Lecture 8:
Training Neural Networks

Overview

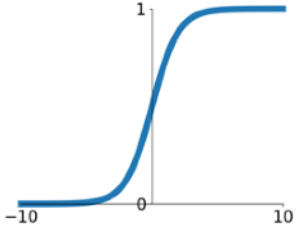
- **One time setup:** activation functions, preprocessing, weight initialization, regularization, gradient checking
- **Training dynamics:** babysitting the learning process, parameter updates, data augmentation, hyperparameter optimization
- **Evaluation:** model ensembles

Recap: Activation Functions

Activation Functions

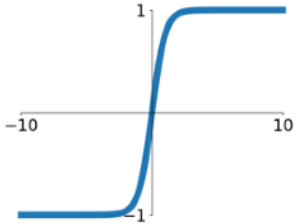
Sigmoid

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



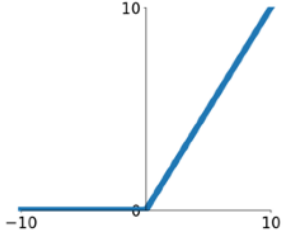
tanh

$$\tanh(x)$$



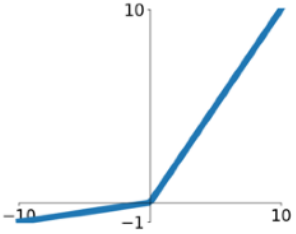
ReLU

$$\max(0, x)$$



Leaky ReLU

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

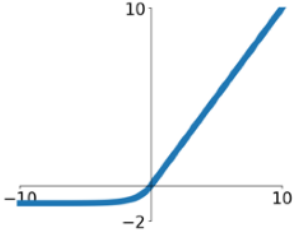


Maxout

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

ELU

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

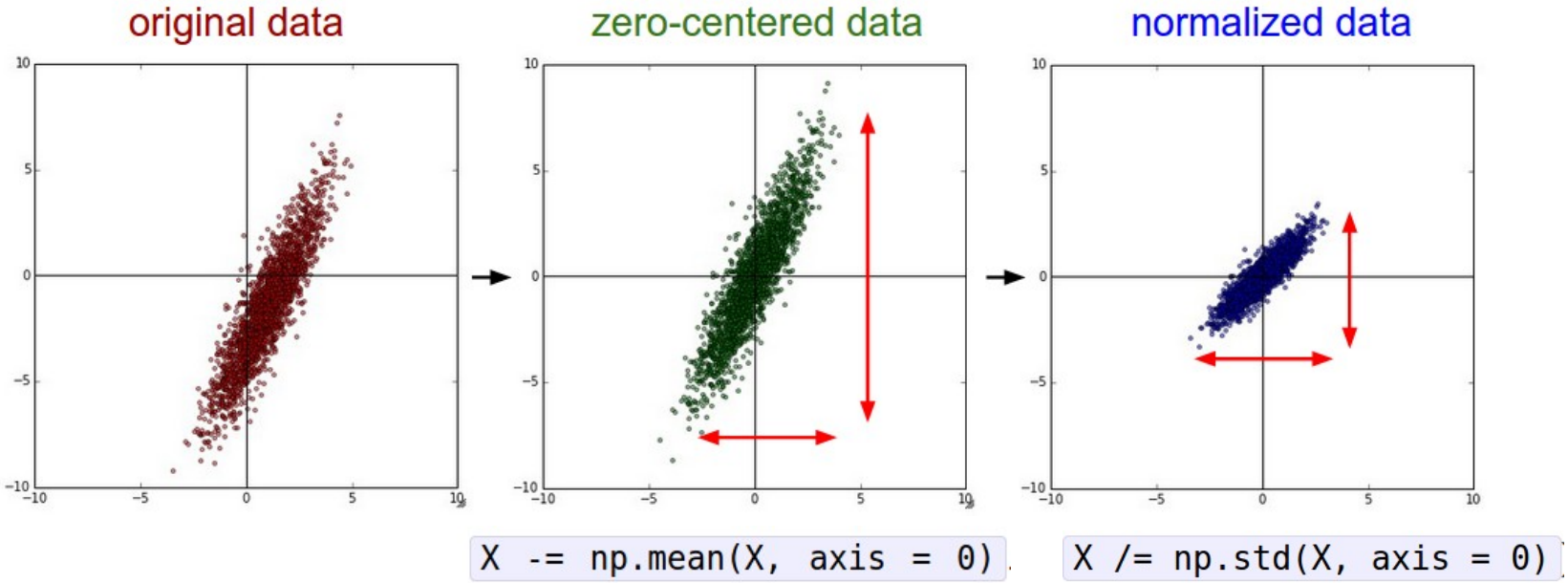


TLDR: In practice:

- Use ReLU. Be careful with your learning rates
- Try out Leaky ReLU / Maxout / ELU / SELU
  - To squeeze out some marginal gains
- Don’t use sigmoid or tanh

