CS 4644-DL / 7643-A: LECTURE 9
DANFEI XU

Topics:

- Convolutional Neural Networks Architectures (cont.)
- Training Neural Networks (Part 1)

Administrative

- PS2/HW2 out: **Difficult assignment. Start early!**

CNN Architectures

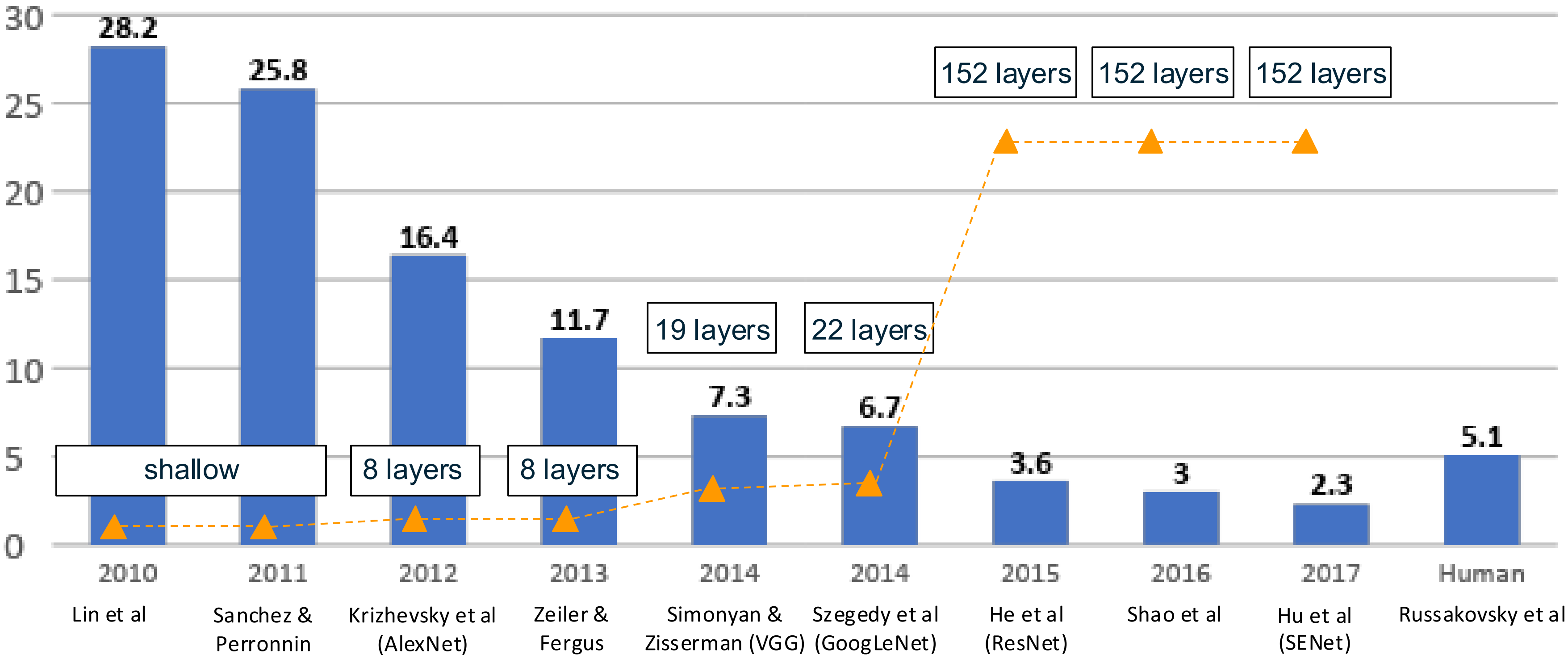
Case Studies

- AlexNet
- VGG
- GoogLeNet
- ResNet

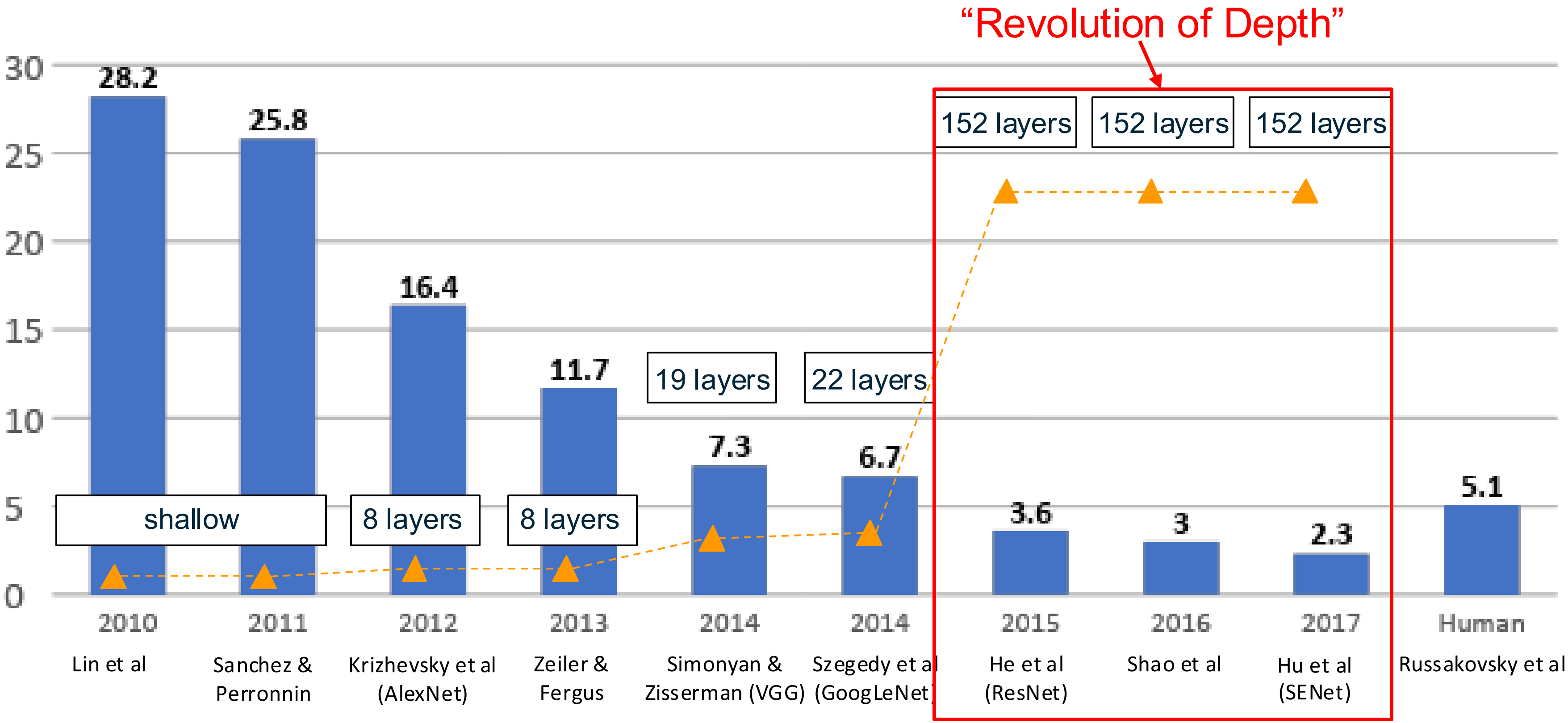
Also....

- SENet
- Wide ResNet
- ResNeXT
- DenseNet
- MobileNets
- NASNet
- EfficientNet

ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



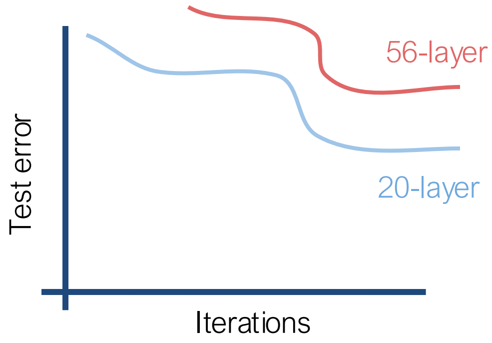
ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners

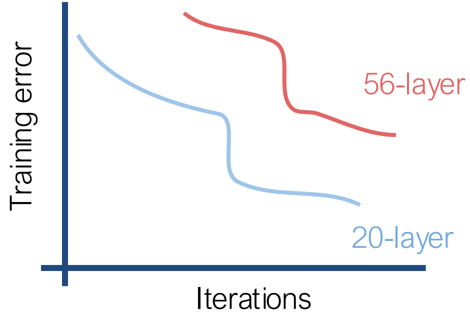


Case Study: ResNet

[He et al., 2015]

What happens when we continue stacking deeper layers on a “plain” convolutional neural network?





56-layer model performs worse on both test and training error
-> The deeper model performs worse, but it’s not caused by overfitting!

Case Study: ResNet

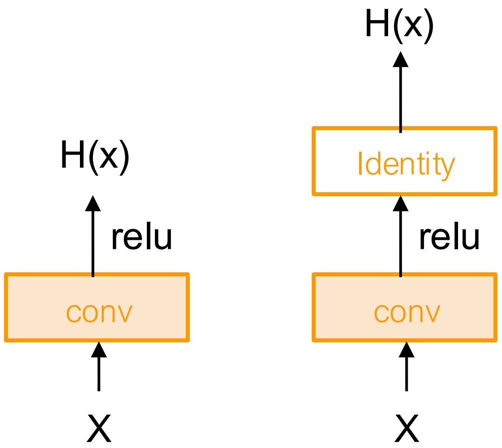
[He et al., 2015]

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

Deeper models are harder to optimize. They don't learn identity functions (no-op) to emulate shallow models

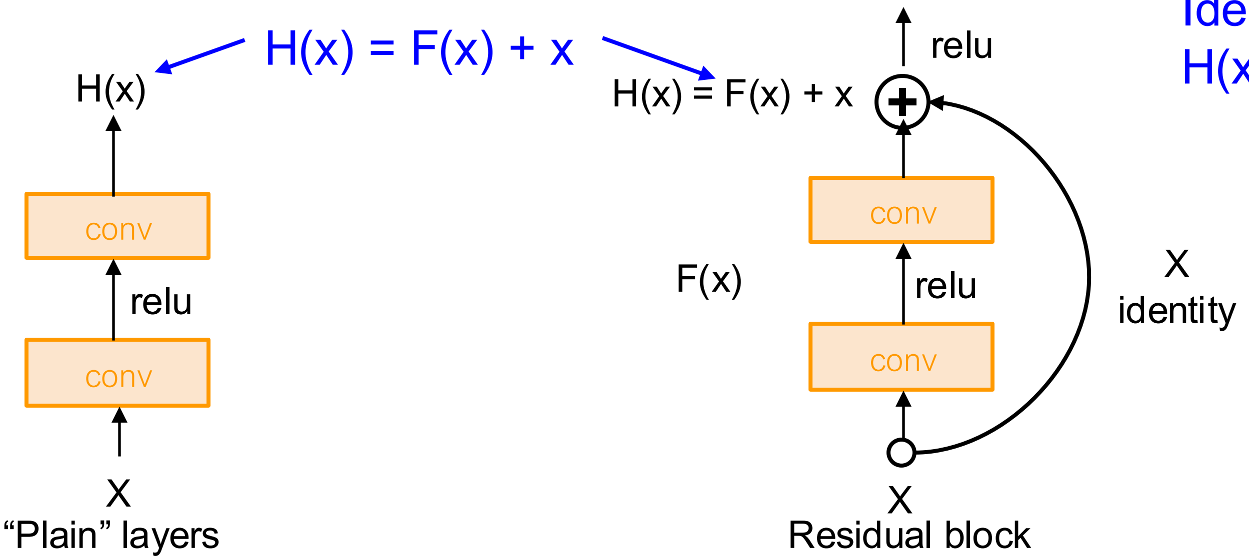
Solution: Change the network so learning identity functions (no-op) as extra layers is easy



Case Study: ResNet

[He et al., 2015]

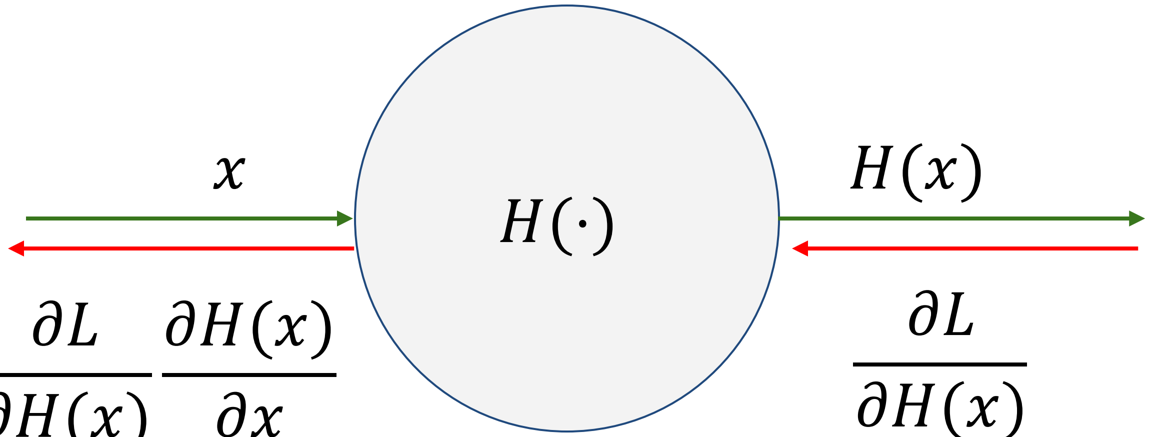
Solution: Change the network so learning identity functions as extra layers is easy



Identity mapping:
$H(x) = x$ if $F(x) = 0$

Use layers to fit **residual** $F(x) = H(x) - x$ instead of $H(x)$ directly

The Vanishing Gradient Problem



Downstream Gradient $\frac{\partial L}{\partial H(x)} \frac{\partial H(x)}{\partial x}$

Upstream Gradient $\frac{\partial L}{\partial H(x)}$

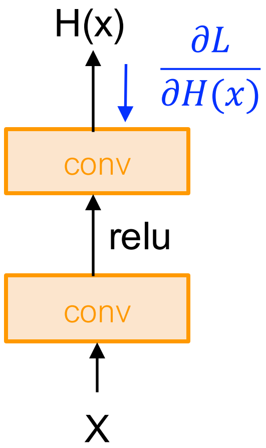
$$H(x) = W^T x + b$$

$$\frac{\partial H(x)}{\partial x} = W^T$$

If W is small, downstream gradient is small.

Each small W in the chain makes gradient *progressively smaller ->*
Vanishing Gadient during backpropagation

Case Study: ResNet

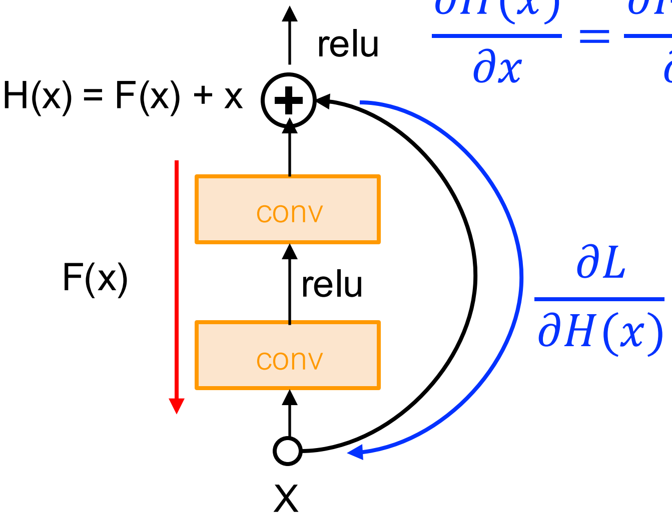


"Plain" layers

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial H(x)} \frac{\partial H(x)}{\partial x}$$

Potentially problematic

$$\frac{\partial L}{\partial H(x)} \frac{\partial F(x)}{\partial x}$$



$$\frac{\partial H(x)}{\partial x} = \frac{\partial F(x)}{\partial x} + 1$$

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial H(x)} \frac{\partial H(x)}{\partial x}$$

