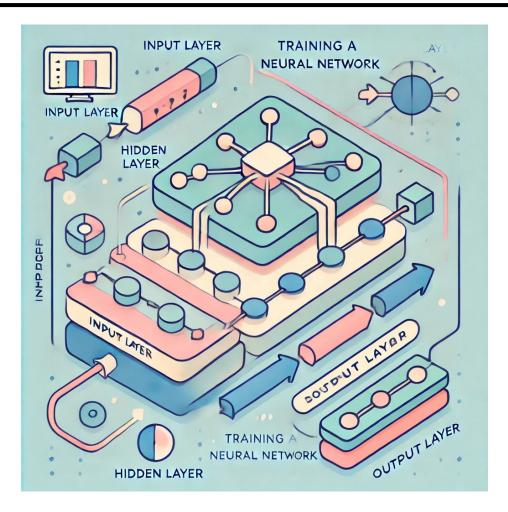
Training Recipes for Neural Nets I



Al604 Deep Learning for Computer Vision Prof. Hyunjung Shim

Slide credit: Justin Johnson, Fei-Fei Li, Ehsan Adeli

Recap: CNN Architectures Summary

Early work (AlexNet -> ZFNet -> VGG) shows that bigger networks work better

GoogLeNet one of the first to focus on **efficiency** (aggressive stem, 1x1 bottleneck convolutions, global avg pool instead of FC layers)

ResNet showed us how to train extremely deep networks – limited only by GPU memory! Started to show diminishing returns as networks got bigger

After ResNet: **Efficient networks** became central: how can we improve the accuracy without increasing the complexity?

Lots of tiny networks aimed at mobile devices: MobileNet, ShuffleNet, etc

Neural Architecture Search promises to automate architecture design

Topics

1. One time setup

Activation functions, data preprocessing, weight initialization, regularization

2. Training dynamics

Learning rate schedules; large-batch training; hyperparameter optimization

3. After training

Model ensembles, transfer learning

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1. One time setup

Activation functions, data preprocessing, weight initialization, regularization

2. Training dynamics

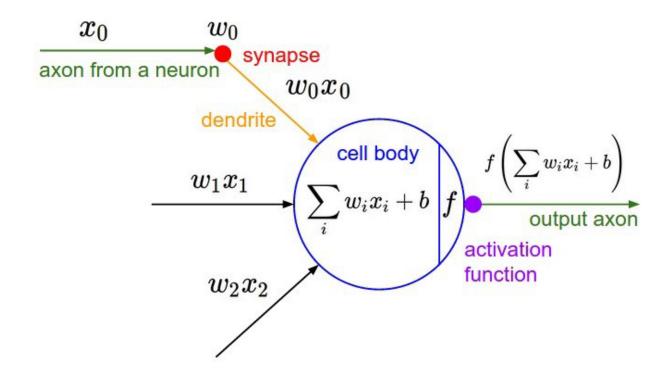
Learning rate schedules; large-batch training; hyperparameter optimization

3. After training

Model ensembles, transfer learning

Activation Functions

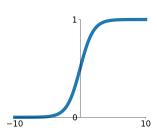
Activation Functions



Activation Functions

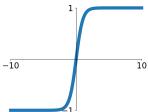
Sigmoid

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



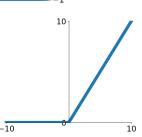
tanh

tanh(x)



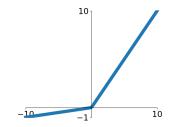
ReLU

 $\max(0, x)$



Leaky ReLU

 $\max(0.1x, x)$

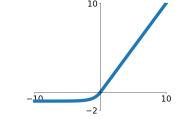


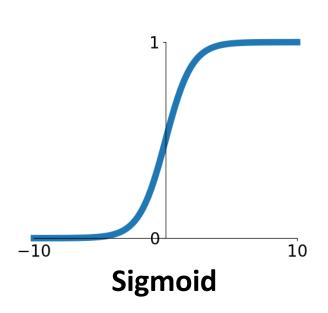
Maxout

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

ELU

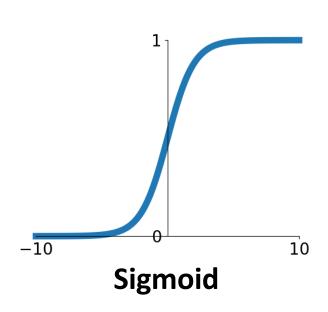
$$\begin{cases} x & x \ge 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$





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

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

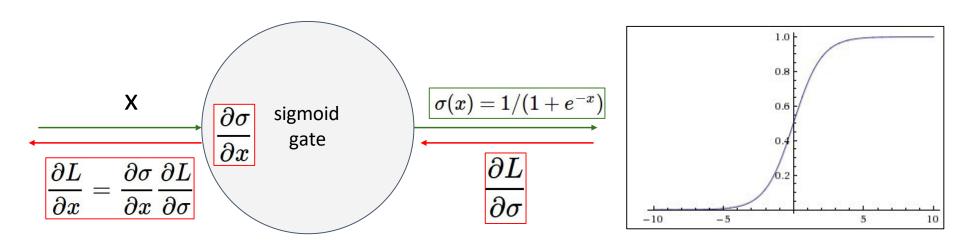


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3 problems:

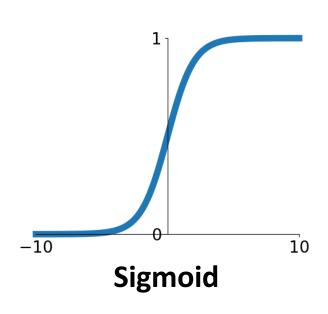
1. Saturated neurons "kill" the gradients



What happens when x = -10?