Recap: Data Preprocessing

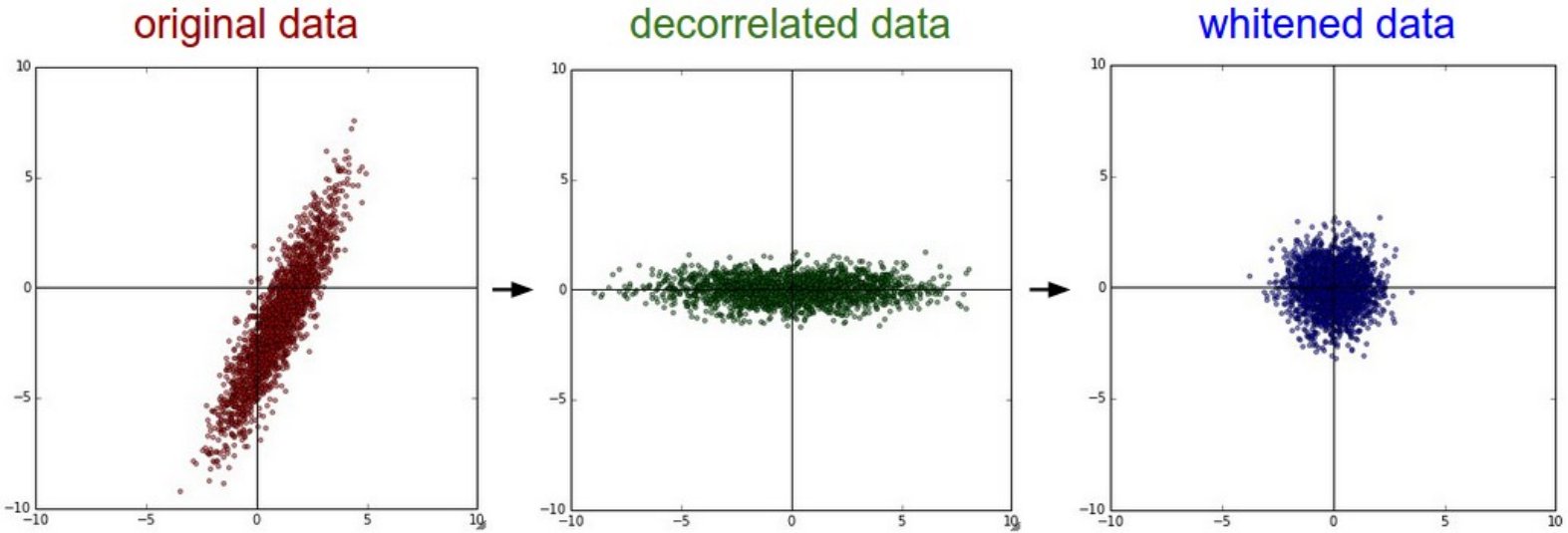
Step 1: Preprocess the data



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

Step 1: Preprocess the data

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



(data has diagonal covariance matrix)

(covariance matrix is the identity matrix)

In practice for Images: center only

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)

Not common to normalize variance, to do PCA or whitening

Recap: Weight Initialization

- 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

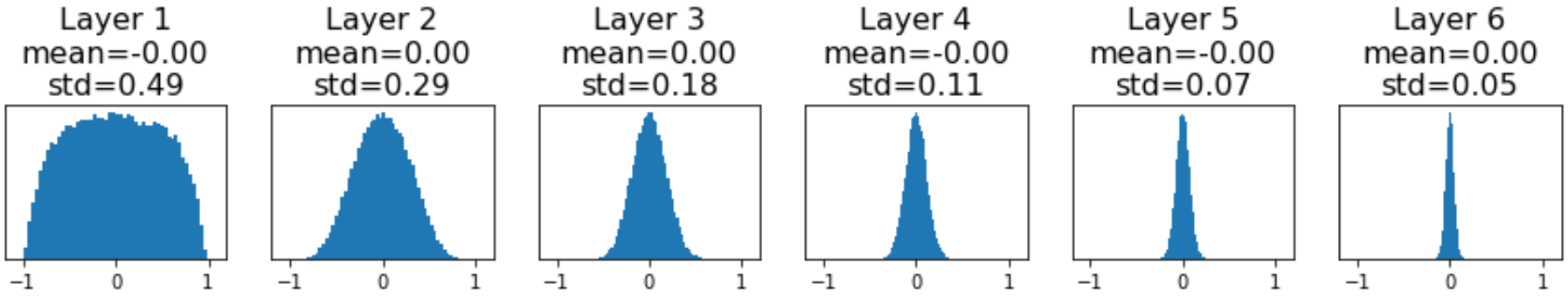
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

A: All zero, no learning =(



Weight Initialization: Activation statistics

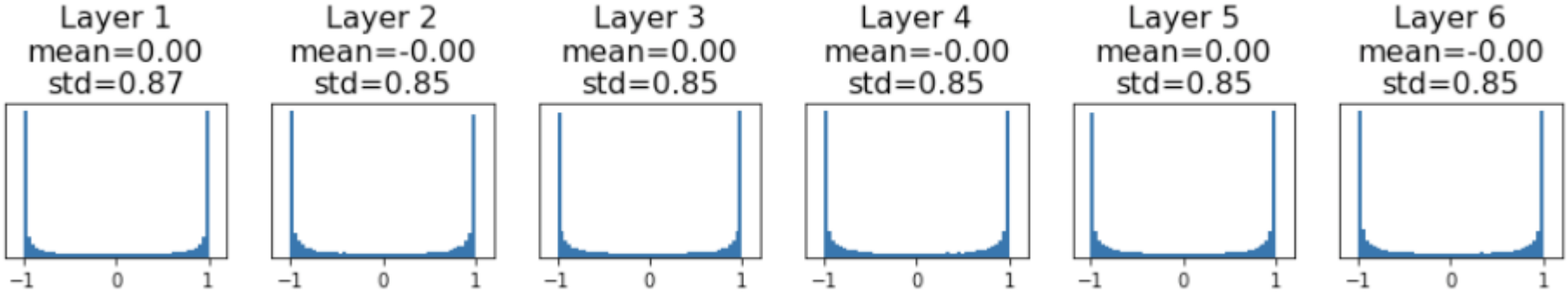
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.05 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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 =(

