CS5841/EE5841 Machine Learning

Lecture 11: Neural Networks, extra details

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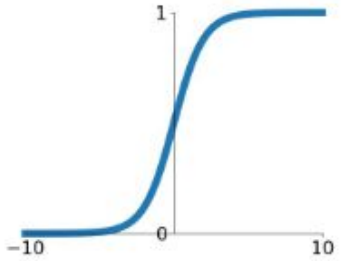
Putting it all together

- Neural networks are multiple layers of linear classifiers
- We train them through optimization with gradient descent methods
- Implementation steps and finer details

Activation functions

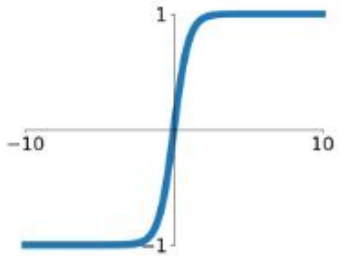
Sigmoid

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



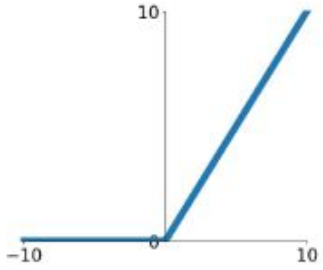
tanh

$$\tanh(x)$$



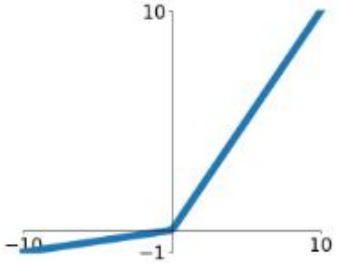
ReLU

$$\max(0, x)$$



Leaky ReLU

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

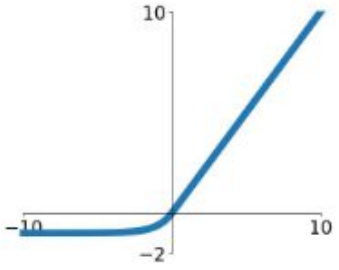


Maxout

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

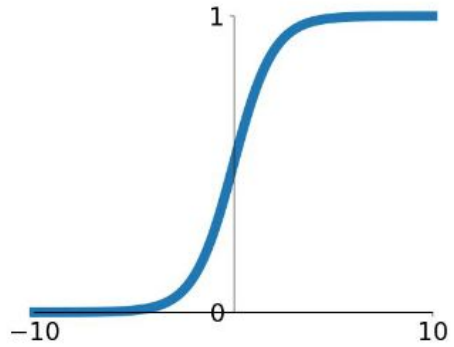
ELU

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



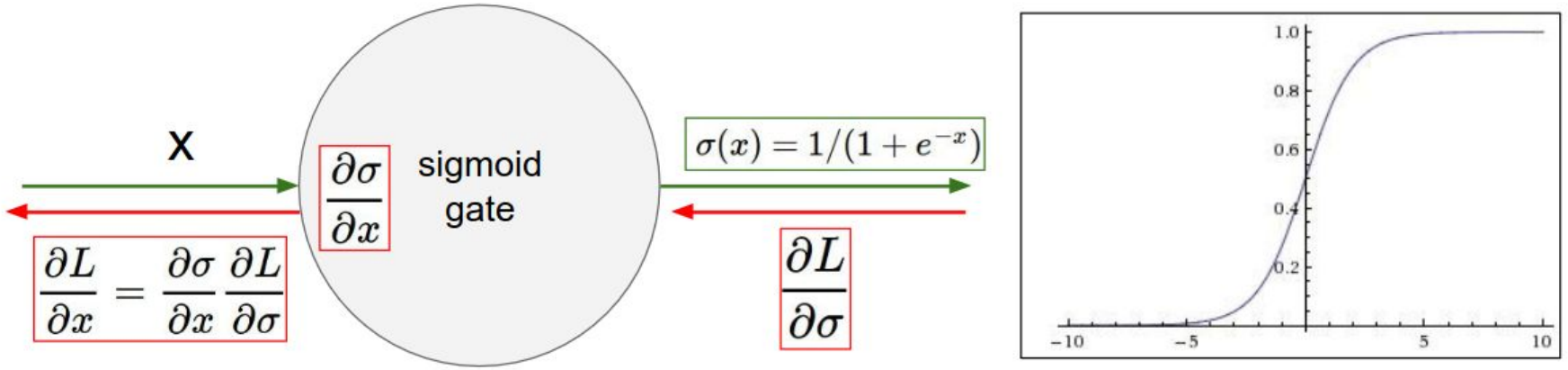
Sigmoid

- Sigmoid is historically popular because of Logistic Regression lineage AND easily interpreted because in range [0,1]
  - What issues could this cause?



Sigmoid

Issue 1: Saturation



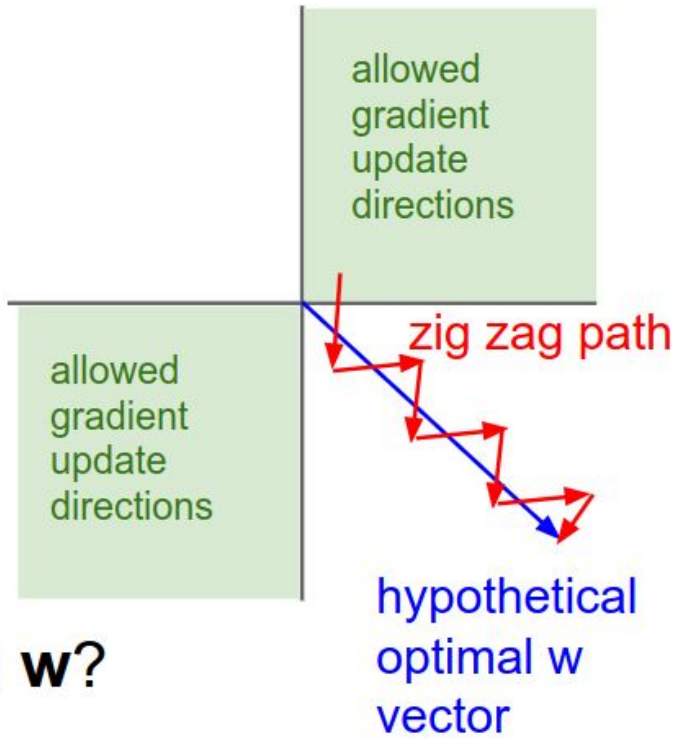
What happens when x = -10?
What happens when x = 0?
What happens when x = 10?

Issue 2: Not zero centered

Consider what happens when the input to a neuron is always positive...

This is somewhat of an edge case and using smaller batch sizes helps prevent it

$$f\left(\sum_i w_i x_i + b\right)$$

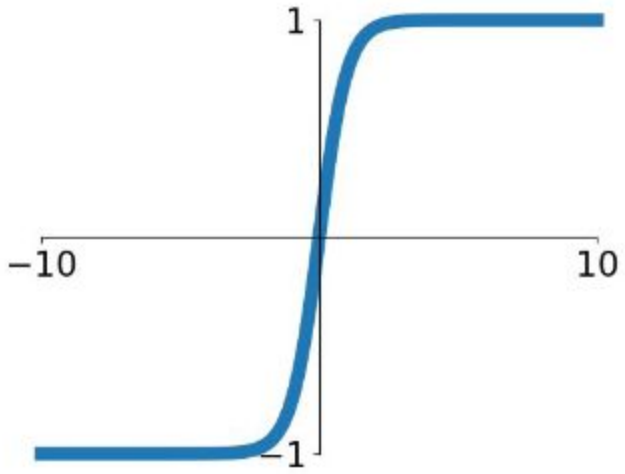


What can we say about the gradients on **w**?

Always all positive or all negative :(

Issue 3: exp() is computationally expensive

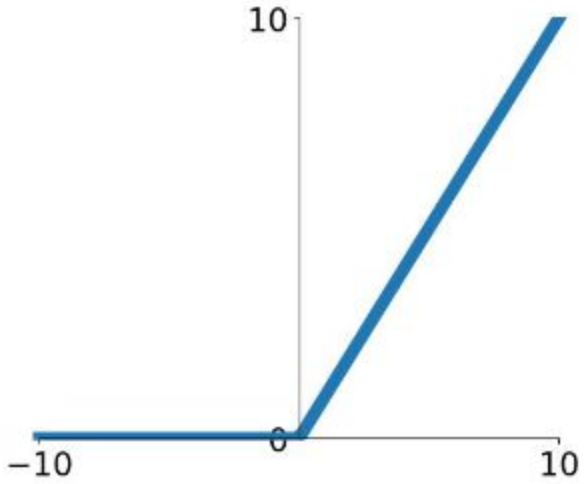
tanh()



tanh(x)

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

ReLU (ie. max(0,x))

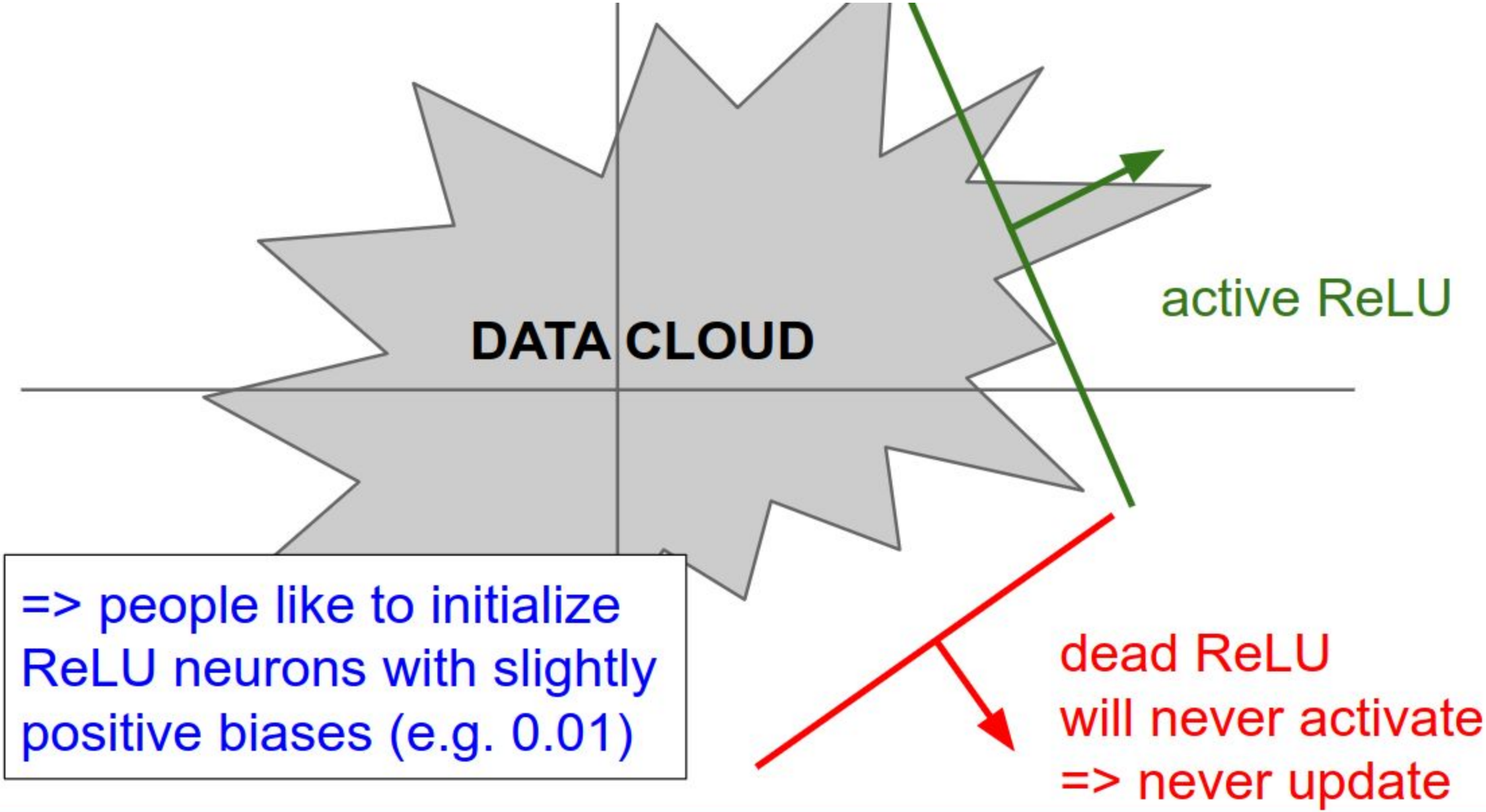


ReLU
(Rectified Linear Unit)

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

- Not zero-centered output
- An annoyance:

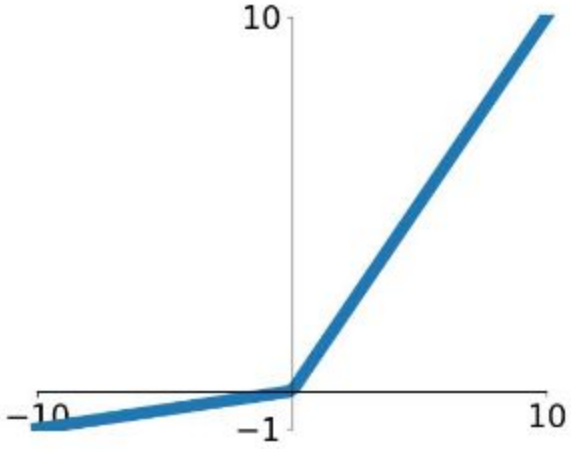
hint: what is the gradient when x < 0?