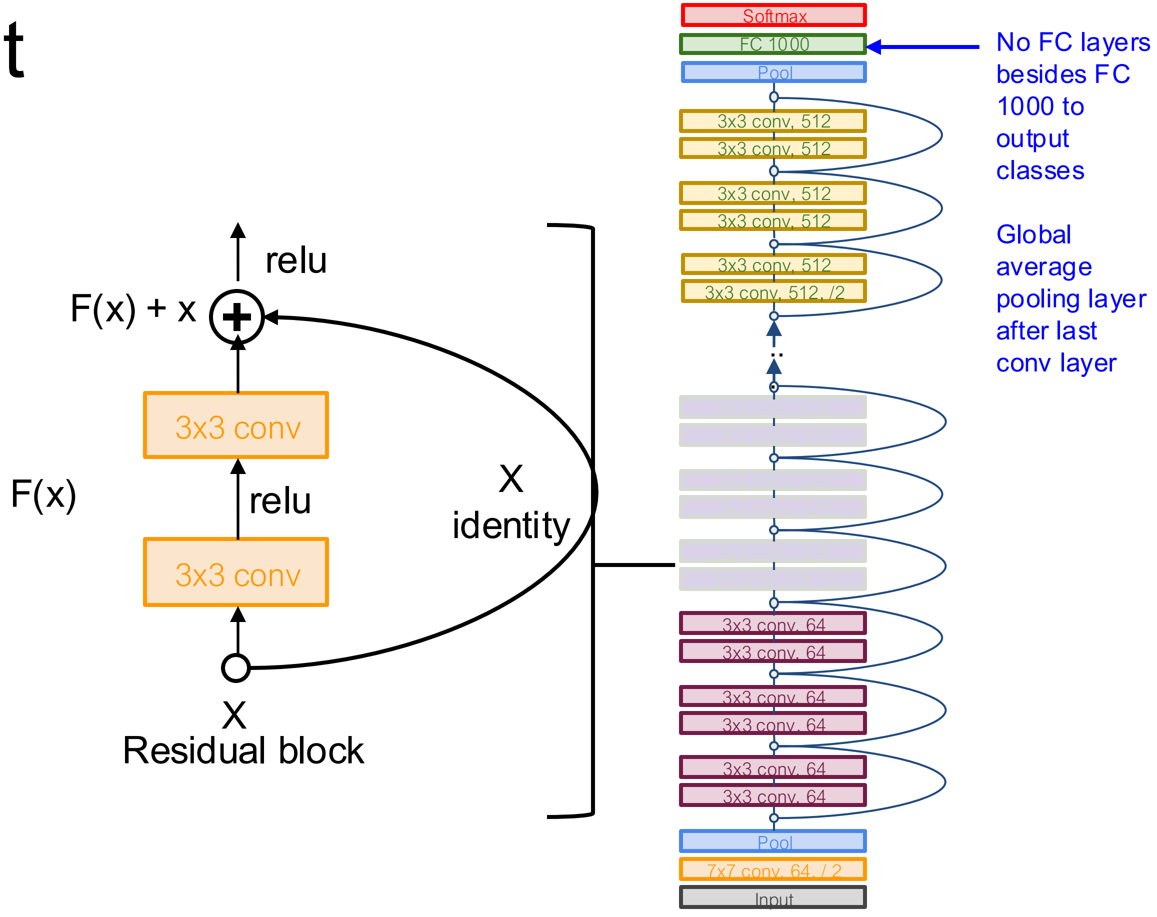
$$= \frac{\partial L}{\partial H(x)} \frac{\partial F(x)}{\partial x} + \frac{\partial L}{\partial H(x)}$$

Direct gradient pathway

Case Study: ResNet

[He et al., 2015]

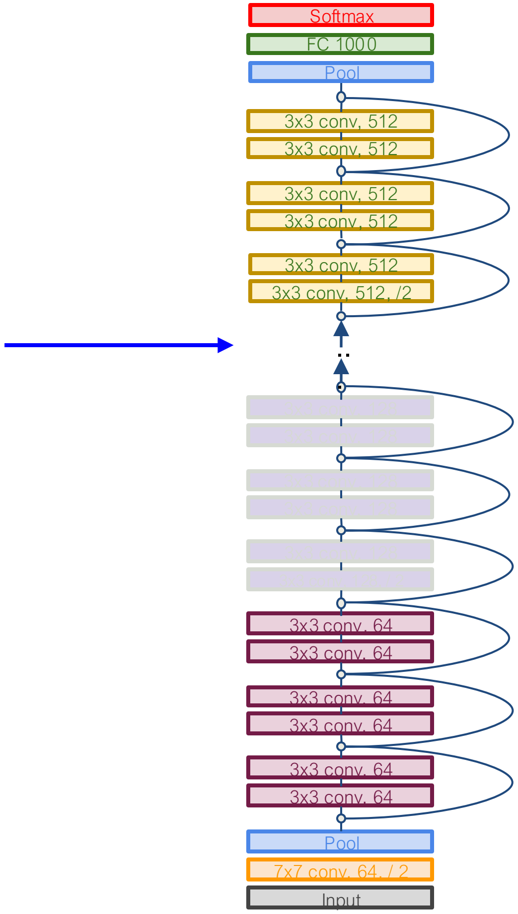
Full ResNet architecture:
- Stack residual blocks
- Every residual block has two 3x3 conv layers
- Periodically, double # of filters and downsample spatially using stride 2 (/2 in each dimension) Reduce the activation volume by half.
- Additional conv layer at the beginning (stem)
- No FC layers at the end (only FC 1000 to output classes)



Case Study: ResNet

[He et al., 2015]

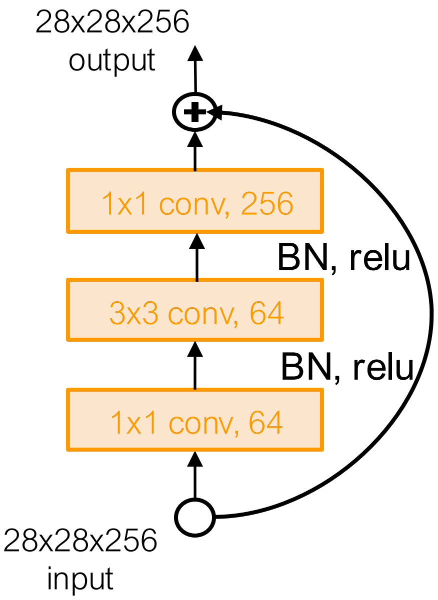
Total depths of 18, 34, 50, 101, or 152 layers for ImageNet



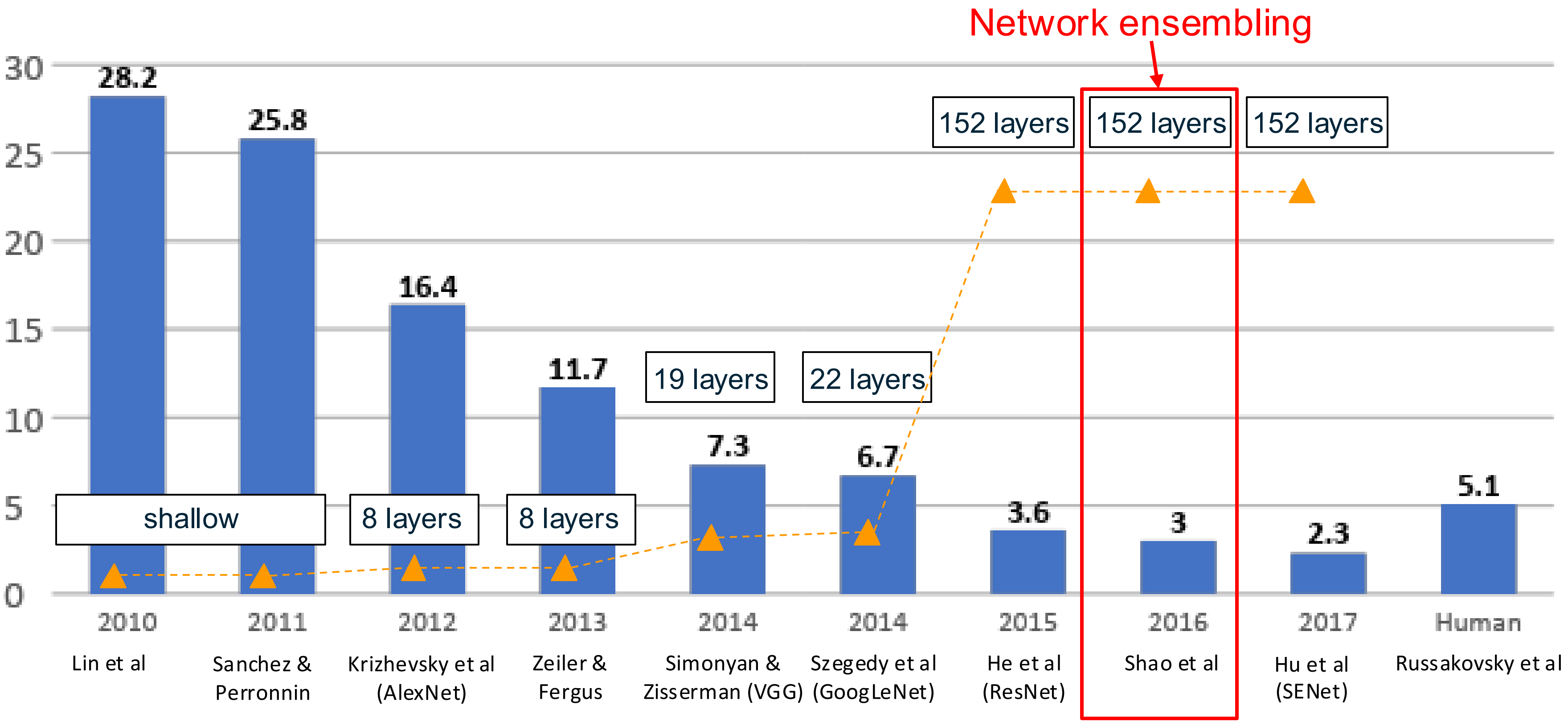
Case Study: ResNet

[He et al., 2015]

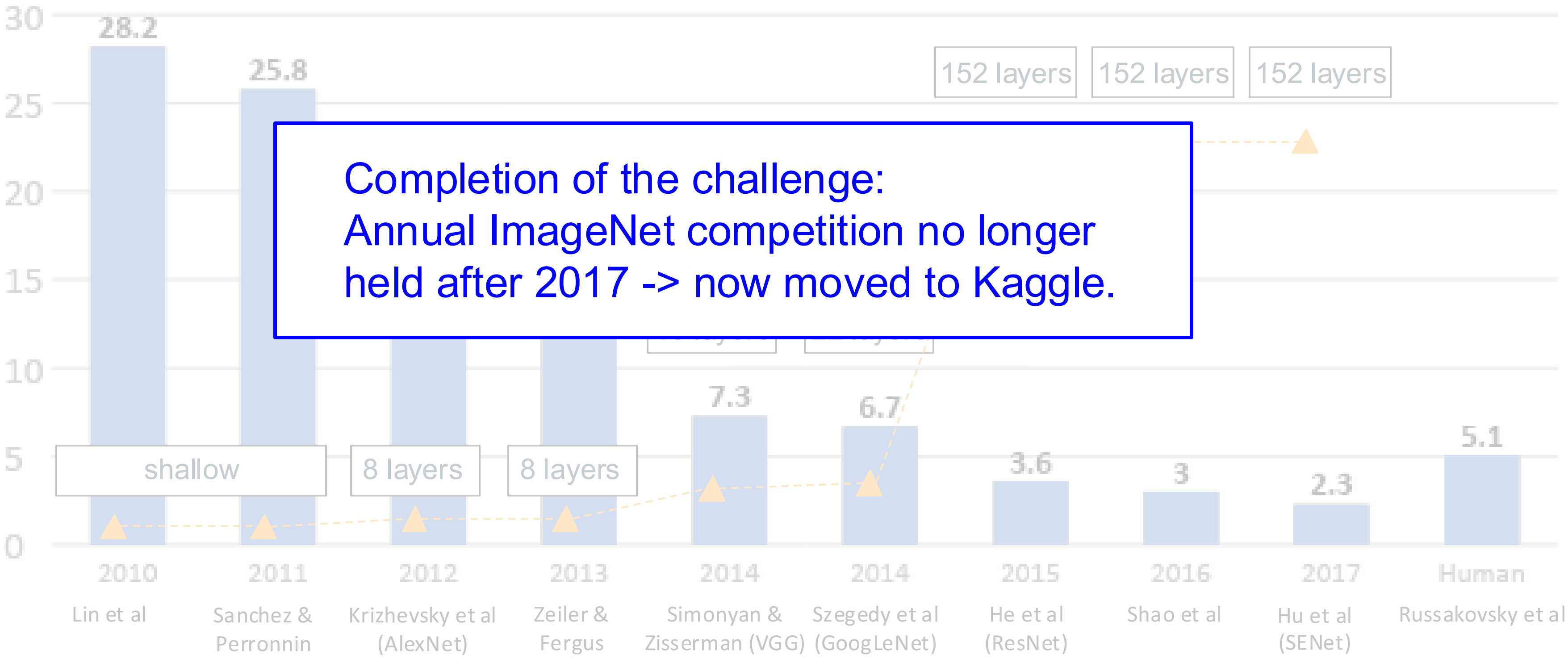
For deeper networks (ResNet-50+), use “bottleneck” layer to improve efficiency (similar to GoogLeNet)



ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



ImageNet Large Scale Visual Recognition Challenge (ILSVRC) winners



Completion of the challenge:
Annual ImageNet competition no longer held after 2017 -> now moved to Kaggle.

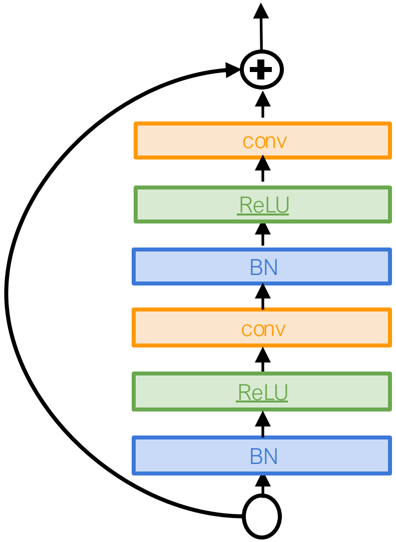
But research into CNN architectures is still flourishing

Improving ResNets...

Identity Mappings in Deep Residual Networks

[He et al. 2016]

- Improved ResNet block design from creators of ResNet
- Creates a more direct path for propagating information throughout network
- Gives better performance

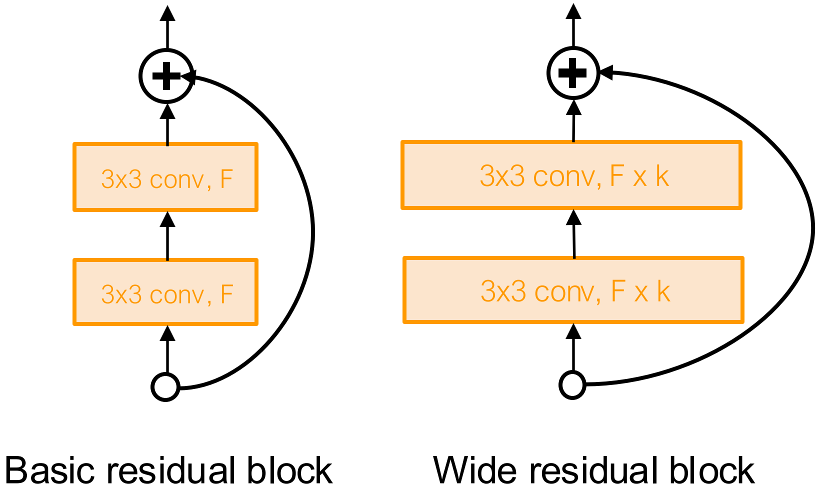


Improving ResNets...

Wide Residual Networks

[Zagoruyko et al. 2016]

- Argues that residuals are the important factor, not depth
- Use wider residual blocks (F x k filters instead of F filters in each layer)
- 50-layer wide ResNet outperforms 152-layer original ResNet
- Increasing width instead of depth more computationally efficient (parallelizable)

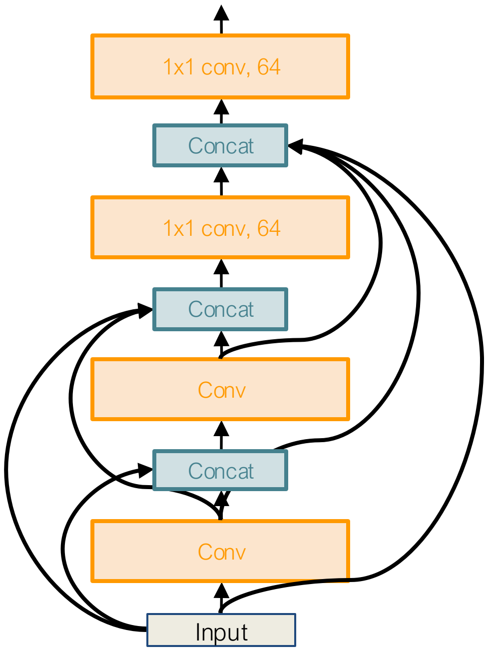


Other ideas...

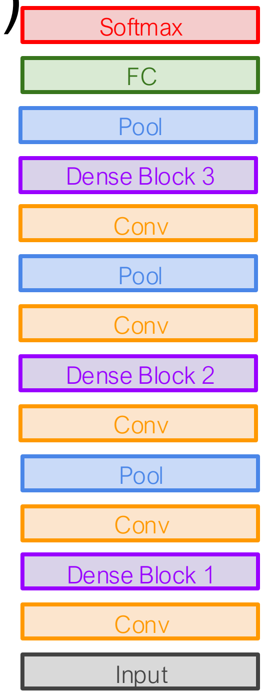
Densely Connected Convolutional Networks (DenseNet)

[Huang et al. 2017]

- Dense blocks where each layer is connected to every other layer through concatenation
- Different way to address vanishing gradient (concat vs. residual) .
- Multi-layer feature aggregation
- Showed that shallow 50-layer network can outperform deeper 152 layer ResNet



Dense Block

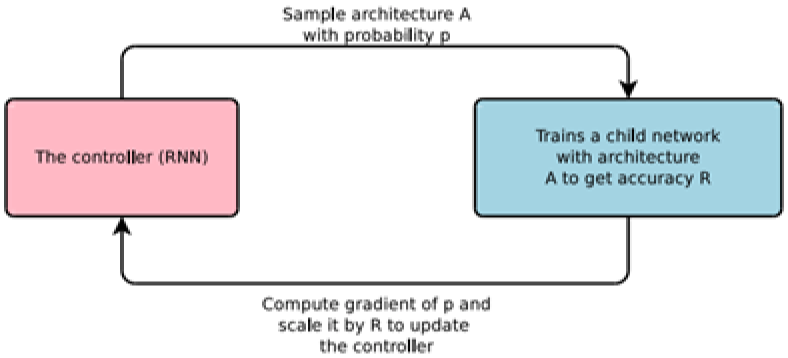


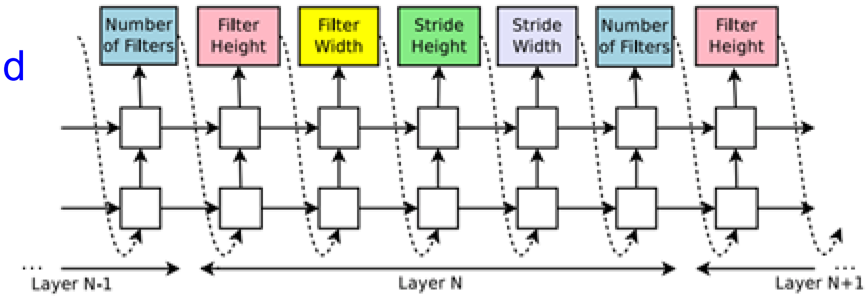
Learning to search for network architectures...