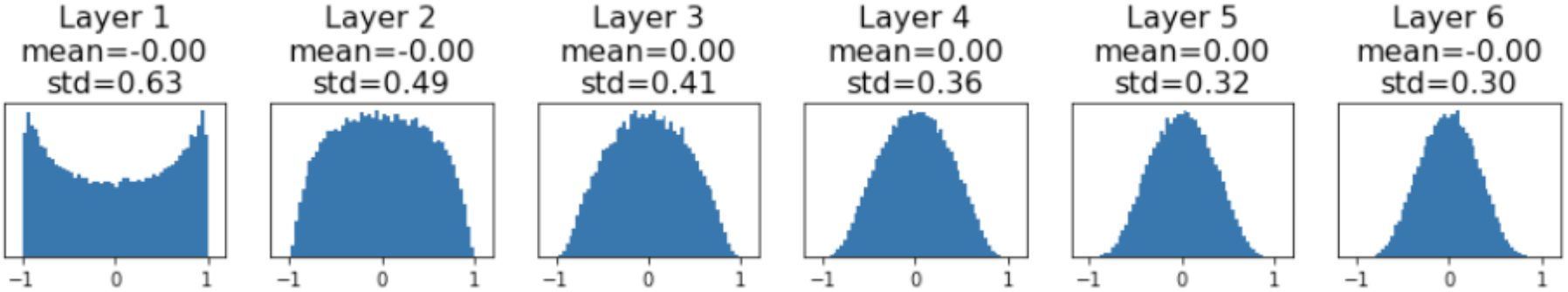


Weight Initialization: “Xavier” Initialization

```
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!



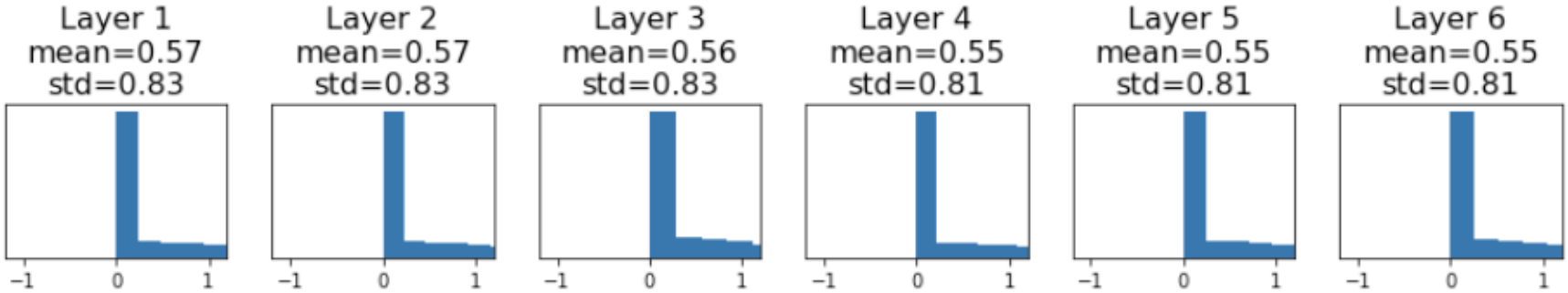
Glorot and Bengio, “Understanding the difficulty of training deep feedforward neural networks”, AISTAT 2010

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!

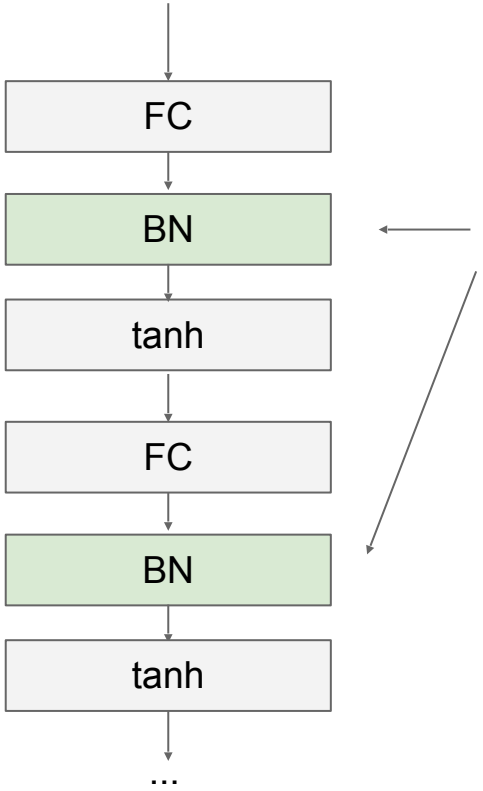


He et al, "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification", ICCV 2015

Recap: Batch Normalization

Batch Normalization

[Ioffe and Szegedy, 2015]



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) 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]

"you want unit Gaussian activations? just make them so."
Not actually "Gaussian". Just zero mean, unit variance.

consider a batch of activations at some layer.
To make each dimension unit normalized,
apply:

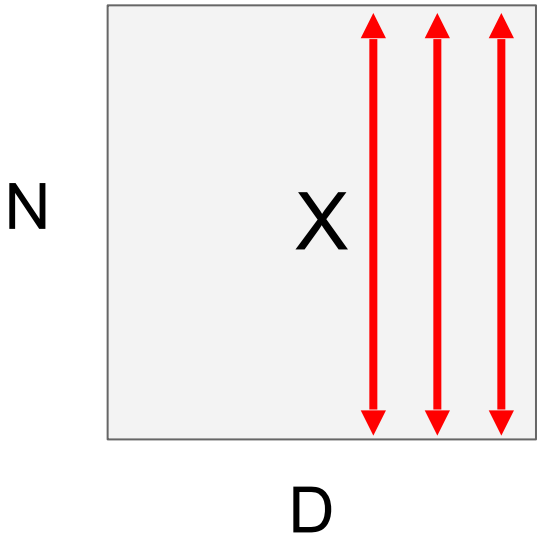
$$\widehat{x}^{(k)} = \frac{x^{(k)} - \mathrm{E}[x^{(k)}]}{\sqrt{\mathrm{Var}[x^{(k)}]}}$$

this is a vanilla differentiable function...

Batch Normalization

[Ioffe and Szegedy, 2015]

"you want unit Gaussian activations?
just make them so." (you want NORMALIZED activations)



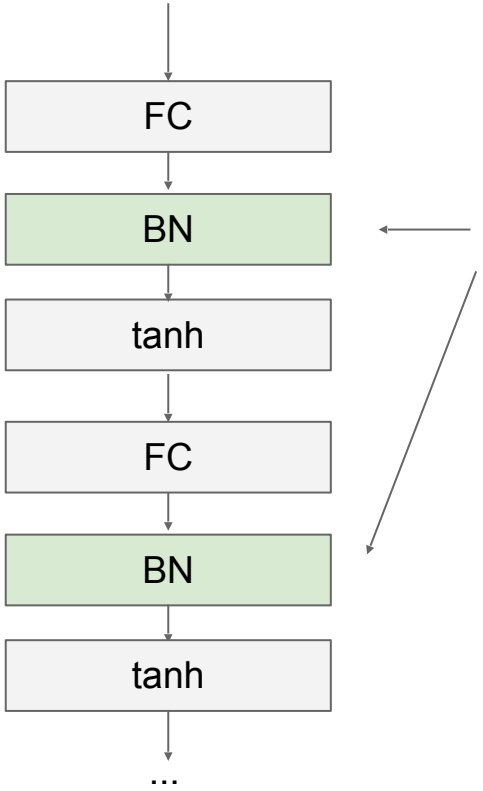
1. compute the empirical mean and variance independently for each dimension.

2. Normalize

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

Batch Normalization

[Ioffe and Szegedy, 2015]



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) 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]