=> people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

Activation Functions

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

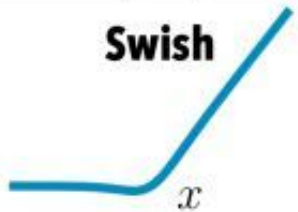
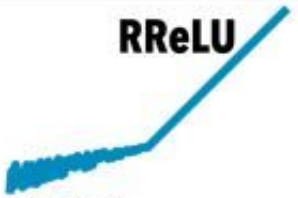


- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

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

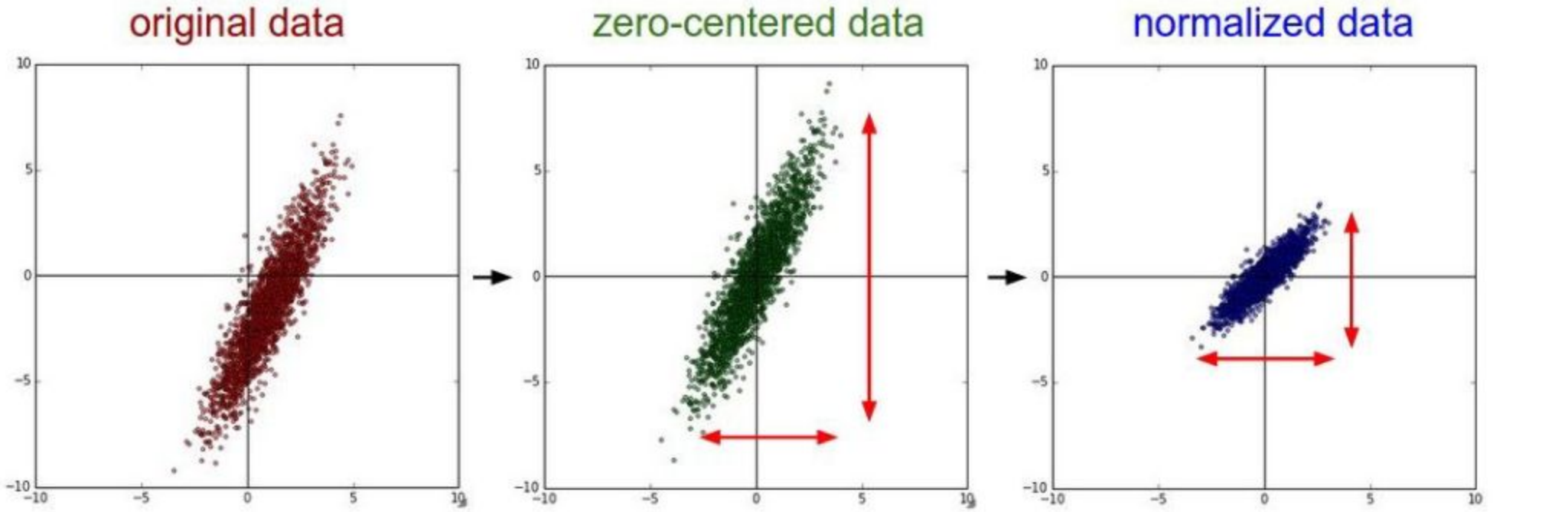
Others

ReLU  $\max(0, x)$	**GELU**  $\frac{x}{2}\left(1+\tanh\left(\sqrt{\frac{2}{\pi}}\left(x+ax^3\right)\right)\right)$	**PReLU**  $\max(0, x)$
ELU  $\begin{cases} x \text{ if } x > 0 \\ \alpha(x \exp x - 1) \text{ if } x < 0 \end{cases}$	**Swish**  $\frac{x}{1+\exp -x}$	**SELU**  $\alpha(\max(0, x)+$ $\min(0, \beta(\exp x - 1)))$
SoftPlus  $\frac{1}{\beta}\log\left(1+\exp(\beta x)\right)$	**Mish**  $x\tanh\left(\frac{1}{\beta}\log\left(1+\exp(\beta x)\right)\right)$	**RReLU**  $\begin{cases} x \text{ if } x \geq 0 \\ ax \text{ if } x < 0 \text{ with } a \sim \Re(l, u) \end{cases}$

General best practices

- ReLU usually works
- Consider Leaky ReLU/Maxout/ELU
- Play with other ones as desired
- Don’t use sigmoid

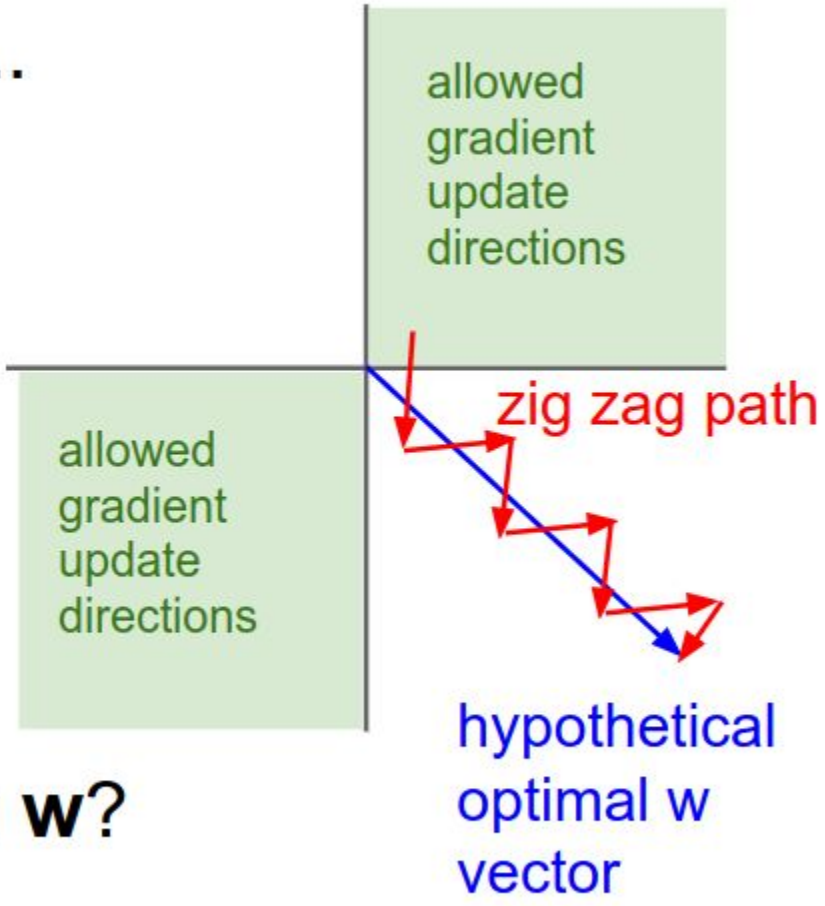
Data preprocessing



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

Remember: Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b\right)$$

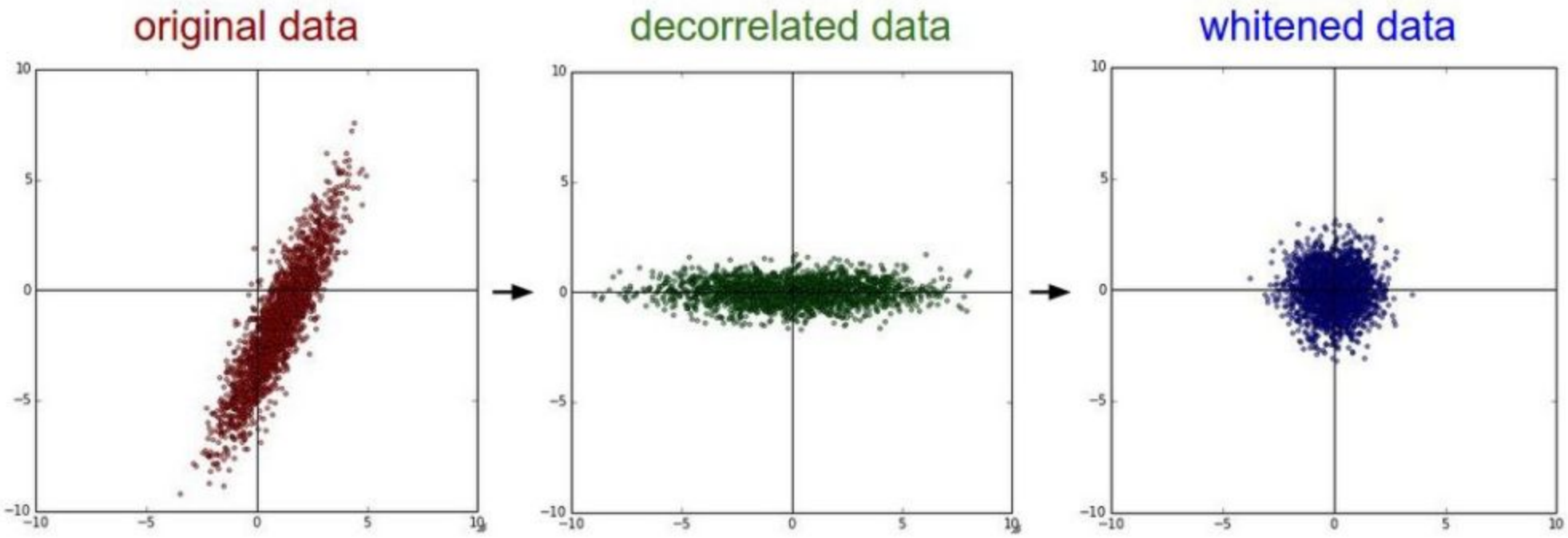


What can we say about the gradients on **w**?

Always all positive or all negative :(

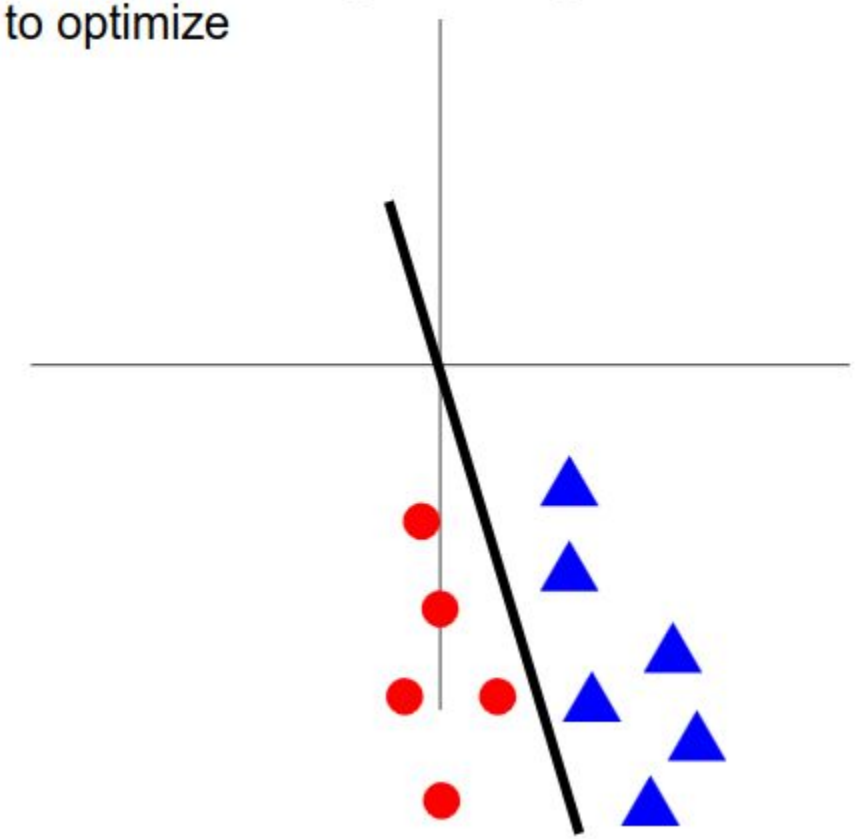
(this is also why you want zero-mean data!)