Neural Architecture Search with Reinforcement Learning (NAS)

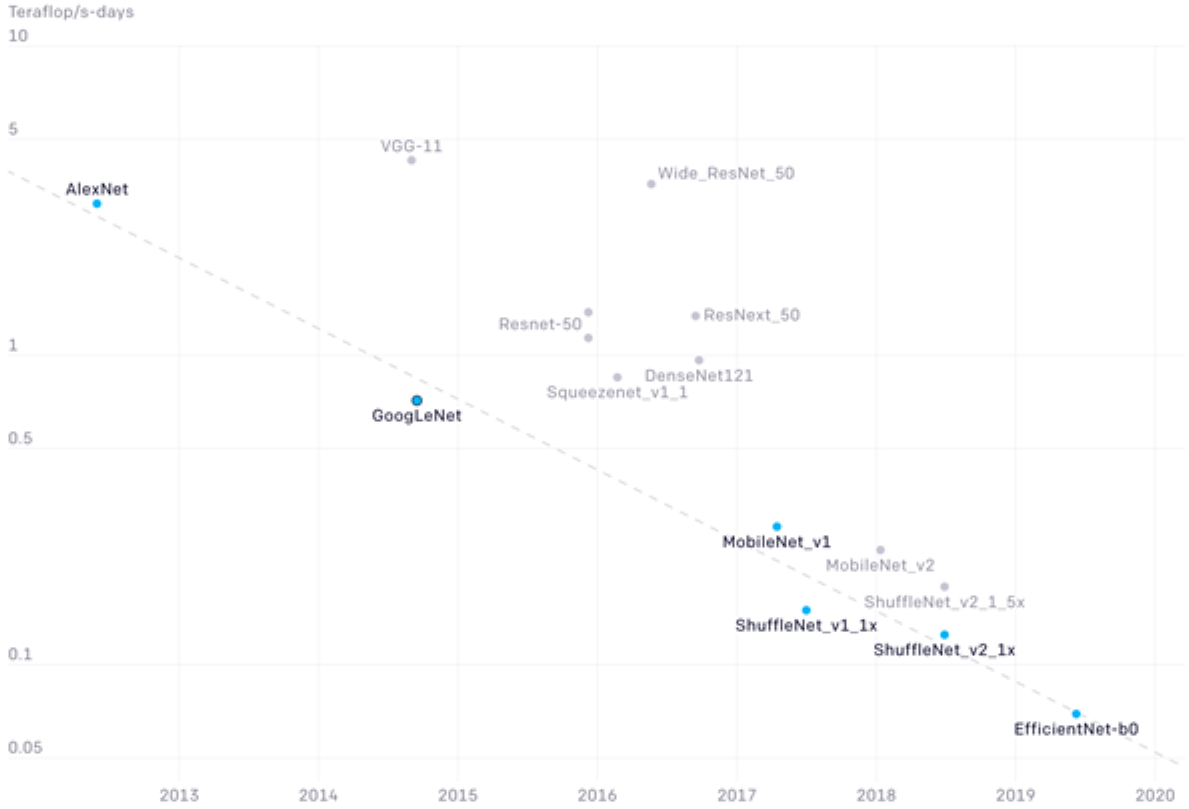
[Zoph et al. 2016]

- "Controller" network that learns to design a good network architecture (output a string corresponding to network design)
- Iterate:
    1) Sample an architecture from search space
    2) Train the architecture to get a "reward" R corresponding to accuracy
    3) Compute gradient of sample probability, and scale by R to perform controller parameter update (i.e. increase likelihood of good architecture being sampled, decrease likelihood of bad architecture)





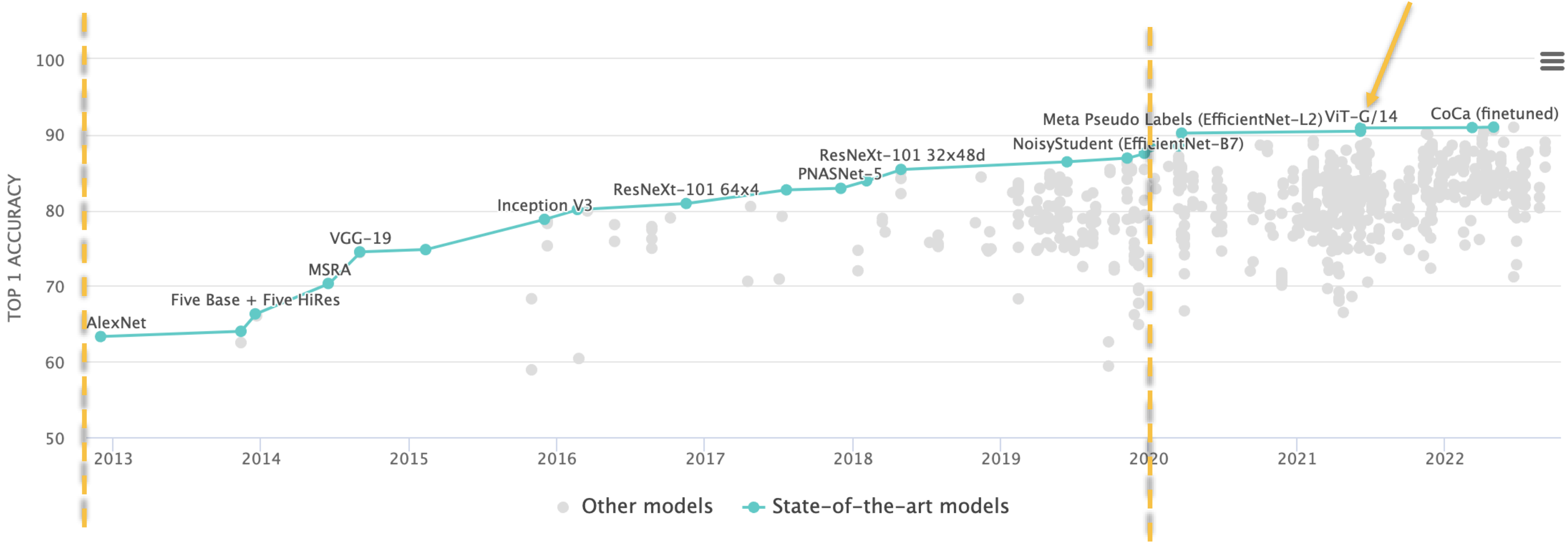
Amount of compute required to reach "AlexNet performance"



https://openai.com/blog/ai-and-efficiency/

Transformer
(later this sem.)

This Lecture



https://paperswithcode.com/sota/image-classification-on-imagenet

What we have learned so far …

Deep Neural Networks:

- What they are (composite parametric, non-linear functions)
- Where they come from (biological inspiration, brief history of ANN)
- How they are optimized, in principle (analytical gradient via computational graphs, backpropagation)
- What they look like in practice (Deep ConvNets)

Next few lectures:

Training Deep Neural Networks

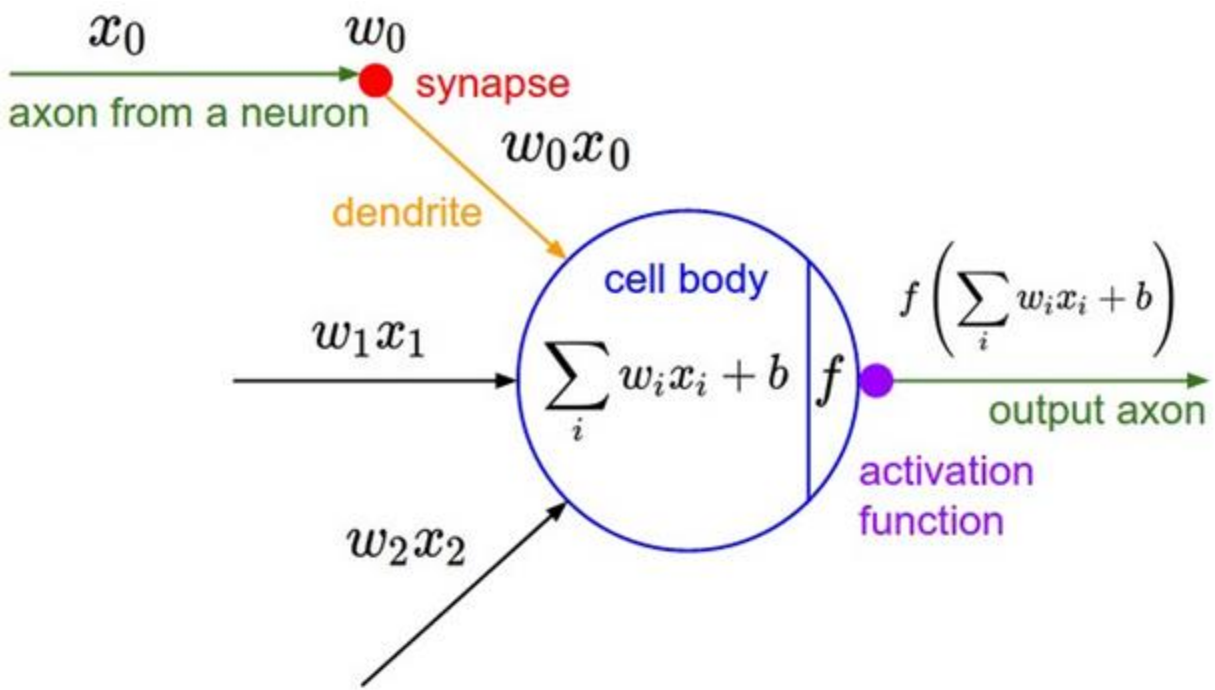
- Details of the non-linear activation functions
- Data normalization
- Weight Initialization
- Batch Normalization
- Regularization
- Advanced Optimization
- Data Augmentation
- Transfer learning
- Hyperparameter Tuning
- Model Ensemble

This lecture:

Training Deep Neural Networks

- Details of the non-linear activation functions
- Data normalization
- Weight Initialization
- Batch Normalization
- Regularization
- Advanced Optimization
- Data Augmentation
- Transfer learning
- Hyperparameter Tuning
- Model Ensemble

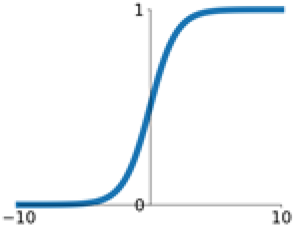
Activation Functions



Activation Functions

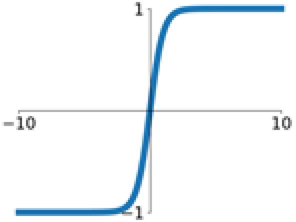
Sigmoid

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



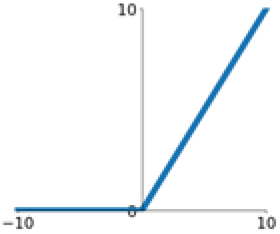
tanh

$$\tanh(x)$$



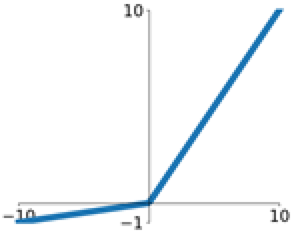
ReLU

$$\max(0, x)$$



Leaky ReLU

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

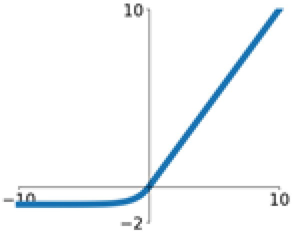


Maxout

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

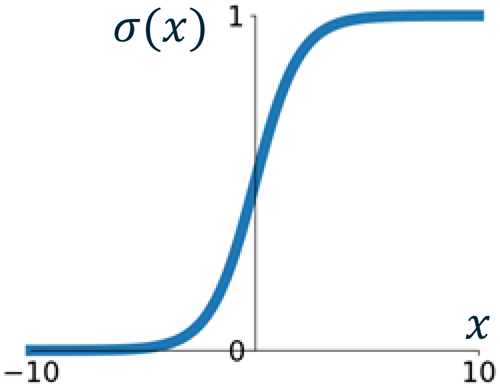
ELU

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



Activation Functions

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

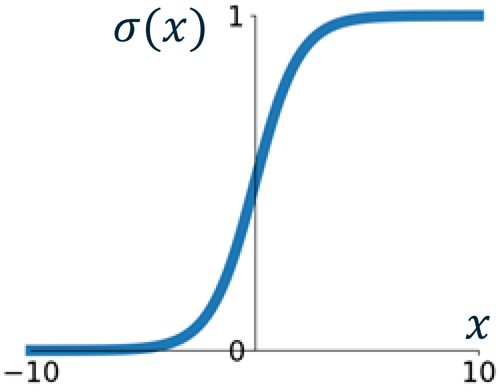


Sigmoid

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

Activation Functions

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

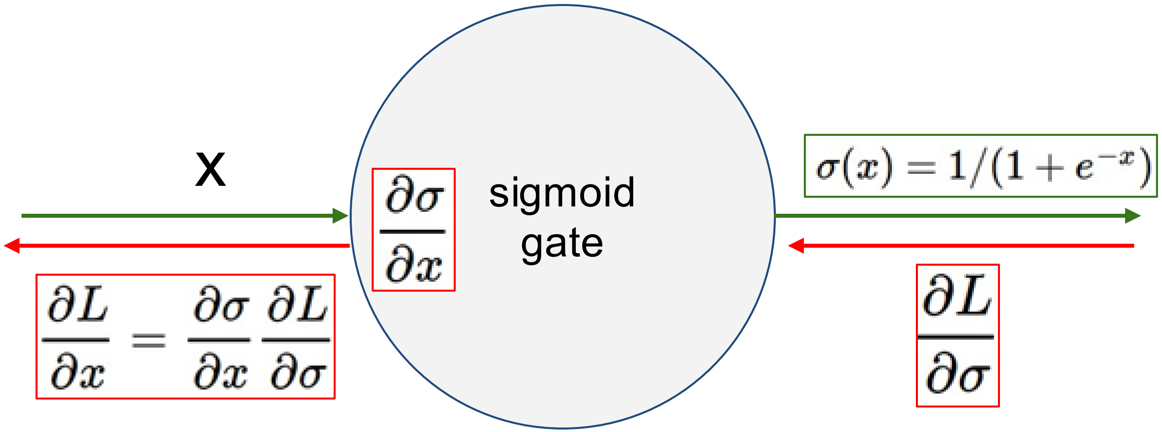


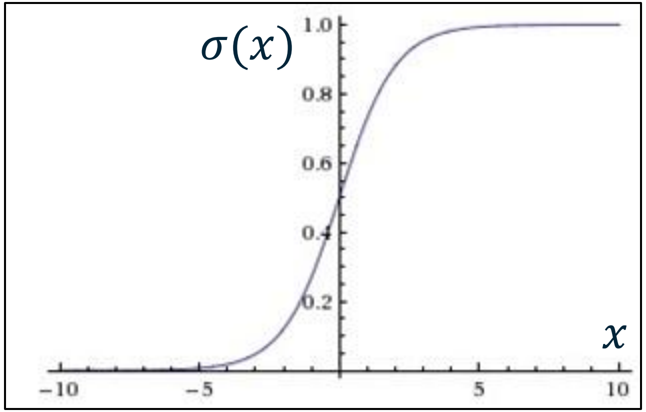
Sigmoid

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

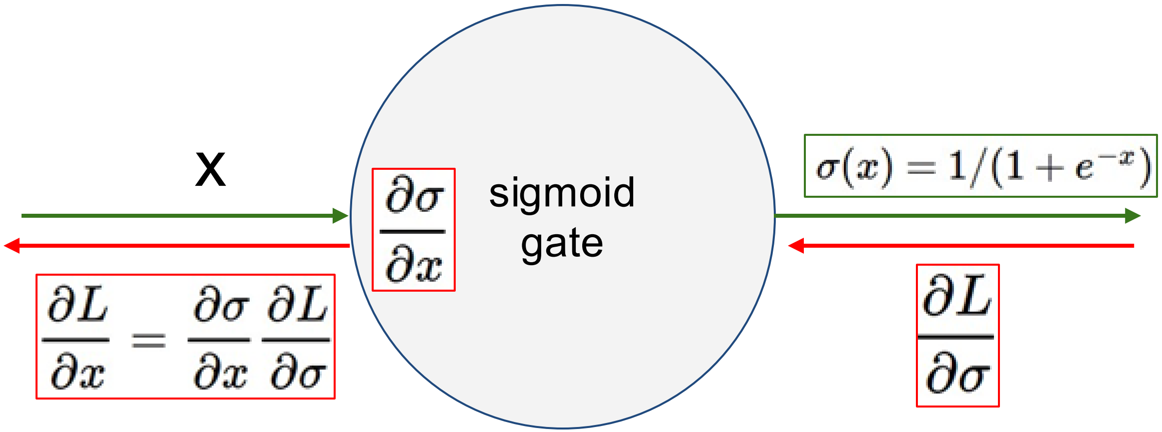
Problems:

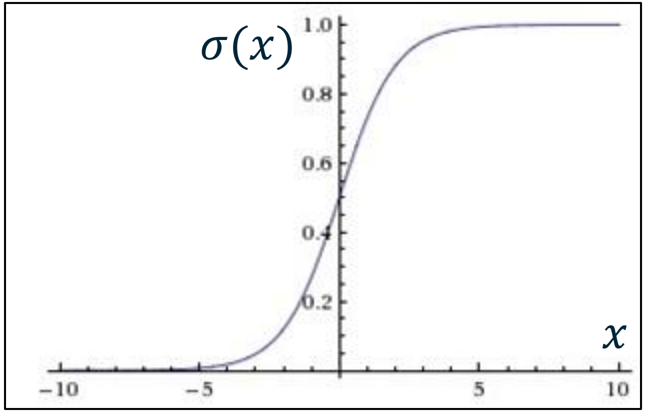
1. Saturated neurons “kill” the gradients





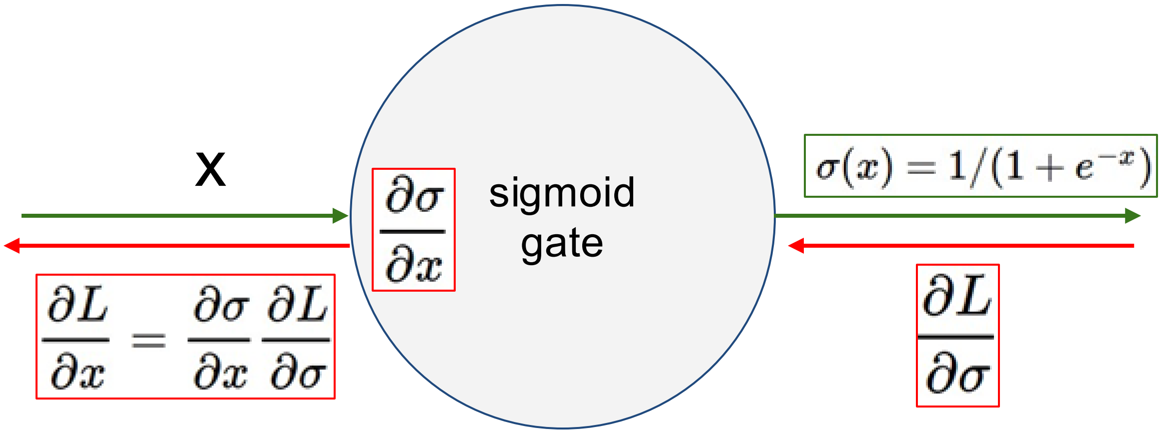
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

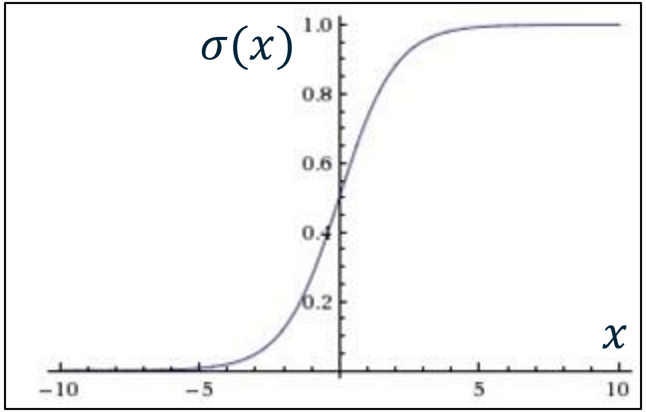




What happens to $\frac{\partial \sigma}{\partial x}$ when $x = -10$?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$



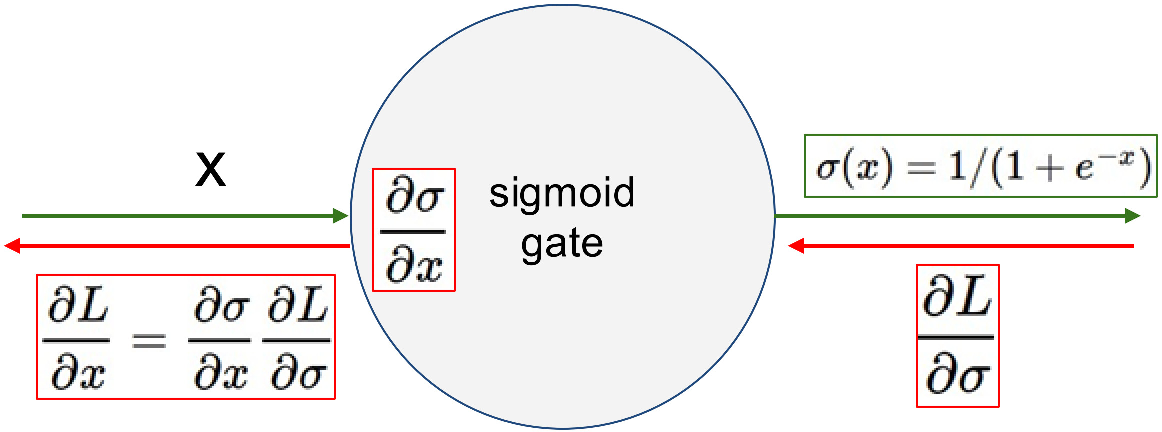


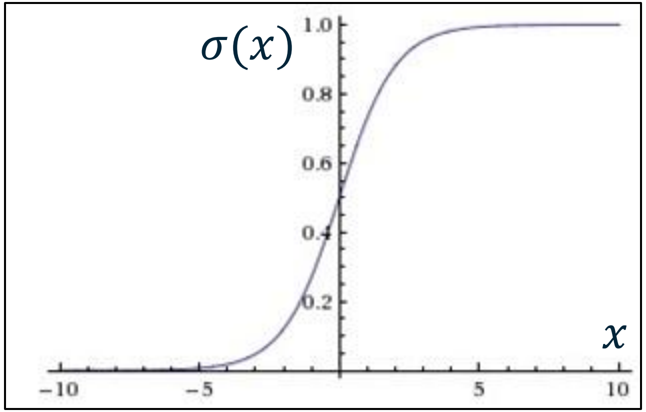
$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

What happens to $\frac{\partial \sigma}{\partial x}$ when $x = -10$?

$$\sigma(x) \;= \sim 0$$

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,) = 0(1-0) \;=\; 0$$

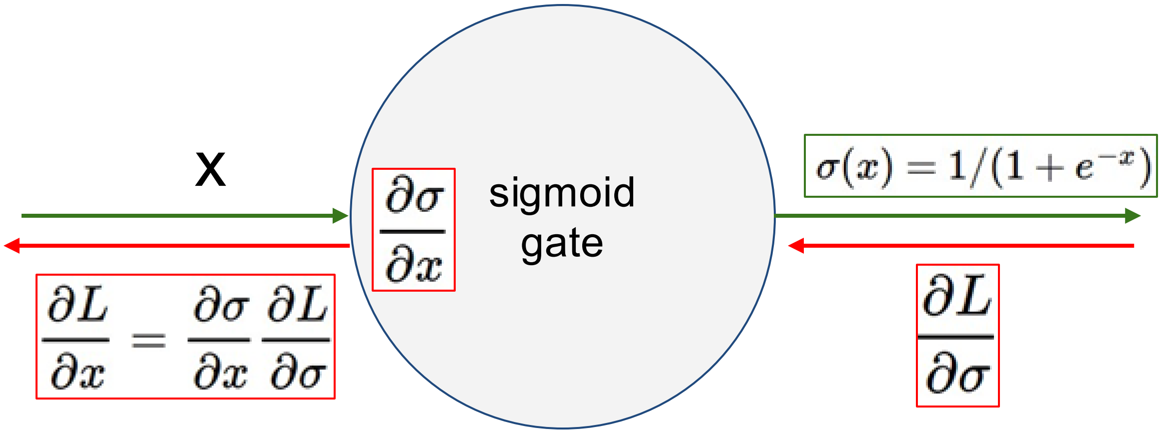


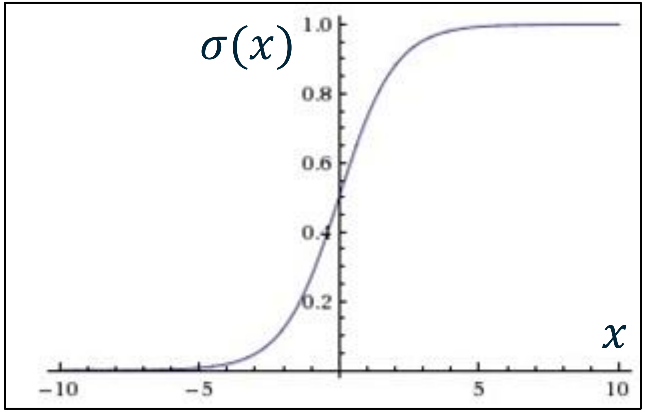


What happens when x = -10?

What happens when x = 10?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$





What happens when x = -10?

What happens when x = 10?

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

$$\sigma(x) \ = \sim 1 \qquad \frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,) = 1(1-1) \ = \ 0$$

x

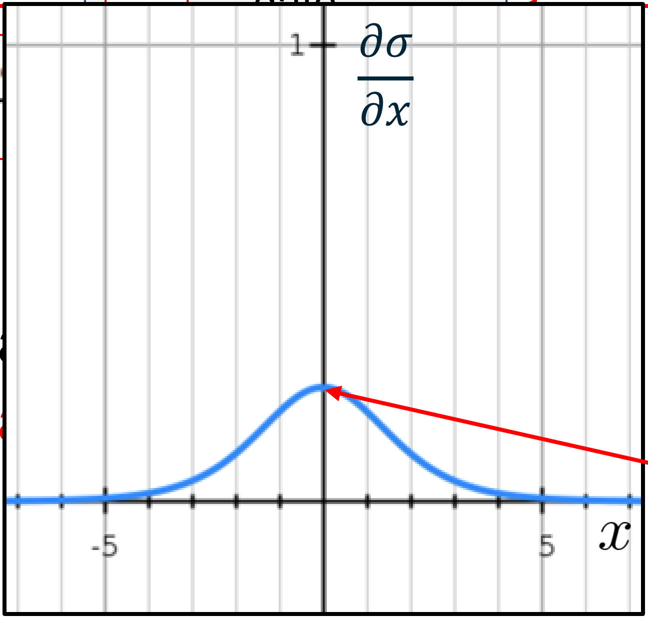
$\partial\sigma$

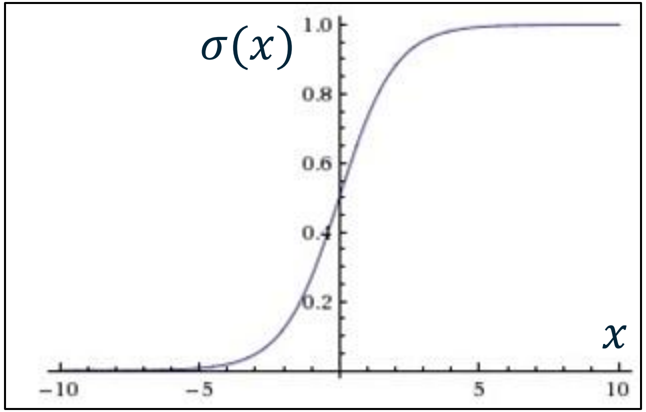
sigmoid gate

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

$\frac{\partial L}{\partial x} = \frac{\partial \sigma}{\partial x}$

$\frac{\partial L}{\partial \sigma}$



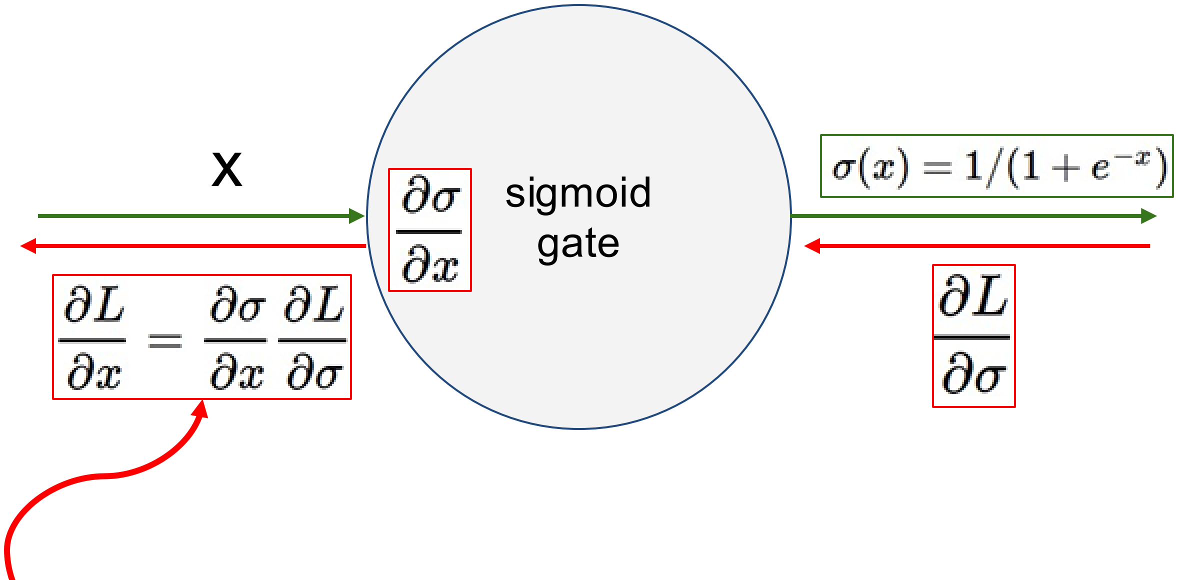


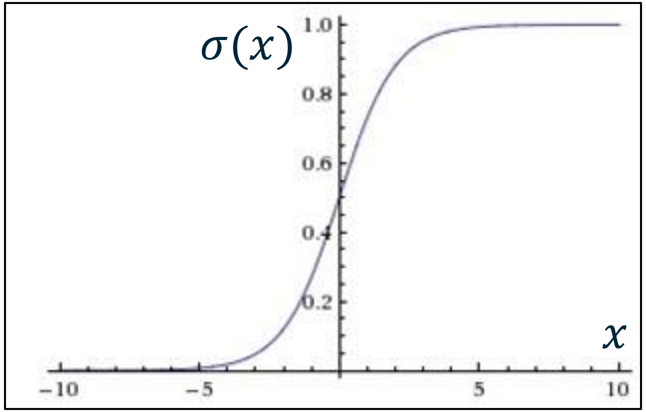
What h

What h

$$\frac{\partial\sigma(x)}{\partial x} = \sigma(x)\,(1-\sigma(x)\,)$$

Non-zero but small (~0.269): still problematic, causes vanishing gradient





$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x)\,(1 - \sigma(x)\,)$$

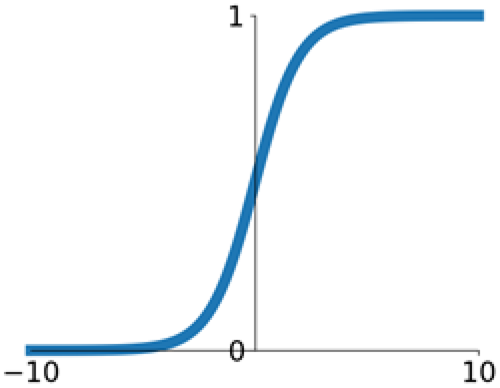
Why is this a problem?

If all the gradients flowing back is small, the weights will change slowly / never change (aka “Vanishing Gradient”)

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial \sigma(x)} \frac{\partial \sigma(x)}{\partial x}$$

Activation Functions

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



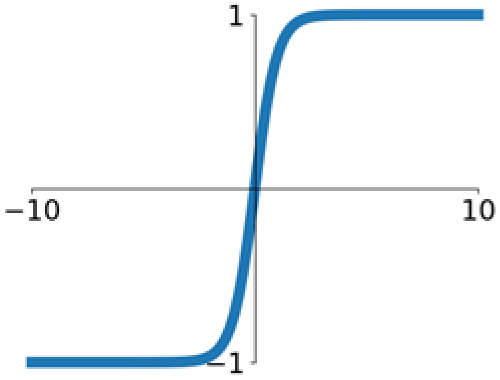
Sigmoid

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

Problems:

1. **Saturated neurons "kill" the gradients**
2. exp() is a bit compute expensive

Activation Functions

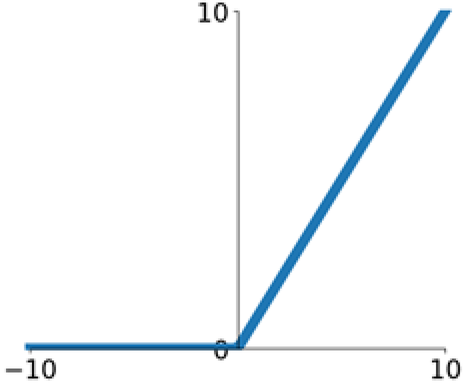


tanh(x)

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

[LeCun et al., 1991]

Activation Functions

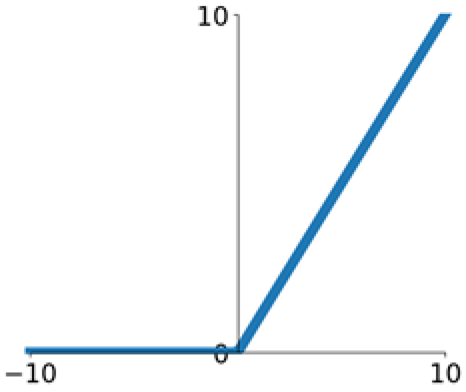


ReLU
(Rectified Linear Unit)

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

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

Activation Functions



ReLU
(Rectified Linear Unit)

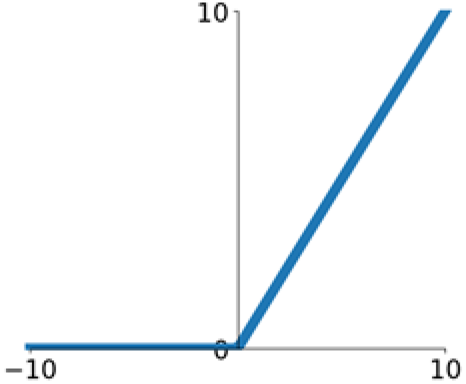
- Computes **f(x) = max(0,x)**

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

- An annoyance:

hint: what is the gradient when x < 0?