Normalize:

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

And then allow the network to squash the range if it wants to:

$$y^{(k)} = \gamma^{(k)}\widehat{x}^{(k)} + \beta^{(k)}$$

Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\mathrm{Var}[x^{(k)}]}$$

$$\beta^{(k)} = \mathrm{E}[x^{(k)}]$$

to recover the identity mapping.

Batch Normalization

[Ioffe and Szegedy, 2015]

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$;
Parameters to be learned: γ, β

Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m} x_i \qquad \text{// mini-batch mean}$$

$$\sigma^2_{\mathcal{B}} \leftarrow \frac{1}{m}\sum_{i=1}^{m}(x_i - \mu_{\mathcal{B}})^2 \qquad \text{// mini-batch variance}$$

$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

Batch Normalization

[Ioffe and Szegedy, 2015]

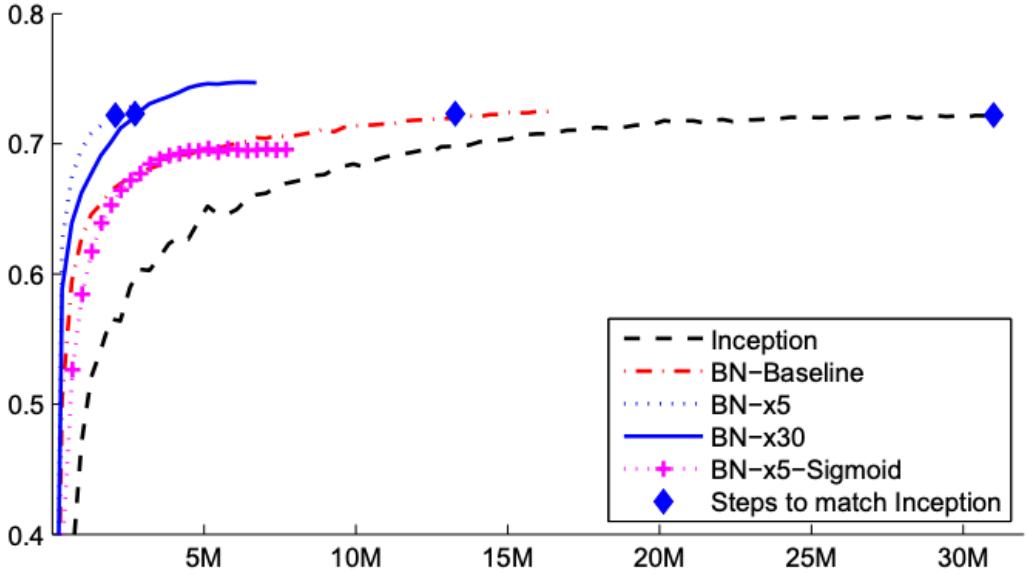


Figure 2: *Single crop validation accuracy of Inception and its batch-normalized variants, vs. the number of training steps.*

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

Batch Normalization

[Ioffe and Szegedy, 2015]

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$$y_i \leftarrow \gamma\widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i) \qquad \text{// scale and shift}$$

Note: At test time BatchNorm layer functions differently:

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

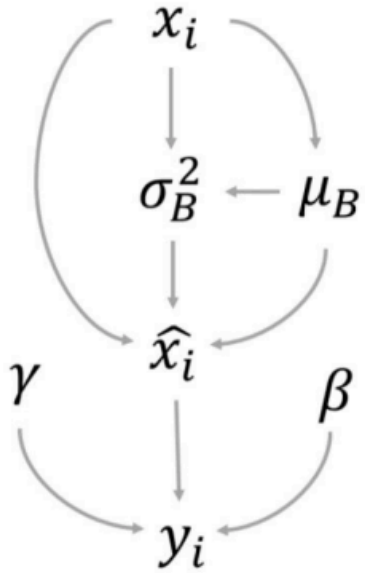
(e.g. can be estimated during training with running averages)

