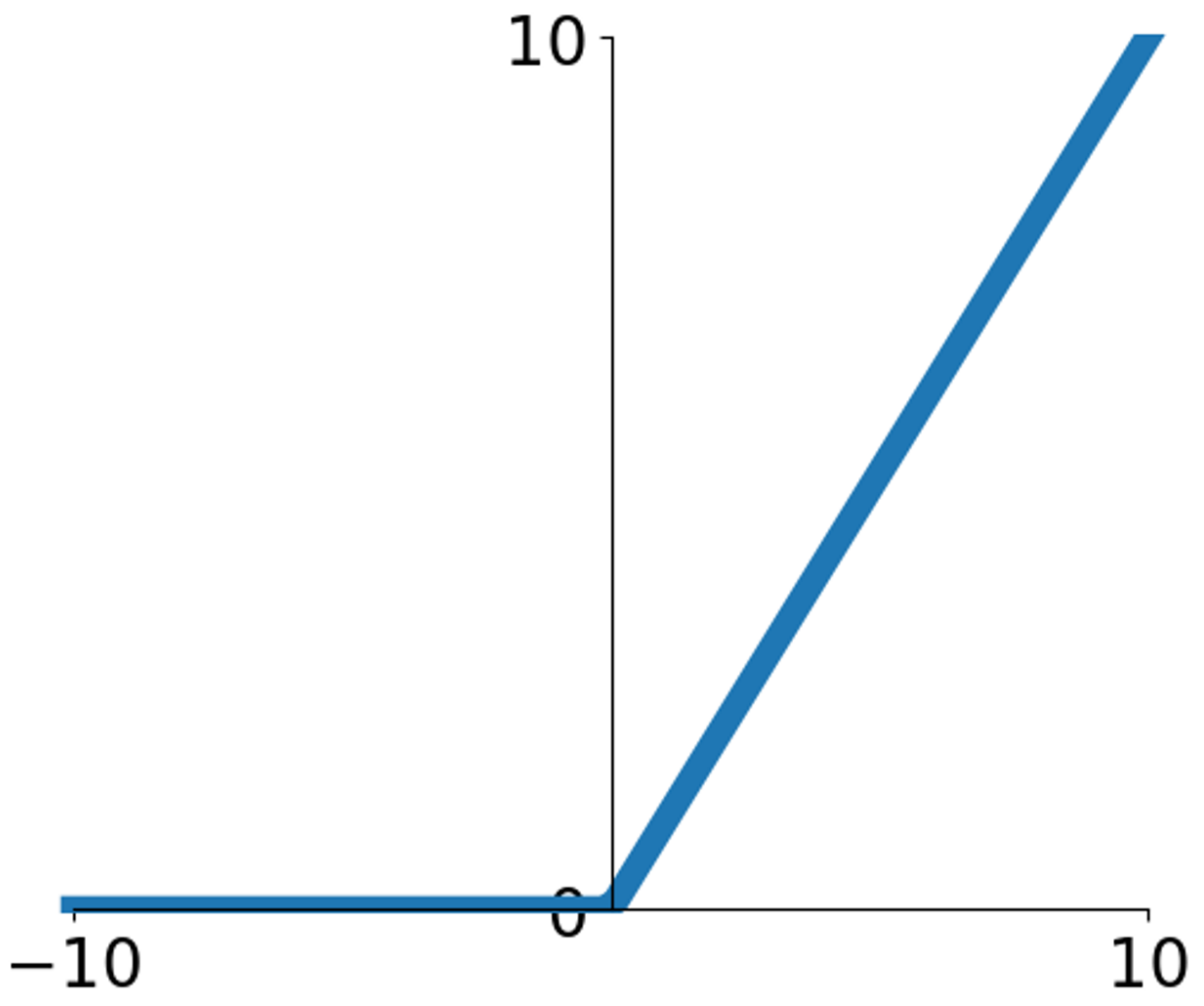
Activation Functions: tanh



tanh(x)

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

Activation Functions: ReLU

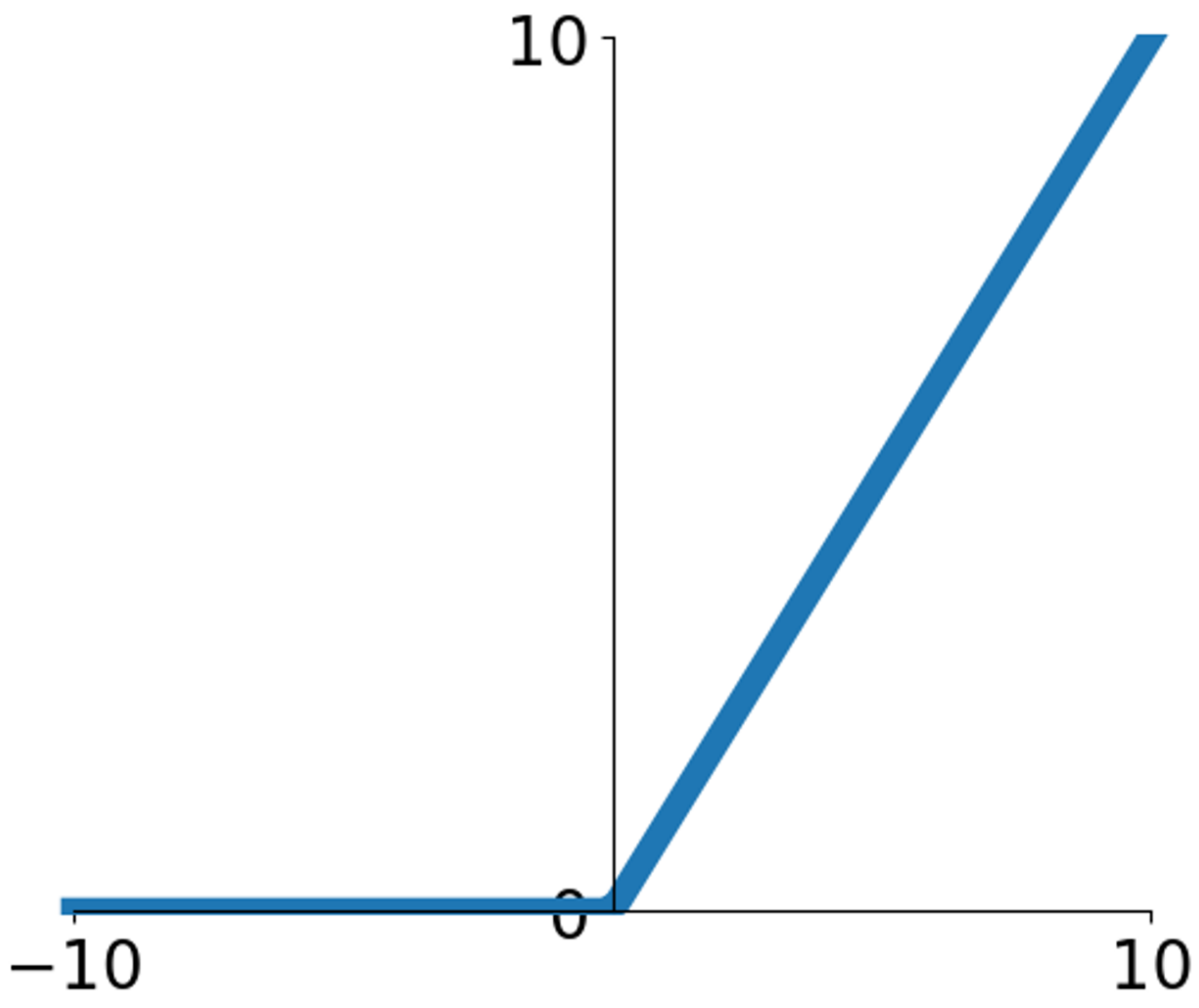


ReLU
(Rectified Linear Unit)

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

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

Activation Functions: ReLU



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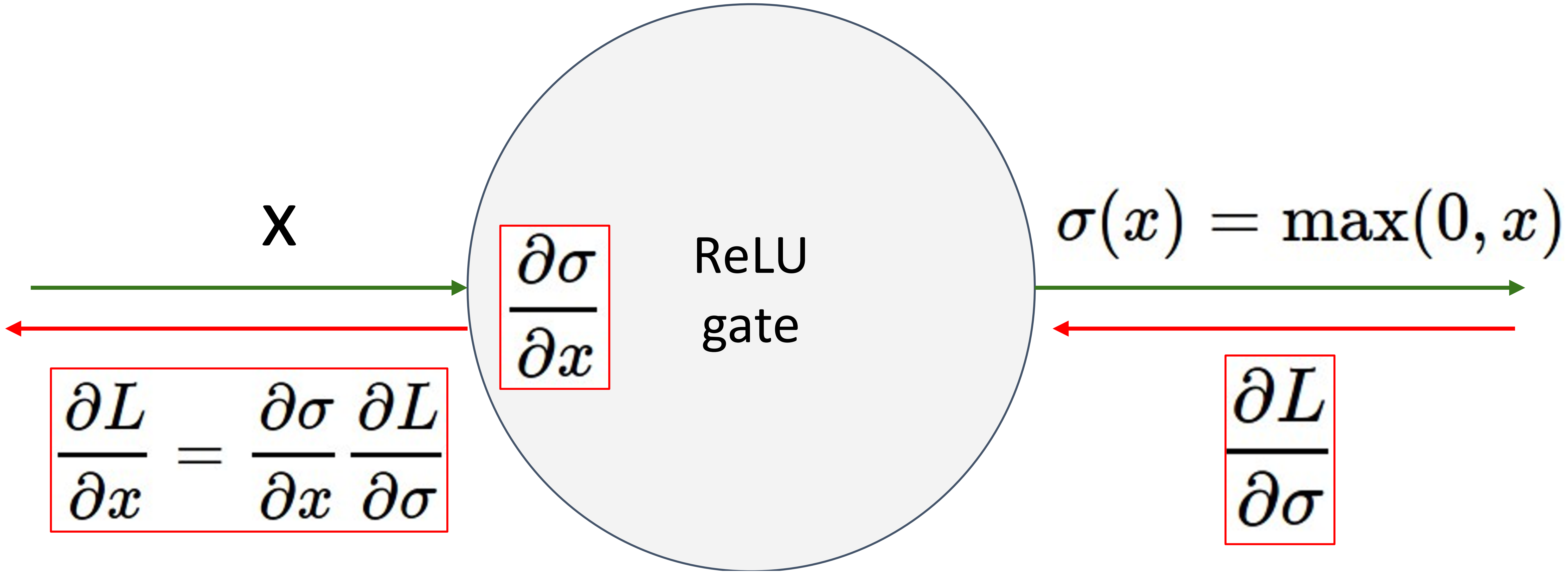
$$f(x) = \max(0, x)$$

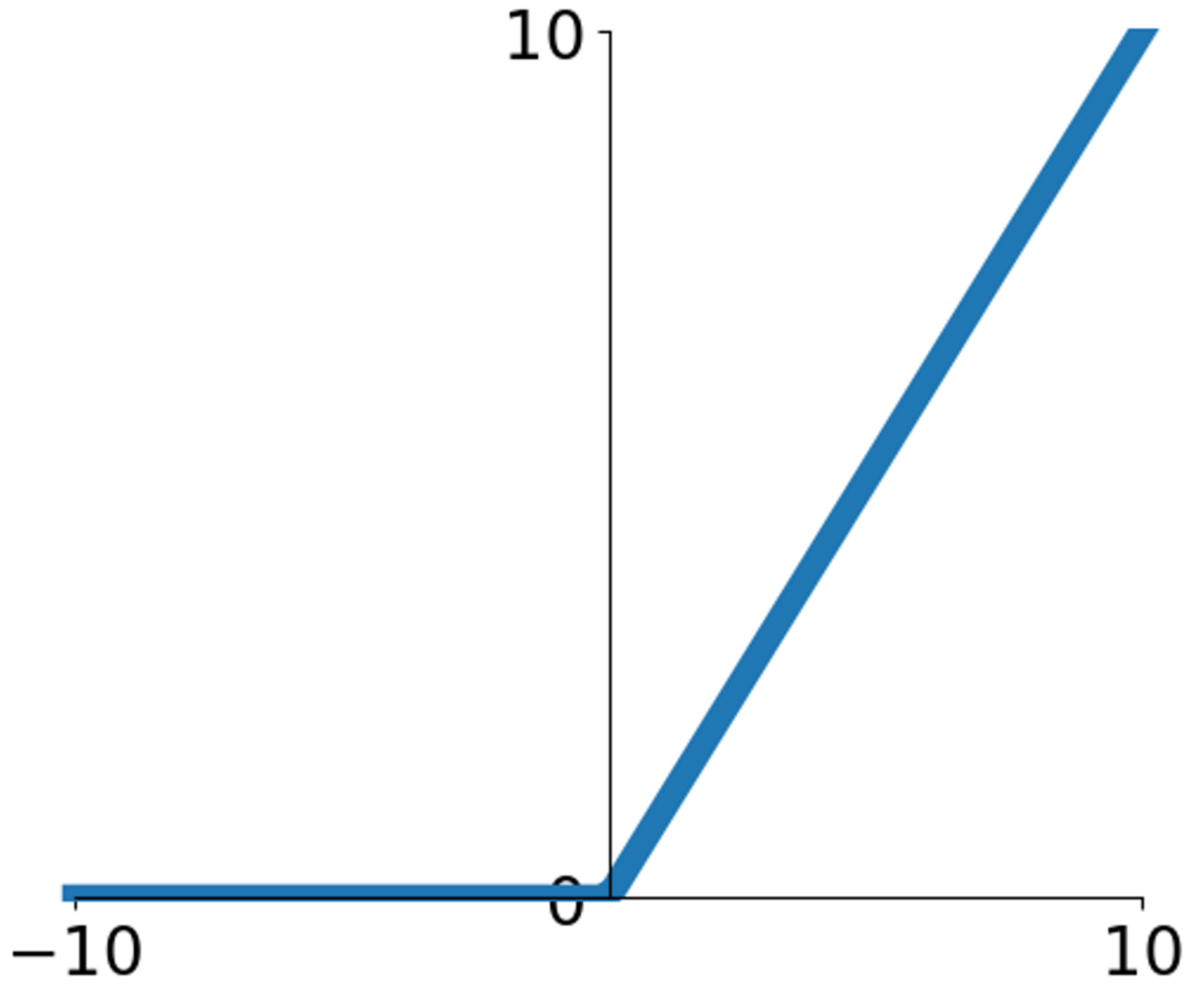
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid and tanh in practice (e.g. 6x)

- Not zero-centered output
- An annoyance:

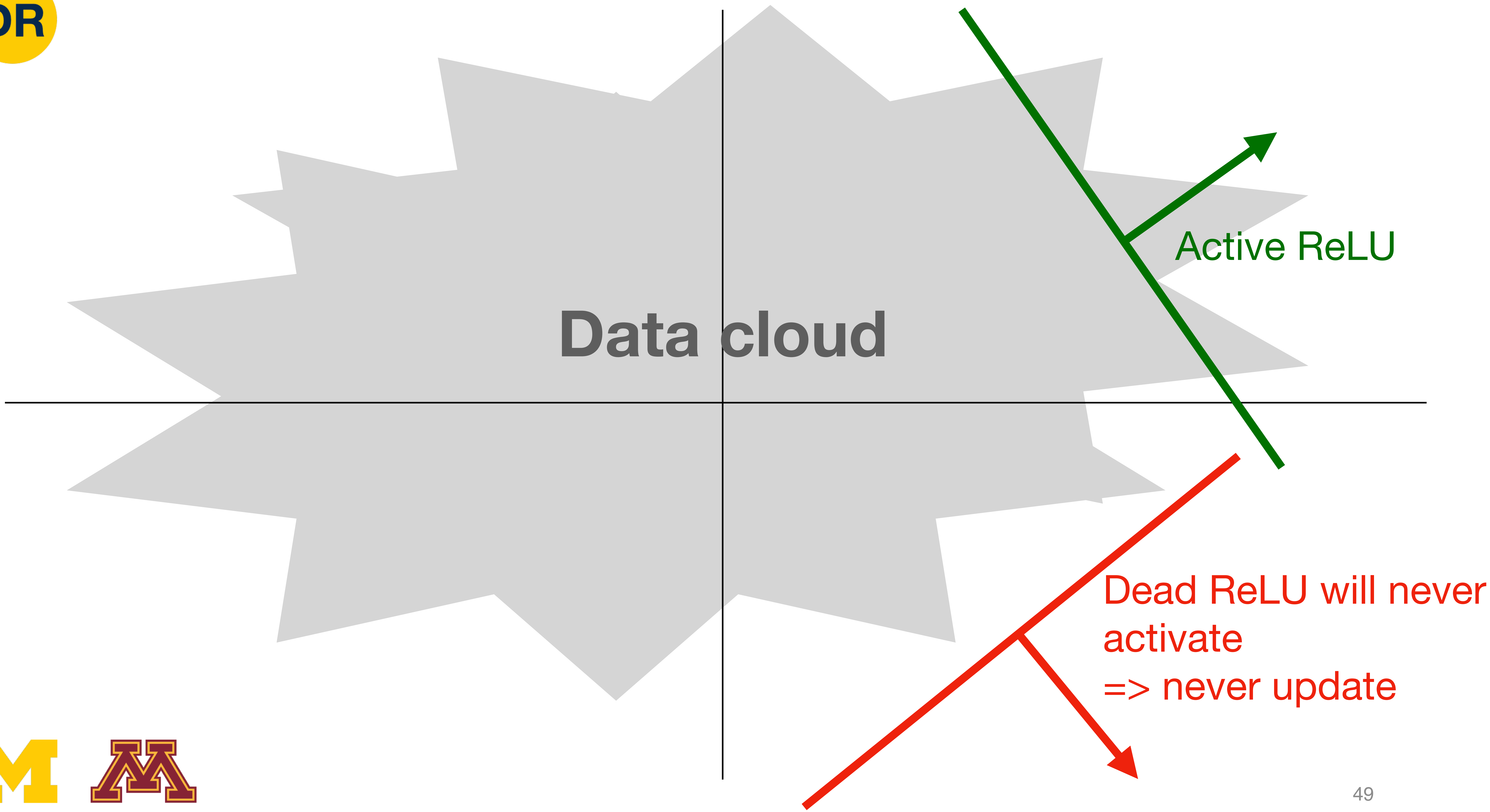
Hint: what is the gradient when x<0?

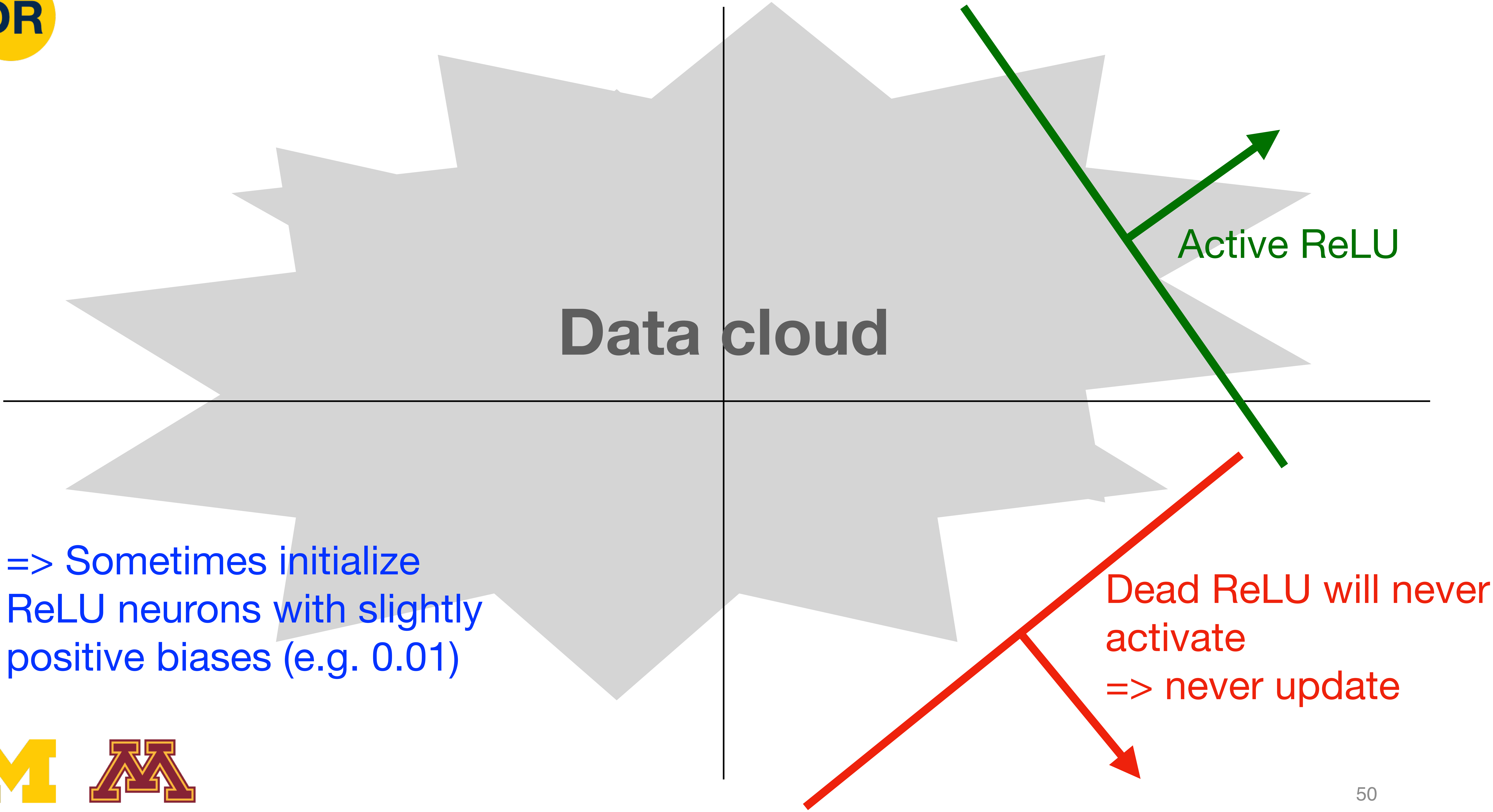
Activation Functions: ReLU





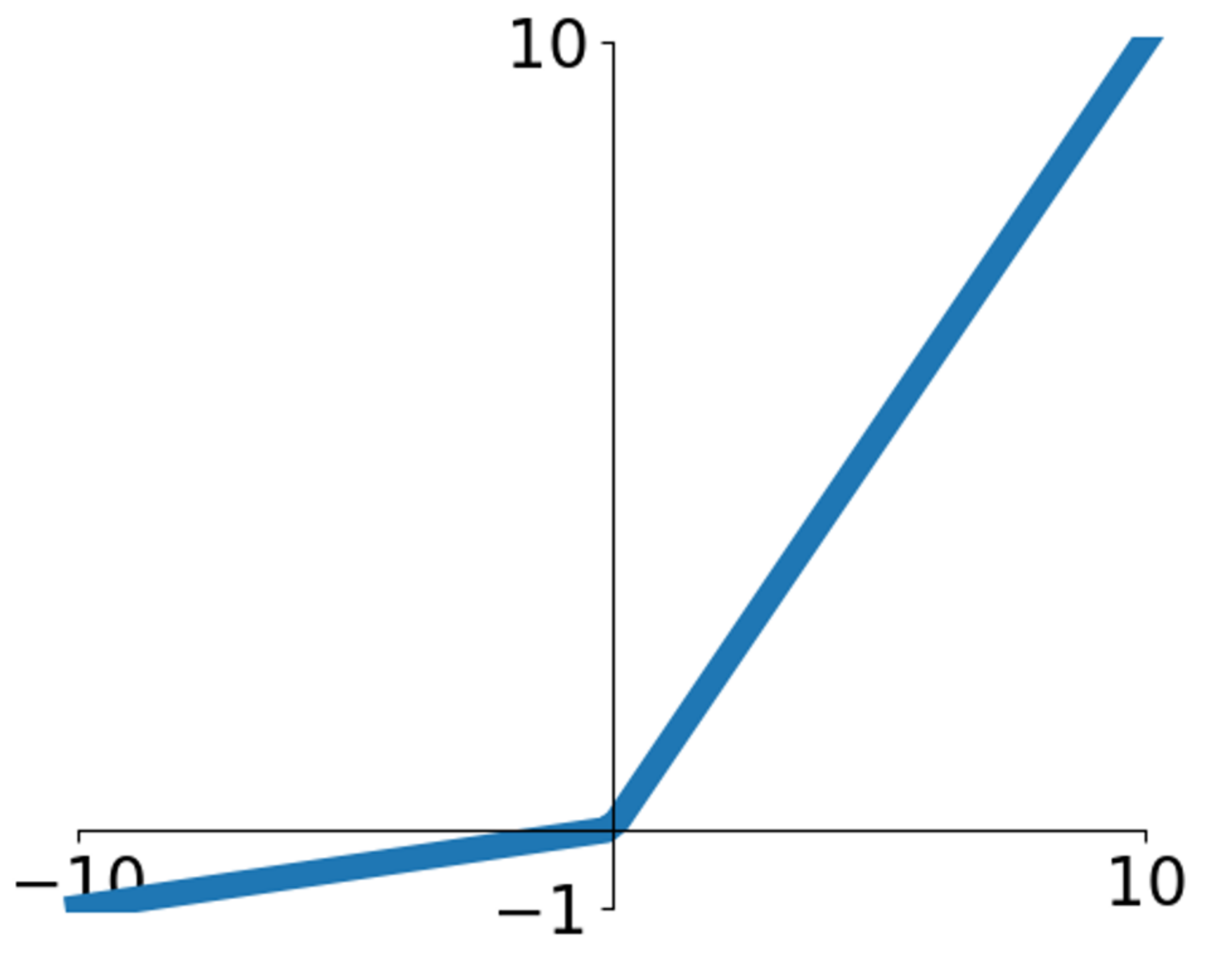
- What happens when x = -10?
- What happens when x = 0?
- What happens when x = 10?


Data cloud
Active ReLU
Dead ReLU will never
activate
=> never update



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

Activation Functions: Leaky ReLU



Leaky ReLU

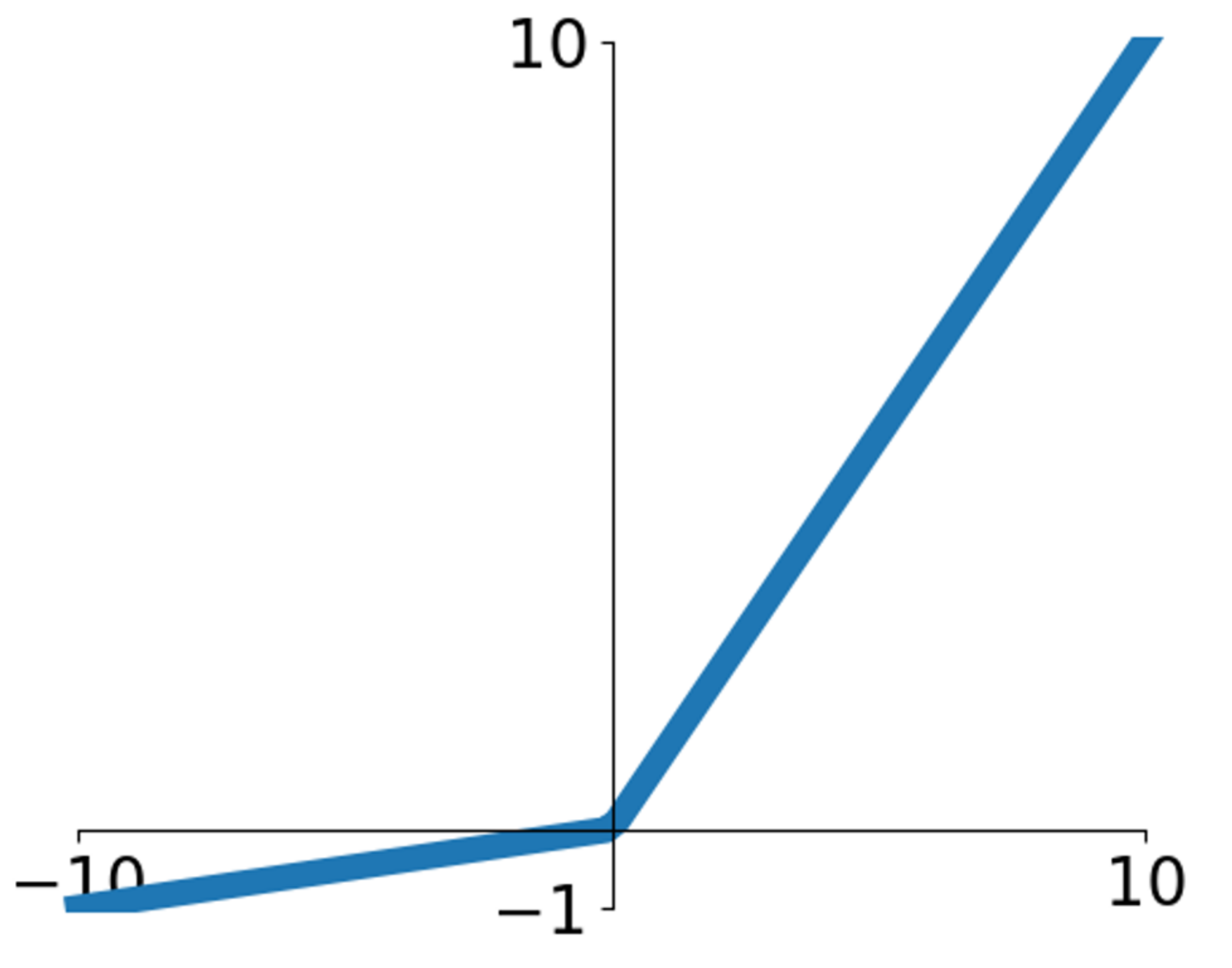
$$f(x) = \max(\alpha x, x)$$

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

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

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

Activation Functions: Leaky ReLU



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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