Activation Functions



ReLU
(Rectified Linear Unit)

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

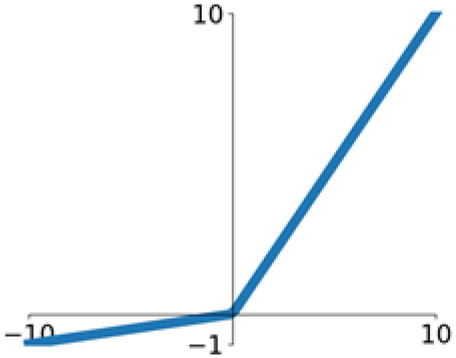
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

- An annoyance:

hint: what is the gradient when x < 0?
Always 0 -> no update in weights -> stays 0, A.K.A. “dead ReLU”

Activation Functions

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



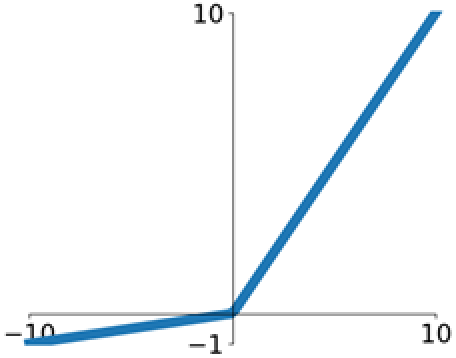
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

Activation Functions

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



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

Leaky ReLU

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

Parametric Rectifier (PReLU)

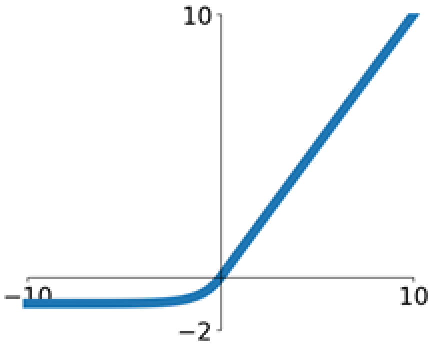
$$f(x) = \max(\alpha x, x)$$

backprop into \alpha
(parameter)

Activation Functions

[Clevert et al., 2015]

Exponential Linear Units (ELU)



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

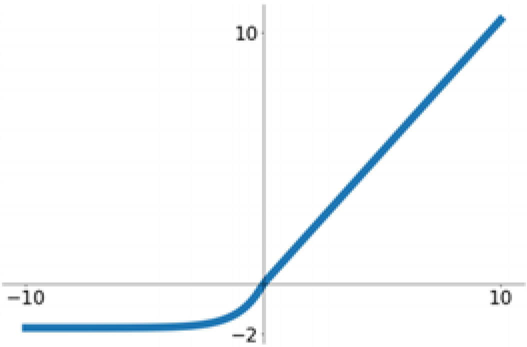
(Alpha default = 1)

- All benefits of ReLU
- Negative saturation encodes presence of features (all goes to $-\alpha$), not magnitude
- Similar in backprop (αe^x when x is negative)
- Compared with Leaky ReLU: smooth gradient at 0 (no kink), better optimization landscape

Activation Functions

[Klambauer et al. ICLR 2017]

Scaled Exponential Linear Units (SELU)



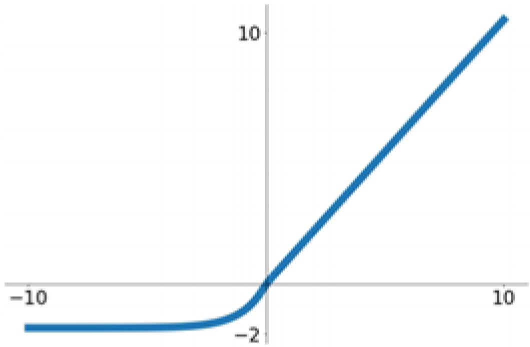
$$f(x) = \begin{cases} \lambda x & \text{if } x > 0 \\ \lambda\alpha(e^x - 1) & \text{otherwise} \end{cases}$$

- Scaled version of ELU that works better for deep networks
- "Self-normalizing" property: under certain condition, the output of a feedforward network stays around zero-mean and unit variance

Activation Functions

[Klambauer et al. ICLR 2017]

Scaled Exponential Linear Units (SELU)



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

α = 1.6732632423543772848170429916717
λ = 1.0507009873554804934193349852946

- Scaled version of ELU that works better for deep networks
- "Self-normalizing" property: under certain condition, the output of a feedforward network stays around zero-mean and unit variance

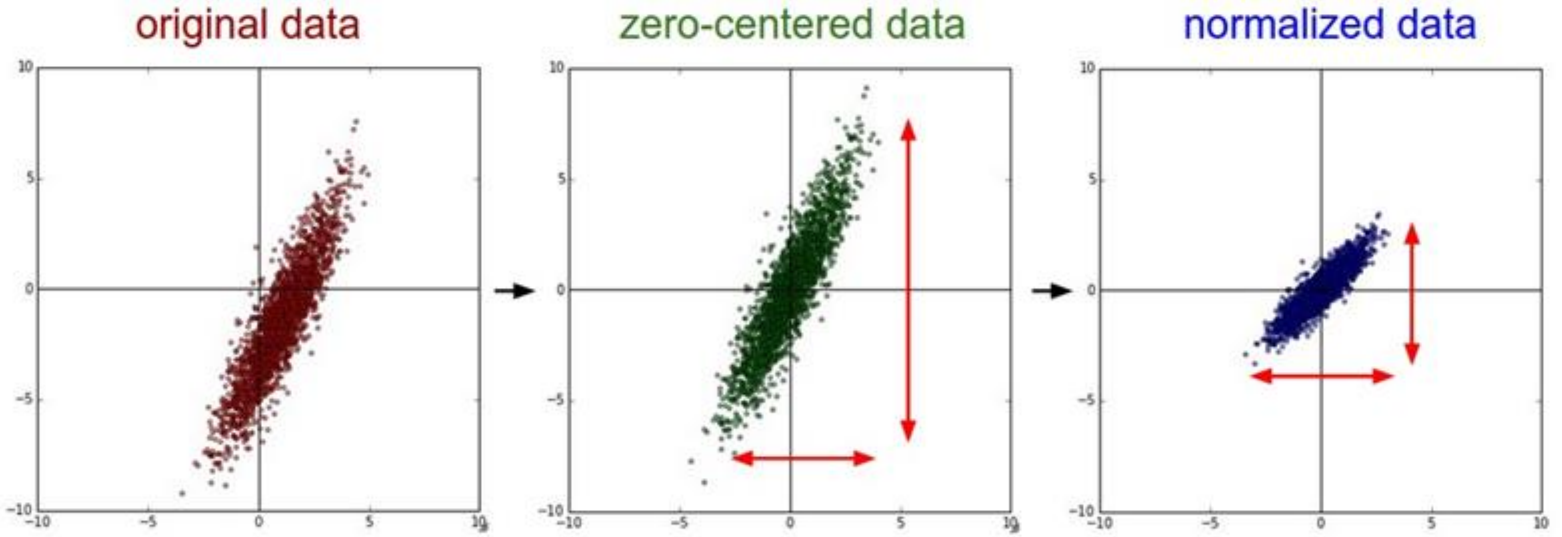
(Klambauer et al, Self-Normalizing Neural Networks, ICLR 2017)

TLDR: In practice:

- Many possible choices beyond what we've talked here, but …
- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / ELU / SELU / GELU
  - To squeeze out some marginal gains
- Don't use sigmoid or tanh

Data Preprocessing

Data Preprocessing



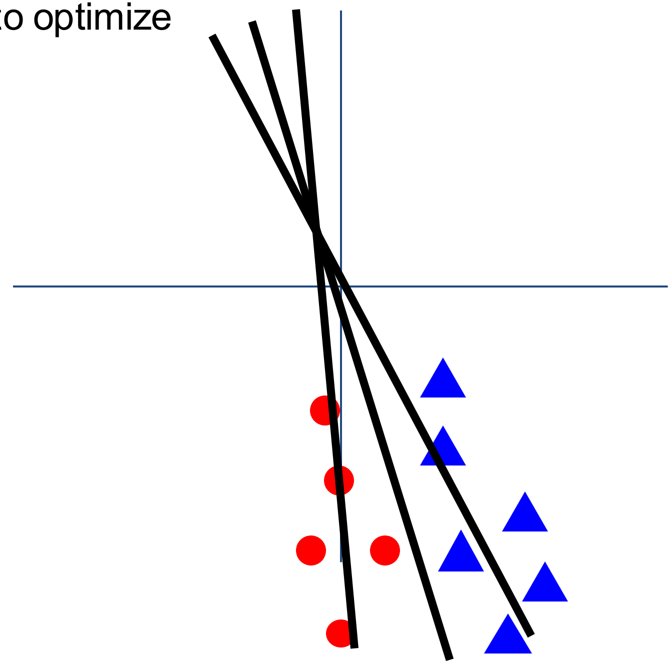

```
X -= np.mean(X, axis = 0)
```

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

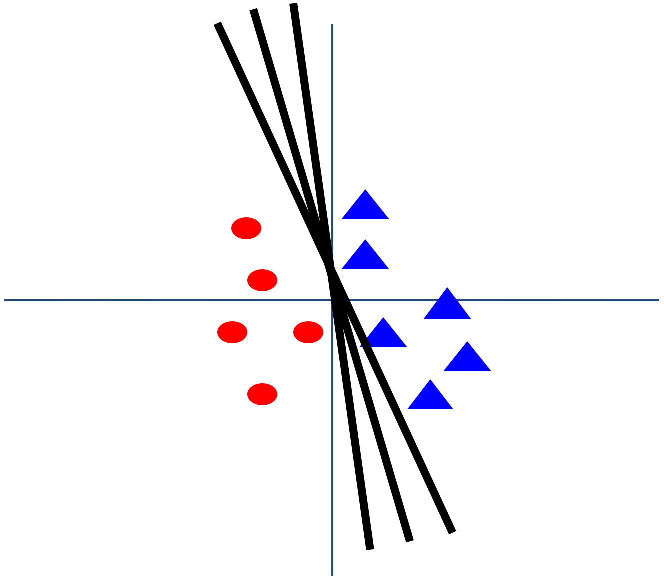
(Assume X [NxD] is data matrix, each example in a row)

Data Preprocessing: example in linear classifier

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

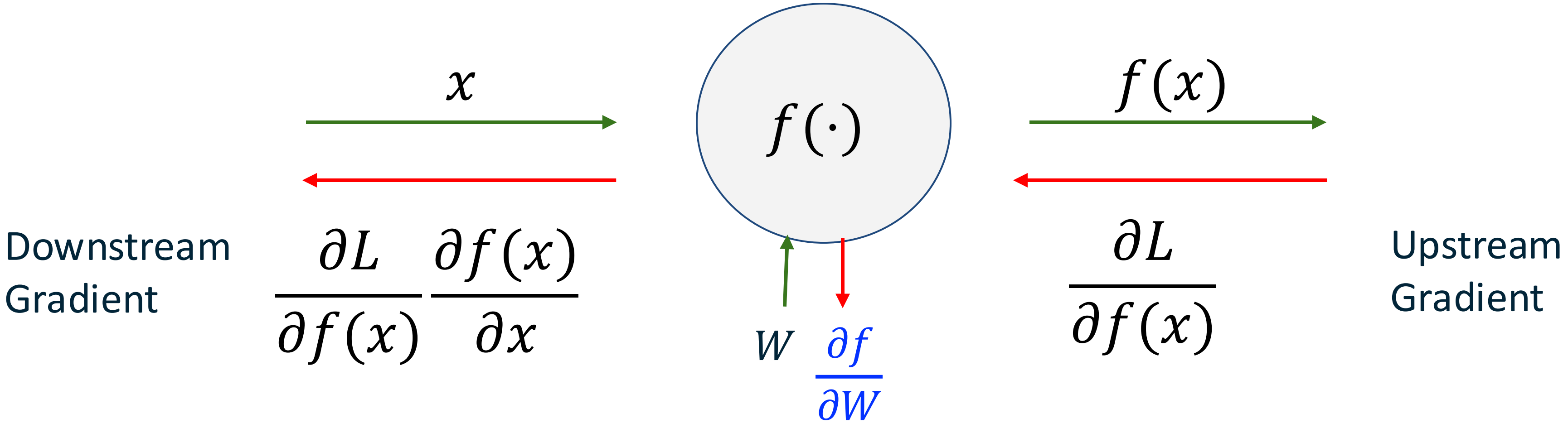


After normalization: less sensitive to small changes in weights; easier to optimize



Many different reasons why we might want to normalize the input!

Another example: Input magnitude affects gradient magnitude

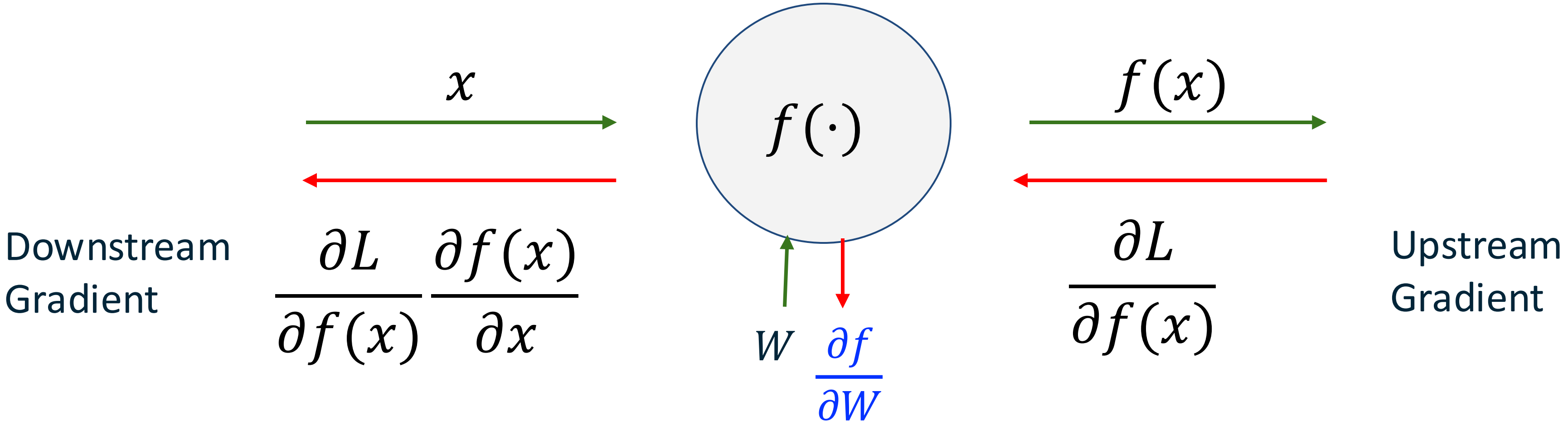


$$f(x) = W^T x + b$$

$$\frac{\partial f}{\partial W} =?$$

Many different reasons why we might want to normalize the input!

Another example: Input magnitude affects gradient magnitude



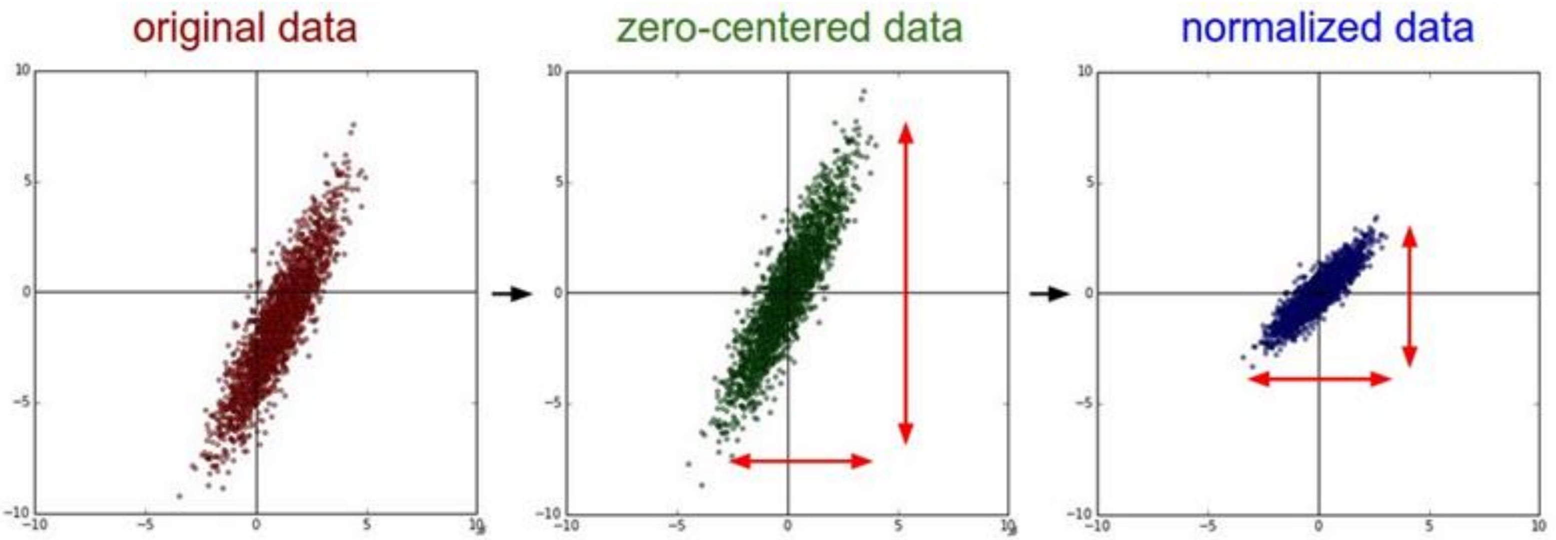
$$f(x) = W^T x + b$$

$$\frac{\partial f}{\partial W} = x$$

Magnitude of input x directly affects the gradients to weights $\frac{\partial f}{\partial W}$!