Batch Normalization

[Ioffe and Szegedy, 2015]

Forward pass:

$$\mu_B = \frac{1}{m}\sum x_i$$
$$\sigma_B^2 = \frac{1}{m}\sum (x_i - \mu_B)^2$$
$$\hat{x}_i = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$
$$y_i = \gamma \hat{x}_i + \beta$$

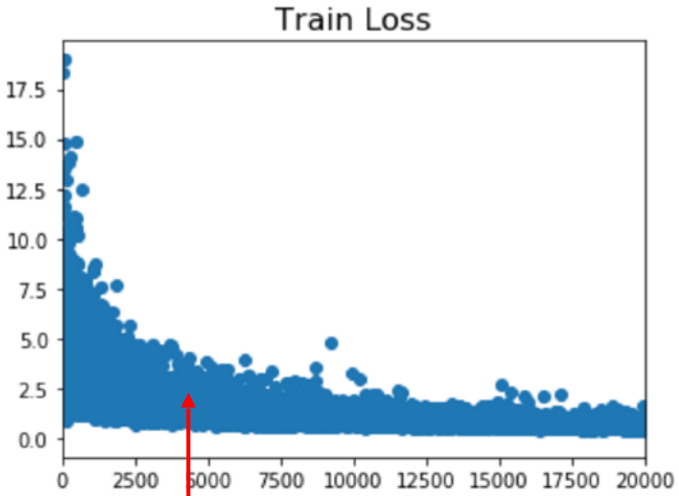


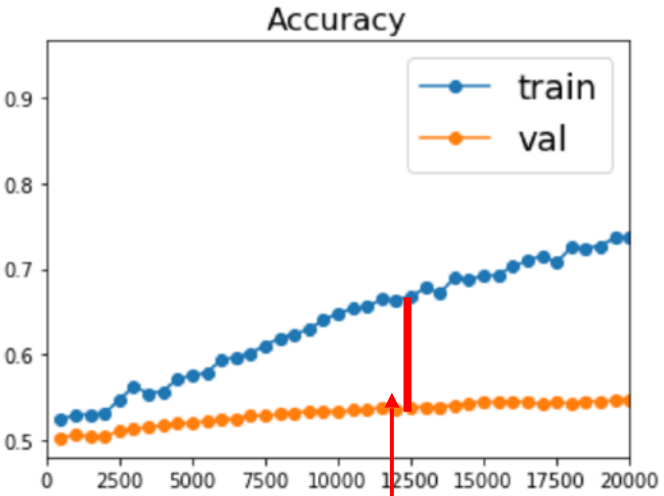
Backward pass:

$$\frac{\partial l}{\partial x_i} = \frac{\partial l}{\partial \sigma_B^2}\frac{\partial \sigma_B^2}{\partial x_i} + \frac{\partial l}{\partial \mu_B}\frac{\partial \mu_B}{\partial x_i} + \frac{\partial l}{\partial \hat{x}_i}\frac{\partial \hat{x}_i}{\partial x_i}$$

Training vs. Test Error

Beyond Training Error

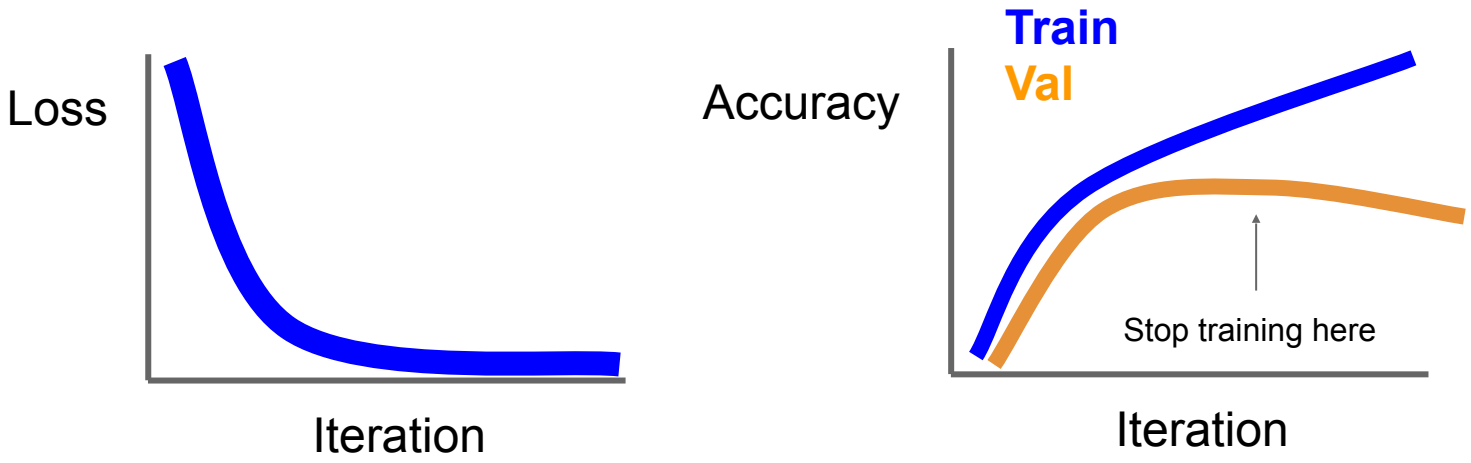




Better optimization algorithms help reduce training loss

But we really care about error on new data - how to reduce the gap?

Early Stopping: Always do this



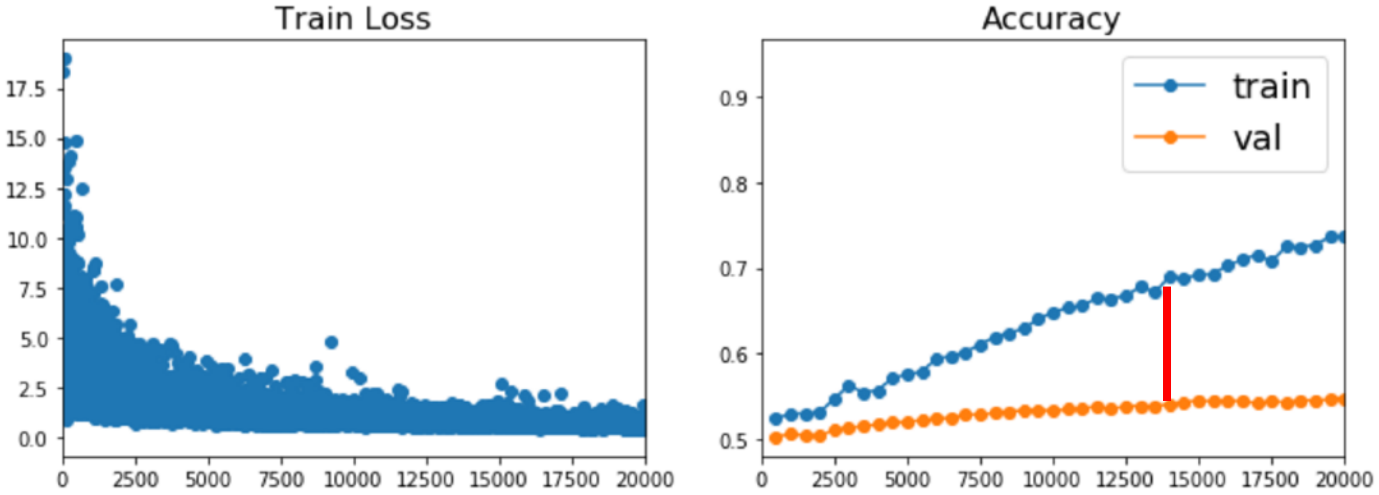
Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot that worked best on val

Model Ensembles

1. Train multiple independent models
2. At test time average their results
   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

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:

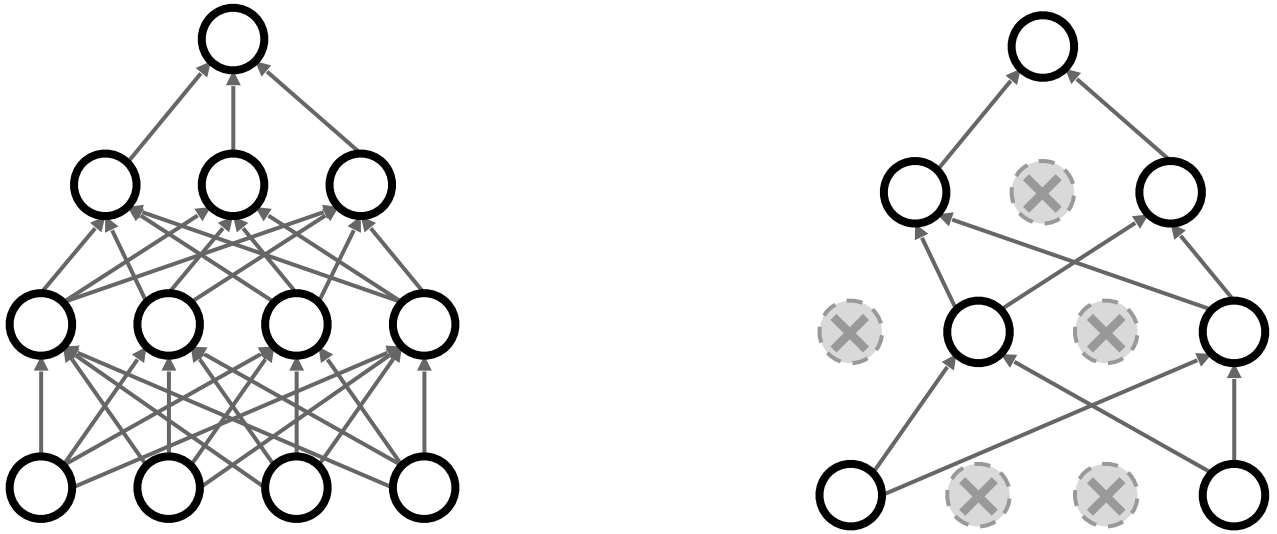
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

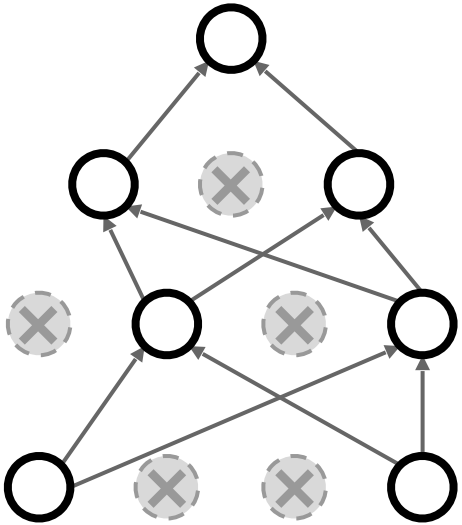


Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

Regularization: Dropout

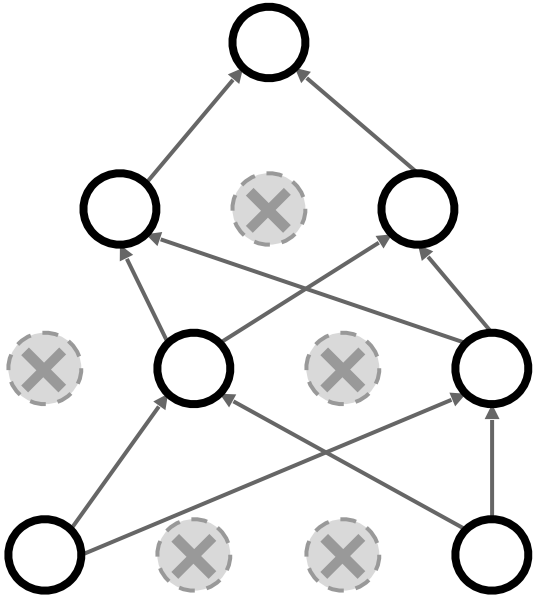
```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