What happens when x = 0?

What happens when x = 10?

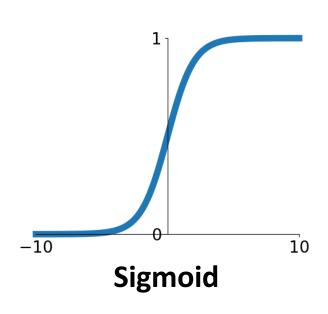


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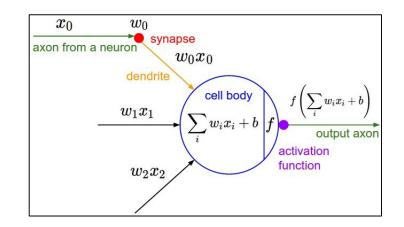
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3 problems:

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

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

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

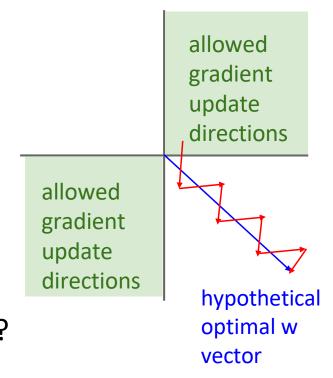


What can we say about the gradients on w?

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

$$f\left(\sum_i w_i x_i + b
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What can we say about the gradients on w? Always all positive or all negative :(



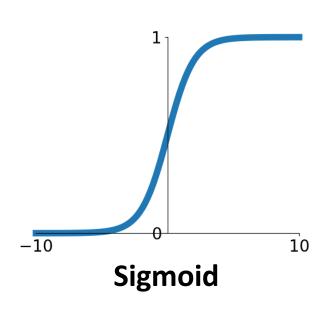
Consider what happens when the input to a neuron is always positive...

$$f\left(\sum_i w_i x_i + b
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What can we say about the gradients on w? Always all positive or all negative :(
(For a single element! Minibatches help)

allowed gradient update directions

allowed gradient update directions hypothetical optimal weector

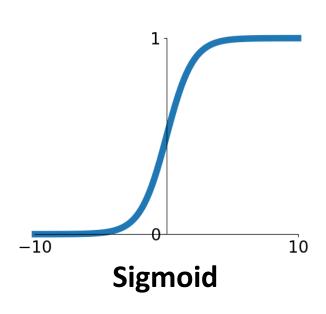


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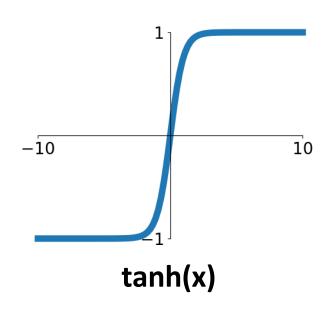
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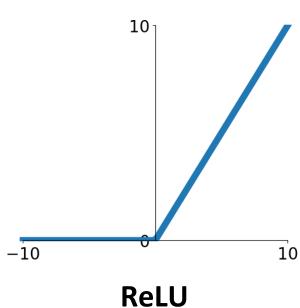
3 problems:

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

Activation Functions: Tanh



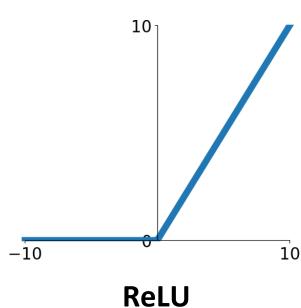
- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(



(Rectified Linear Unit)

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

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



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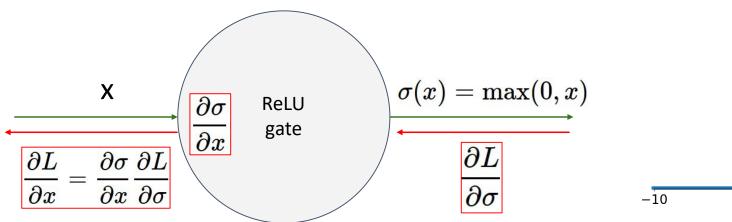
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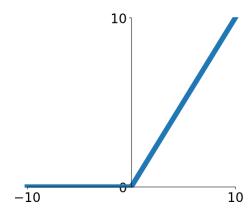
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- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?