Other practices

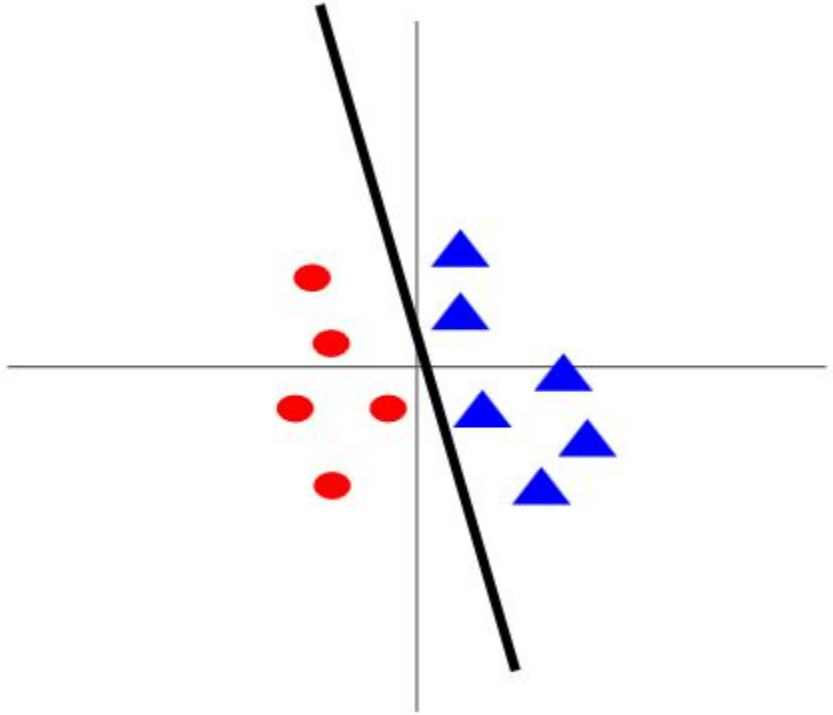


Preprocessing effects

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



Other data specific pre-processing

For images:

- Subtract mean image
- Subtract per-channel mean
- Subtract per-channel mean and divide by per-channel std
- Typically don’t do PCA or whitening

Weight initialization

- Random
  - Works pretty well for small networks
  - Values must be small
  - zero mean, e-2 std typical
  - Problematic with big networks

Weight Initialization: Activation statistics

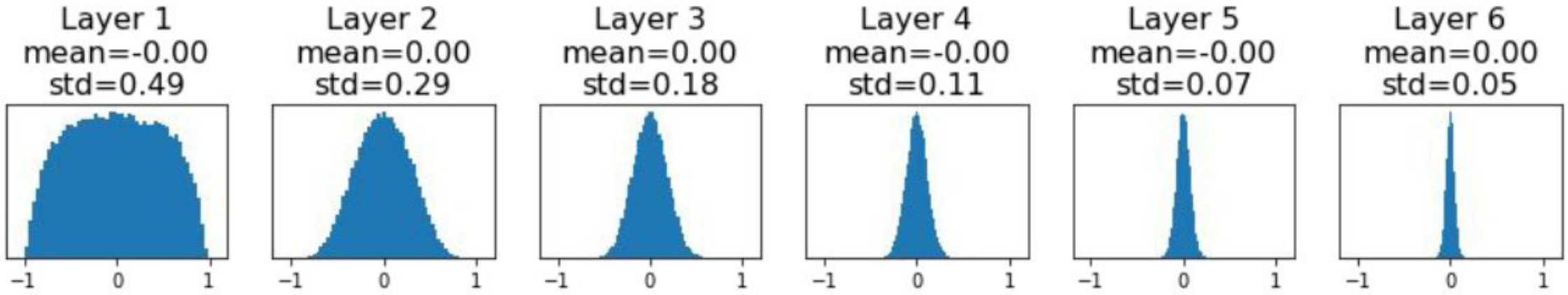
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

A: All zero, no learning =(



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Weight Initialization: Activation statistics

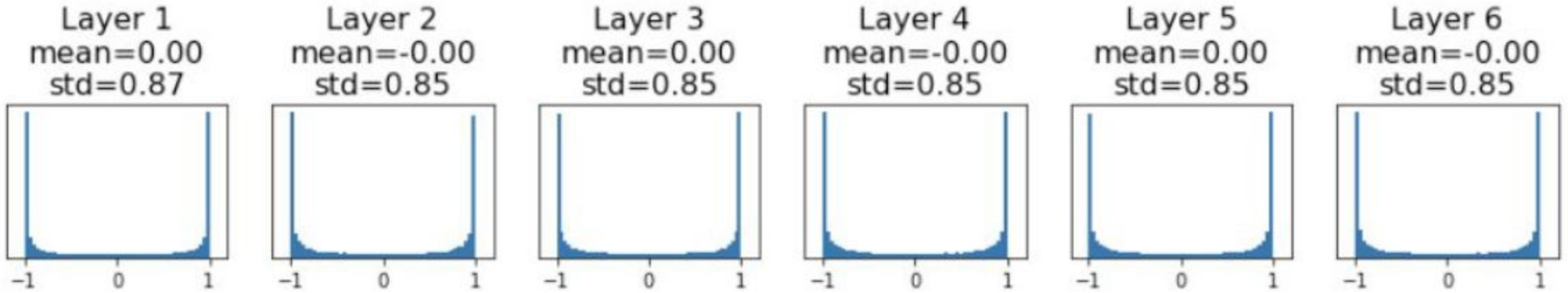
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

A: Local gradients all zero, no learning =(



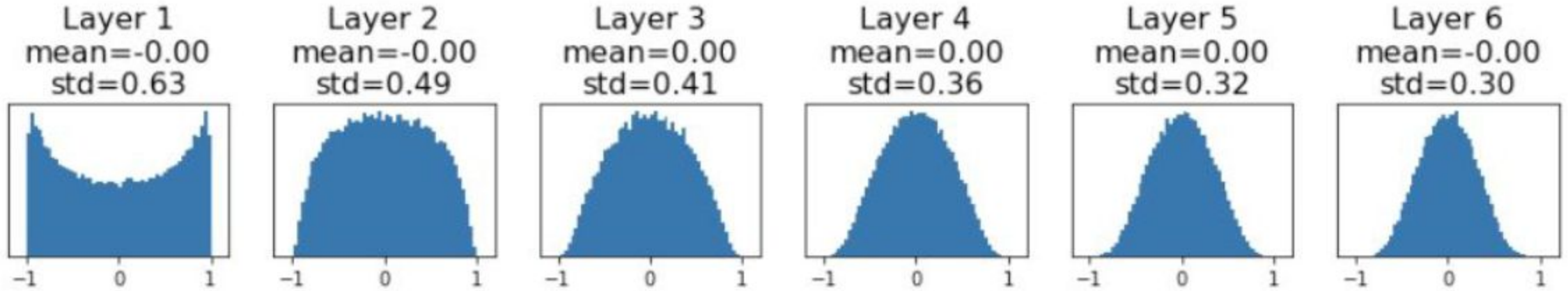
Weight Initialization: "Xavier" Initialization

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

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

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

For conv layers, Din is kernel_size^2 * input_channels



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

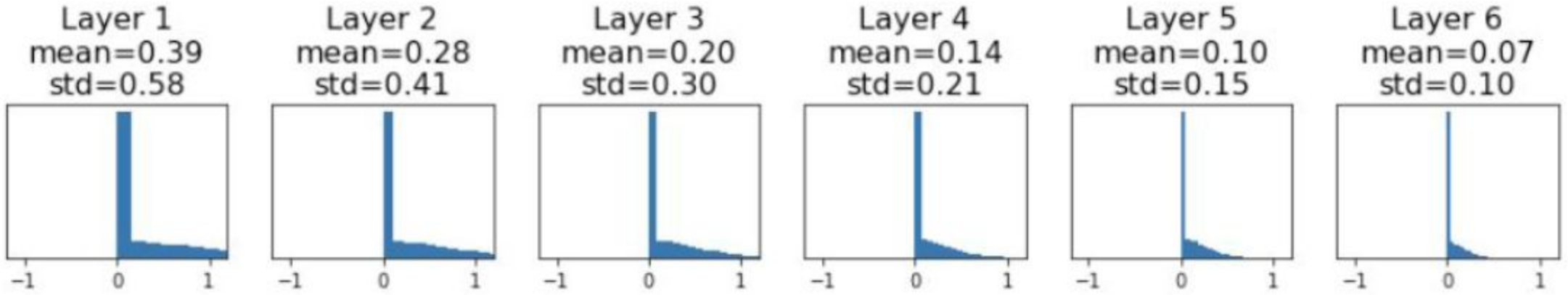
Weight Initialization: What about ReLU?