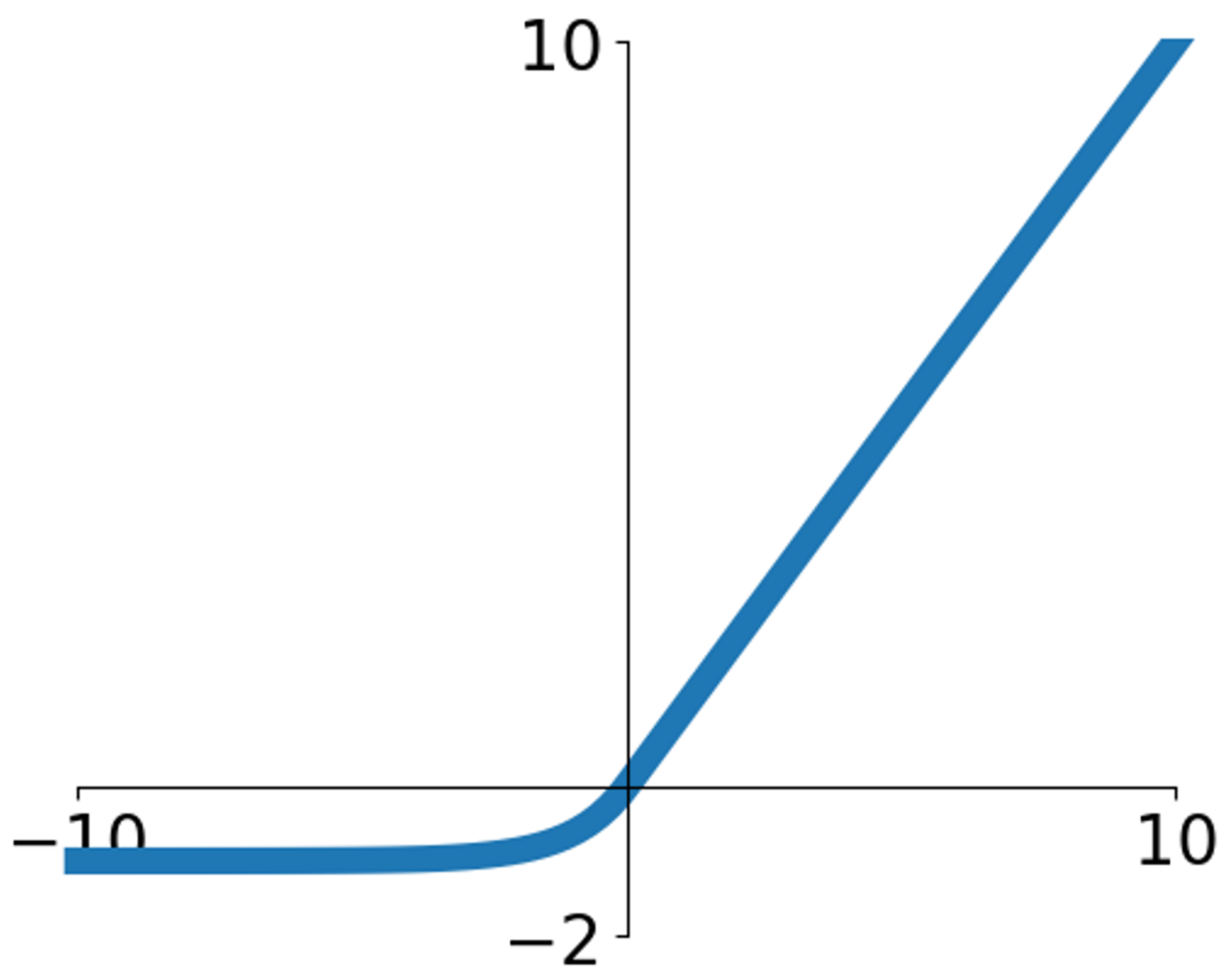
Parametric ReLU (PReLU)

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

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)

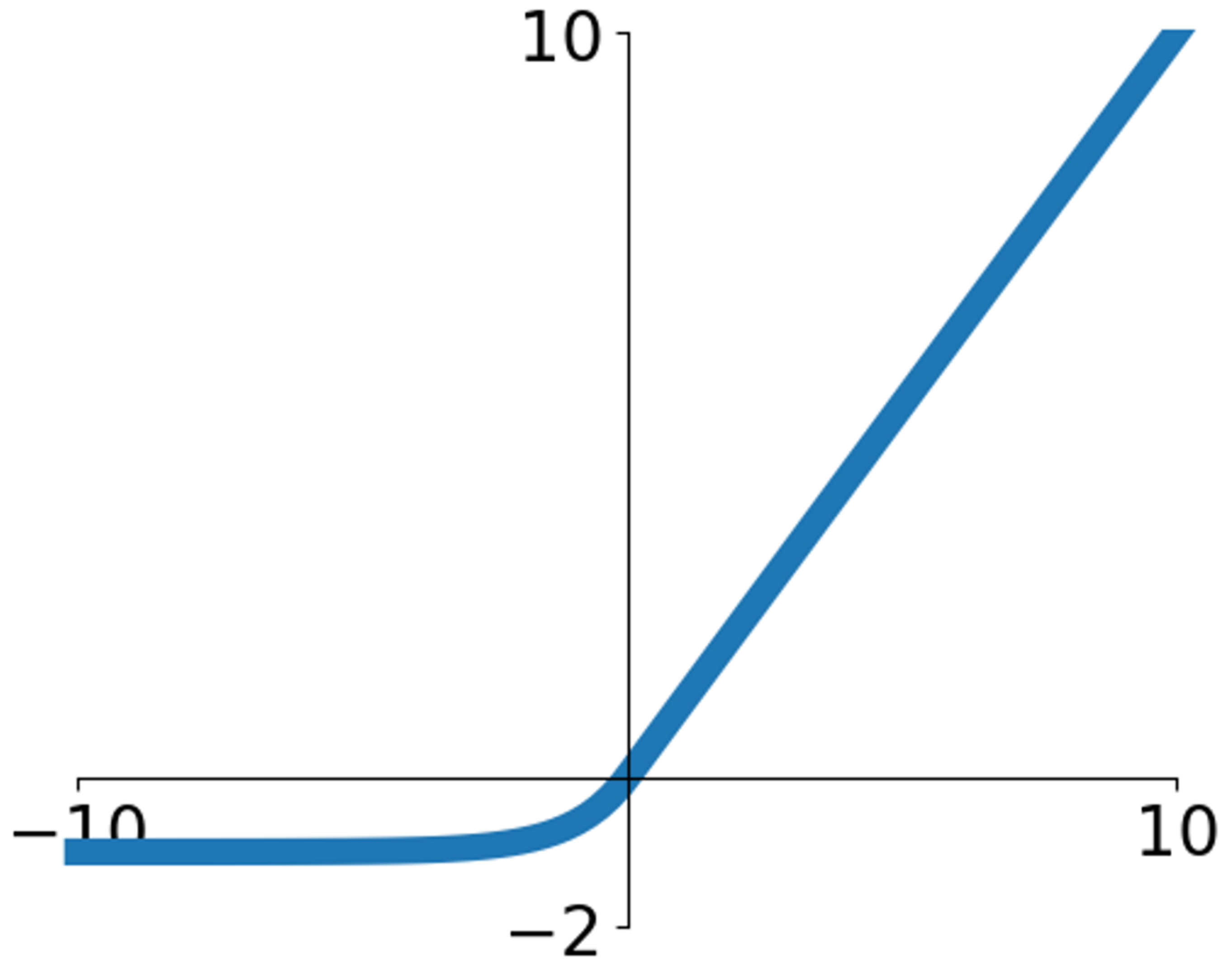


$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(e^x - 1) & \text{if } x \leq 0 \end{cases}$$

(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)



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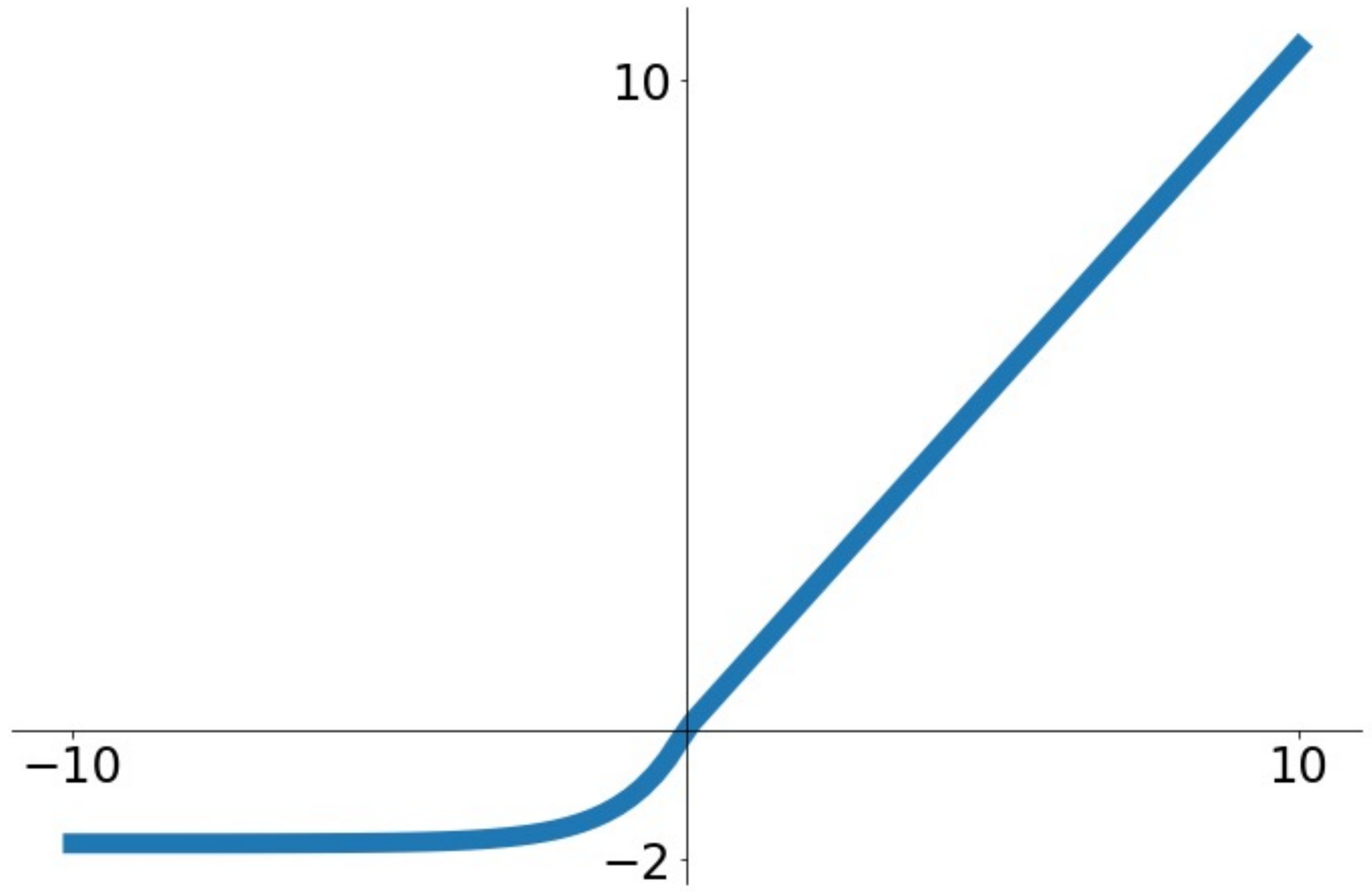
(Default $\alpha = 1$)

- 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)



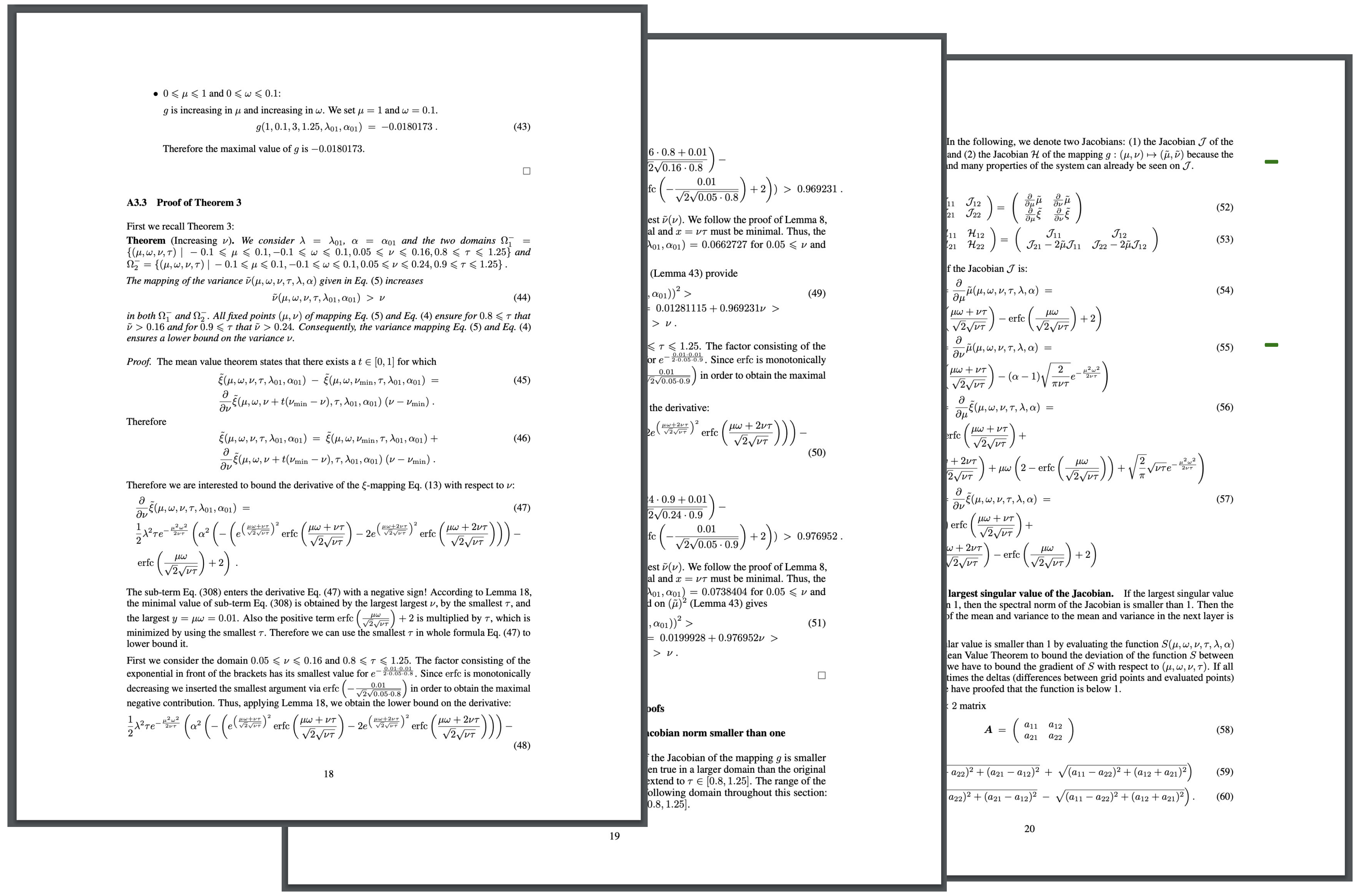
- Scaled version of ELU that works better for deep networks "Self-Normalizing" property; can train deep SELU networks without BatchNorm

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

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

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

Activation Functions: Scale Exponential Linear Unit (SELU)