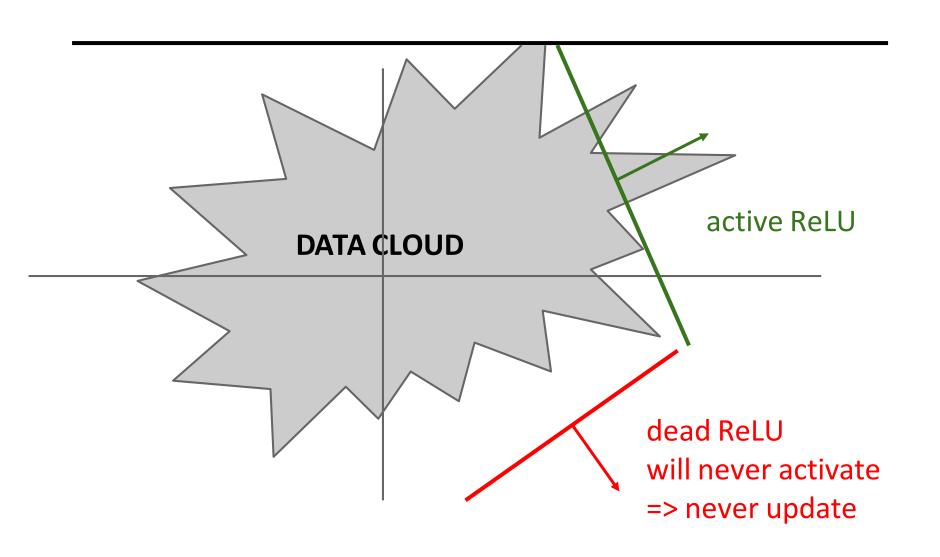


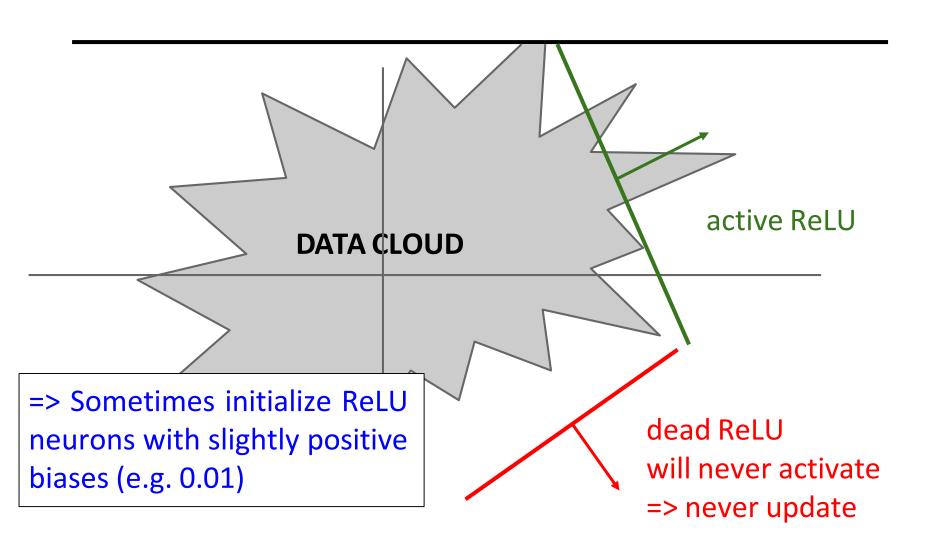


What happens when x = -10?

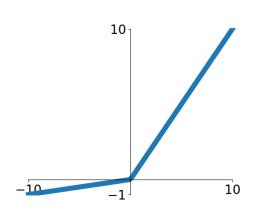
What happens when x = 0?

What happens when x = 10?





Activation Functions: Leaky ReLU

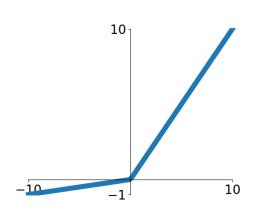


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- will not "die".

Leaky ReLU

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

Activation Functions: Leaky ReLU

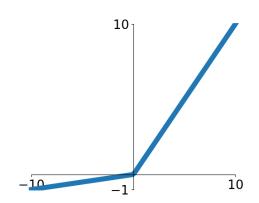


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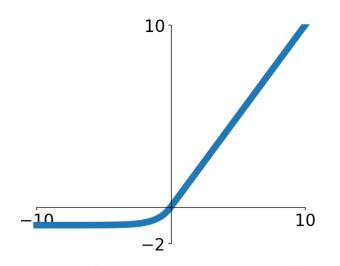
Parametric Rectifier (PReLU)

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

backprop into \alpha (parameter)

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

Activation Functions: Exponential Linear Unit (ELU)

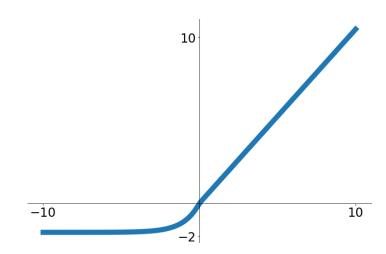


$$f(x) = \begin{cases} x & \text{if } x > 0\\ \alpha \ (\exp(x) - 1) & \text{if } x \le 0 \end{cases}$$
(Default alpha=1)

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

Computation requires exp()

Activation Functions: Scaled Exponential Linear Unit (SELU)

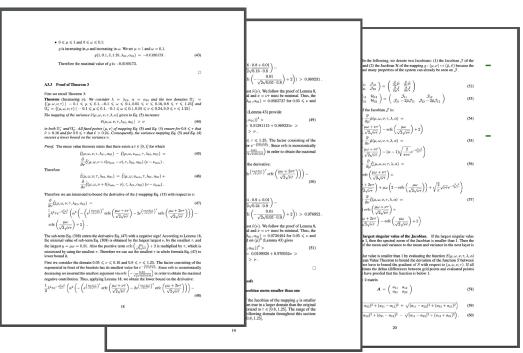


$$selu(x) = \begin{cases} \lambda x & \text{if } x < 0 \\ \lambda (\alpha e^x - \alpha) & \text{otherwise} \end{cases}$$

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

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

Activation Functions: Scaled Exponential Linear Unit (SELU)