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

Change from tanh to ReLU

Xavier assumes zero centered activation function

Activations collapse to zero again, no learning =(



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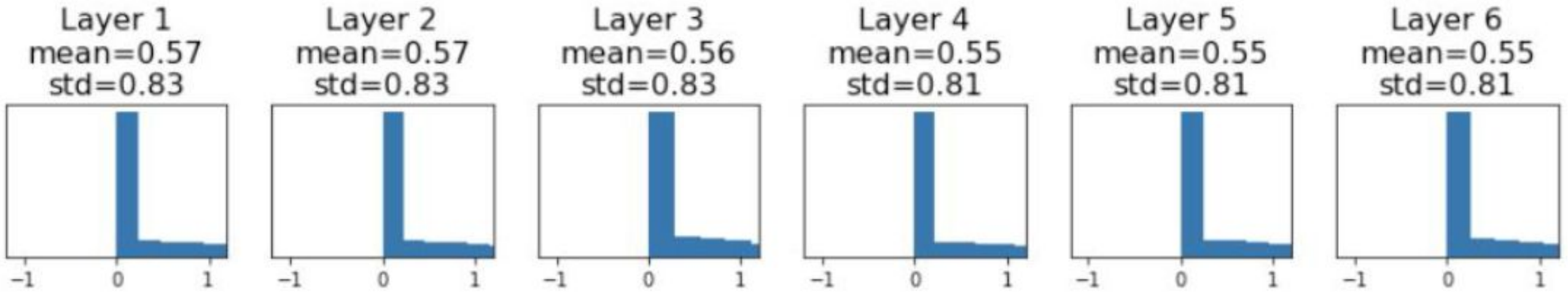
Weight Initialization: Kaiming / MSRA Initialization

```
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)

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



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

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

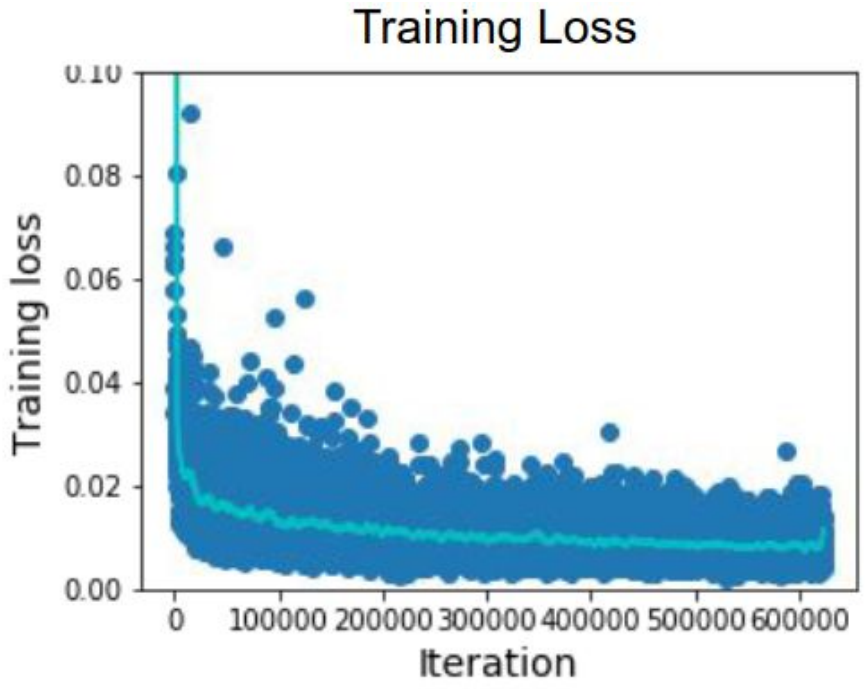
Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

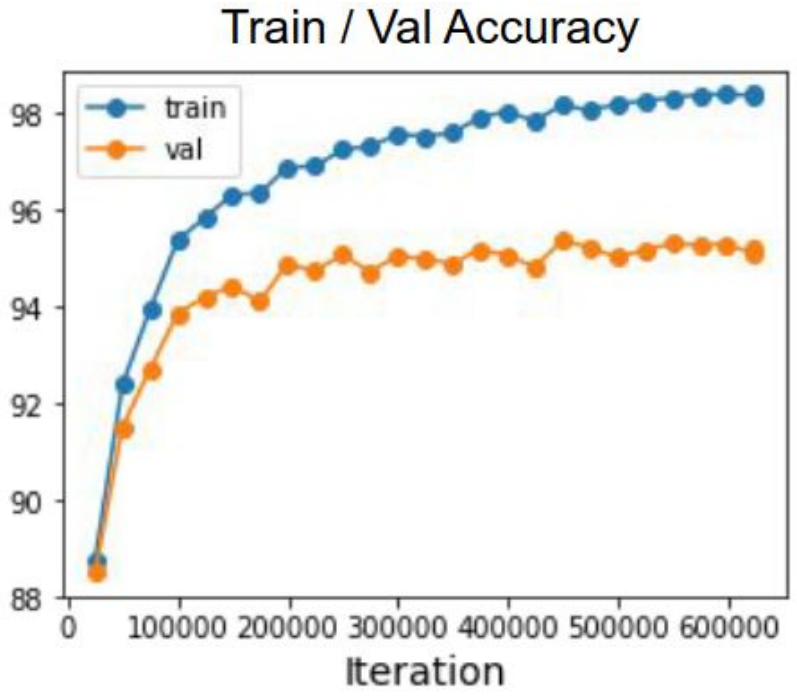
All you need is a good init, Mishkin and Matas, 2015

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

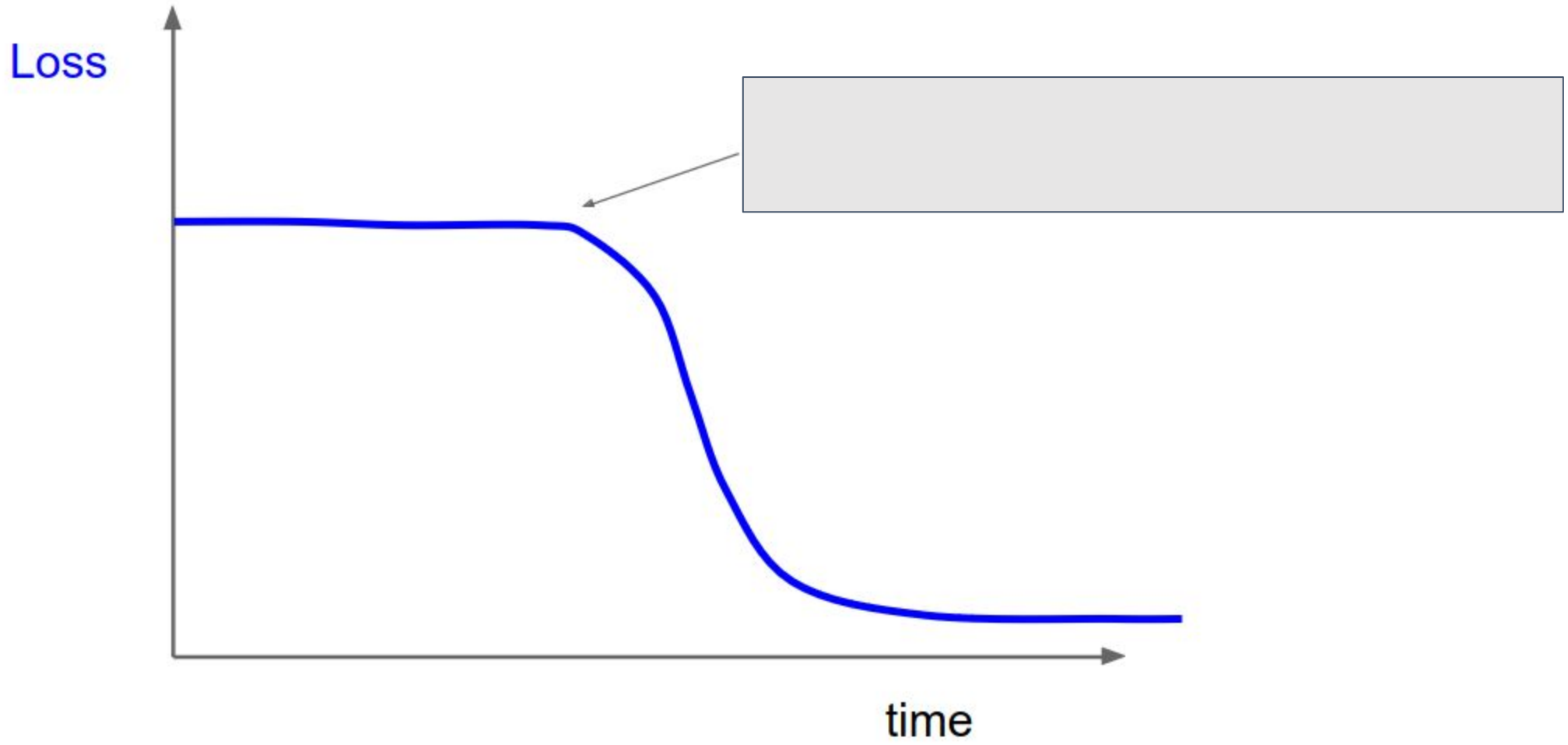
The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks, Frankle and Carbin, 2019

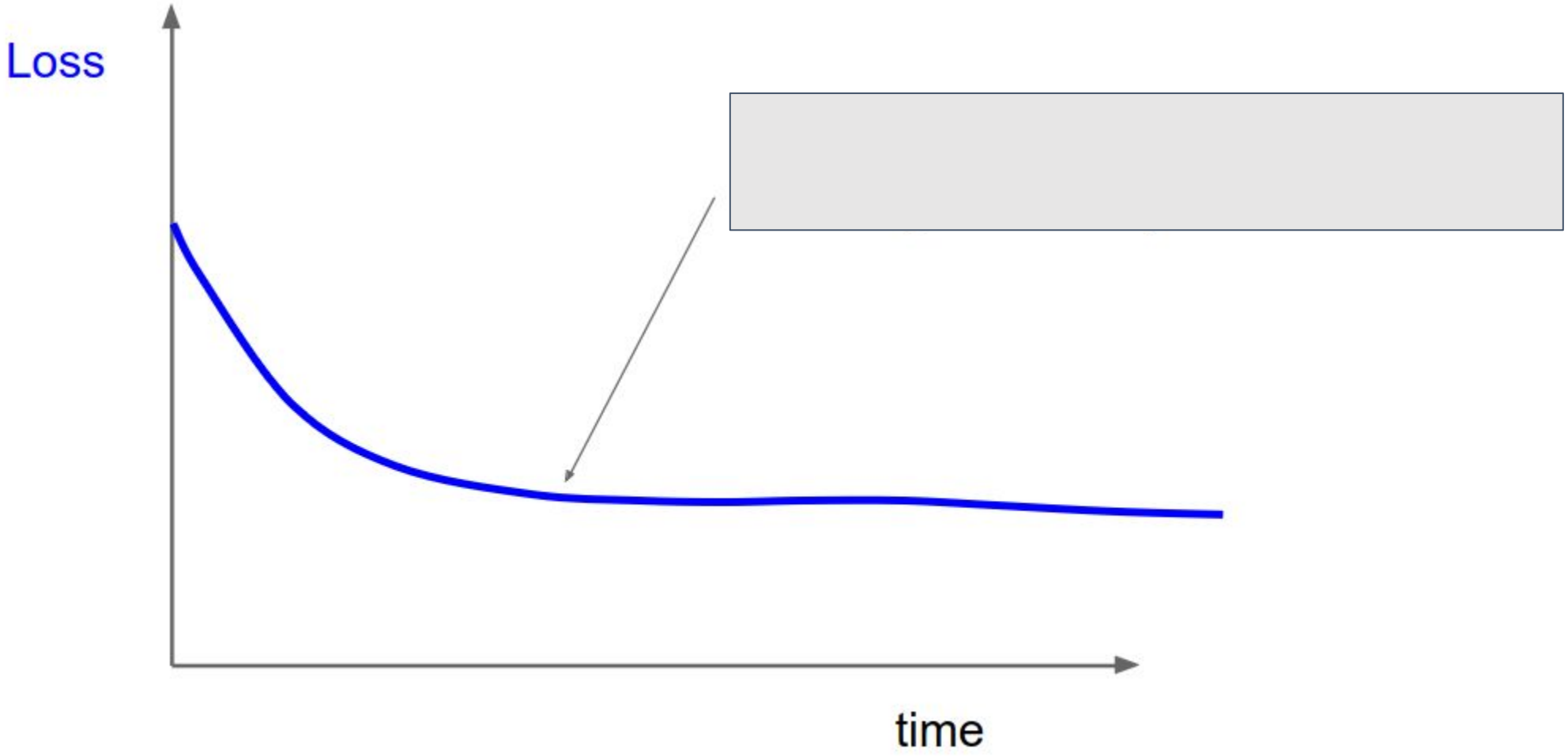
Reading loss curves

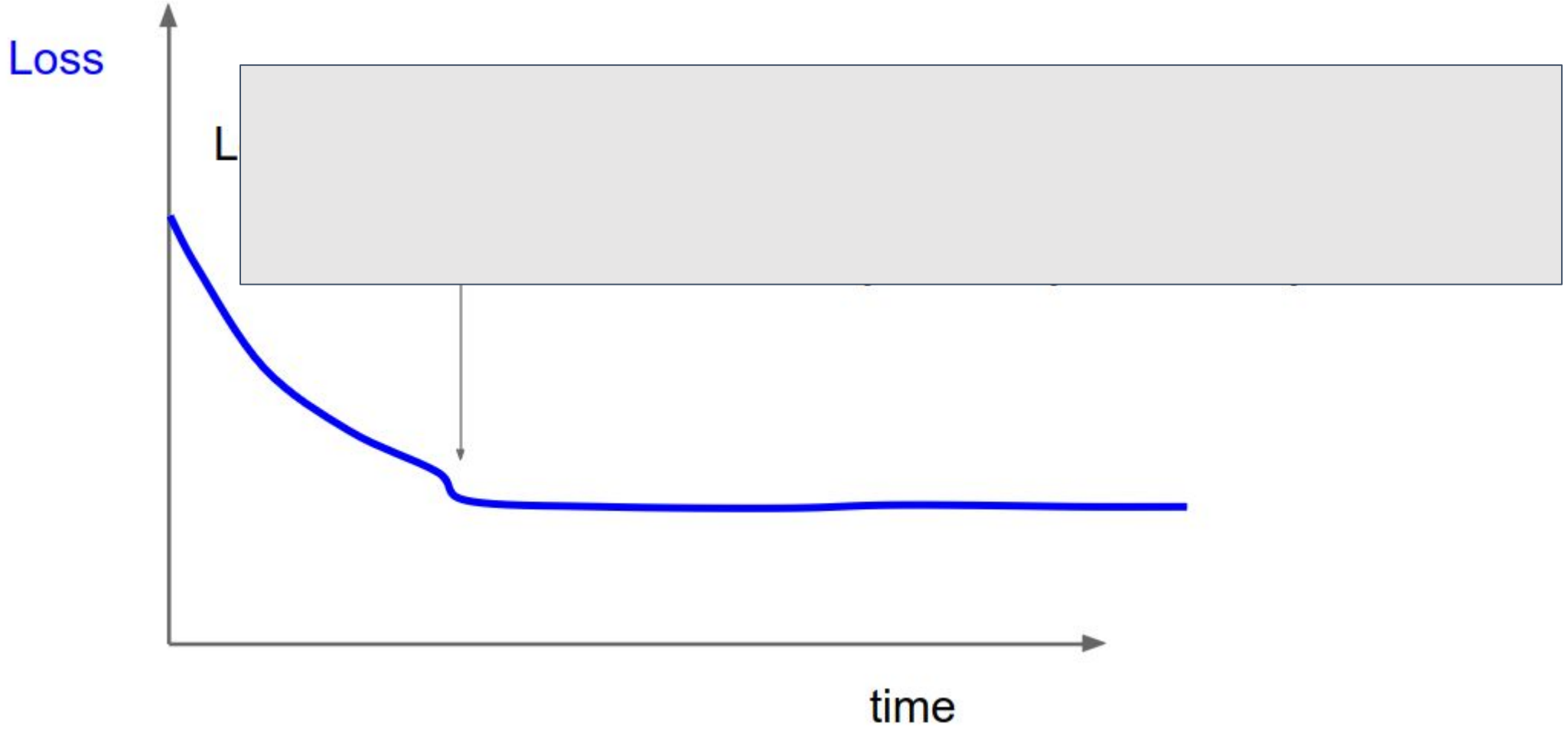


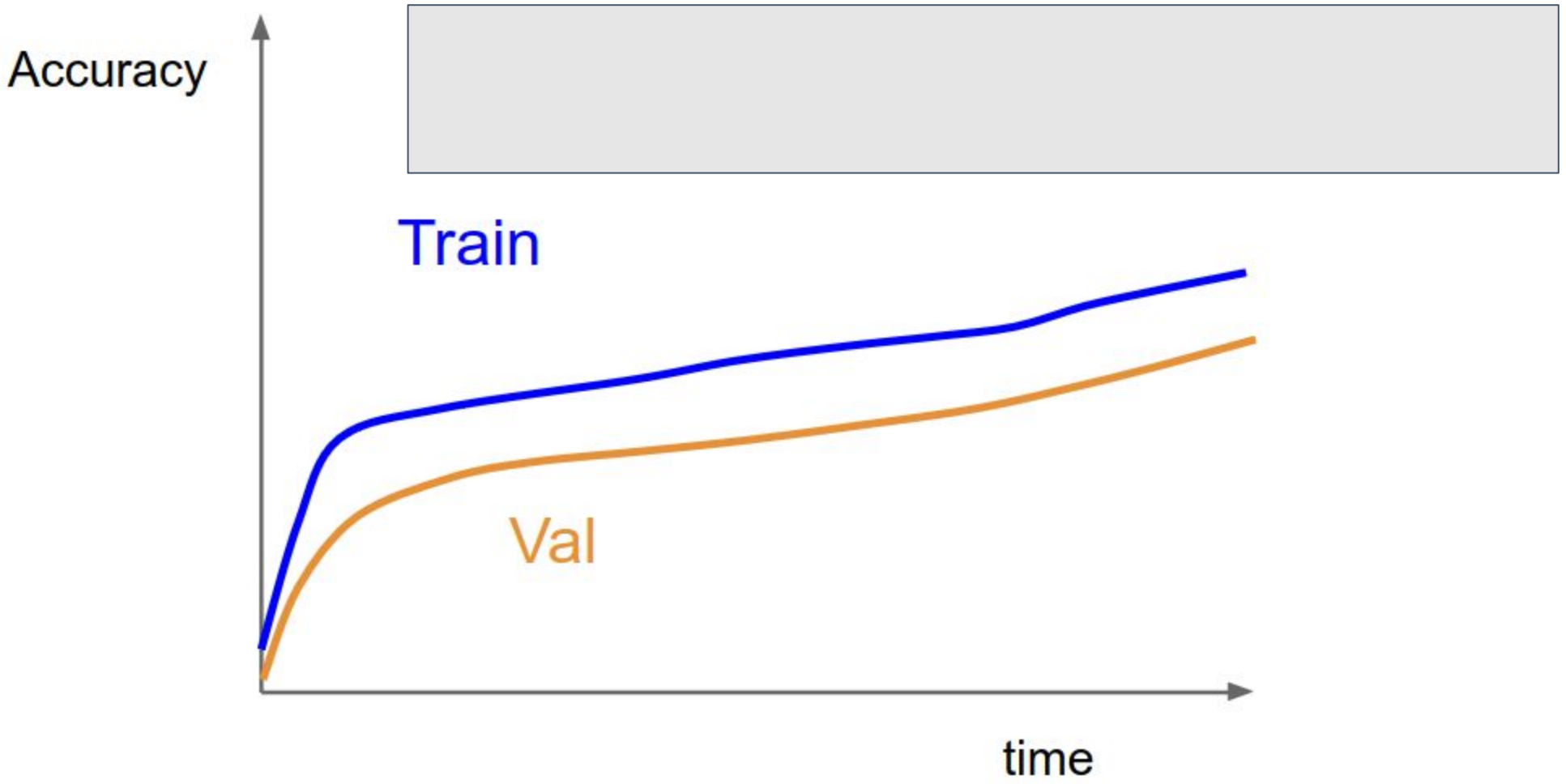


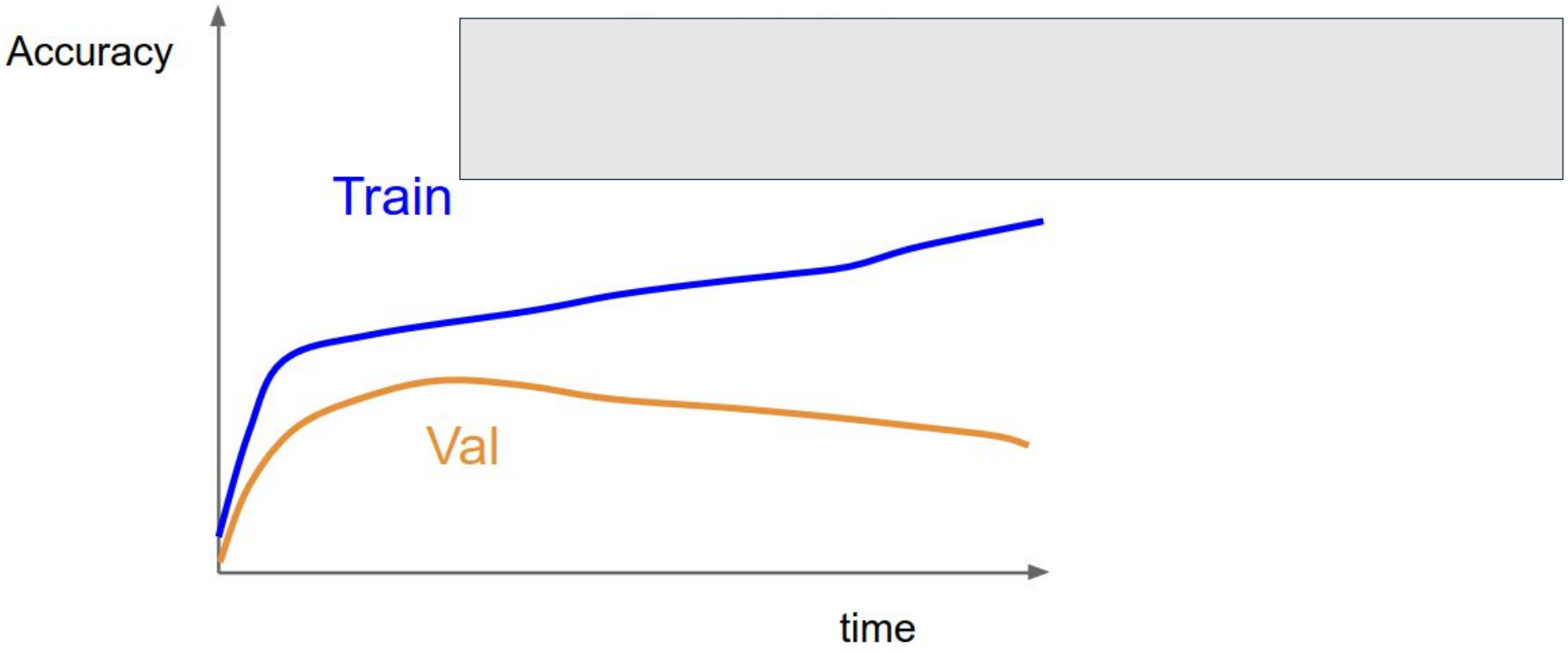
Losses may be noisy, use a scatter plot and also plot moving average to see trends better

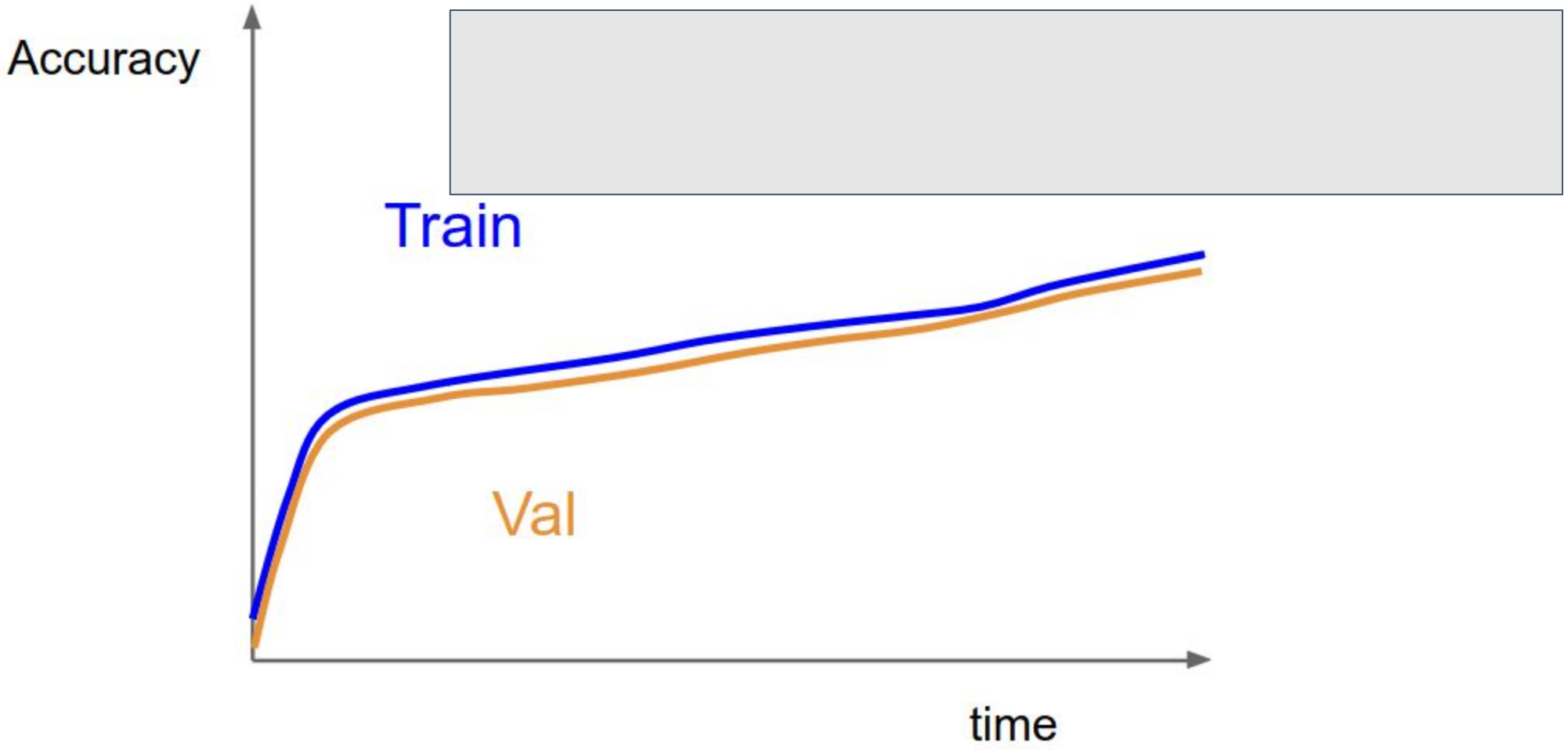

Loss
time


Loss
time


Loss
L
time


Accuracy
Train
Val
time

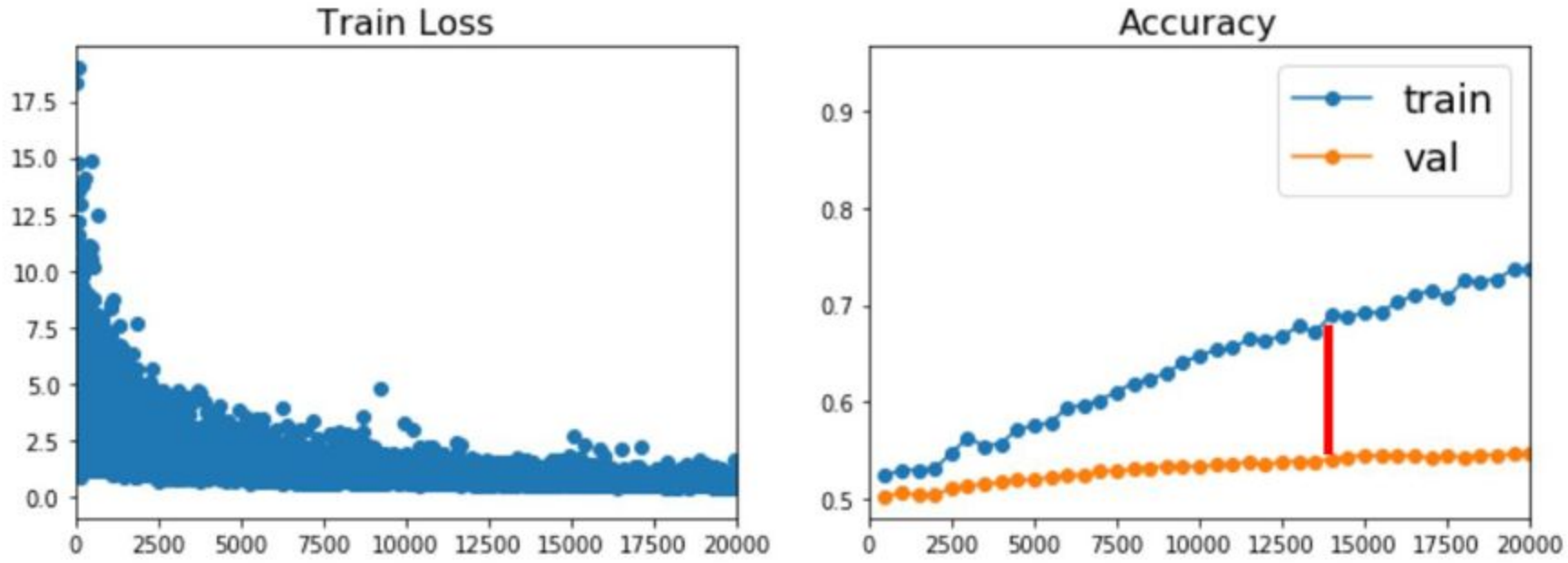

Accuracy
Train
Val
time


Accuracy
Train
Val
time

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer
Step 6: Look at loss curves
Step 7: GOTO step 5

How to improve single-model performance?



Regularization

Regularization: Add term to loss

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

In common use:

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

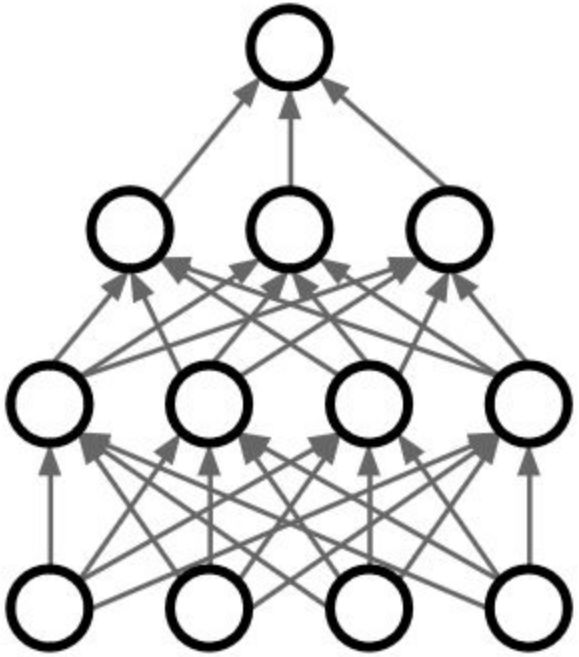
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

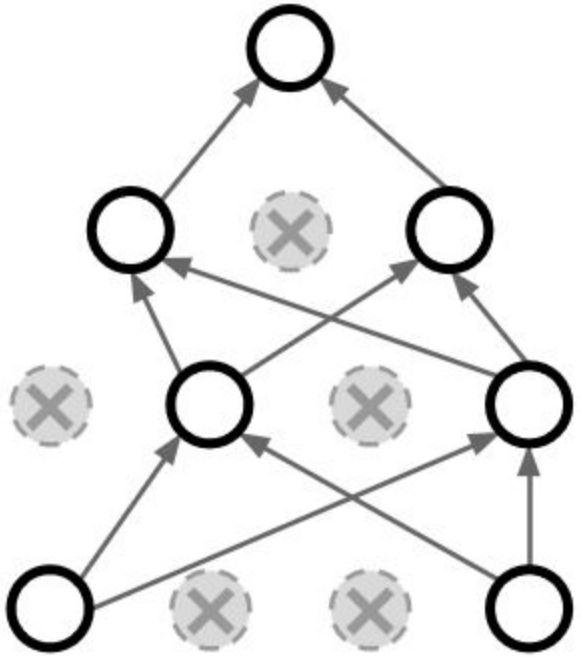
Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

Regularization: Dropout

In each forward pass, randomly set some neurons to zero

Probability of dropping is a hyperparameter; 0.5 is common



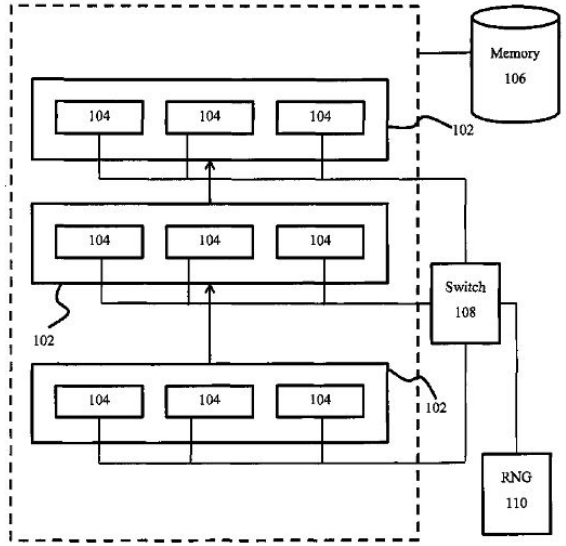