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



Regularization: Dropout

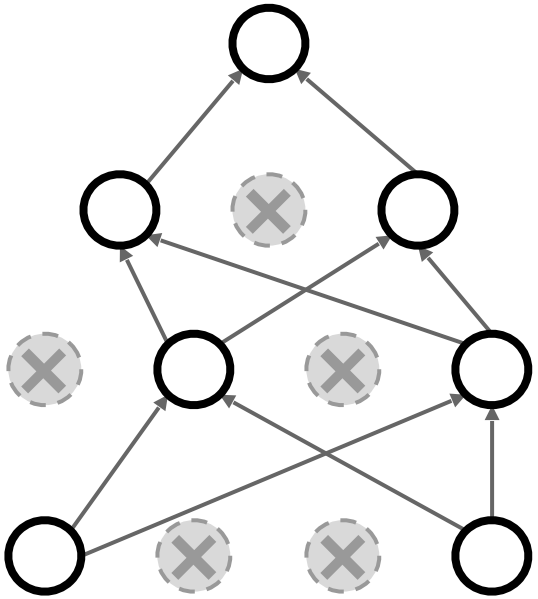
How can this possibly be a good idea?



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

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

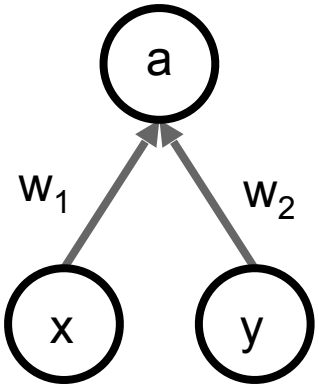
But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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

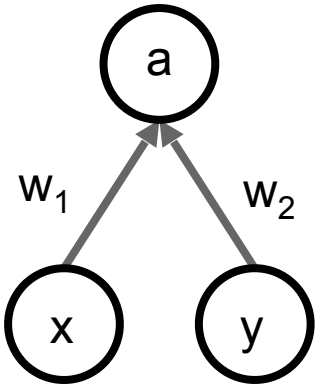
Consider a single neuron.



Dropout: Test time

Want to approximate the integral

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



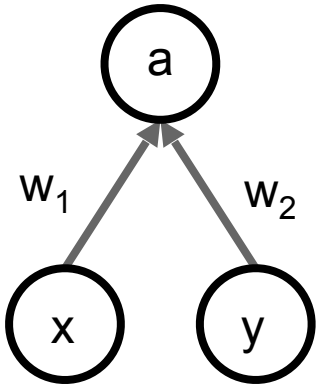
Consider a single neuron.

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

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: $E\big[a\big] = w_1 x + w_2 y$

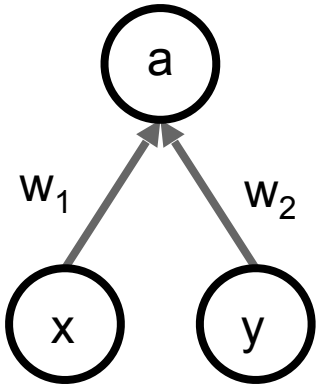
During training we have:

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

Dropout: Test time

Want to approximate the integral

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



Consider a single neuron.