Data Preprocessing

Gaussian normalization is very commonly used

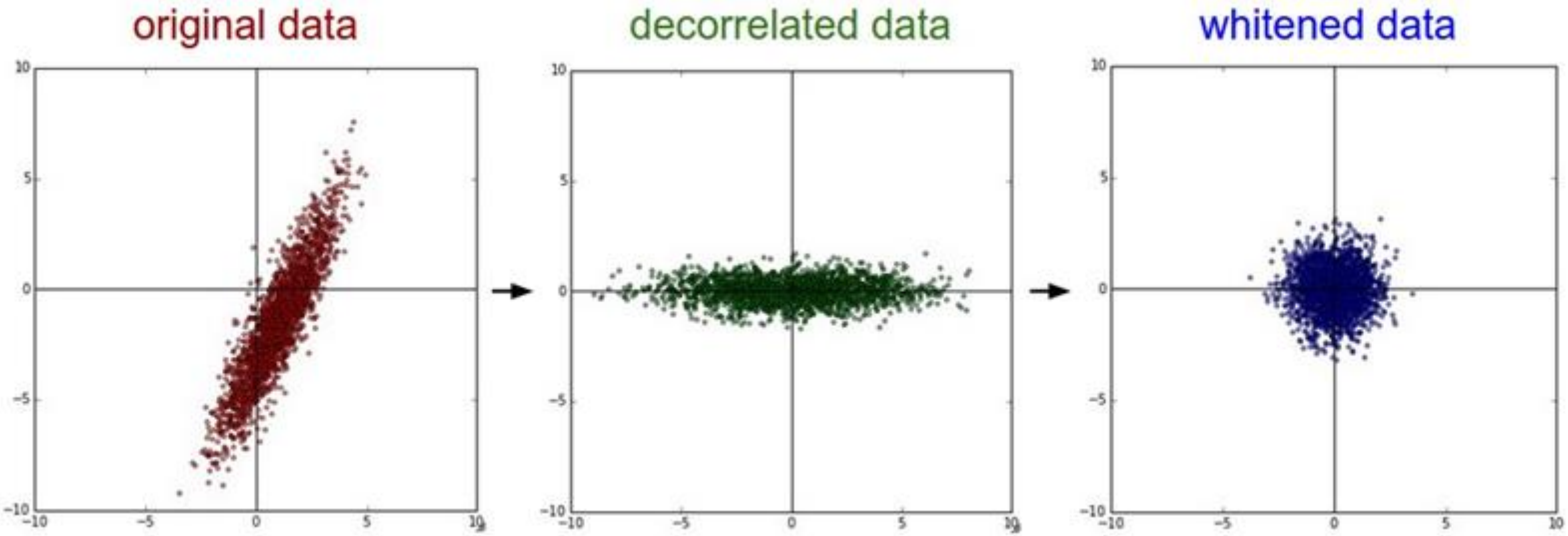



```
X -= np.mean(X, axis = 0)
```

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

Data Preprocessing

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



(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

Examples: images

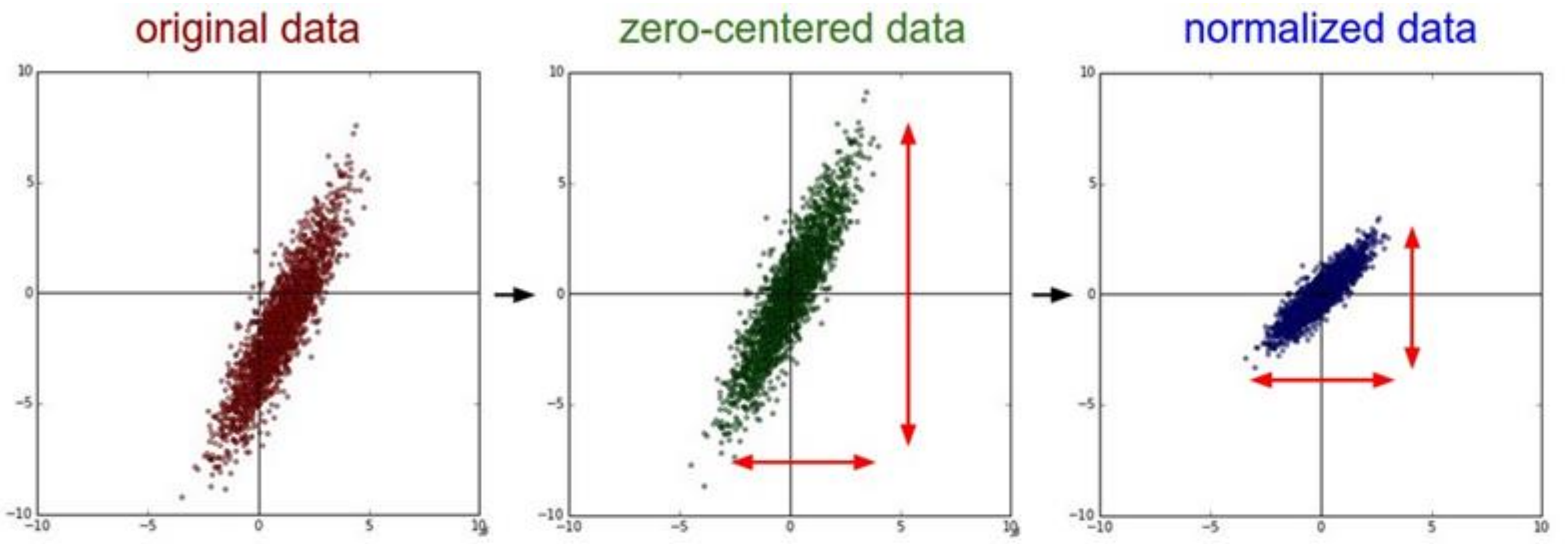
e.g. consider CIFAR-10 example with [32,32,3] images

- Default: Normalize to [0, 1] float (from uint8)
- Subtract the per-pixel mean(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)

Examples: other domains

- **Natural language processing:** Normalize word embeddings like Word2Vec or GloVe vectors so that they have a unit norm
- **Graph Neural Networks (GNN):** the feature vector of a node might be scaled by the inverse of its degree or the square root of its degree.
- **Audio data**: Spectral normalize waveforms to ensure that the frequency components are on a similar scale.
- **Reinforcement learning**: reward can be normalized to stabilize learning.

Data Preprocessing




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

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

What about intermediate features inside the NN after the input?

Batch Normalization

[Ioffe and Szegedy, 2015]

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

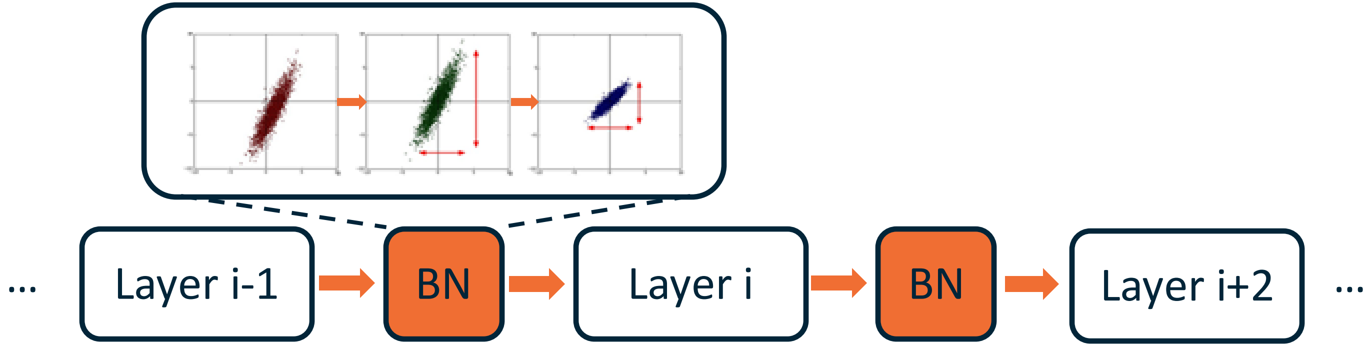
consider a **batch of activations** x at some layer. To make each dimension zero-mean unit-variance, apply:

$$\hat{x} = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x]}}$$

this is a vanilla differentiable function...

Batch Normalization

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



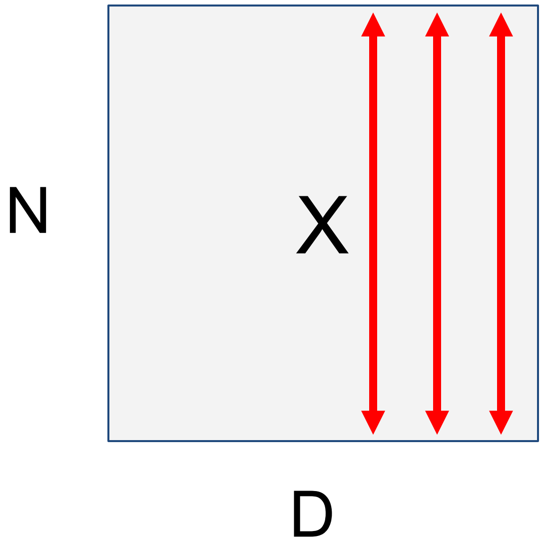
$$\hat{x} = \frac{x - \mathrm{E}[x]}{\sqrt{\mathrm{Var}[x]}}$$

Batch Normalization

$x \rightarrow \boxed{\text{BN}} \rightarrow \hat{x}$

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



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

Per-batch mean, shape is D

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

Per-batch var, shape is D

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

Normalized x, Shape is N x D

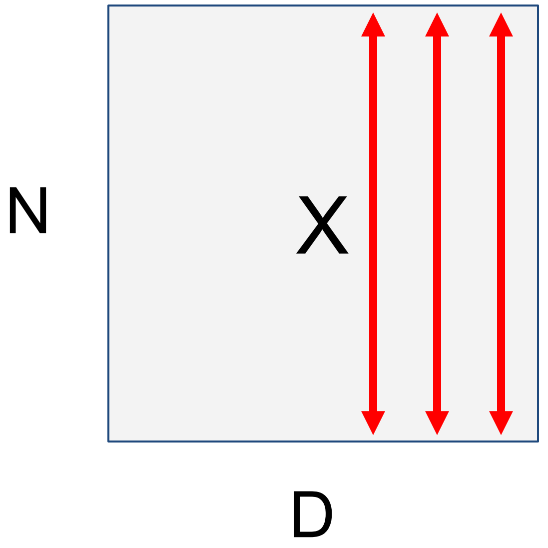
(Prevent div by 0 err)

Batch Normalization

$x \rightarrow \boxed{\text{BN}} \rightarrow \hat{x}$

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



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

Per-batch mean, shape is D

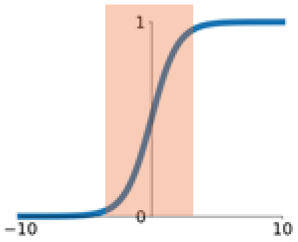
$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-batch var, shape is D

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

Normalized x, Shape is N x D

Problem: What if zero-mean, unit variance is too hard of a constraint? E.g., inserting a BN before sigmoid will constrain it to (mostly) linear regime

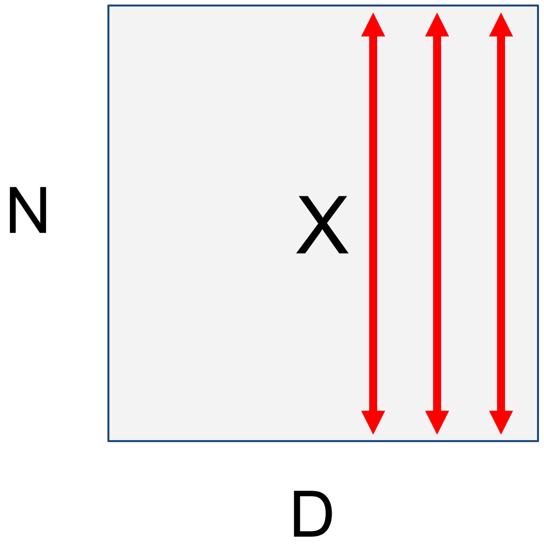


Batch Normalization

$x \rightarrow \boxed{\text{BN}} \rightarrow \hat{x}$

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



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

Per-batch mean,
shape is D

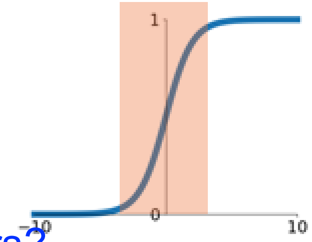
$$\sigma_j^2 = \frac{1}{N} \sum_{i=1}^{N} (x_{i,j} - \mu_j)^2$$

Per-batch var,
shape is D

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

Normalized x,
Shape is N x D

Problem: What if zero-mean, unit variance is too hard of a constraint?
E.g., inserting a BN before sigmoid will constrain it to (mostly) linear regime



Can we learn the normalization parameters?

Batch Normalization

$x \rightarrow \boxed{\text{BN}} \rightarrow y$

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

γ, β: $\mathbb{R}^D$

We want to give the model a chance to **adjust batchnorm** if the default is not optimal.

Learning $\gamma = \sigma$ and $\beta = \mu$ will recover the original input batch!

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

Per-batch mean, shape is D

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

Per-batch var, shape is D

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

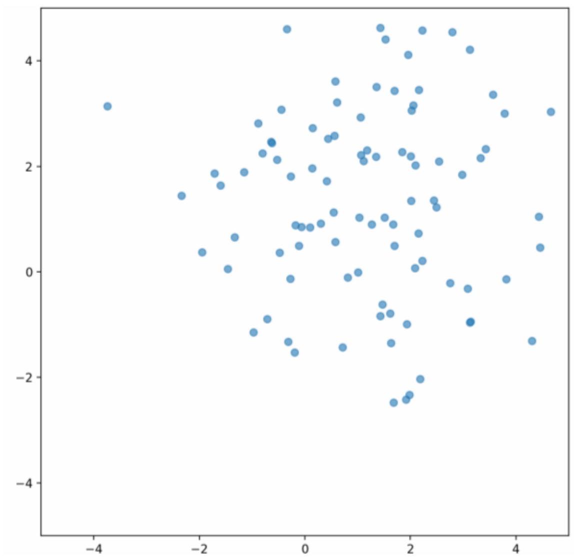
Normalized x, Shape is N x D

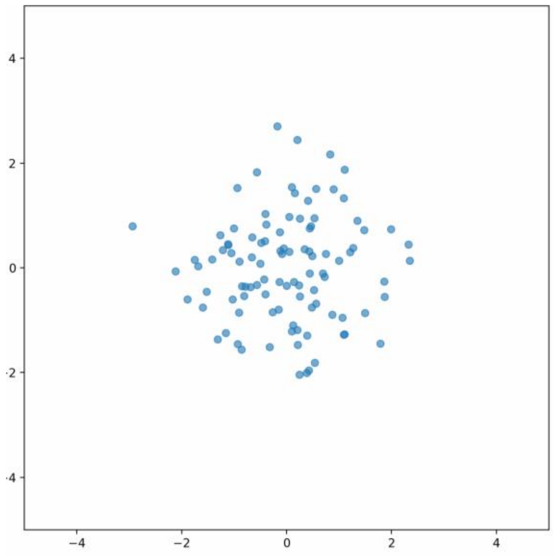
$$y_{i,j} = \underline{\gamma_j}\hat{x}_{i,j} + \underline{\beta_j}$$

Output, Shape is N x D

Initialize $\gamma = 1, \beta = 0$

What does it look like?





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

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

$\gamma = [2, 1.5], \beta = [1, -1]$

Batch Normalization: Test-Time

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

Input: $x : N \times D$

Learnable scale and shift parameters:

γ, β: $\mathbb{R}^D$

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

Per-batch mean, shape is D

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

Per-batch var, shape is D

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

Normalized x, Shape is N x D

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

Output, Shape is N x D

Batch Normalization: Test-Time

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

Input: $x : N \times D$

Learnable scale and shift parameters:

$\gamma, \beta : \mathbb{R}^D$

Activations become fixed after training. Can calculate training set-wide statistics for inference-time normalization.

At training time, do moving average to save compute.