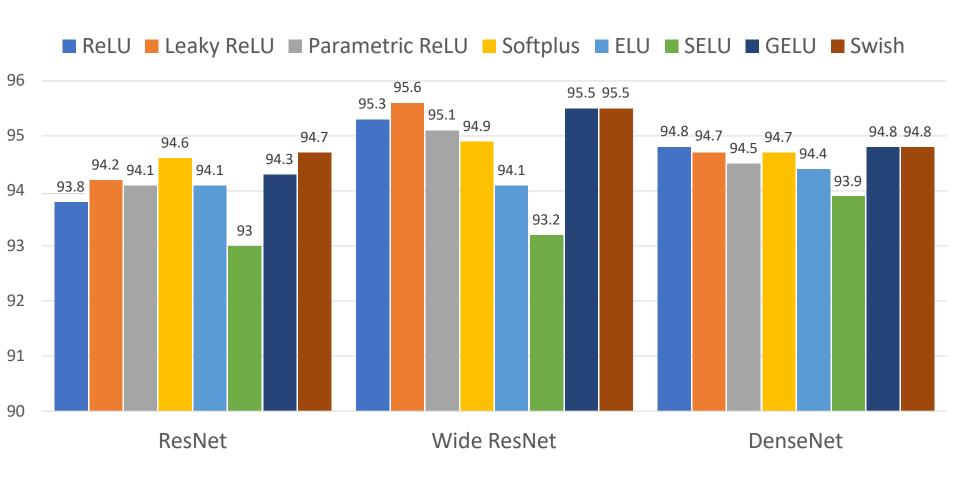
Scaled version of ELU that works better for deep networks "Self-Normalizing" property; can train deep SELU networks without BatchNorm

Derivation takes 91 pages of math in appendix...

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

Accuracy on CIFAR10

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

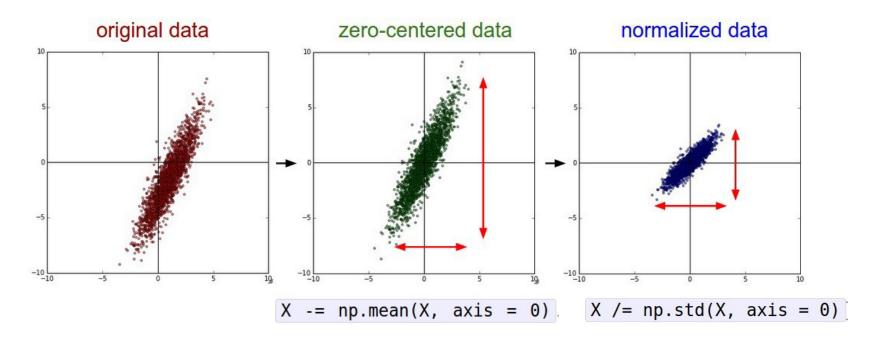


Activation Functions: Summary

- 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

Data Preprocessing

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...

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

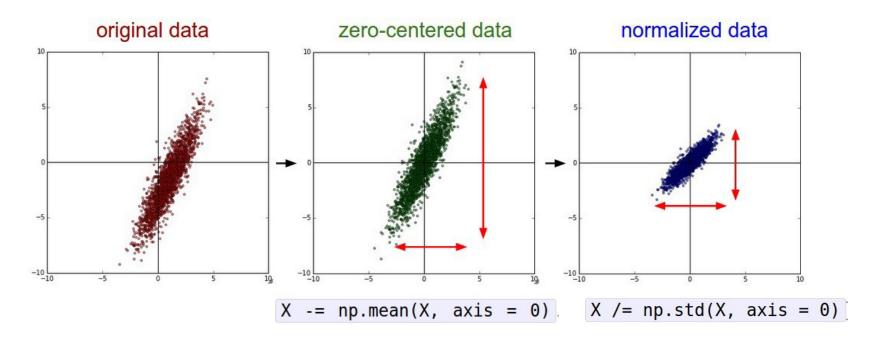
What can we say about the gradients on w? Always all positive or all negative :(
(this is also why you want zero-mean data!)

allowed gradient update directions

allowed gradient update directions

hypothetical optimal w vector

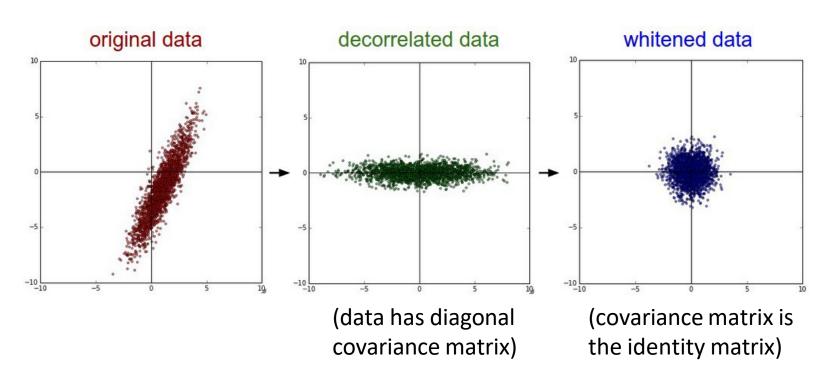
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Data Preprocessing

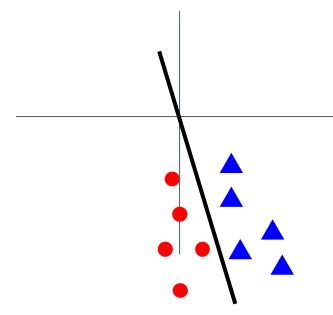
In practice, you may also see PCA and Whitening of the data