Srivastava et al, "Dropout: A simple way to prevent neural networks from overfitting", JMLR 2014

US009406017B2

(57) **ABSTRACT**

A system for training a neural network. A switch is linked to feature detectors in at least some of the layers of the neural network. For each training case, the switch randomly selectively disables each of the feature detectors in accordance with a preconfigured probability. The weights from each training case are then normalized for applying the neural network to test data.



(12) **United States Patent**
Hinton et al.

(10) **Patent No.: US 9,406,017 B2**
(45) **Date of Patent: Aug. 2, 2016**

(54) **SYSTEM AND METHOD FOR ADDRESSING OVERFITTING IN A NEURAL NETWORK**

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(73) Assignee: **Google Inc.**, Mountain View, CA (US)

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 369 days.

(21) Appl. No.: **14/015,768**

(22) Filed: **Aug. 30, 2013**

(65) **Prior Publication Data**

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Related U.S. Application Data

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(51) **Int. Cl.**
G06N 3/08 (2006.01)
G06N 3/04 (2006.01)

(52) **U.S. Cl.**
CPC ***G06N 3/082*** (2013.01); ***G06N 3/0454*** (2013.01)

(58) **Field of Classification Search**
CPC G06N 3/082
See application file for complete search history.

(56) **References Cited**

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(Continued)

Primary Examiner — Kakali Chaki
Assistant Examiner — Kevin W Figueroa
(74) *Attorney, Agent, or Firm* — Fish & Richardson P.C.

(57) **ABSTRACT**

A system for training a neural network. A switch is linked to feature detectors in at least some of the layers of the neural network. For each training case, the switch randomly selectively disables each of the feature detectors in accordance with a preconfigured probability. The weights from each training case are then normalized for applying the neural network to test data.

24 Claims, 2 Drawing Sheets

Michigan Tech

Regularization: Dropout

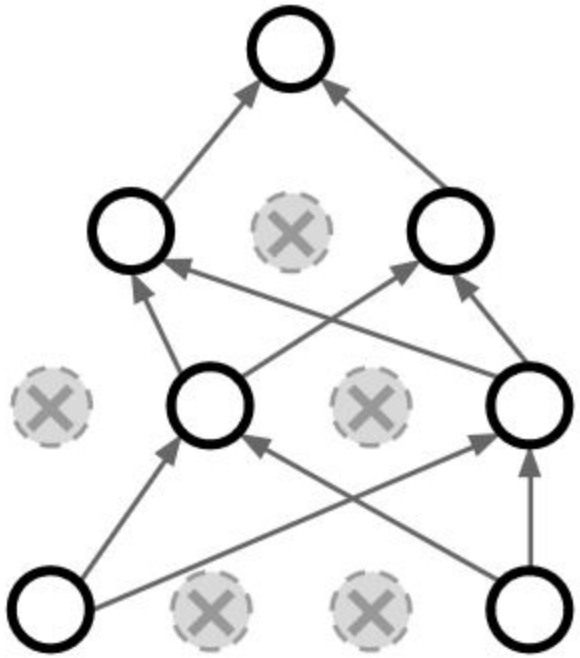
```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