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

During training we have:

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

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 train time

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)

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

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

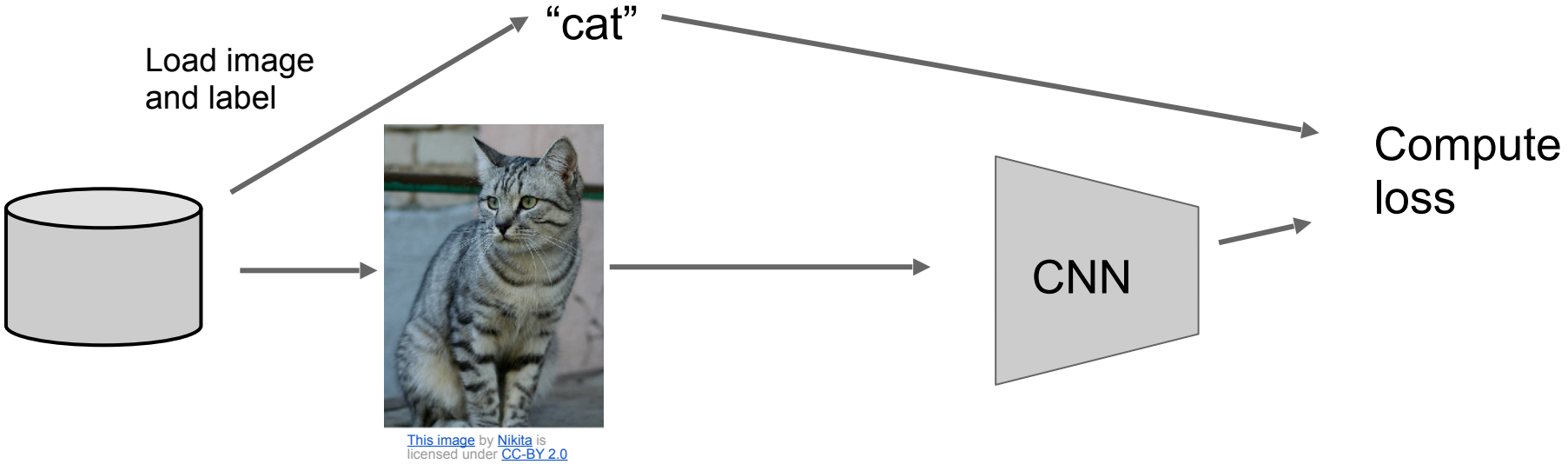
$$y = f(x) = E_z\big[f(x, z)\big] = \int p(z) f(x, z) dz$$

Example: Batch Normalization

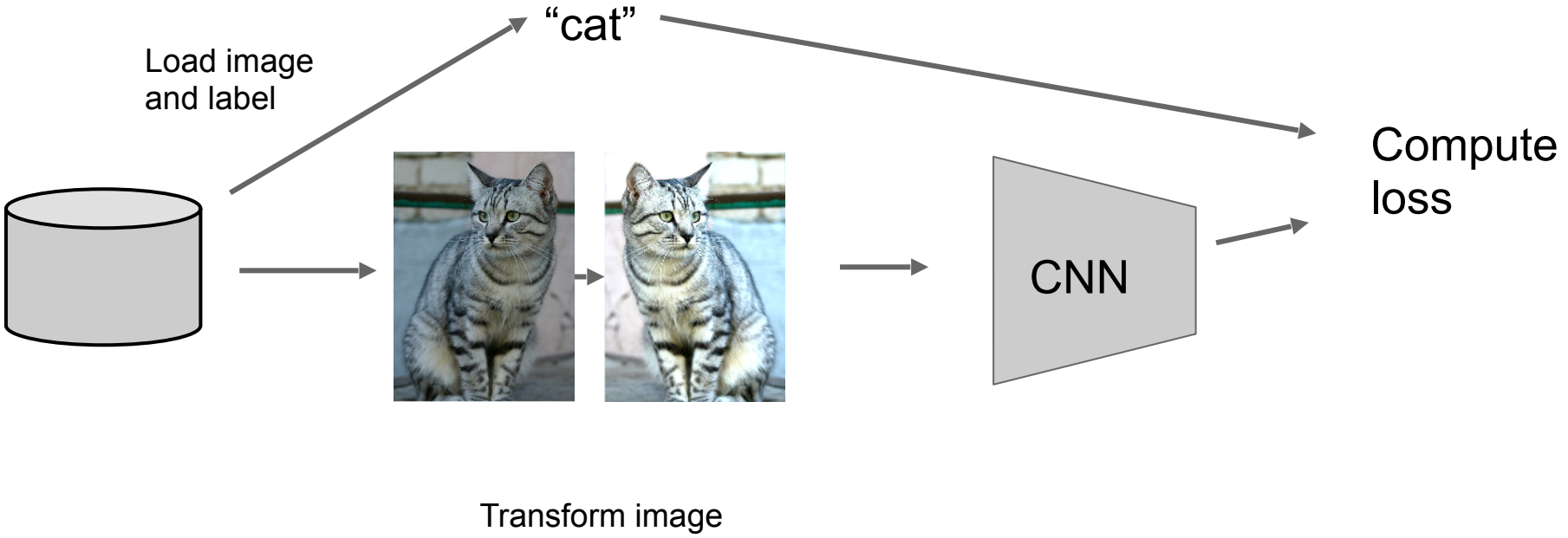
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