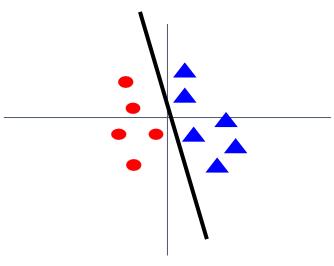


Data Preprocessing

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



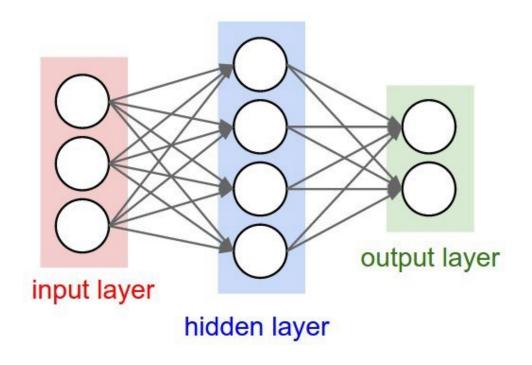


Data Preprocessing for Images

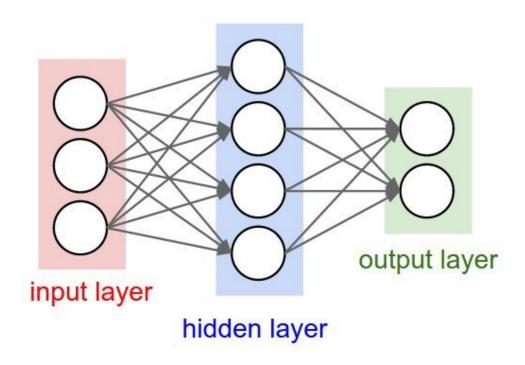
```
e.g. consider CIFAR-10 example with [32,32,3] images
```

- 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



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



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

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

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

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

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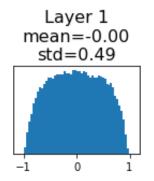
Works ~okay for small networks, but problems with deeper networks.