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

Per-batch mean, shape is D

Per-batch var, shape is D

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

Normalized x, Shape is N x D

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

Output, Shape is N x D

Batch Normalization: Test-Time

Input: $x : N \times D$

Learnable scale and shift parameters:

$\gamma, \beta: \mathbb{R}^D$

$\mu_j =$ (Moving) average of values seen during training

Per-batch mean, shape is D

$\sigma_j^2 =$ (Moving) average of values seen during training

Per-batch var, shape is D

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

Normalized x, Shape is N x D

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

Output, Shape is N x D

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

```python
import numpy as np

class BatchNorm:
    def __init__(self, num_features, eps=1e-5, momentum=0.1):
        self.num_features = num_features
        self.eps = eps
        self.momentum = momentum

        # Learnable parameters
        self.gamma = np.ones(num_features)  # Scale parameter
        self.beta = np.zeros(num_features)  # Shift parameter

        # Running statistics (used for inference)
        self.running_mean = np.zeros(num_features)
        self.running_var = np.ones(num_features)
```

You can think of gamma and beta as the layer parameters

```python
import numpy as np

class BatchNorm:
    def __init__(self, num_features, eps=1e-5, momentum=0.1):
        self.num_features = num_features
        self.eps = eps
        self.momentum = momentum

        # Learnable parameters
        self.gamma = np.ones(num_features)  # Scale parameter
        self.beta = np.zeros(num_features)  # Shift parameter

        # Running statistics (used for inference)
        self.running_mean = np.zeros(num_features)
        self.running_var = np.ones(num_features)

    def forward(self, X, training=True):
        if training:
            # Training mode
            batch_mean = np.mean(X, axis=0)
            batch_var = np.var(X, axis=0)

            # Update running statistics
            self.running_mean = (1 - self.momentum) * self.running_mean + self.momentum * batch_mean
            self.running_var = (1 - self.momentum) * self.running_var + self.momentum * batch_var

            # Normalize
            X_norm = (X - batch_mean) / np.sqrt(batch_var + self.eps)
```

Use batch statistics during training

Keep running dataset statistics

```python
import numpy as np

class BatchNorm:
    def __init__(self, num_features, eps=1e-5, momentum=0.1):
        self.num_features = num_features
        self.eps = eps
        self.momentum = momentum

        # Learnable parameters
        self.gamma = np.ones(num_features)  # Scale parameter
        self.beta = np.zeros(num_features)  # Shift parameter

        # Running statistics (used for inference)
        self.running_mean = np.zeros(num_features)
        self.running_var = np.ones(num_features)

    def forward(self, X, training=True):
        if training:
            # Training mode
            batch_mean = np.mean(X, axis=0)
            batch_var = np.var(X, axis=0)

            # Update running statistics
            self.running_mean = (1 - self.momentum) * self.running_mean + self.momentum * batch_mean
            self.running_var = (1 - self.momentum) * self.running_var + self.momentum * batch_var

            # Normalize
            X_norm = (X - batch_mean) / np.sqrt(batch_var + self.eps)
        else:
            # Inference mode
            X_norm = (X - self.running_mean) / np.sqrt(self.running_var + self.eps)

        # Scale and shift
        return self.gamma * X_norm + self.beta
```

Use running statistics during testing

Apply learned scale and shift parameters

Batch Normalization

[Ioffe and Szegedy, 2015]

Q: Should you put batchnorm before or after ReLU?
A: Topic of debate. Original paper says BN->ReLU. Now most commonly ReLU->BN. If BN-> ReLU and zero mean, ReLU kills half of the activations, but in practice makes insignificant differences.

Q: Should you normalize the **input** (e.g., images) with batchnorm?
A: No, you already have the fixed & correct dataset statistics, no need to do batchnorm.

Q: How many parameters does a batchnorm layer have?
A: Input dimension * 4: beta, gamma, moving average mu, moving average sigma. Only beta and gamma are trainable parameters.

Batch Normalization

[Ioffe and Szegedy, 2015]

- Makes deep networks **much** easier to train!
  - If you are interested in the theory, read https://arxiv.org/abs/1805.11604
  - TL;DR: makes optimization landscape smoother
- Allows higher learning rates, faster convergence
- More useful in deeper networks
- Networks become more robust to initialization
- More robust to range of input
- Zero overhead at test-time: can be fused with conv!
- Behaves differently during training and testing: this is a very common source of bugs!
- Needs large batch size to calculate accurate stats

Batch Normalization for ConvNets

Batch Normalization for **fully-connected** networks

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

Normalize

$$\mu, \sigma: 1 \times D$$
$$\gamma, \beta: 1 \times D$$
$$y = \gamma(x - \mu)/\sigma + \beta$$

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

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

Normalize

$$\mu, \sigma: 1 \times C \times 1 \times 1$$
$$\gamma, \beta: 1 \times C \times 1 \times 1$$
$$y = \gamma(x - \mu)/\sigma + \beta$$

Keep the spatial equivariance property of conv: all locations should be normalized in similar ways

Layer Normalization

Batch Normalization for fully-connected networks

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

Normalize

$$\mu, \sigma: 1 \times D$$

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

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

Ba, Kiros, and Hinton, "Layer Normalization", arXiv 2016

Layer Normalization for fully-connected networks

Same behavior at train and test!

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

Normalize

$$\mu, \sigma: N \times 1$$

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

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

More flexible (can use N = 1!), works well with sequence models (RNN, Transformers)

Instance Normalization

Batch Normalization for convolutional networks

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

Normalize

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

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

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

Instance Normalization for convolutional networks

Same behavior at train / test!

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

Normalize

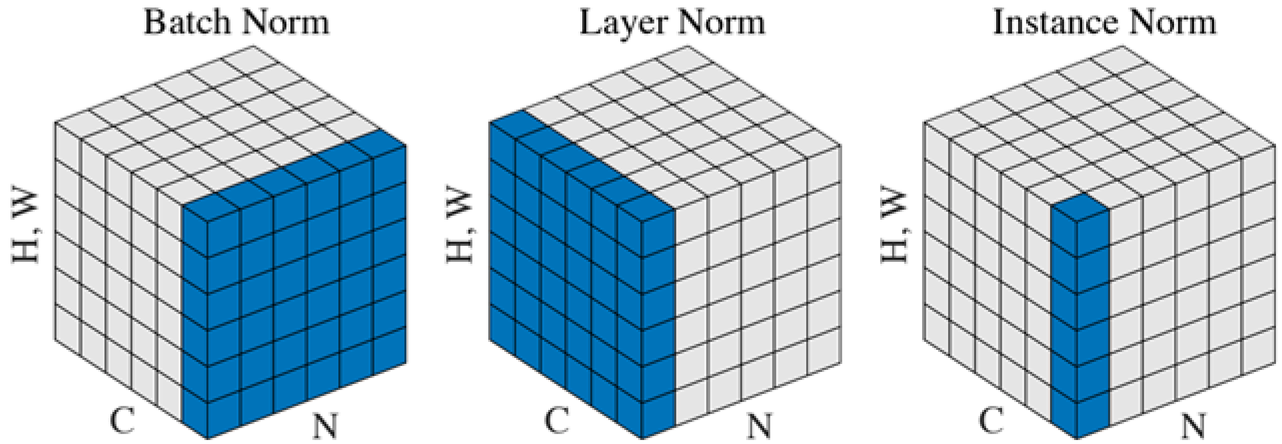
$$\boldsymbol{\mu}, \boldsymbol{\sigma}: N \times C \times 1 \times 1$$

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

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

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

Comparison of Normalization Layers



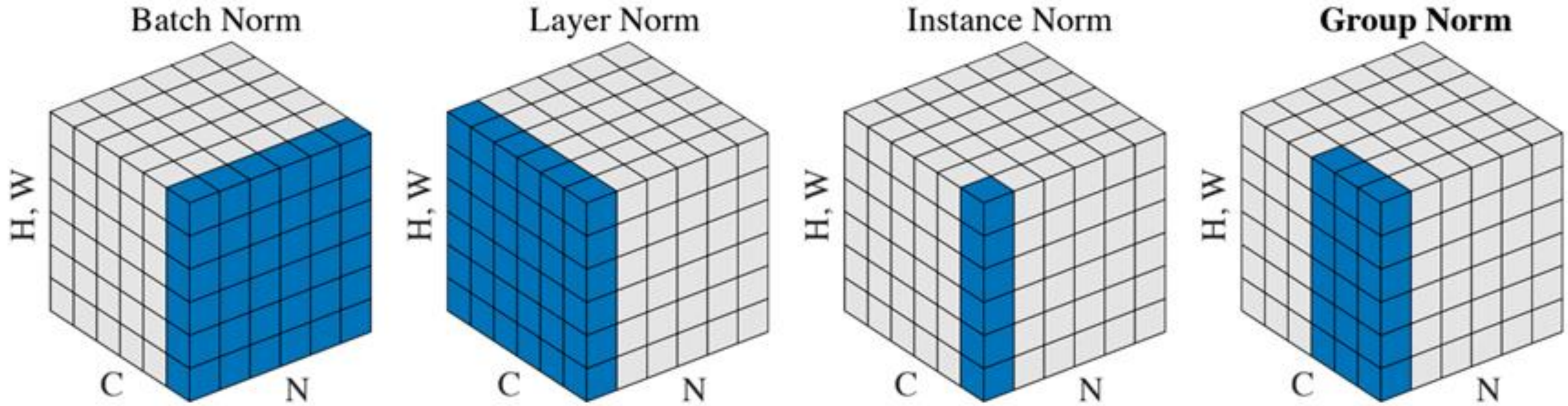
N x C x H x W -> 1 x C x 1 x 1

N x C x H x W -> N x 1 x 1 x 1

N x C x H x W -> N x C x 1 x 1

Wu and He, “Group Normalization”, ECCV 2018

Group Normalization



N x C x H x W ->
1 x C x 1 x 1

N x C x H x W ->
N x 1 x 1 x 1

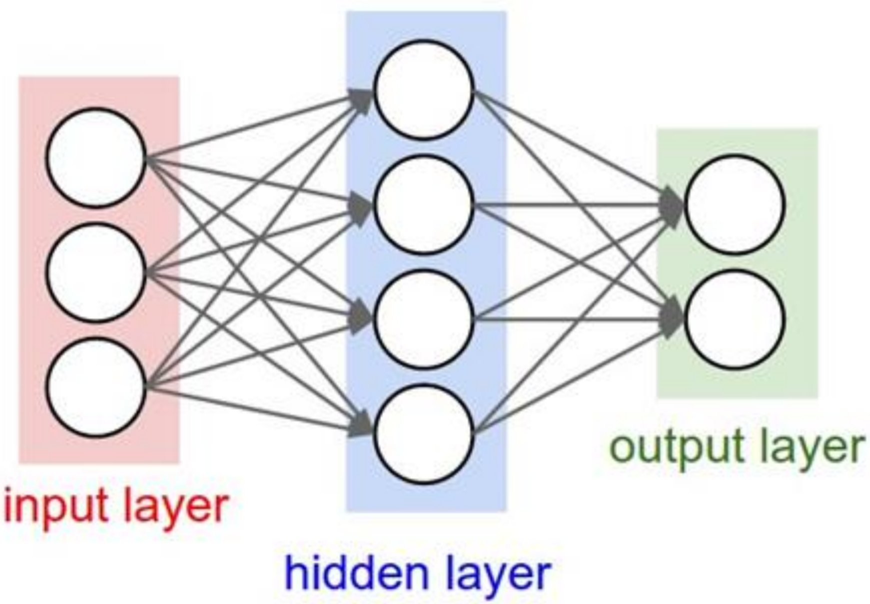
N x C x H x W ->
N x C x 1 x 1

N x C x H x W ->
N x C/G x 1 x 1

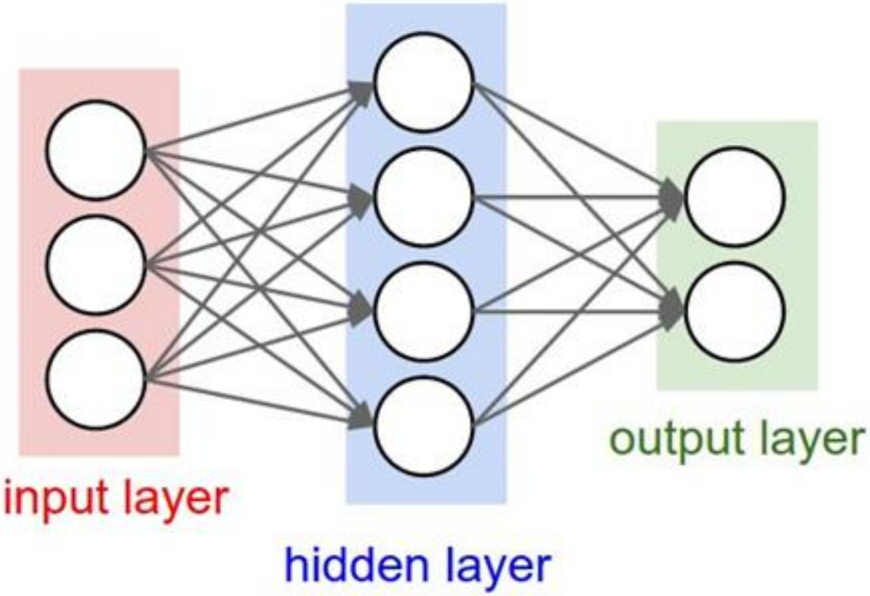
Wu and He, “Group Normalization”, ECCV 2018

Weight Initialization

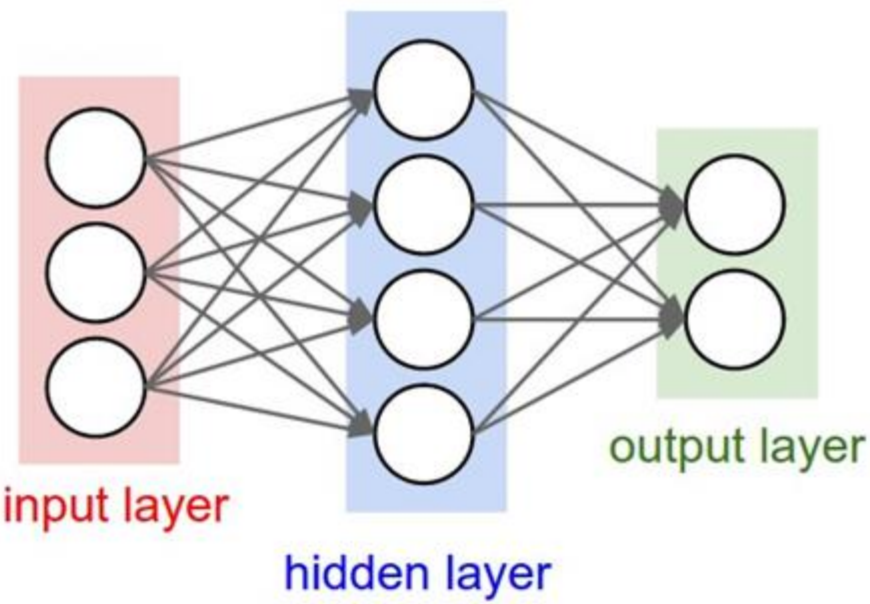
- Q: what happens when W=same initial value is used?



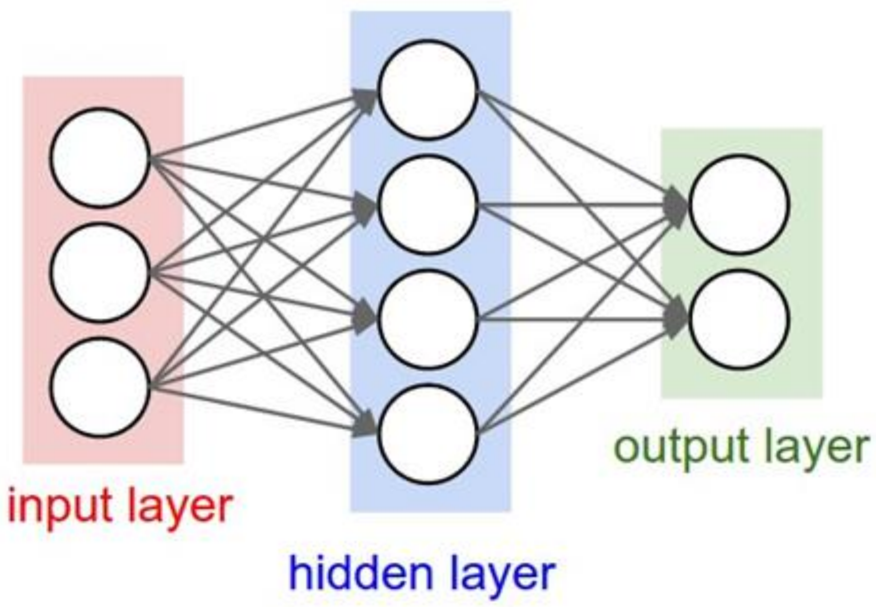
- Q: what happens when W=same initial value is used?
- A: All output will be the same! $w_1^T x = w_2^T x$ if $w_1 = w_2$



- Q: what if $w_1 = 0$ and $w_2 = 100000$?
- A: Output will have extremely different values! Vanishing / exploding gradient



Weight initialization: goal is to **maintain both diversity and variance** of layer output throughout the network, at least at the beginning of the training