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)
```

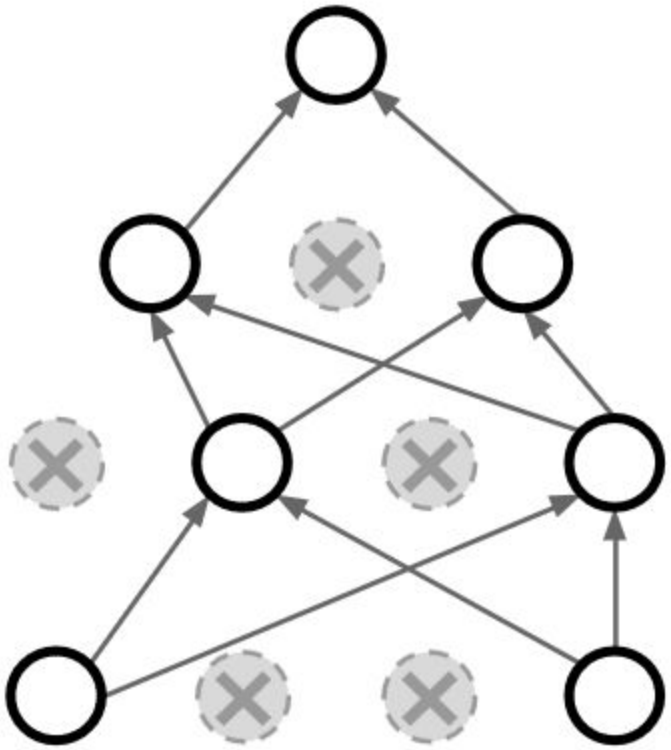
Example forward pass with a 3-layer network using dropout



Michigan Tech

Regularization: Dropout

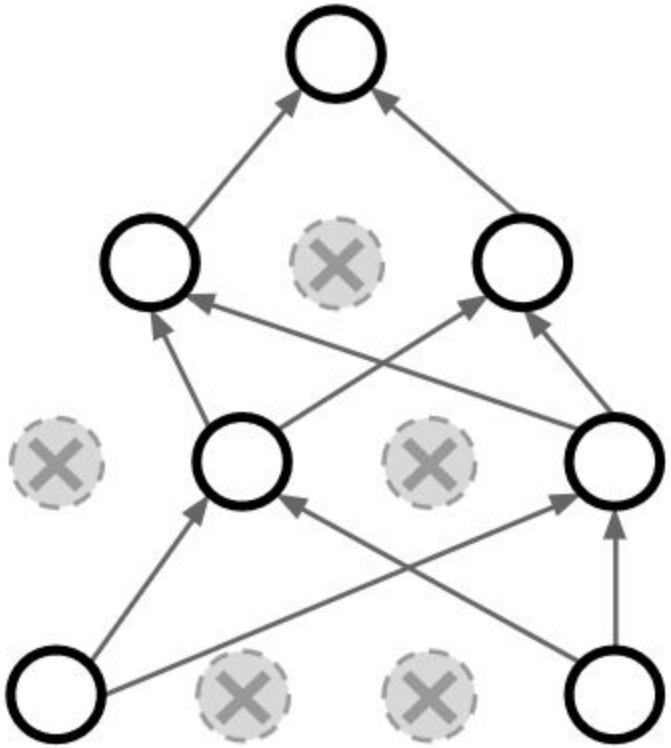
How can this possibly be a good idea?



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

Regularization: Dropout

How can this possibly be a good idea?



Another interpretation:

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

Each binary mask is one model

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

Dropout: Test time

Dropout makes our output random!

Output (label) Input (image)

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

Random mask

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

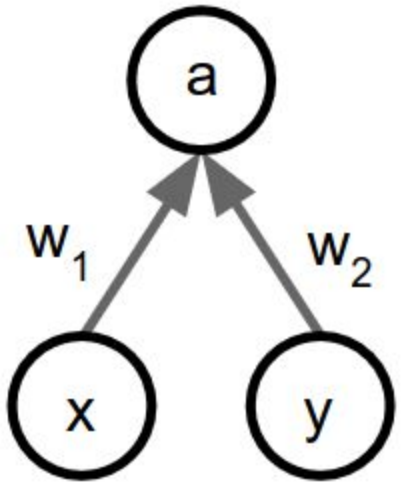
$$y = f(x) = E_z\left[f(x, z)\right] = \int p(z) f(x, z) dz$$

But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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



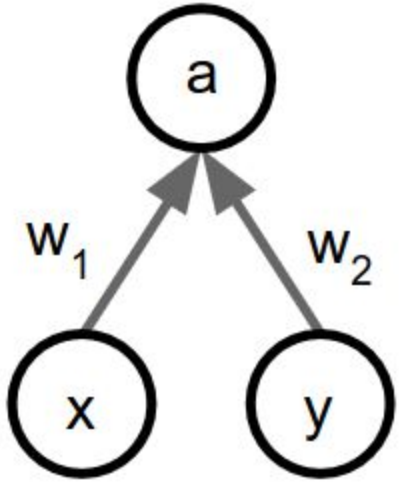
Consider a single neuron.

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

Dropout: Test time

Want to approximate the integral

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



Consider a single neuron.

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

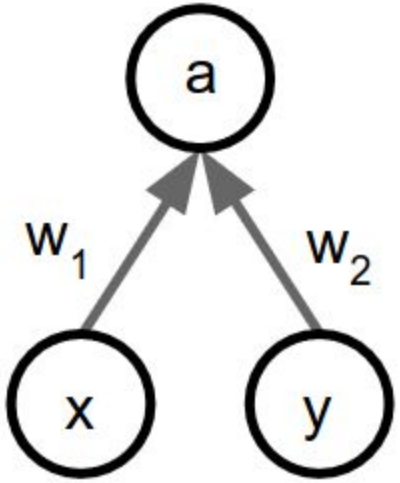
During training we have:

$$\begin{aligned} E\big[a\big] =& \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0y) \\ &+ \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y) \\ =& \frac{1}{2}(w_1 x + w_2 y) \end{aligned}$$

Dropout: Test time

Want to approximate the integral

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



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At test time, **multiply** by dropout probability

Dropout: Test time

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

At test time all neurons are active always
=> We must scale the activations so that for each neuron:
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
```

test time is unchanged!