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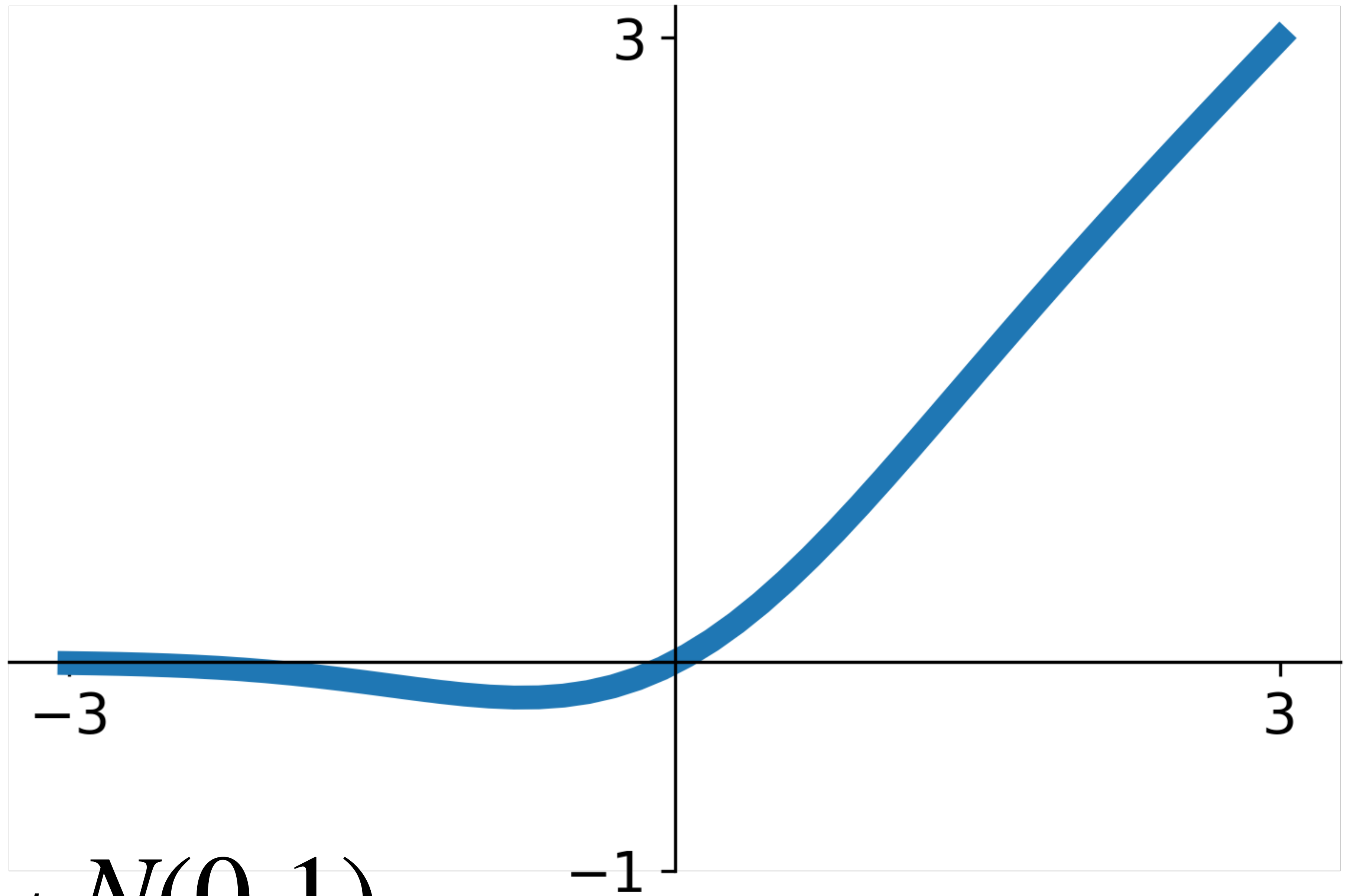
- Scaled version of ELU that works better for deep networks "Self-Normalizing" property; can train deep SELU networks without BatchNorm

- Derivation takes 91 pages of math in appendix…

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

Activation Functions: Gaussian Error Linear Unit (GELU)



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

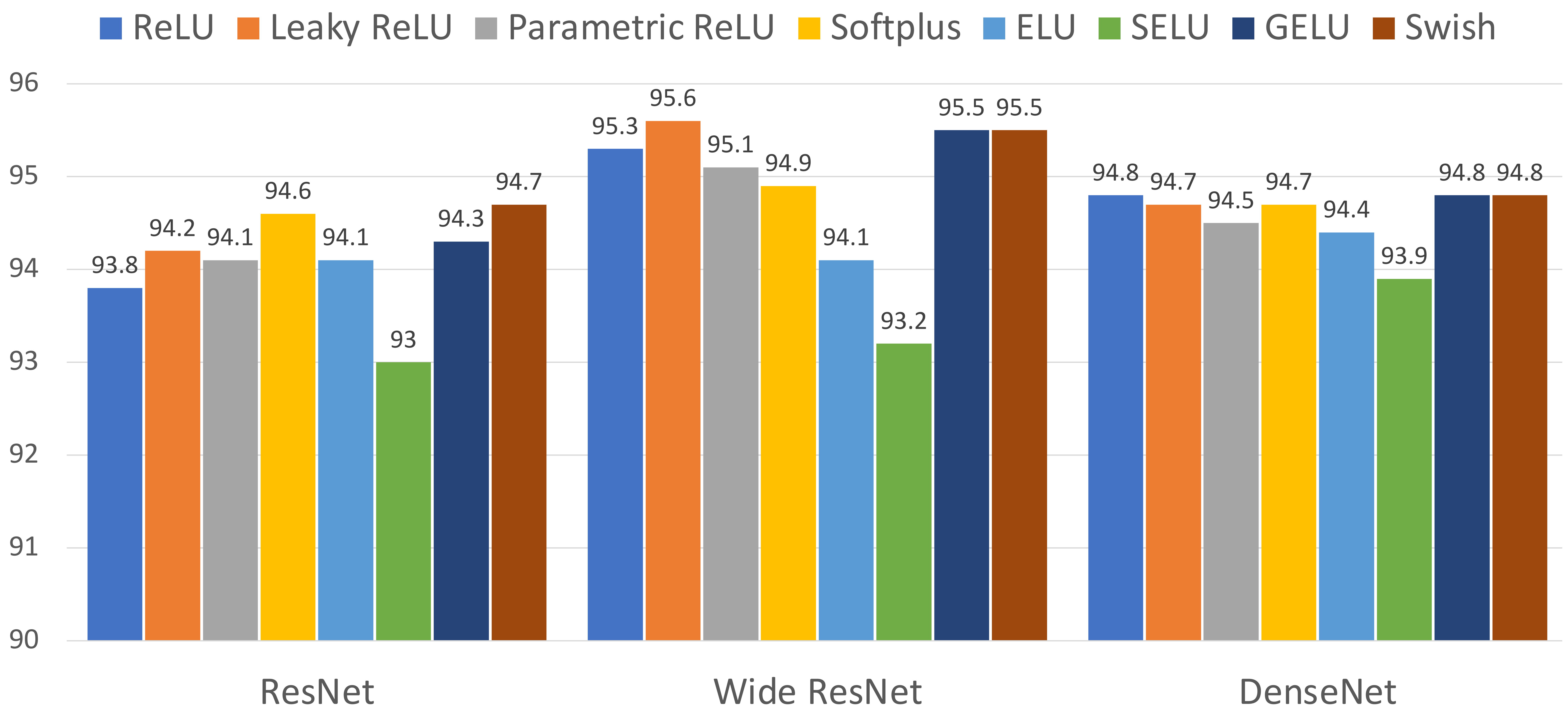
$$\text{gelu}(x) = xP(X \le x) = \frac{x}{2}(1 + \text{erf}(x/\sqrt{2}))$$

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

- **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)

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

Accuracy on CIFAR10



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

Activation Functions: Summary

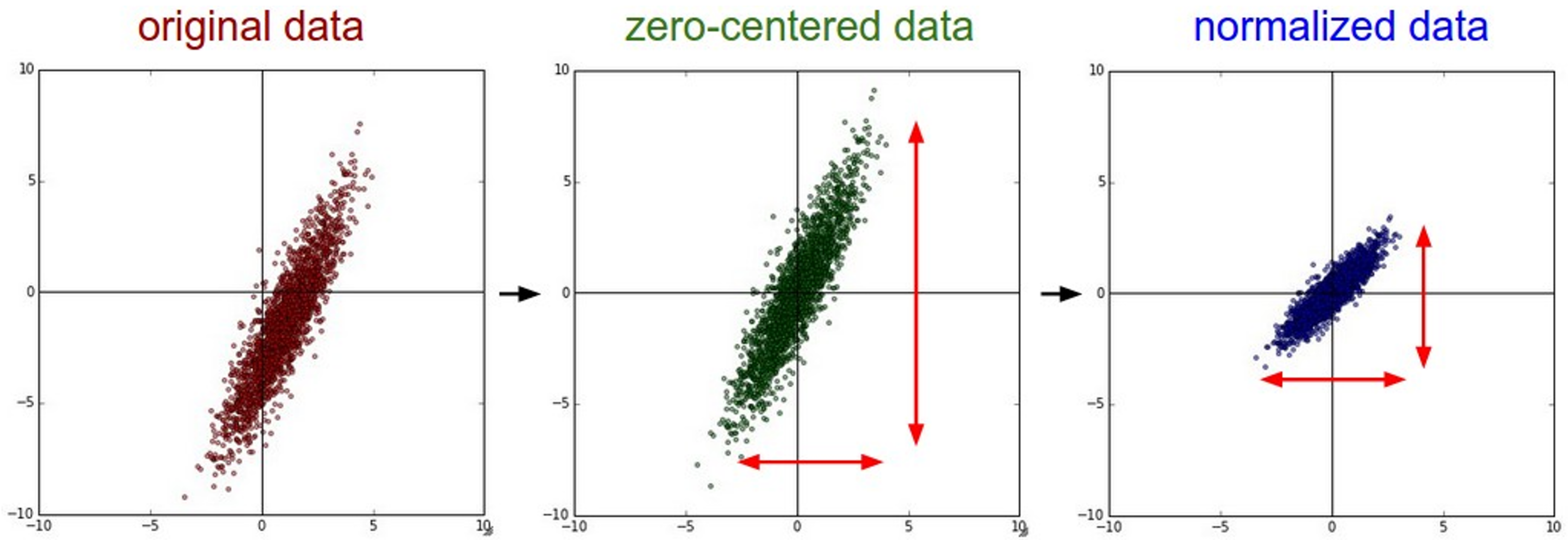
- Don't think too hard. Just use **ReLU**
- Try out **Leaky ReLU / ELU / SELU / GELU** if you need to squeeze that last 0.1%
- Don't use sigmoid or tanh

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

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

Data preprocessing

Data preprocessing



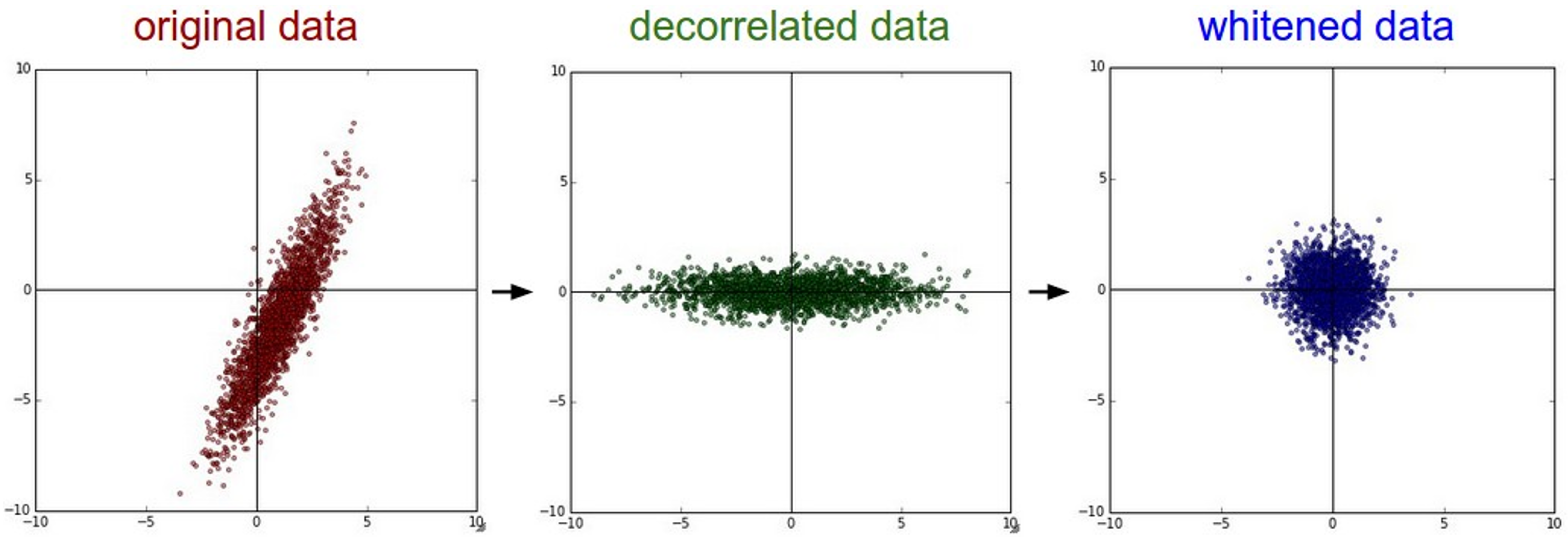

```
X -= np.mean(X, axis = 0)
```

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

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

Data preprocessing

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

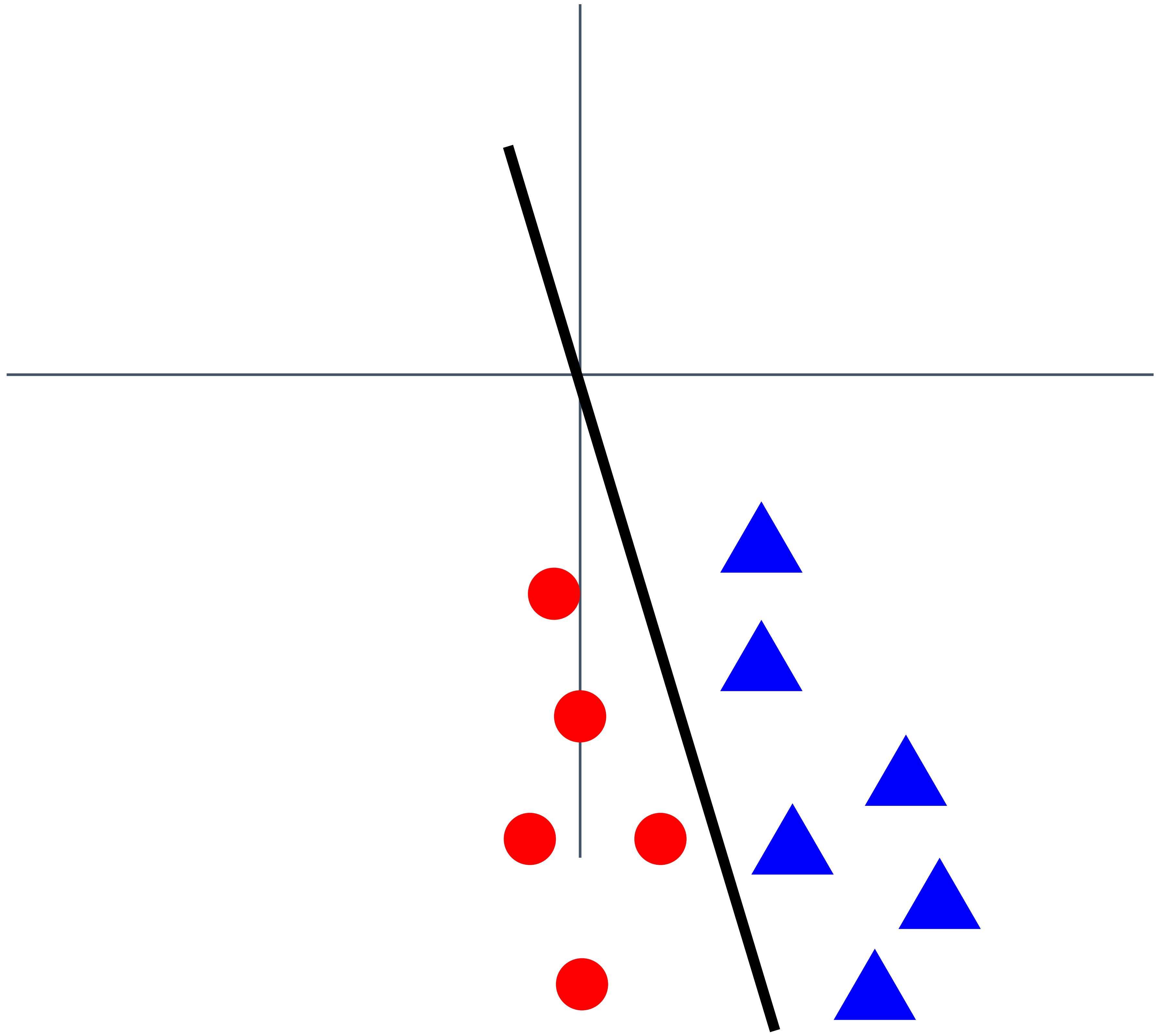


(Data has diagonal covariance matrix)