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

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

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

```
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

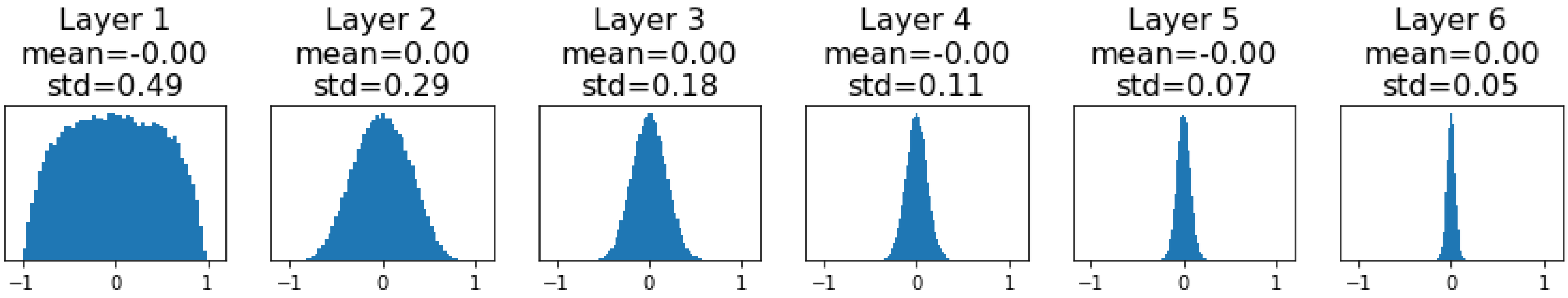
What will happen to the activations for the last layer?

Weight Initialization: Activation statistics

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

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

All activations tend to zero for deeper network layers



Visualize distribution of activations

Weight Initialization: Activation statistics

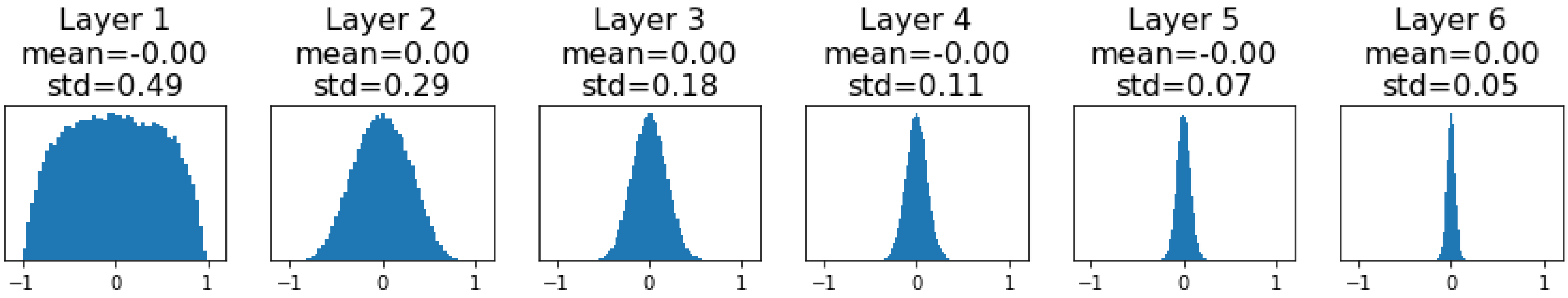
```python
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

Hint: $\frac{\partial L}{\partial w} = x^T \left(\frac{\partial L}{\partial y}\right)$



Visualize distribution of activations

Weight Initialization: Activation statistics

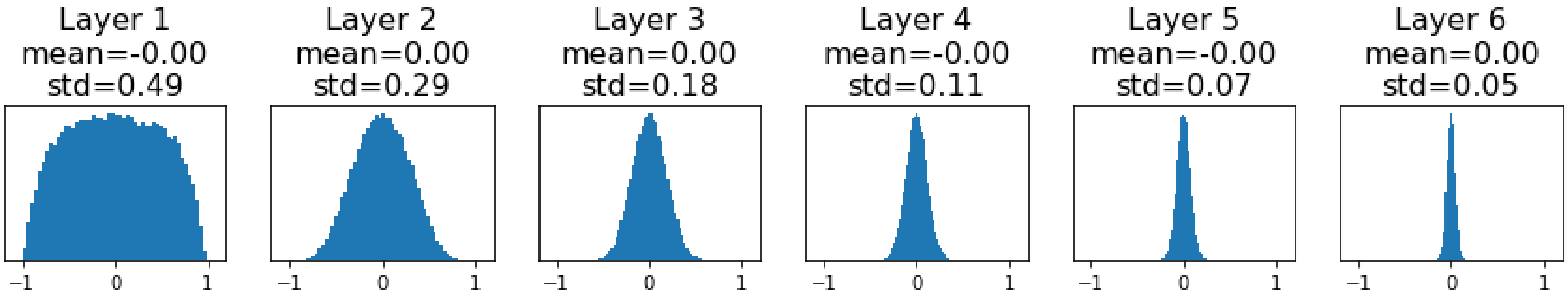
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

A: Very small, slow learning



Visualize distribution of activations

Weight Initialization: Activation statistics

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

Increase std of initial weights from 0.01 to 0.05

Initialize with higher values

What will happen to the activations for the last layer?

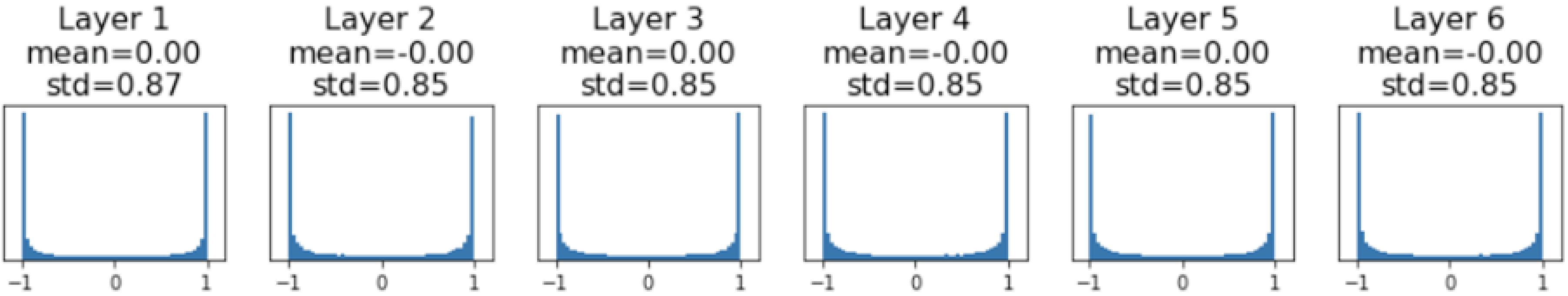
Weight Initialization: Activation statistics

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

Increase std of initial weights from 0.01 to 0.05

All activations saturate

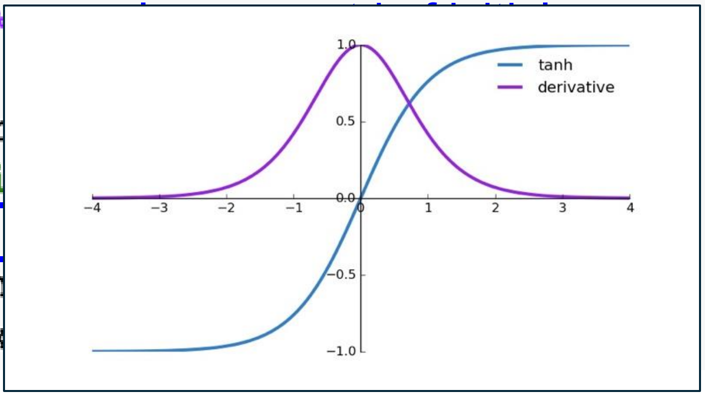
Q: What do the gradients look like?



Visualize distribution of activations

Weight Initialization: Activation statistics

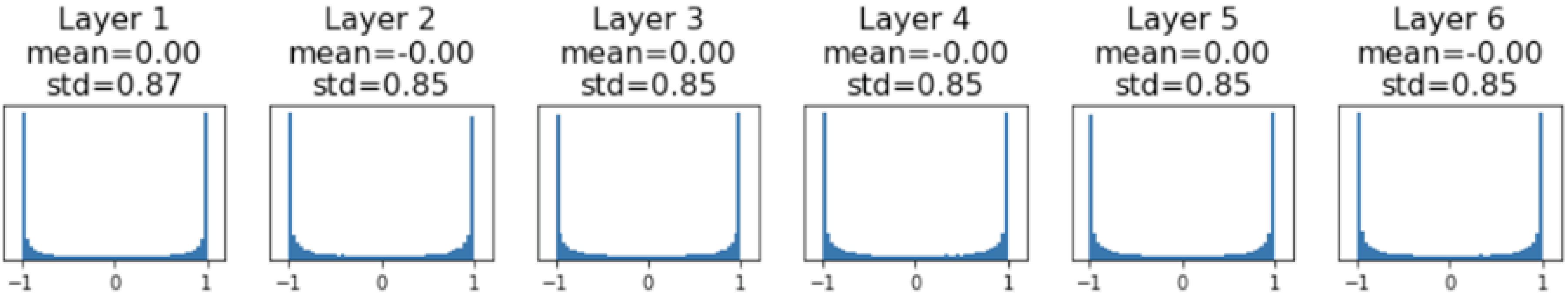
```
dims = [4096] *
hs = []
x = np.random.r
for Din, Dout i
    W = 0.05 *
    x = np.tanh
    hs.append(x
```



All activations saturate

Q: What do the gradients look like?

A: For tanh, large value -> small gradient



Visualize distribution of activations

Weight Initialization: Activation statistics

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

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

More generally, *gradient explosion* (high w-> high output -> high gradient).

Visualize distribution of activations

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)

Assume each input contribute similarly to output
more number of weights needs -> small weight multiplier

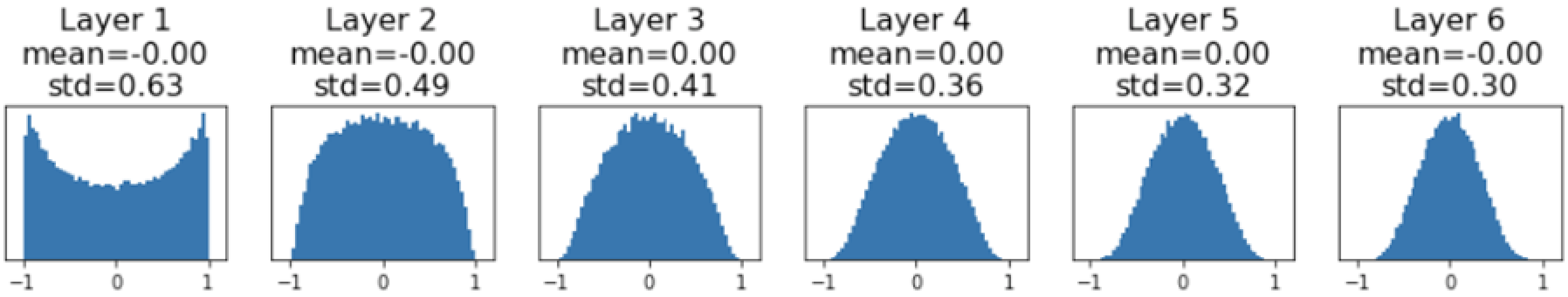
Glorot and Bengio, "Understanding the difficulty of training deep feedforward neural networks", AISTAT 2010

Weight Initialization: "Xavier" Initialization

```python
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

Visualize distribution of activations

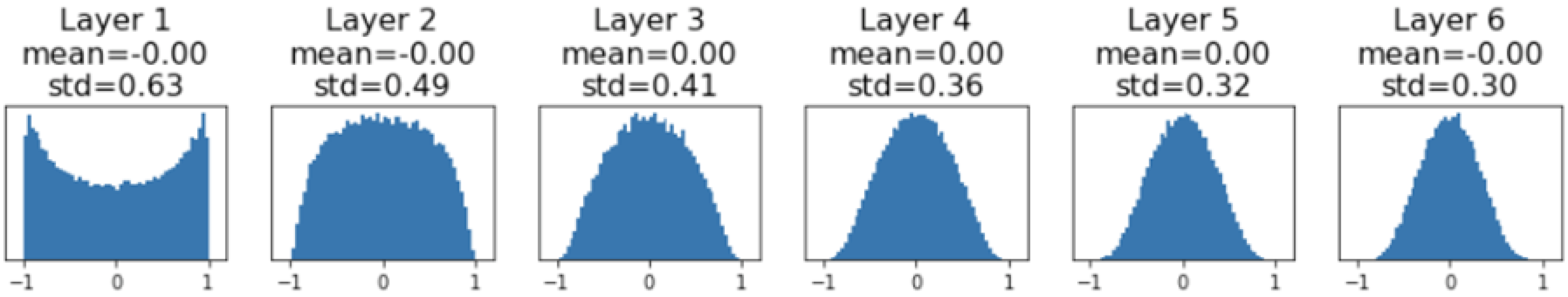
Weight Initialization: “Xavier” Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels



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

Visualize distribution of activations

Weight Initialization: “Xavier” Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

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

Weight Initialization: “Xavier” Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= \ldots=Var(x_{Din})$

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

Weight Initialization: "Xavier" Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= \ldots=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

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

Weight Initialization: "Xavier" Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= \ldots =Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din})$
[substituting value of y]

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

Weight Initialization: “Xavier” Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= \ldots =Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din})$
$= \Sigma\, Var(x_iw_i) = Din\, Var(x_iw_i)$
[Assume all x_i, w_i are iid] $\sigma^2_{X+Y} = \sigma^2_X + \sigma^2_Y$

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

Weight Initialization: “Xavier” Initialization

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

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

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

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

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $\mathrm{Var}(x_1) = \mathrm{Var}(x_2)= \ldots=\mathrm{Var}(x_{Din})$

We want: $\mathrm{Var}(y) = \mathrm{Var}(x_i)$

$$\begin{aligned}\mathrm{Var}(y) &= \mathrm{Var}(x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}) \\ &= Din\ \mathrm{Var}(x_iw_i) \\ &= Din\ \mathrm{Var}(x_i)\ \mathrm{Var}(w_i)\end{aligned}$$

[Assume all x_i, w_i are zero mean]

$$\mathrm{Var}(XY) = E(X^2Y^2) - (E(XY))^2 = \mathrm{Var}(X)\mathrm{Var}(Y) + \cancel{\mathrm{Var}(X)(E(Y))^2} + \cancel{\mathrm{Var}(Y)(E(X))^2}$$

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

Weight Initialization: "Xavier" Initialization

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

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

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

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= \ldots=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$$
\begin{aligned}
Var(y) &= Var(x_1w_1+x_2w_2+\ldots+x_{Din}w_{Din}) \\
&= Din\ Var(x_iw_i) \\
&= Din\ Var(x_i)\ Var(w_i)
\end{aligned}
$$

[Assume all x_i, w_i are iid]

So, $Var(y) = Var(x_i)$ only when $Var(w_i) = 1/Din$

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

Weight Initialization: What about ReLU?

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

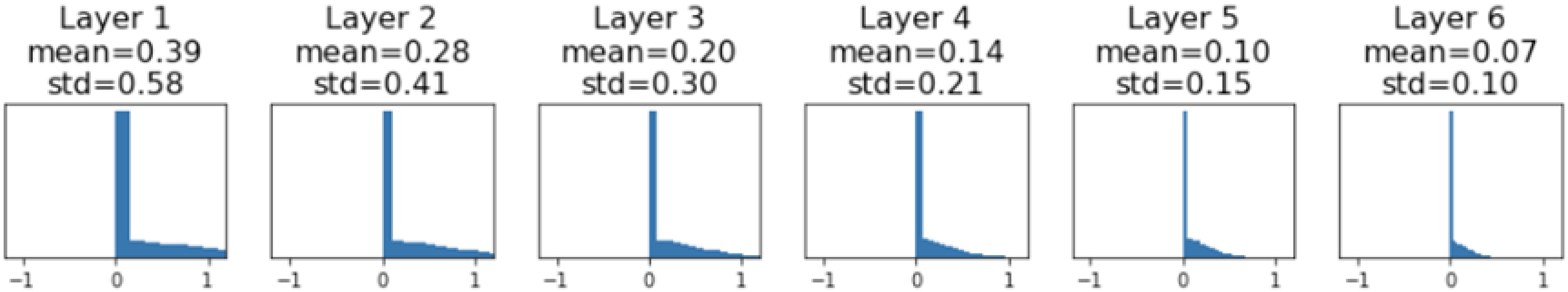
Change from tanh to ReLU

Weight Initialization: What about ReLU?

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

Change from tanh to ReLU

Xavier assumes zero centered activation function



Visualize distribution of activations

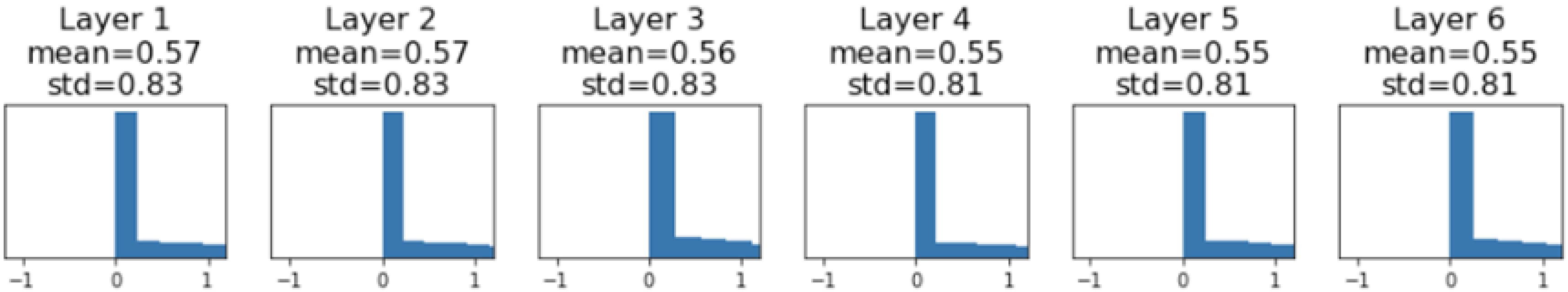
Weight Initialization: Kaiming / MSRA Initialization

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

ReLU correction: std = sqrt(2 / Din)

Issue: Half of the activation get killed.

Solution: make the non-zero output variance twice as large as input



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

Visualize distribution of activations

Proper initialization is still 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

Summary

Training Deep Neural Networks

- Details of the non-linear activation functions
  - Sigmoid, Tanh, ReLU, LeakyRELU, ELU, SELU
- Data normalization
  - Zero-centering, image normalization
- Batch normalization
  - BN, Instance Norm, Layer Norm, Group Norm
- Weight Initialization
  - Constant init, random init, Xavier Init, Kaiming Init