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

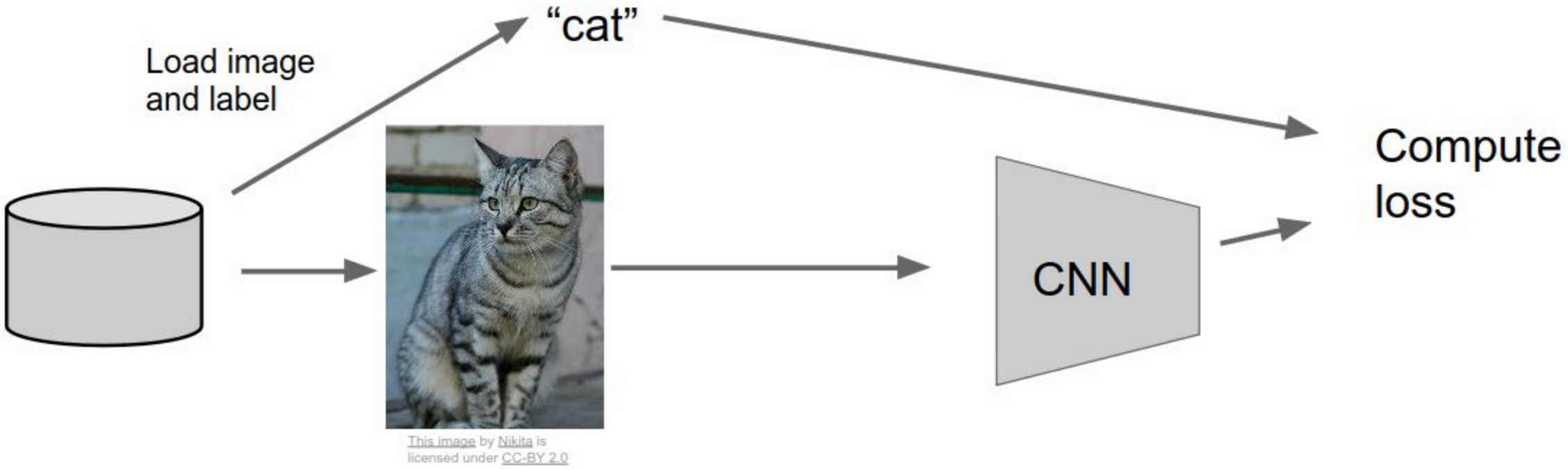
$$y = f(x) = E_z\left[f(x, z)\right] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

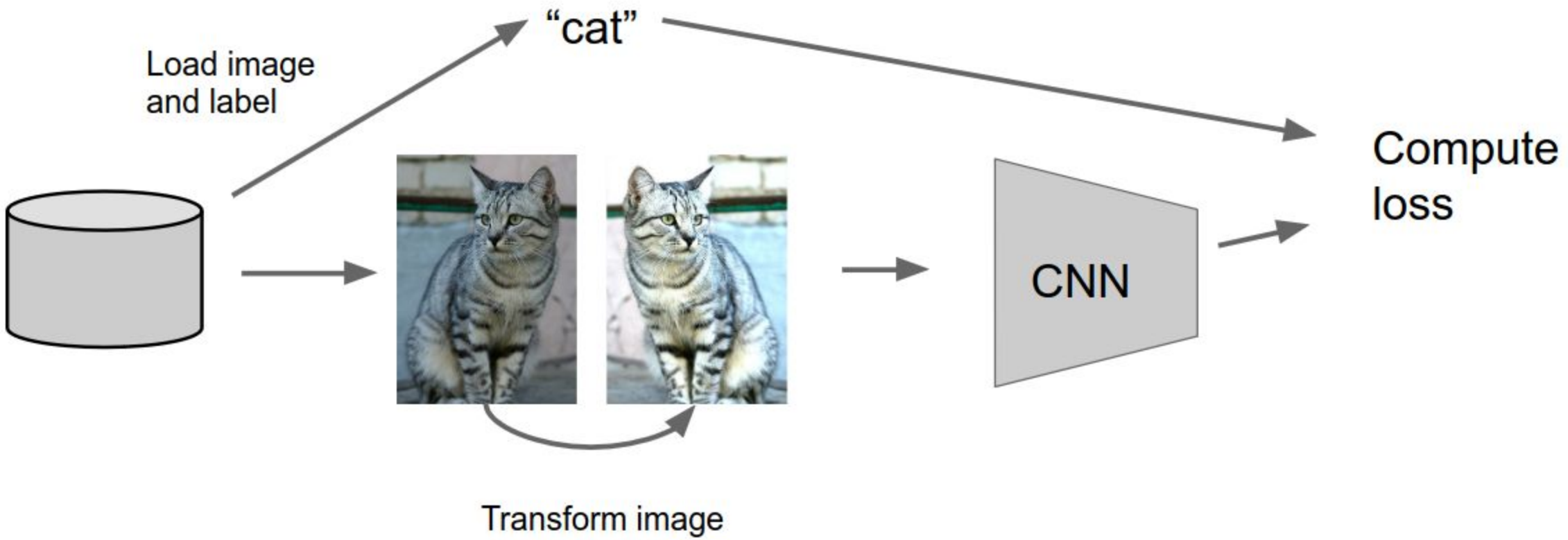
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Regularization: Data Augmentation



Regularization: Data Augmentation



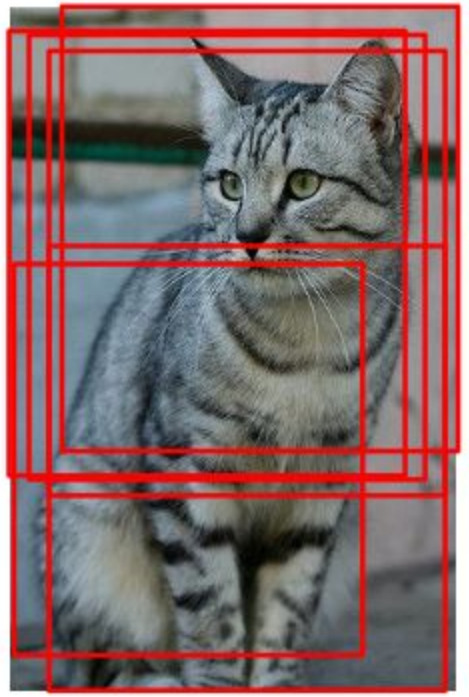
Data Augmentation

Random crops and scales

Training: sample random crops / scales

ResNet:

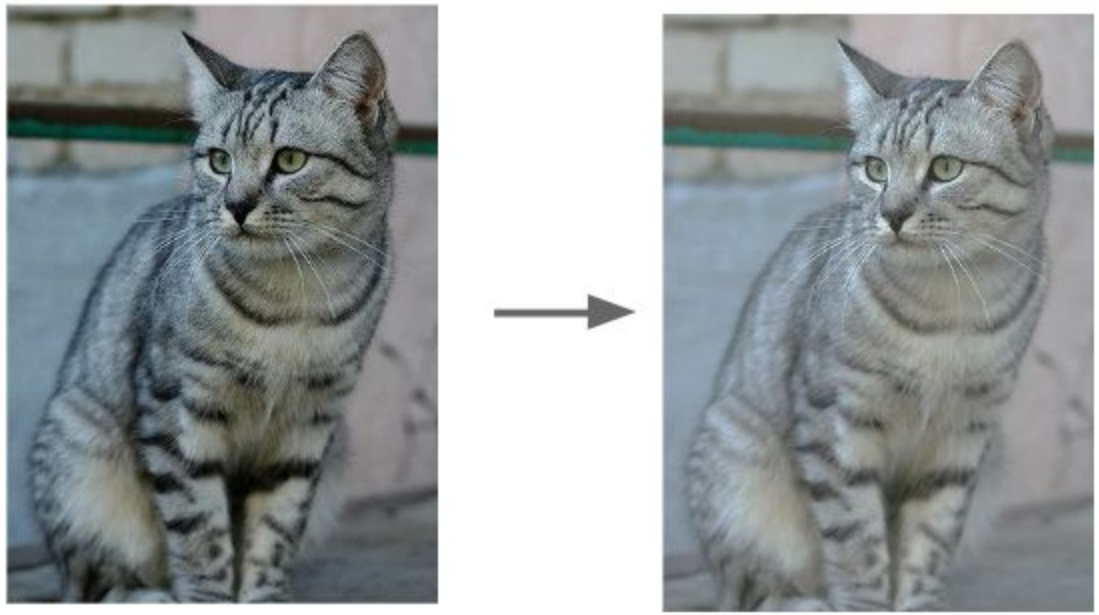
1. Pick random L in range [256, 480]
2. Resize training image, short side = L
3. Sample random 224 x 224 patch



Data Augmentation

Color Jitter

Simple: Randomize
contrast and brightness



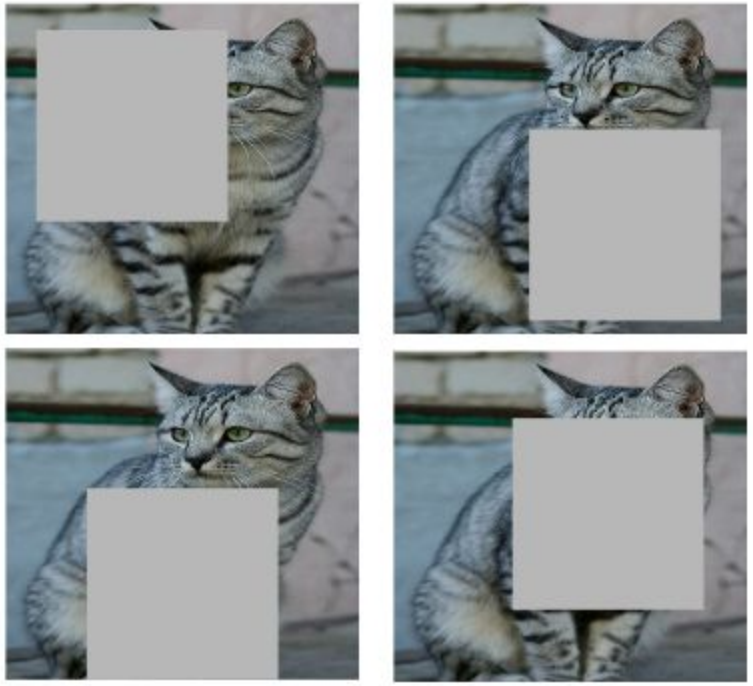
Regularization: Cutout

Training: Set random image regions to zero

Testing: Use full image

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout



Works very well for small datasets like CIFAR, less common for large datasets like ImageNet

DeVries and Taylor, "Improved Regularization of Convolutional Neural Networks with Cutout", arXiv 2017

Regularization: Mixup

Training: Train on random blends of images

Testing: Use original images

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
Stochastic Depth
Cutout
Mixup

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

Target label:
cat: 0.4
dog: 0.6

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

Batch Normalization

[Ioffe and Szegedy, 2015]

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

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

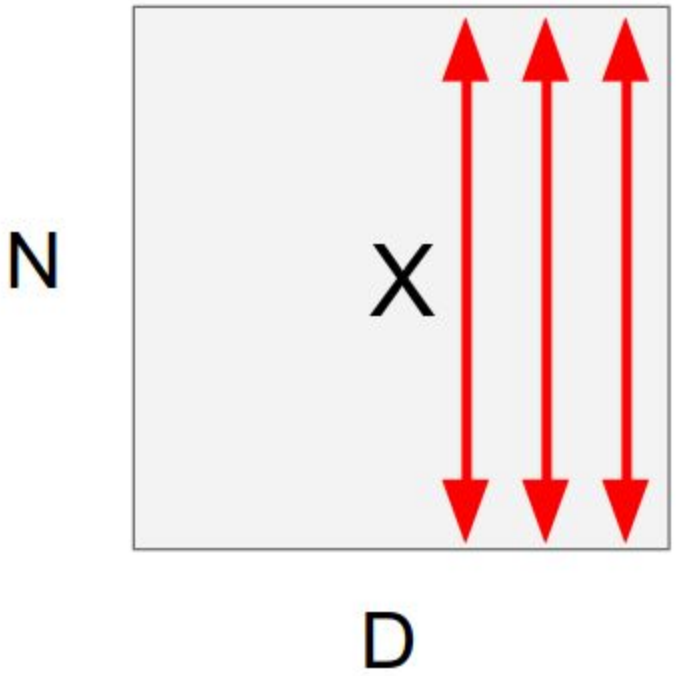
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$



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

Per-channel mean, shape is D

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

Per-channel 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

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$,
$\beta = \mu$ will recover the identity function!