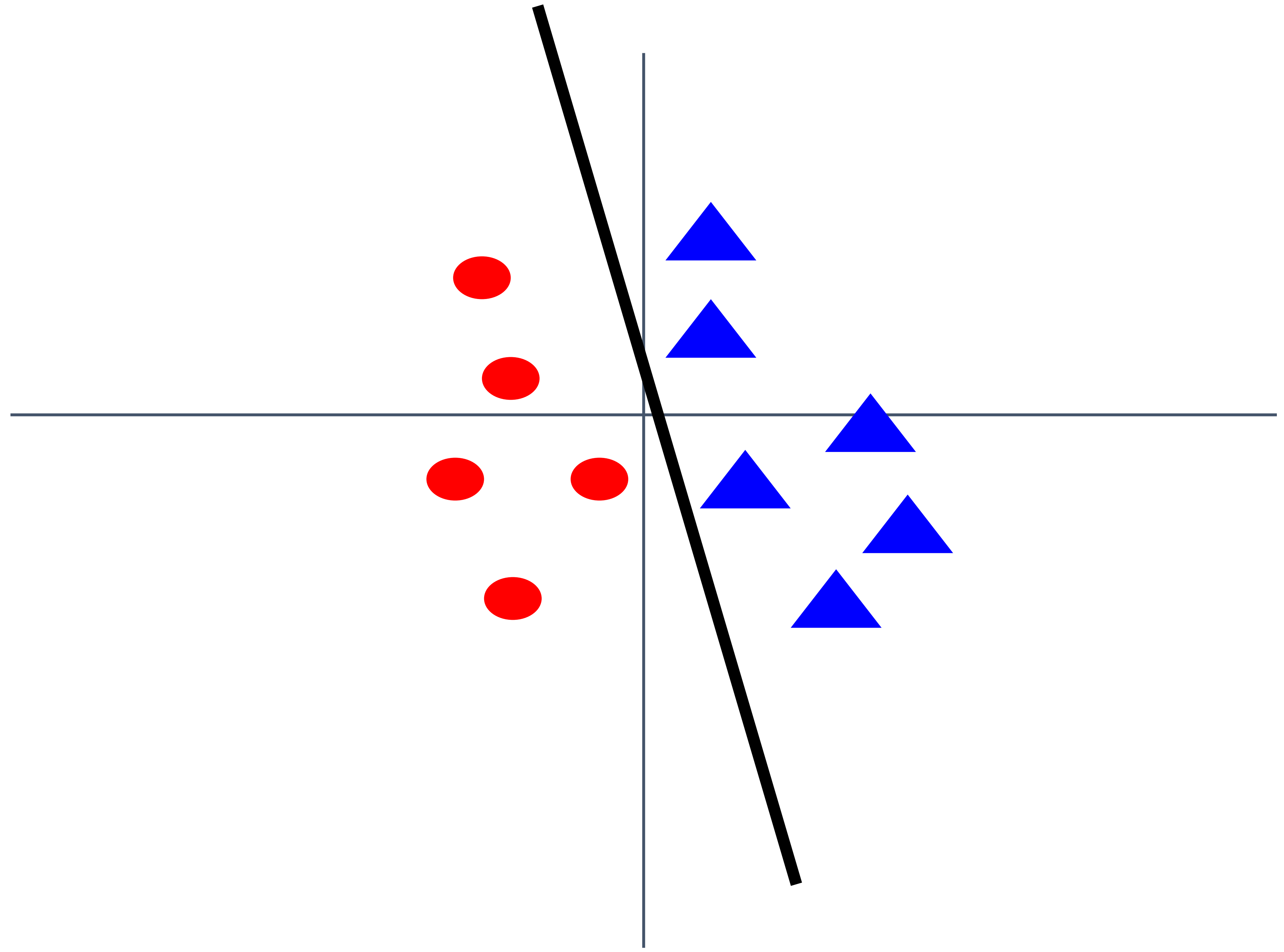
(Covariance matrix is the identity matrix)

Data preprocessing

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



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



Data preprocessing for Images

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

- Subtract the mean image (e.g. AlexNet)
  (mean image = [32, 32, 3] array)

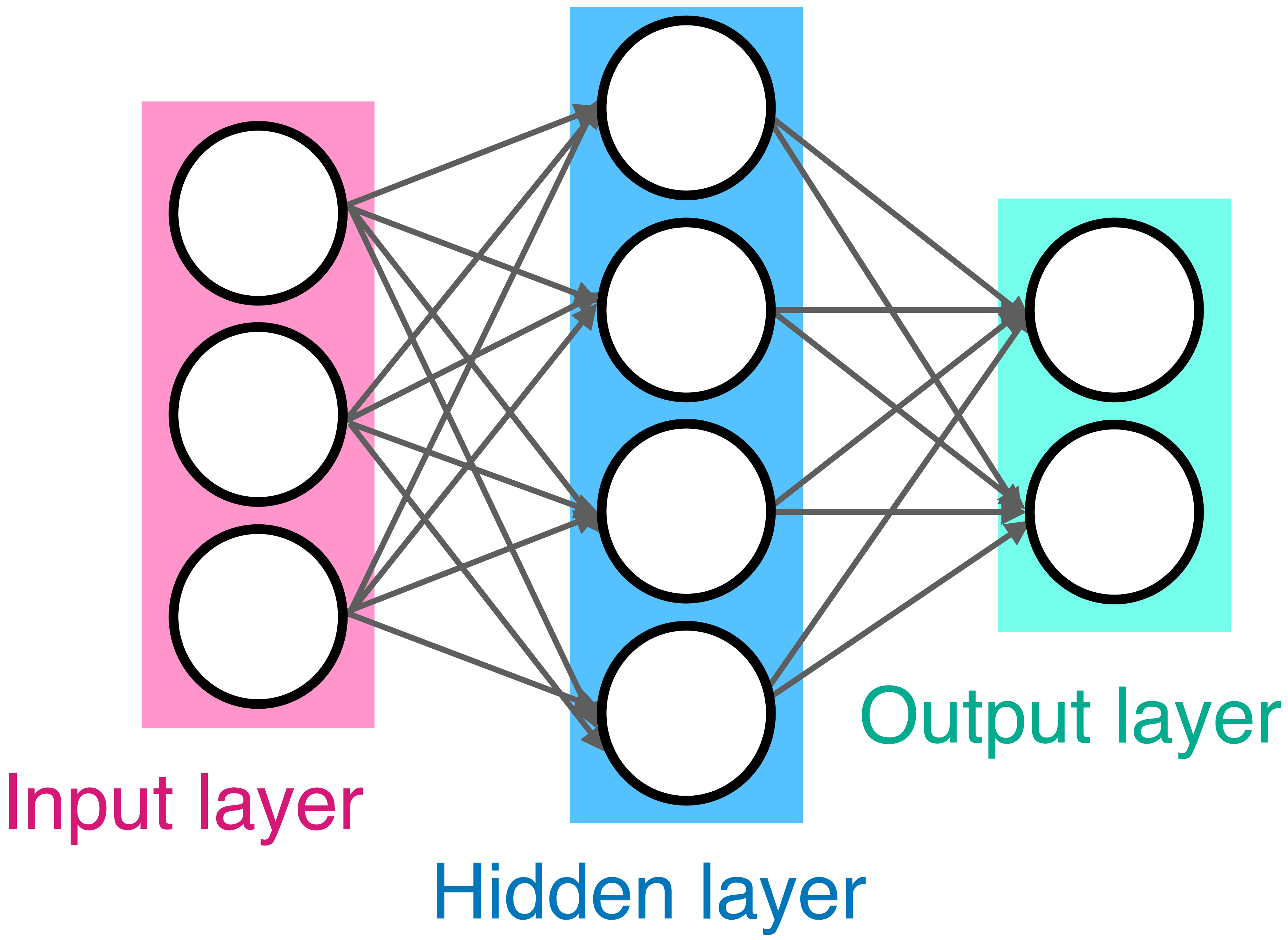
- Subtract per-channel mean (e.g. VGGNet)
  (mean along each channel = 3 numbers)

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

Not common to do PCA or whitening

Weight initialization

Weight initialization



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

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

Weight initialization

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

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

Weight initialization

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

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

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

Weight initialization: Activation statistics

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

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

Weight initialization: Activation statistics

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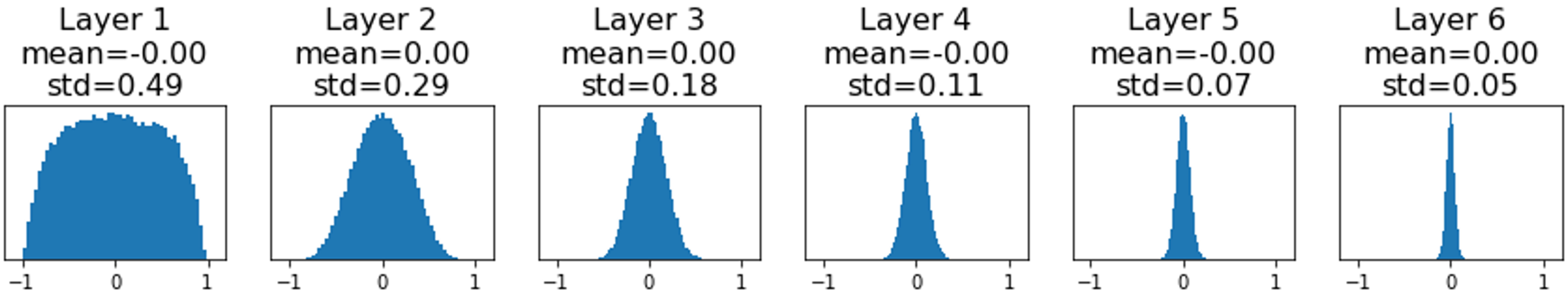
Forward pass for a 6-layer net with hidden size 4096