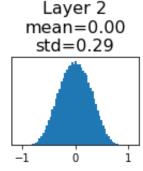
```
dims = [4096] * 7 Forward pass for a 6-layer
hs = [] net with hidden size 4096
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

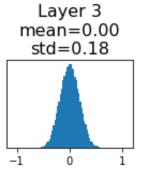
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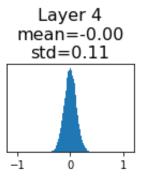
All activations tend to zero for deeper network layers

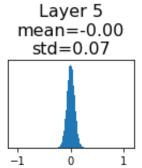
Q: What do the gradients dL/dW look like?

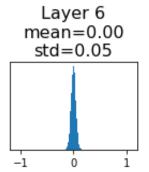










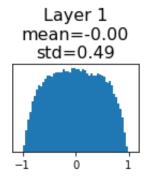


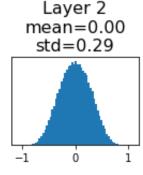
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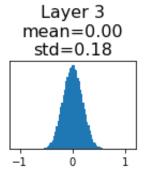
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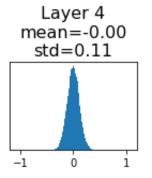
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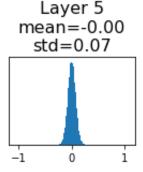
A: All zero, no learning =(

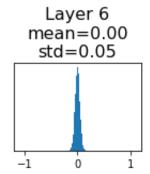






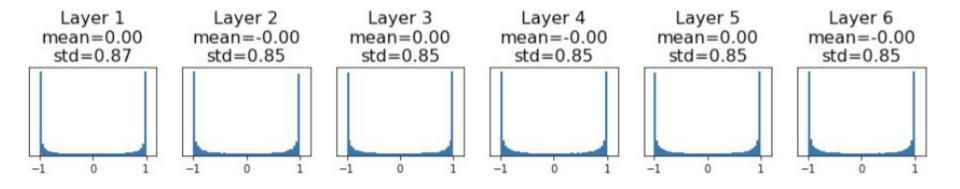






All activations saturate

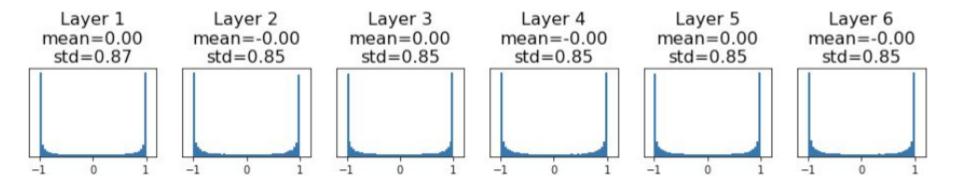
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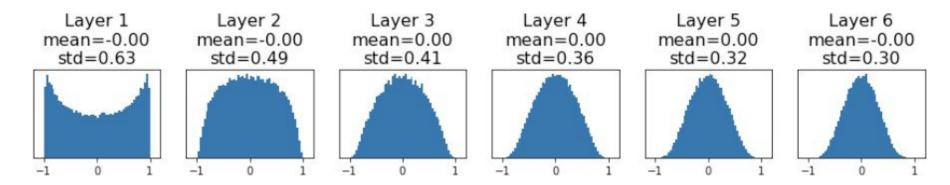
Q: What do the gradients look like?

A: Local gradients all zero, no learning =(



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

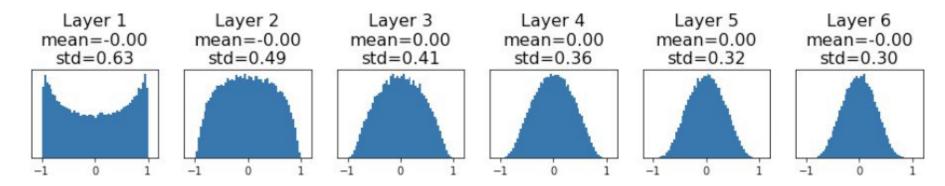
"Just right": Activations are nicely scaled for all layers!



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

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

For conv layers, Din is kernel_size² * input_channels



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

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

Derivation: Variance of output = Variance of input

$$y = Wx y_i = \sum_{j=1}^{D_{in}} x_j w_j$$

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

Derivation: Variance of output = Variance of input

$$y = Wx$$

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

$$Var(y_i) = D_{in}Var(x_iw_j)$$

[Assume x, w are iid]

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

Derivation: Variance of output = Variance of input

$$y = Wx y_i = \sum_{j=1}^{D_{in}} x_j w_j$$

 $Var(y_i) = D_{in}Var(x_iw_i)$

[Assume x, w are iid]

=
$$D_{in} * (E[x_i^2]E[w_i^2] - E[x_i]^2 E[w_i]^2)$$
[Assume x, w independent]

$$= D_{in} * Var[x_i] * Var[w_i]$$

[Assume x, w are zero-mean]

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

Derivation: Variance of output = Variance of input

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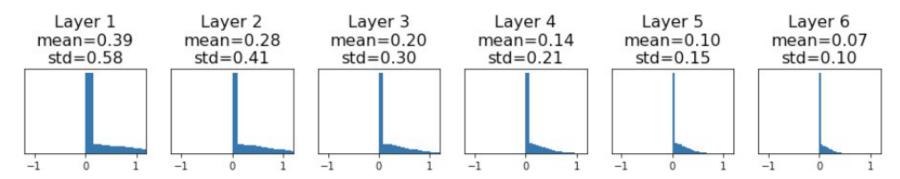
If
$$Var(w_i) = 1/D_{in}$$
 then $Var(y_i) = Var(x_i)$

Weight Initialization: What about ReLU?

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Xavier assumes zero centered activation function

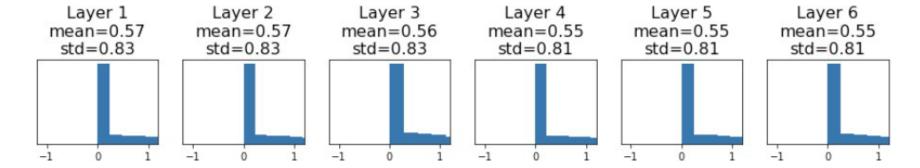
Activations collapse to zero again, no learning =(



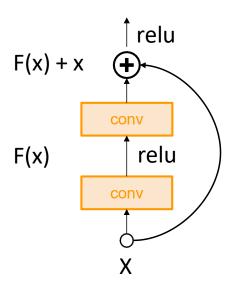
Weight Initialization: Kaiming / MSRA Initialization

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

"Just right" – activations nicely scaled for all layers



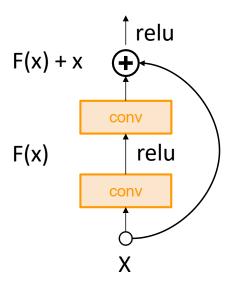
Weight Initialization: Residual Networks



Residual Block

If we initialize with MSRA: then Var(F(x)) = Var(x)But then Var(F(x) + x) > Var(x) - variance grows with each block!

Weight Initialization: Residual Networks

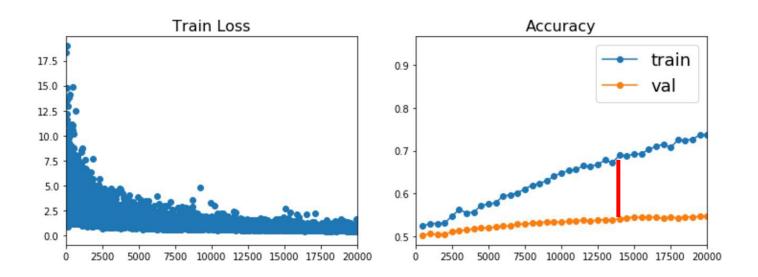


Residual Block

If we initialize with MSRA: then Var(F(x)) = Var(x)But then Var(F(x) + x) > Var(x) - variance grows with each block!

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

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



Regularization

Regularization: Add term to the loss

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

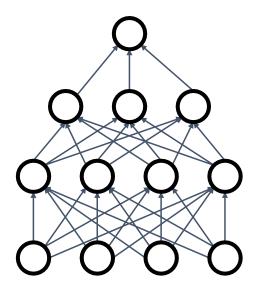
In common use:

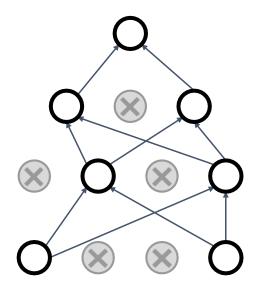
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

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

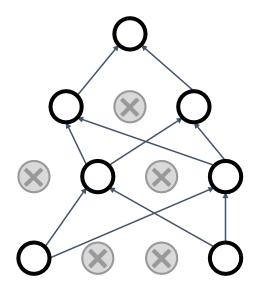
In each forward pass, randomly set some neurons to zero Probability of dropping is a hyperparameter; 0.5 is common

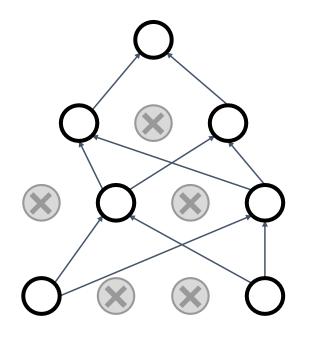