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

Per-channel mean, shape is D

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

Per-channel 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:

$$\gamma, \beta : D$$

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

$$\mu_j = \text{(Running) average of values seen during training}$$

Per-channel mean, shape is D

$$\sigma_j^2 = \text{(Running) average of values seen during training}$$

Per-channel var, shape is D

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

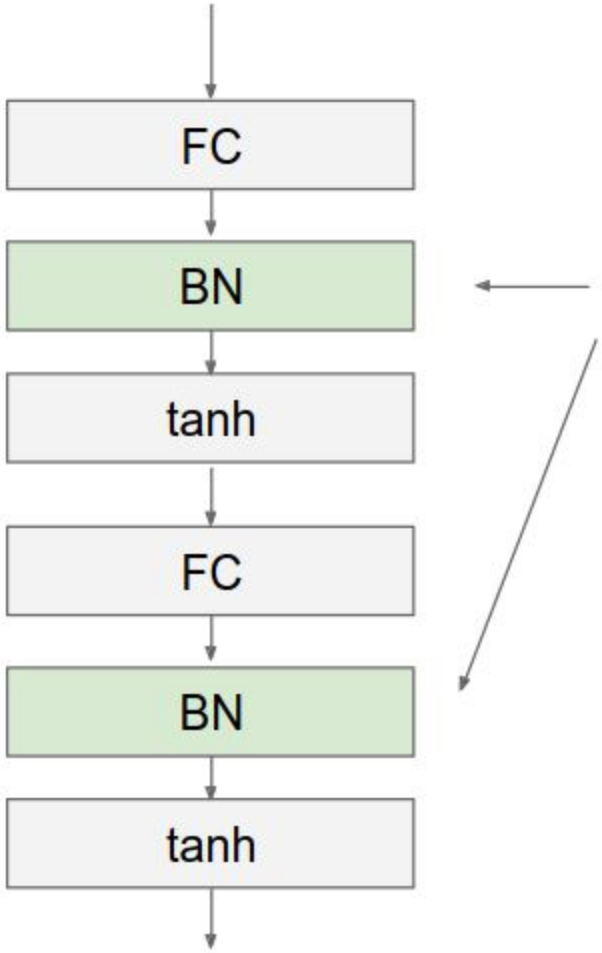
Normalized x, Shape is N x D

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

Output, Shape is N x D

Batch Normalization

[Ioffe and Szegedy, 2015]

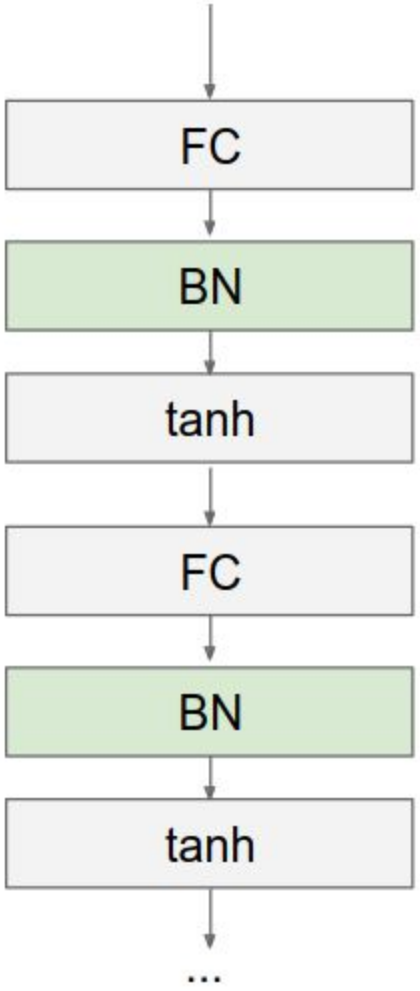


Usually inserted after Fully Connected or Convolutional layers, and before nonlinearity.

$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

Batch Normalization

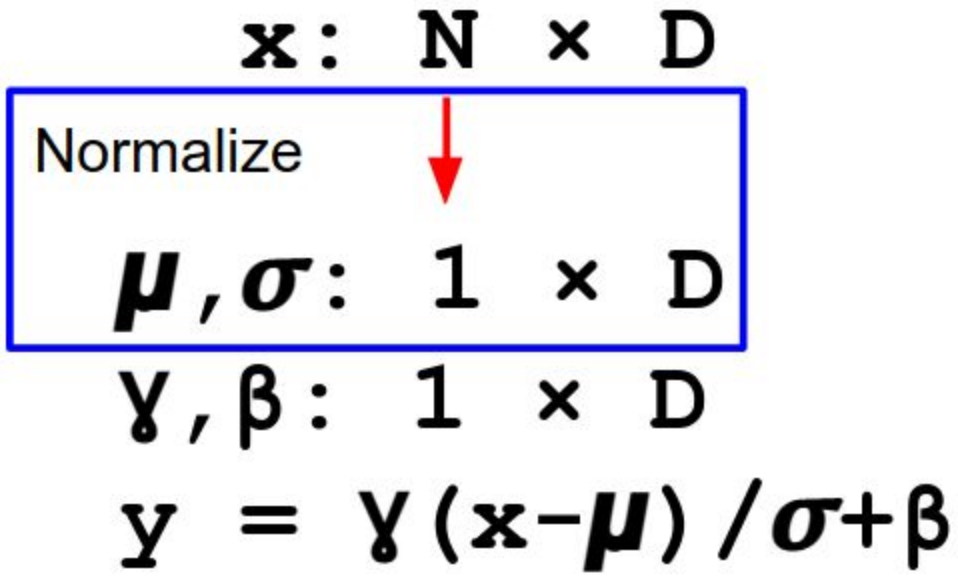
[Ioffe and Szegedy, 2015]



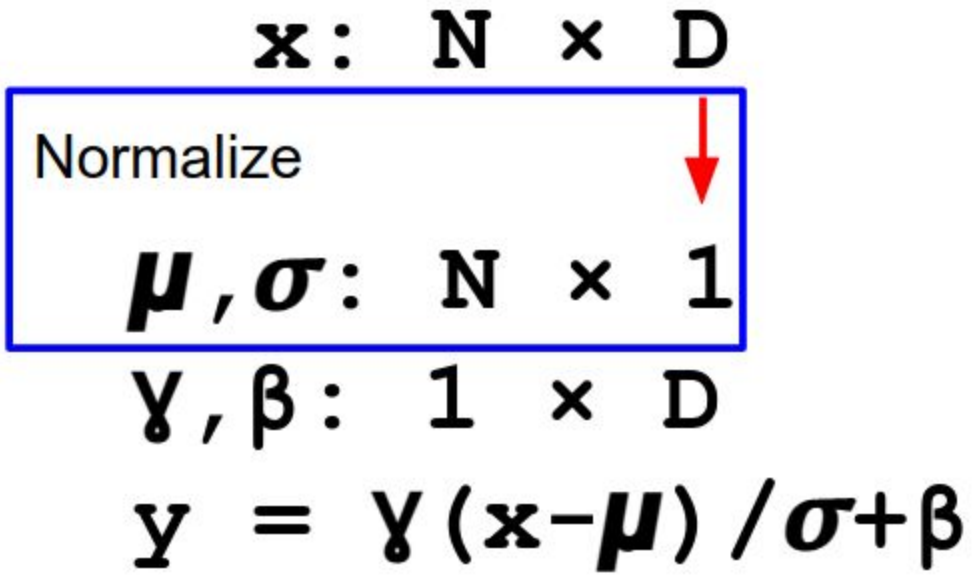
- Makes deep networks **much** easier to train!
- Improves gradient flow
- Allows higher learning rates, faster convergence
- Networks become more robust to initialization
- Acts as regularization during training
- Zero overhead at test-time: can be fused with conv!
- Behaves differently during training and testing: this is a very common source of bugs!

Layer Normalization

Batch Normalization for fully-connected networks



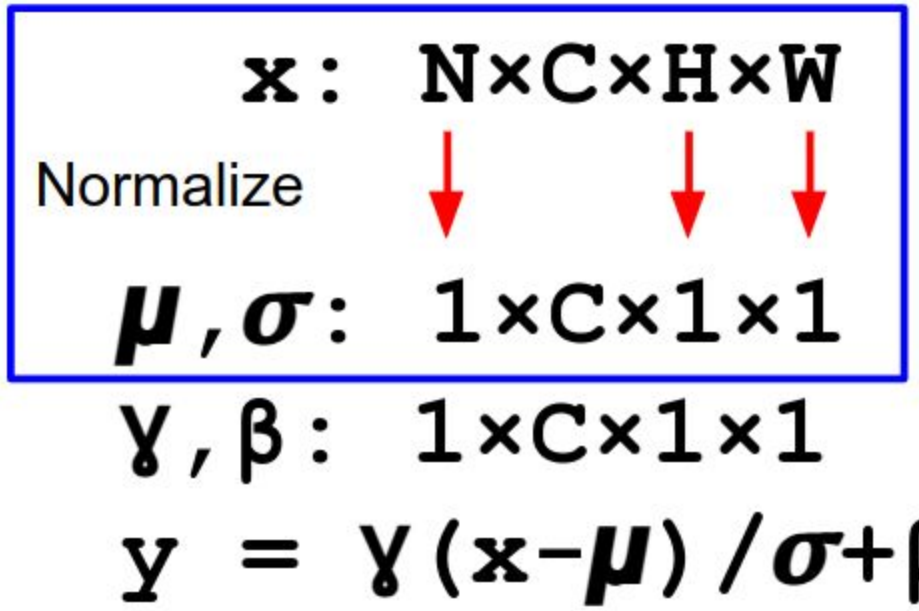
Layer Normalization for fully-connected networks
Same behavior at train and test!
Can be used in recurrent networks



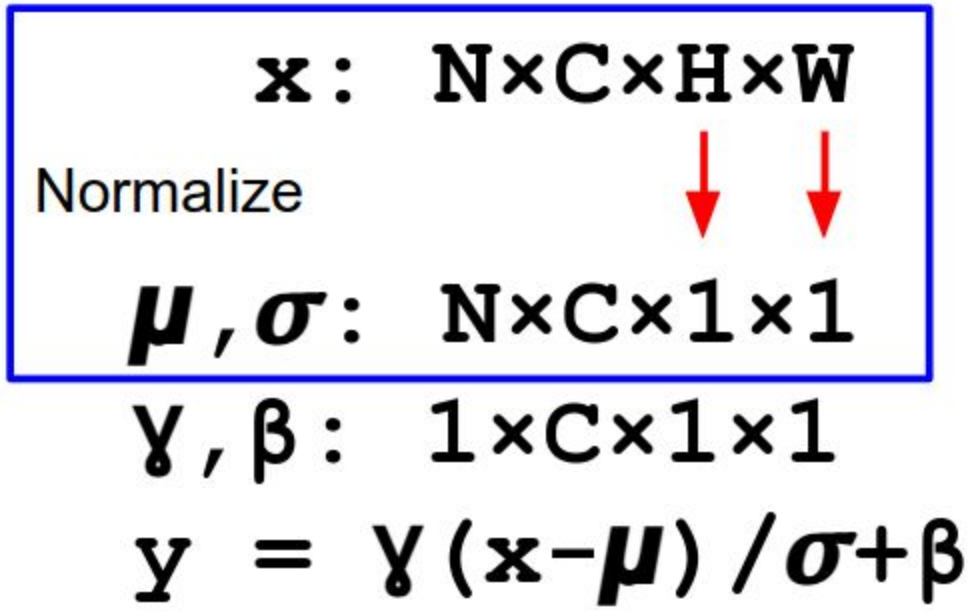
Ba, Kiros, and Hinton, "Layer Normalization", arXiv 2016

Instance Normalization

Batch Normalization for convolutional networks



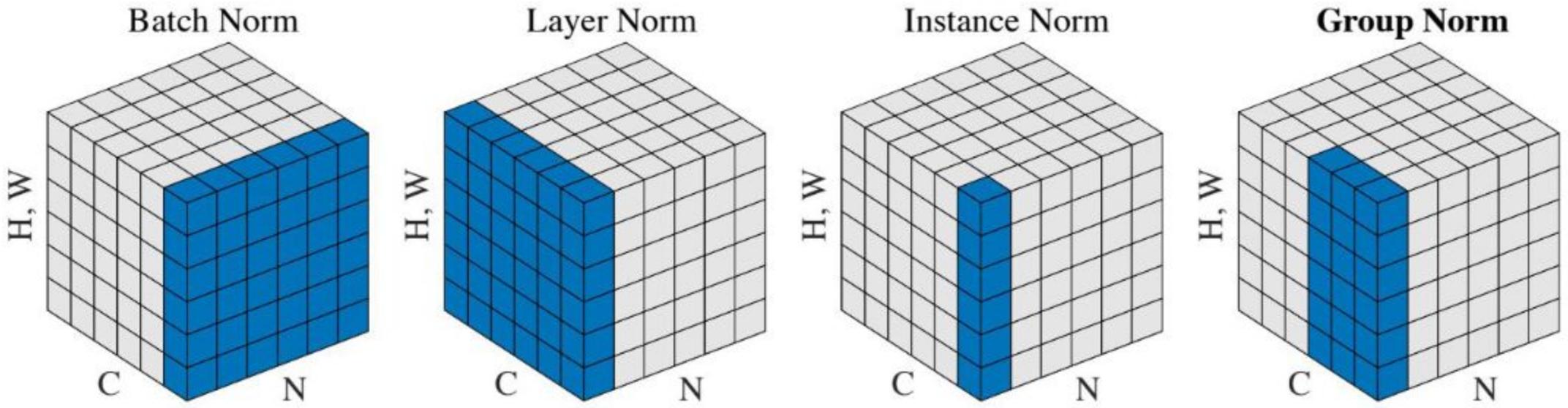
Instance Normalization for convolutional networks
Same behavior at train / test!



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

Michigan Tech

Group Normalization



Wu and He, “Group Normalization”, ECCV 2018

Questions + Comments?

Resources used

http://cs231n.stanford.edu/slides/2023/lecture_2.pdf

http://cs231n.stanford.edu/slides/2023/lecture_3.pdf

http://cs231n.stanford.edu/slides/2023/lecture_4.pdf