All activations tend to zero for deeper network layers

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



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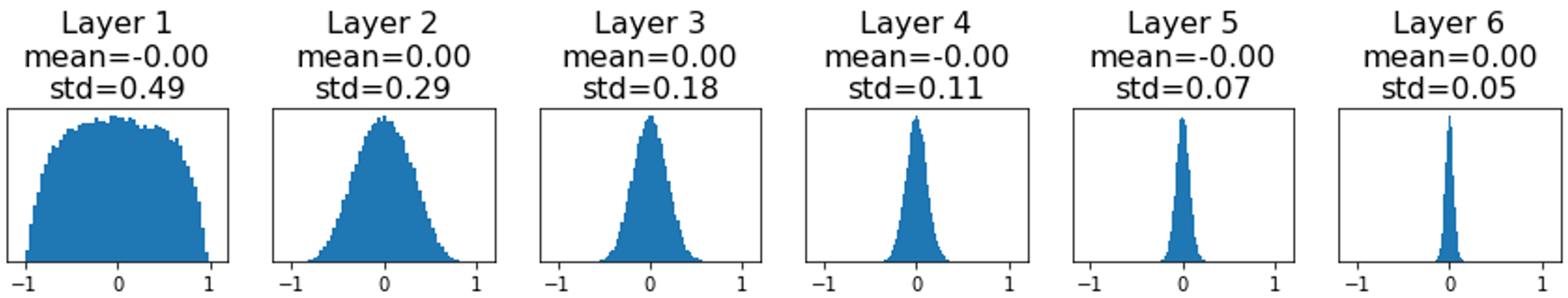
```

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

All activations tend to zero for deeper network layers

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

A: All zero, no learning :(



Weight initialization: Activation statistics

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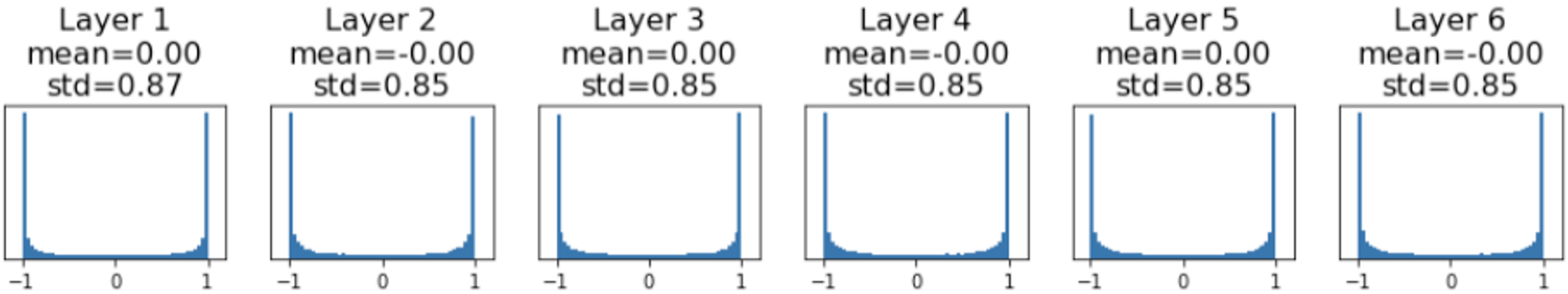
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?



Weight initialization: Activation statistics

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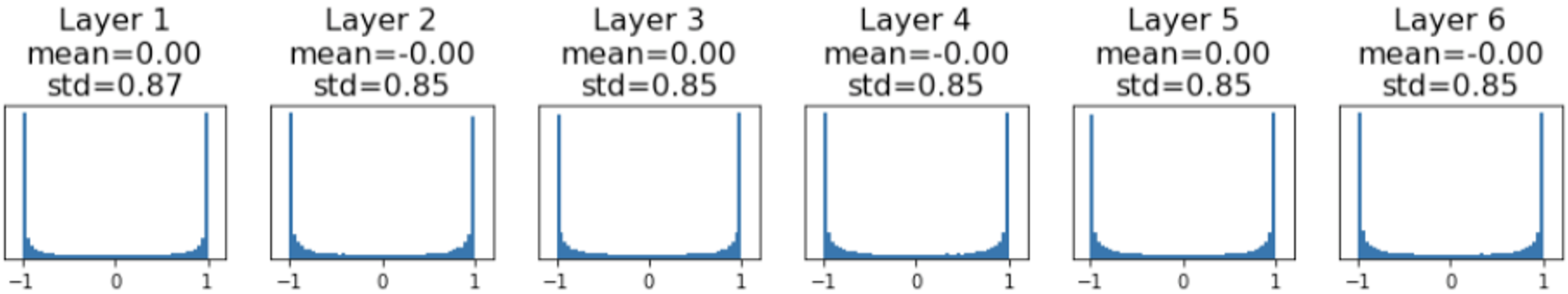
Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

A: Local gradients all zero, no learning :(



Weight initialization: Xavier Initialization

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

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

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

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

Weight initialization: Xavier Initialization

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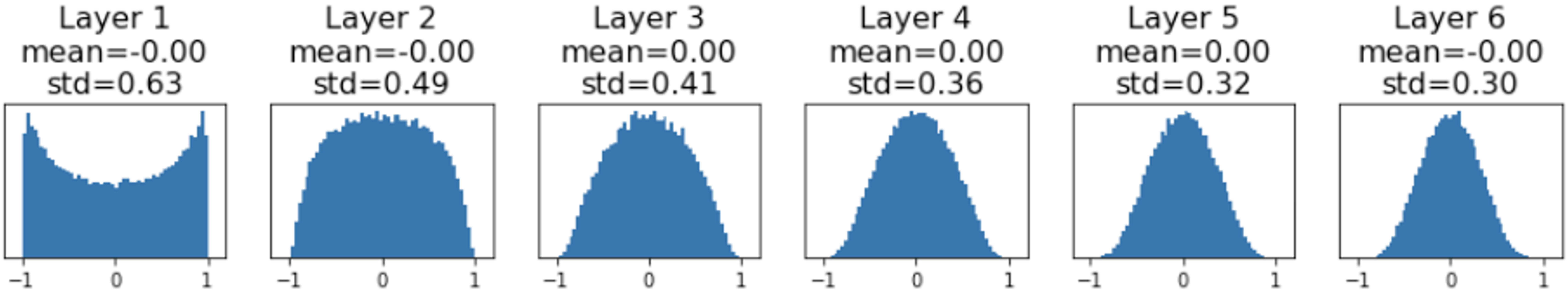

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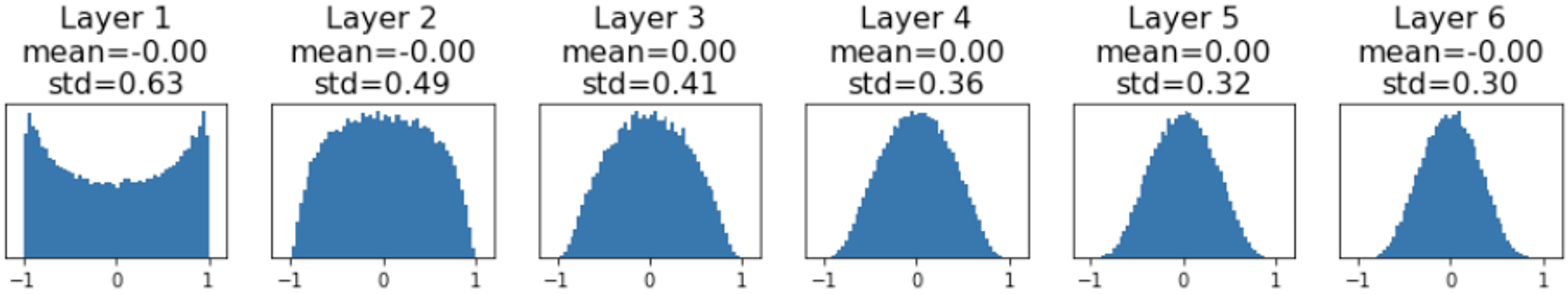
"Just right": Activations are nicely scaled for all layers!

For conv layers, Din is kernel_size^2 x input_channels



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

Weight initialization: Xavier Initialization

"Xavier" initialization:
std $= 1/\sqrt{Din}$

Derivation: Variance of output = Variance of input

$$y = Wx$$

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

$Var(y_i) = Din \times Var(x_i, w_i)$ [Assume x, w are iid]

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

$= Din \times Var(x_i) \times Var(w_i)$ [Assume x, w are zero-mean]

If $Var(w_i) = 1/Din$ then $Var(y_i) = Var(x_i)$

Weight initialization: What about ReLU?

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

Change from tanh to ReLU

Xavier assumes zero centered activation function

Weight initialization: What about ReLU?