```
p = 0.5 # probability of keeping a unit active. higher = less dropout
def train_step(X):
  """ X contains the data """
  # forward pass for example 3-layer neural network
 H1 = np.maximum(0, np.dot(W1, X) + b1)
 U1 = np.random.rand(*H1.shape) < p # first dropout mask
 H1 *= U1 # drop!
 H2 = np.maximum(0, 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)
```

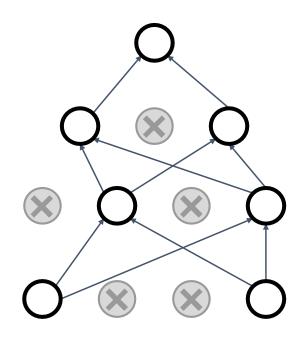
Example forward pass with a 3-layer network using dropout





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





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 makes our output random!

Output Input (label) (image)
$$y = f_W(x,z) \quad \text{Random} \quad \text{mask}$$

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

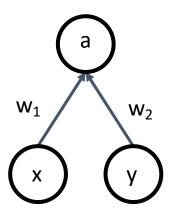
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

But this integral seems hard ...

Want to approximate the integral

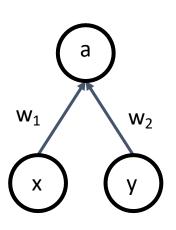
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

Consider a single neuron.



Want to approximate the integral

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

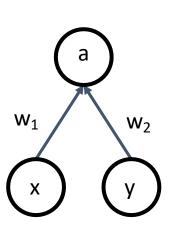


Consider a single neuron.

At test time we have:
$$E[a] = w_1x + w_2y$$

Want to approximate the integral

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



Consider a single neuron.

$$E[a] = w_1 x + w_2 y$$

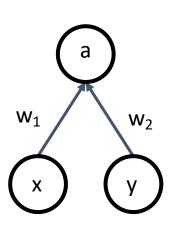
$$E[a] = \frac{1}{4}(w_1 x + w_2 y) + \frac{1}{4}(w_1 x + 0 y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2 y)$$

$$= \frac{1}{2}(w_1 x + w_2 y)$$

Dropout: Test Time

Want to approximate the integral

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



Consider a single neuron.

At test time we have:

During training we have:

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

$$E[a] = w_1 x + w_2 y$$

$$E[a] = \frac{1}{4}(w_1x + w_2y) + \frac{1}{4}(w_1x + 0y) + \frac{1}{4}(0x + 0y) + \frac{1}{4}(0x + w_2y) + \frac{1}{4}(0x + w_2y) + \frac{1}{4}(0x + w_2y)$$

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

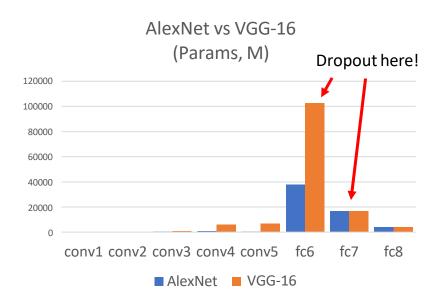
scale at test time

More common: "Inverted dropout"

```
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!
                                                                             Drop and scale
 H1 *= U1 # drop!
  H2 = np.maximum(0, np.dot(W2, H1) + b2)
                                                                            during training
  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)
                                                                     test time is unchanged!
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
```

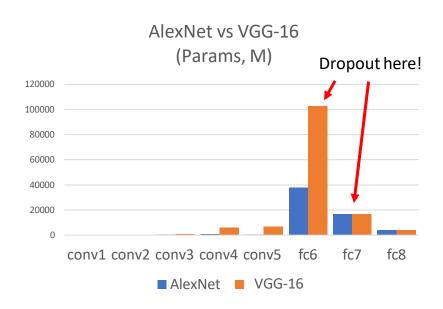
Dropout architectures

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



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!

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

Example: Batch Normalization

Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

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)

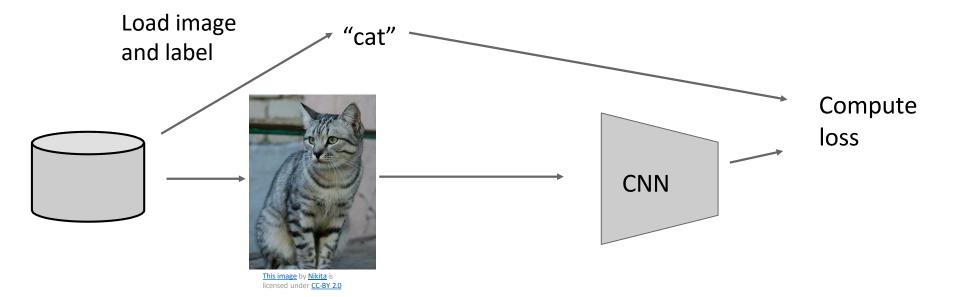
$$y = f(x) = E_z[f(x,z)] = \int p(z)f(x,z)dz$$

Example: Batch Normalization

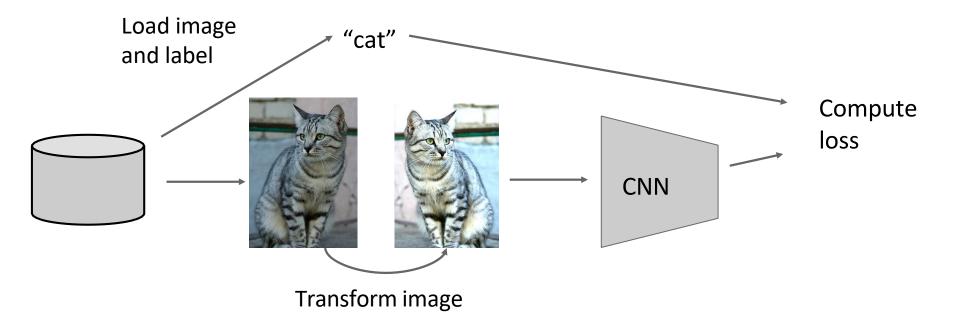
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Data Augmentation



Data Augmentation



Data Augmentation: Horizontal Flips



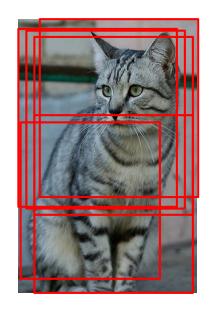


Data Augmentation: Random Crops and Scales

Training: sample random crops / scales

ResNet:

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

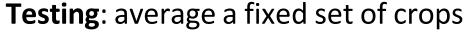


Data Augmentation: Random Crops and Scales

Training: sample random crops / scales

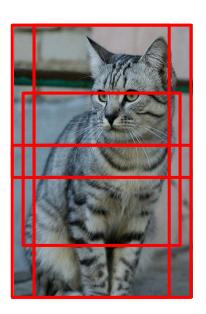
ResNet:

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



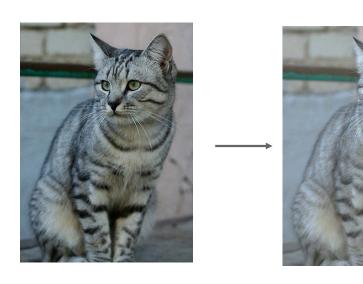
ResNet:

- 1. Resize image at 5 scales: {224, 256, 384, 480, 640}
- 2. For each size, use 10 224 x 224 crops: 4 corners + center, + flips



Data Augmentation: Color Jitter

Simple: Randomize contrast and brightness



More Complex:

- Apply PCA to all [R, G, B] pixels in training set
- Sample a "color offset" along principal component directions
- 3. Add offset to all pixels of a training image

(Used in AlexNet, ResNet, etc)

Data Augmentation: Get creative for your problem!

Random mix/combinations of:

- translation
- rotation
- stretching
- shearing,
- lens distortions, ... (go crazy)

Training: Add some randomness

Testing: Marginalize over randomness

Examples:

Dropout

Batch Normalization

Data Augmentation

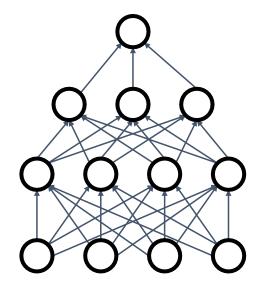
Regularization: DropConnect

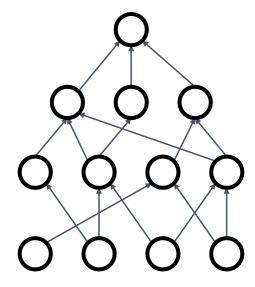
Training: Drop random connections between neurons (set weight=0)

Testing: Use all the connections

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect





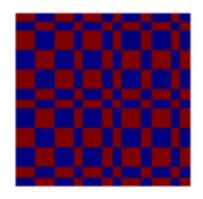
Regularization: Fractional Pooling

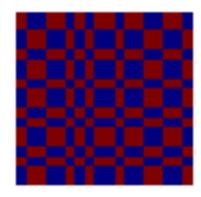
Training: Use randomized pooling regions

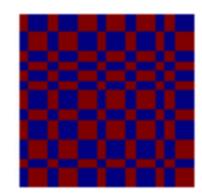
Testing: Average predictions over different samples

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling







Regularization: Stochastic Depth

Training: Skip some residual blocks in ResNet

Testing: Use the whole network

Examples:

Dropout

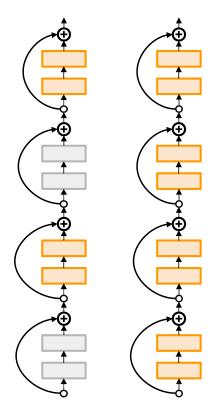
Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth



Regularization: Cutout

Training: Set random images regions to 0

Testing: Use the whole 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

Regularization: Mixup

Training: Train on random blends of images

Testing: Use original images

1.0 0.8 0.6 0.4 0.2 0.0 0.2 0.4 0.6 0.8 1.0

Sample blend probability from a beta distribution Beta(a, b) with a=b≈0 so blend weights are close to 0/1

Examples:

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







CNN Target label: cat: 0.4 dog: 0.6

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

Regularization: Mixup

Training: Train on random blends of images

Testing: Use original images

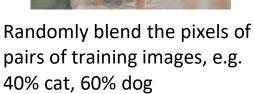
Examples:

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









CNN Target label: cat: 0.4 dog: 0.6

Regularization: CutMix

Training: Train on local mixture of images

Testing: Use original images

Examples:

Mixup

CutMix

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







CNN Target label: cat: 0.2 dog: 0.8

Randomly composite the patch and image from pairs of training images, e.g. 20% cat, 80% dog (proportional to the regional size)

Regularization

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

CutMix

- Consider dropout for large fullyconnected layers
- Batch normalization and data augmentation almost always a good idea
- Try cutout/mixup/cutMix especially for small classification datasets

Next Time: Training Neural Networks