```
dims = [4096] * 7
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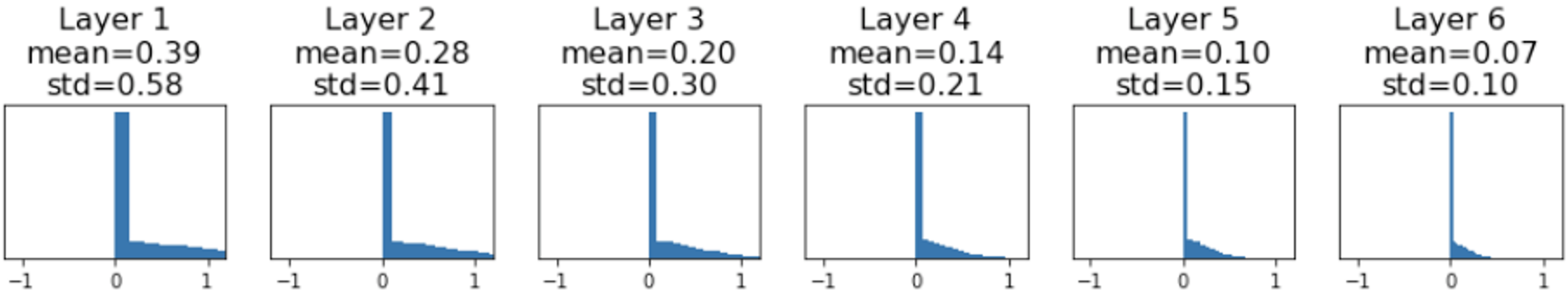
```

Change from tanh to ReLU

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning :(

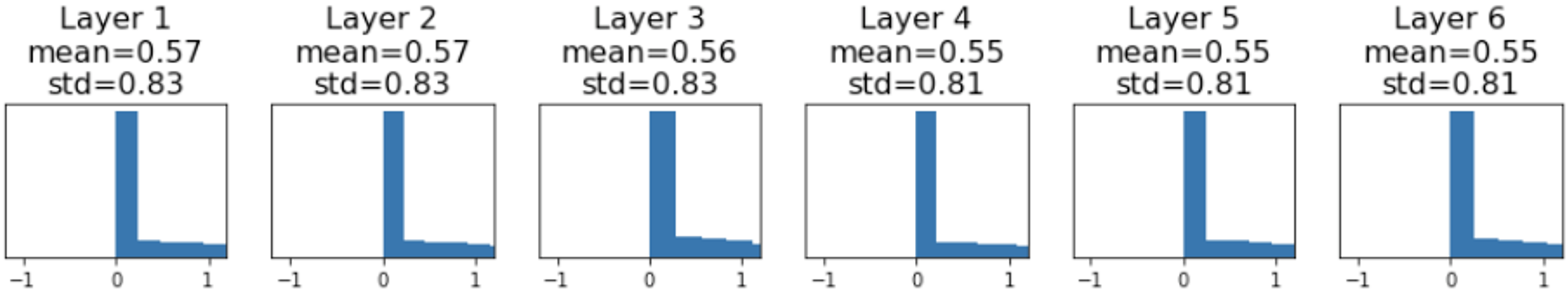


Weight initialization: Kaiming / MSRA initialization

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

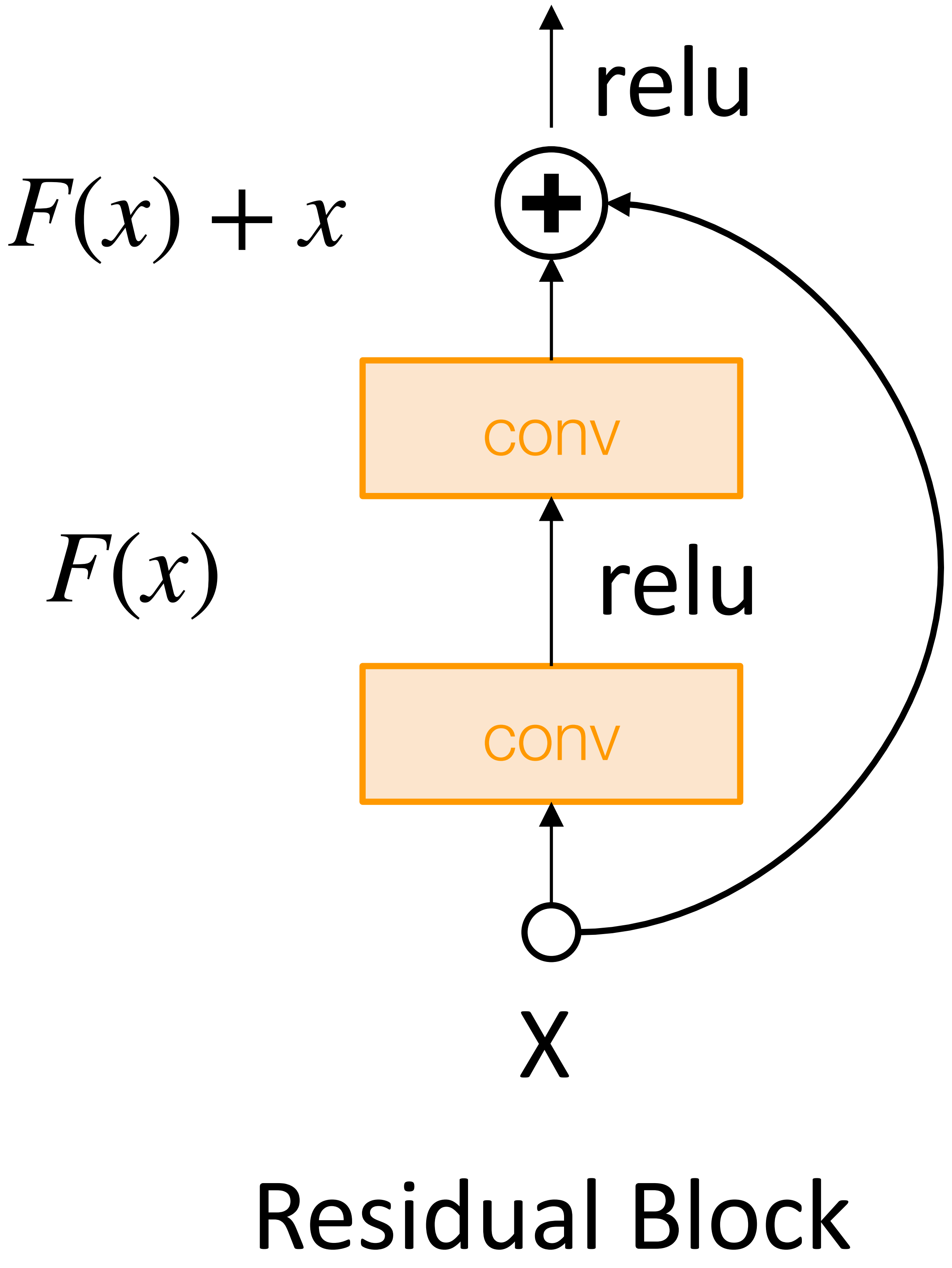
ReLU correction: std = sqrt(2 / Din)

"Just right" - activations nicely scaled for all layers



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

Weight initialization: Residual Networks

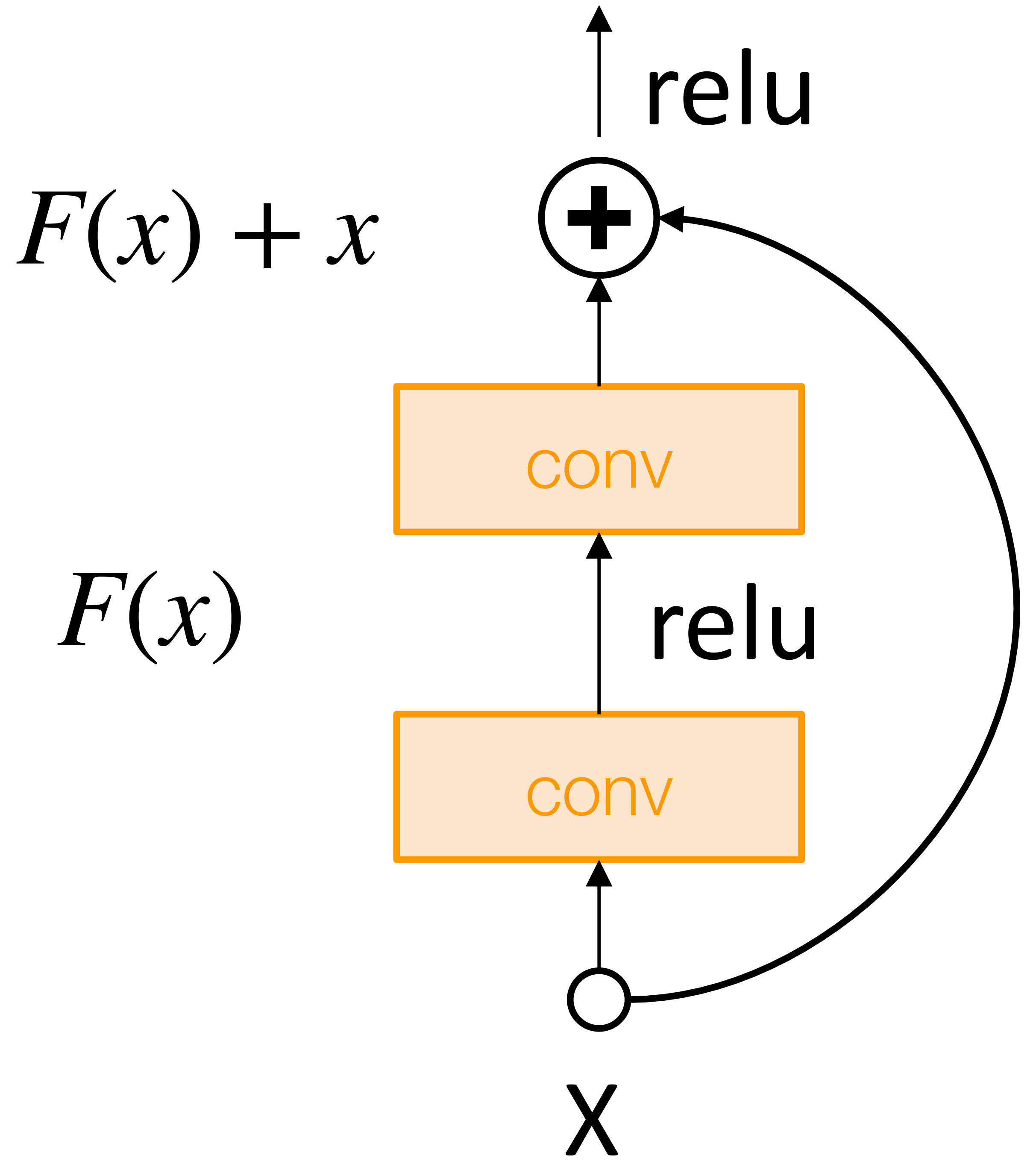


If we initialize with MSRA: then
$Var(F(x)) = Var(x)$

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

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

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!

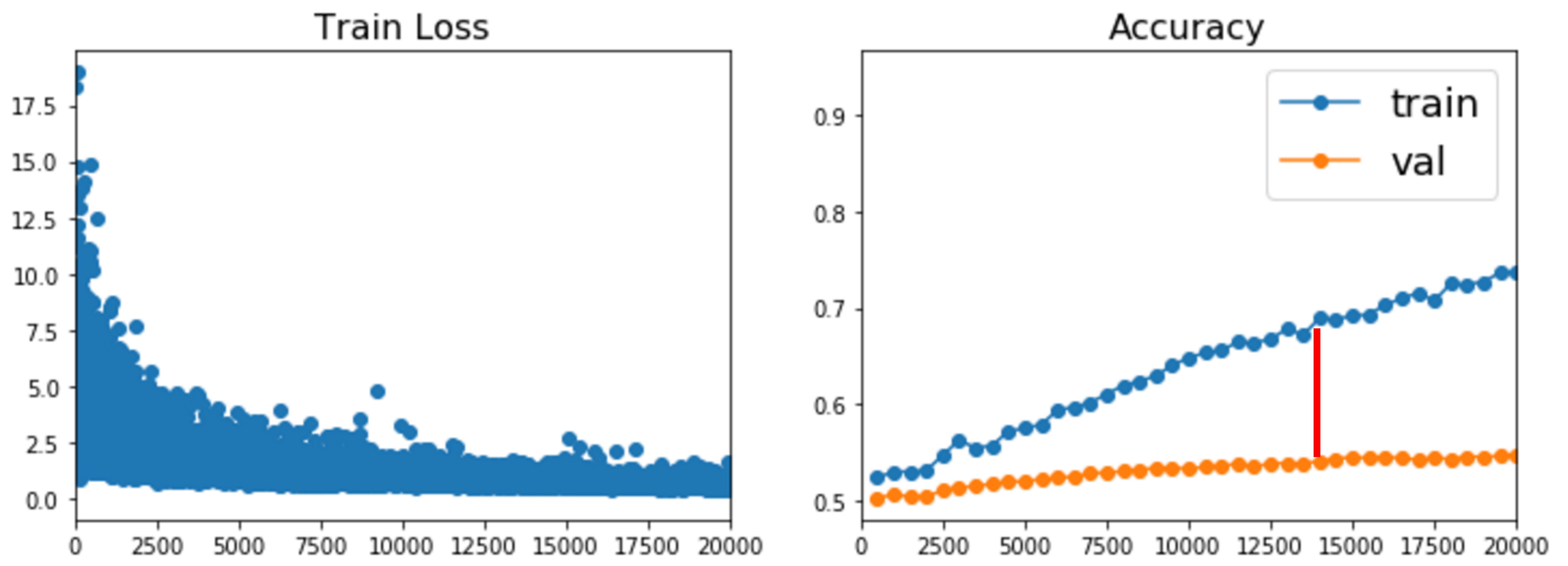
Solution: Initialize first conv with MSRA, initialize second conv to zero. Then
$Var(F(x) + x) = Var(x)$

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

Proper initialization is an active area of research

- *Understanding the difficulty of training deep feedforward neural networks* by Glorot and Bengio, 2010
- *Exact solutions to the nonlinear dynamics of learning in deep linear neural networks* by Saxe et al, 2013
- *Random walk initialization for training very deep feedforward networks* by Sussillo and Abbott, 2014
- *Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification* by He et al., 2015
- *Data-dependent Initializations of Convolutional Neural Networks* by Krähenbühl et al., 2015
- *All you need is a good init*, Mishkin and Matas, 2015
- *Fixup Initialization: Residual Learning Without Normalization*, Zhang et al, 2019
- *The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks*, Frankle and Carbin, 2019

Now your model is training … but it overfits!



Regularization

Regularization: Add term to the loss

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

In common use:

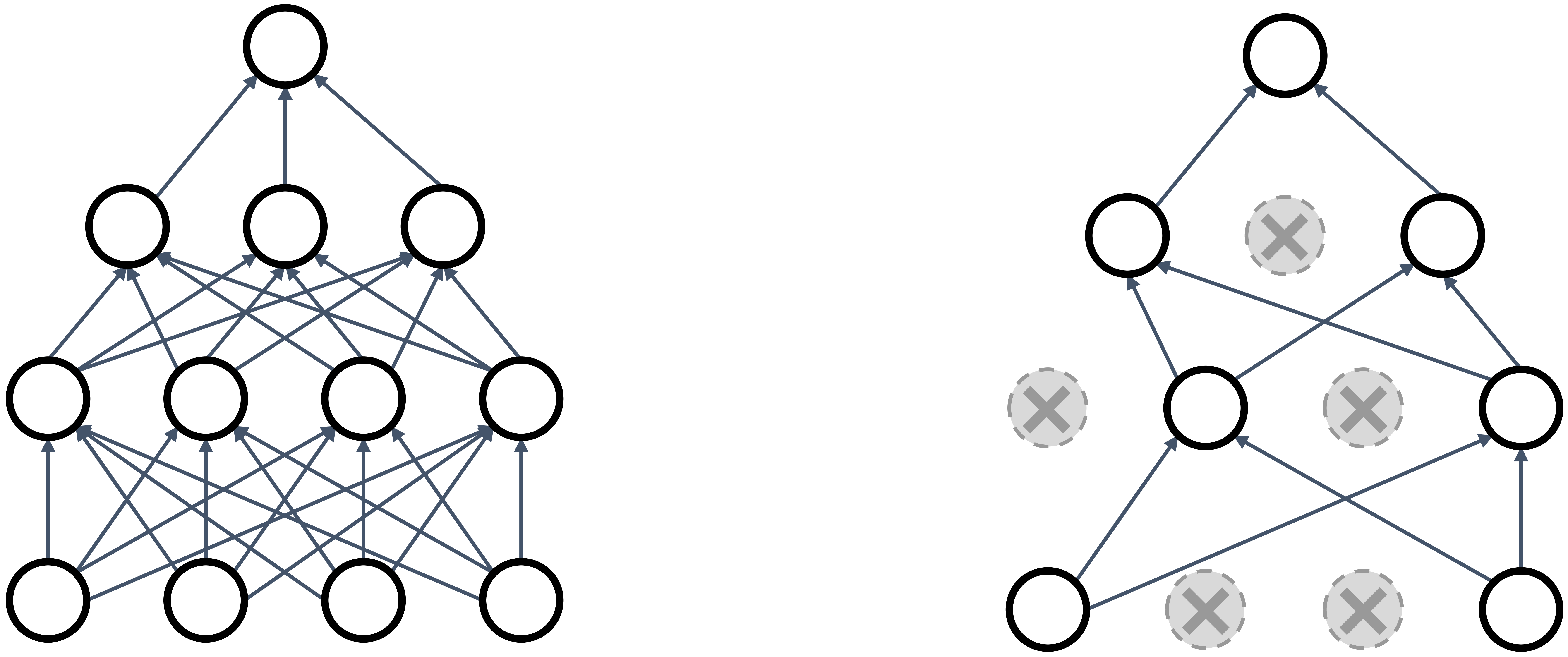
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

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

Regularization: Dropout

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



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

Regularization: Dropout

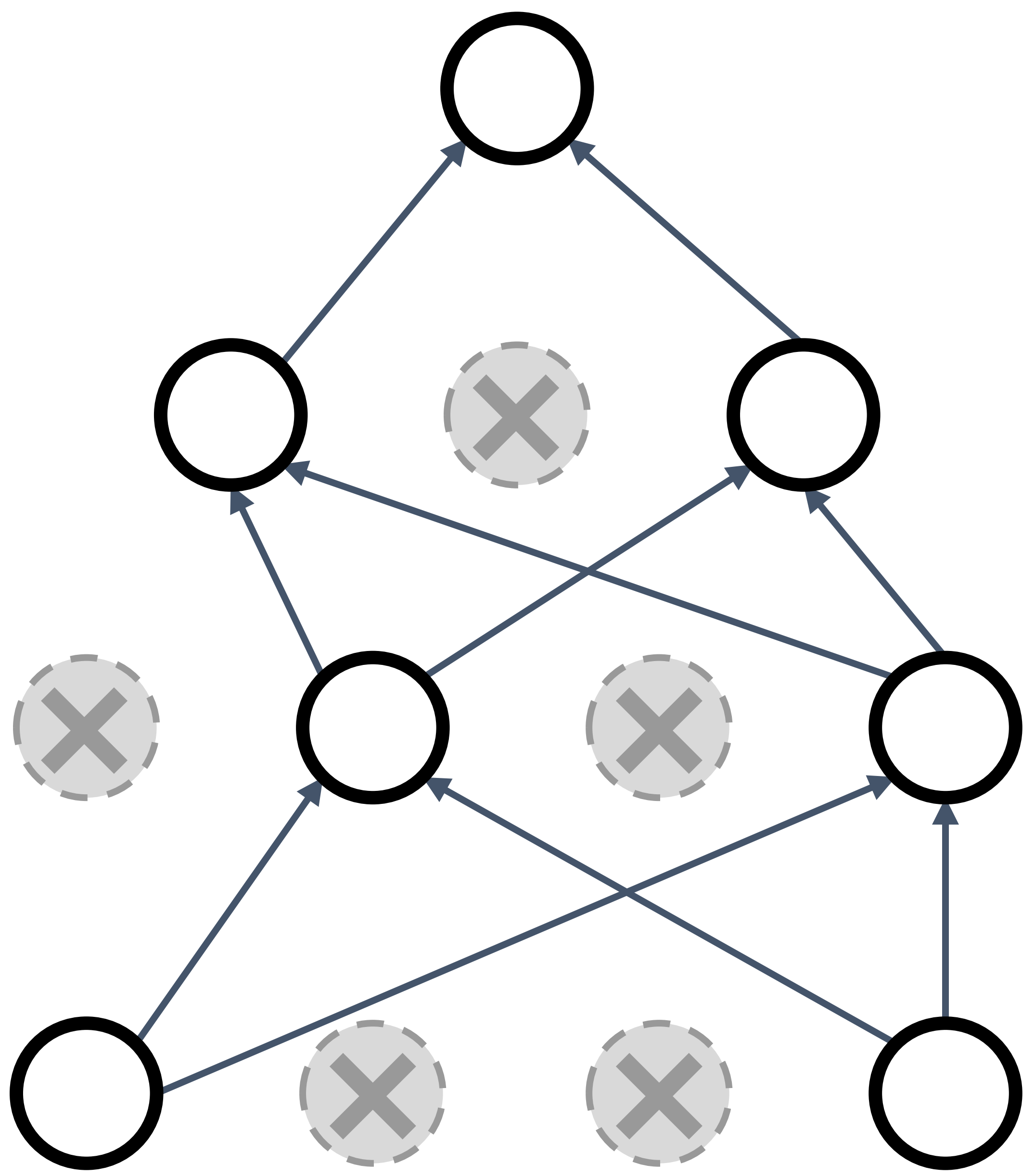
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

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

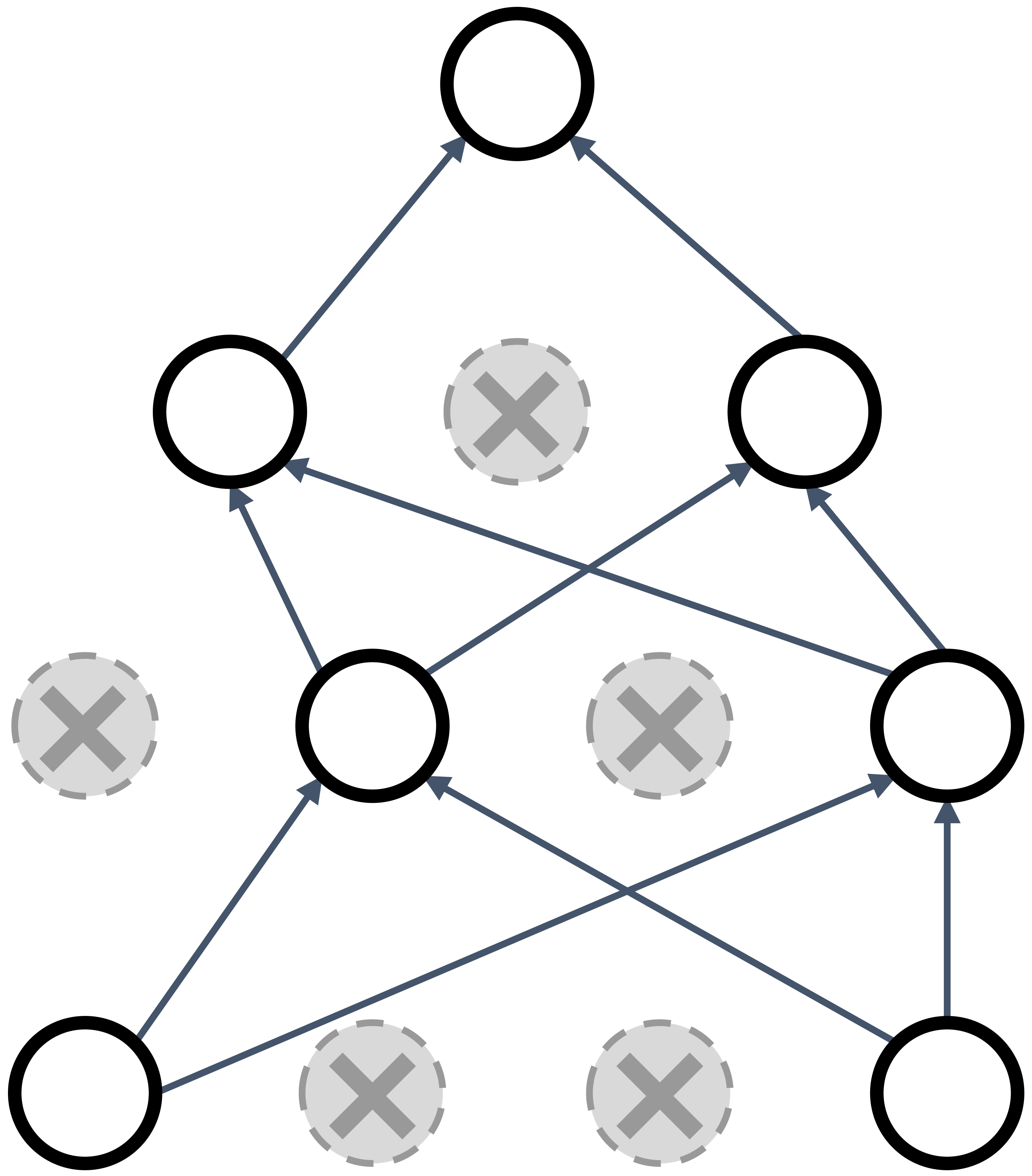
  # forward pass for example 3-layer neural network
  H1 = np.maximum(0, np.dot(W1, X) + b1)
  U1 = np.random.rand(*H1.shape) < p # first dropout mask
  H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
  U2 = np.random.rand(*H2.shape) < p # second dropout mask
  H2 *= U2 # drop!
  out = np.dot(W3,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

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

Example forward pass with a 3-layer network using dropout

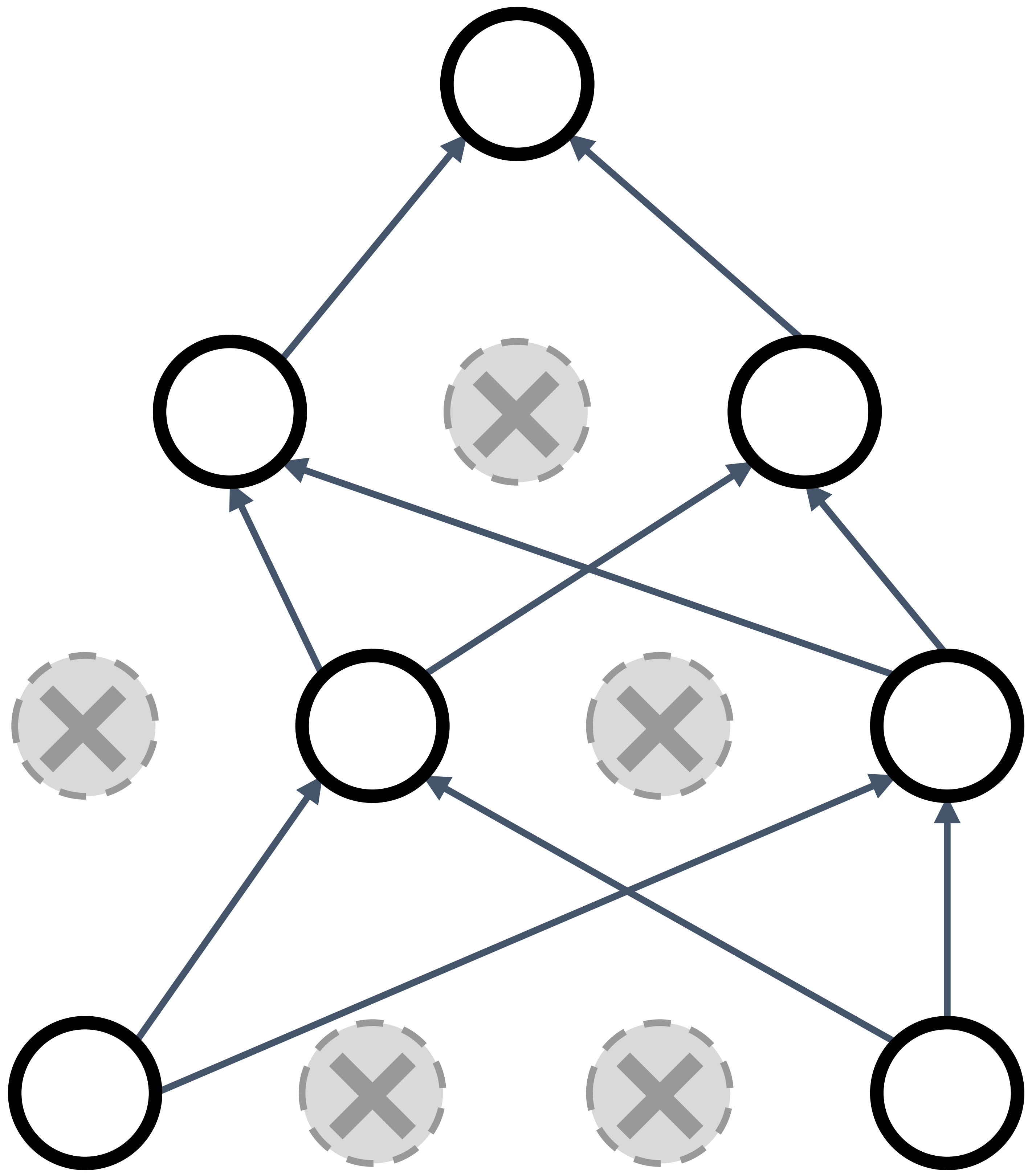


Regularization: Dropout



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

Regularization: Dropout



Another interpretation:

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

Each binary mask is one model

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

Dropout: Test time

Dropout makes our output random!

Random mask

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

Output label — Input image

Want to “average out” the randomness at test-time

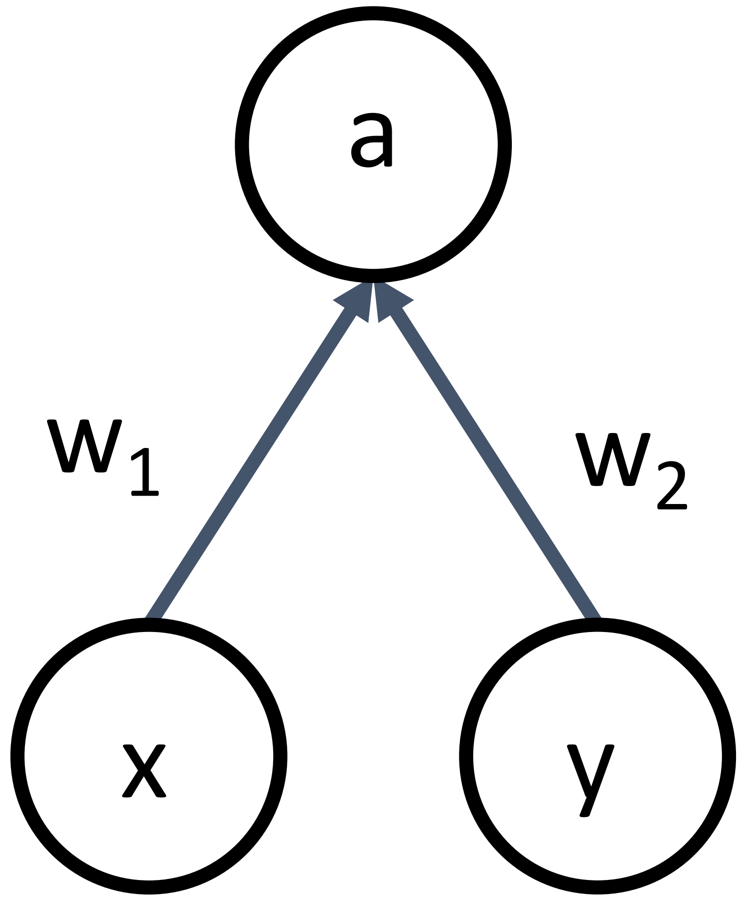
$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z) f(x, z) dz$$

But this integral seems hard…

Dropout: Test time

Want to approximate the integral

$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z)f(x, z)dz$$



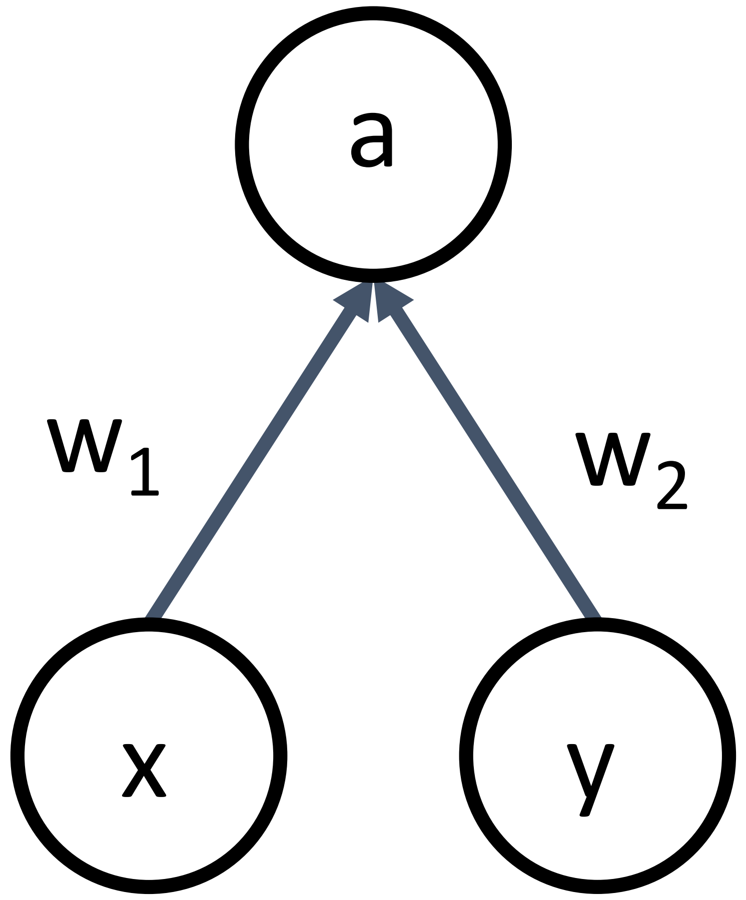
Consider a single neuron:

At test time we have: $\mathbb{E}[a] = w_1x + w_2y$

Dropout: Test time

Want to approximate the integral

$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z) f(x, z) dz$$



Consider a single neuron:

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

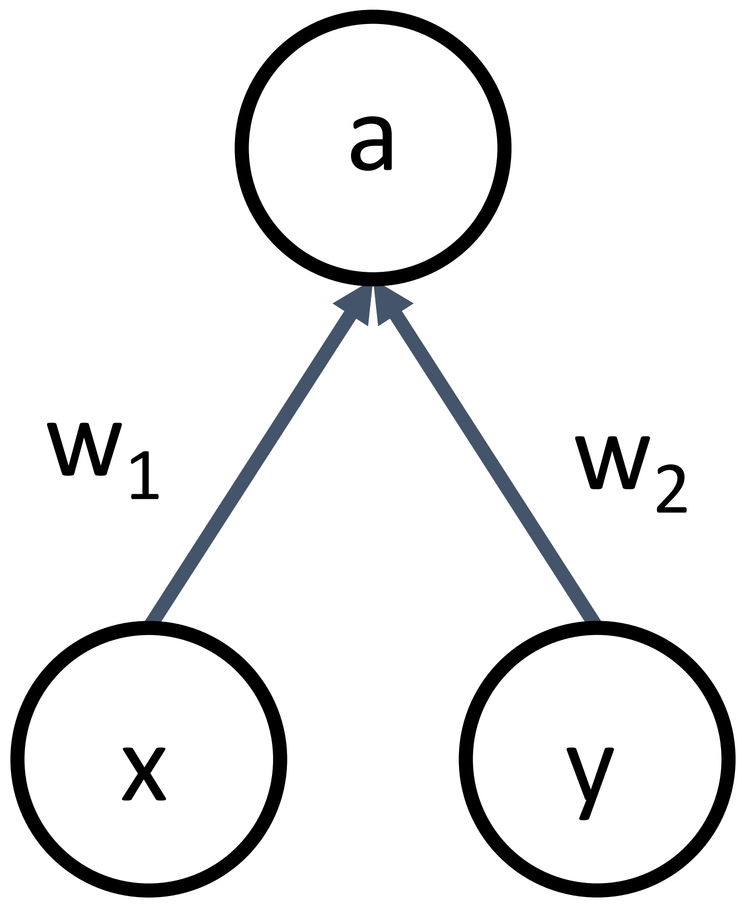
During training time we have:

$$\mathbb{E}[a] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y) = \frac{1}{2}(w_1 x + w_2 y)$$

Dropout: Test time

Want to approximate the integral

$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z) f(x, z) dz$$



Consider a single neuron:

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During training time we have: $$\mathbb{E}[a] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y) = \frac{1}{2}(w_1 x + w_2 y)$$

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

Dropout: Test time

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

At test time all neurons are active always

=> We must scale the activations so that for each neuron:
Output at test time = Expected output at training time

Dropout Summary

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

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

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

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

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

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

Drop in forward pass

Scale at test time

More common: “Inverted dropout”

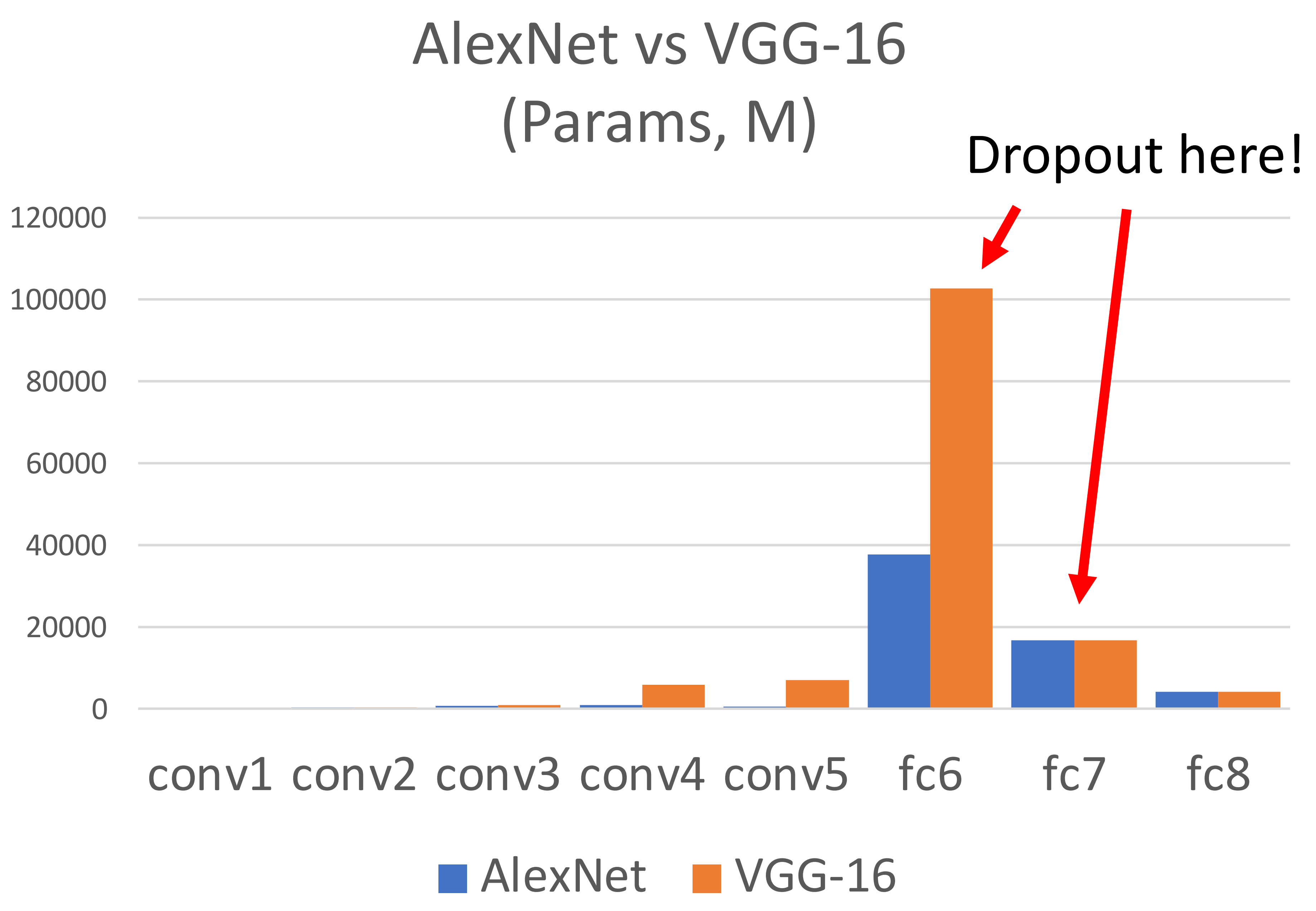
```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

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

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

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

Drop and scale during training

test time is unchanged!

Dropout architectures

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



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

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z)f(x, z)dz$$

Regularization: A common pattern

Training: Add some kind of randomness

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

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

Testing: Average out randomness (sometimes approximate)

$$y = f(x, z) = \mathbb{E}_z[f(x, z)] = \int p(z)f(x, z)dz$$

Example: Batch Normalization

Training: Normalize using stats from random mini batches

Testing: Use fixed stats to normalize

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