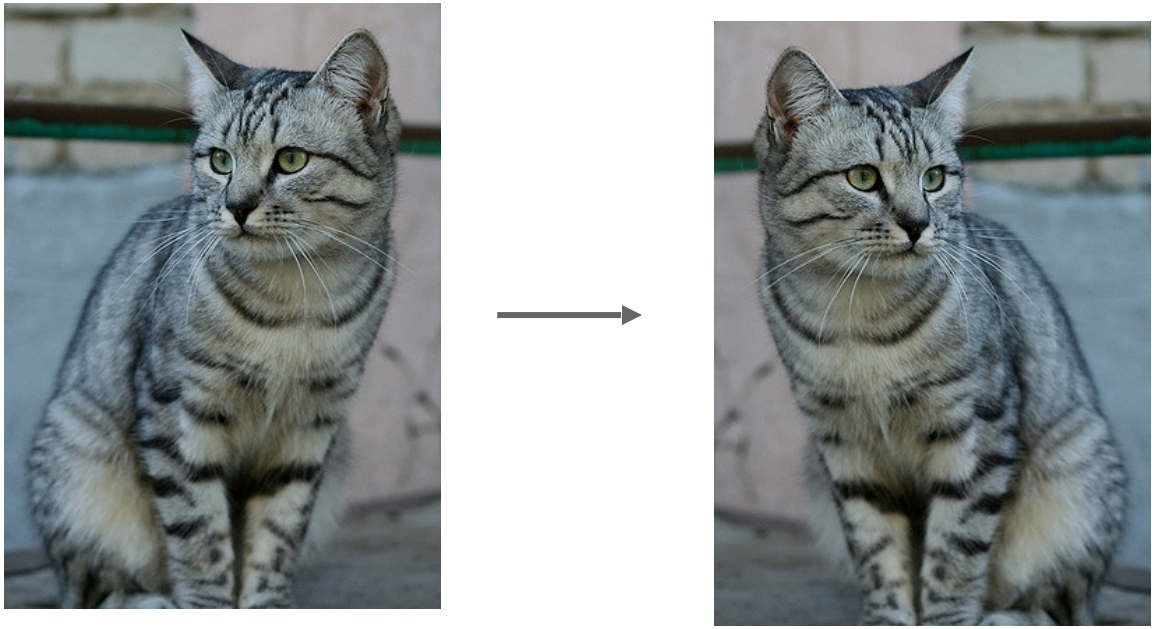
Regularization: Data Augmentation



Regularization: Data Augmentation



Data Augmentation
Horizontal Flips

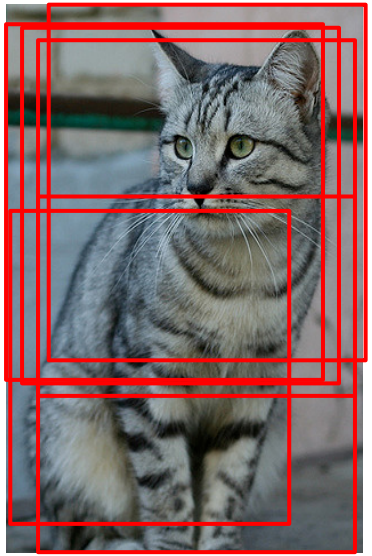


Data Augmentation
Random crops and scales

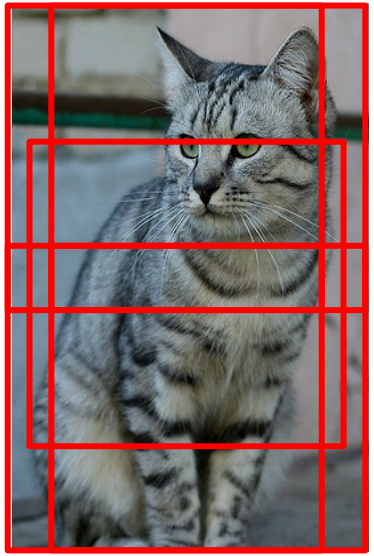
Training: sample random crops / scales

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
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

Testing: average a fixed set of crops

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

Data Augmentation
Color Jitter

Simple: Randomize contrast and brightness

More Complex:

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

(As seen in *[Krizhevsky et al. 2012],* ResNet, etc)

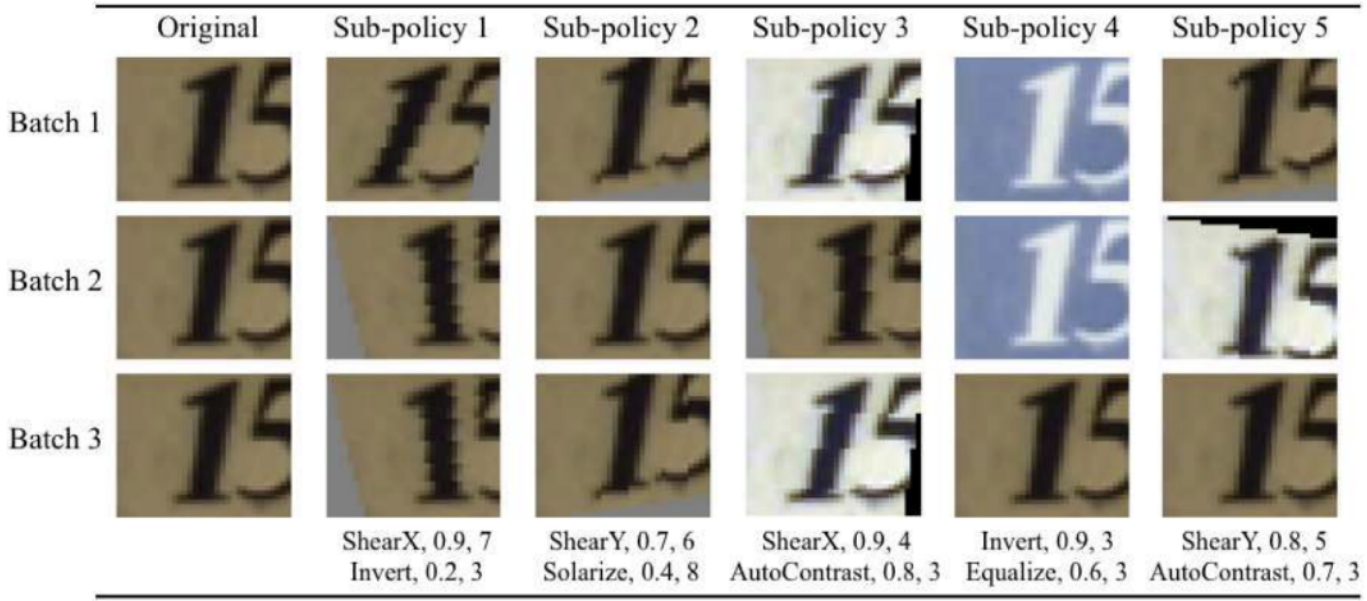
Data Augmentation

Get creative for your problem!

Examples of data augmentations:

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

Automatic Data Augmentation



Cubuk et al., “AutoAugment: Learning Augmentation Strategies from Data”, CVPR 2019

Regularization: A common pattern

Training: Add random noise

Testing: Marginalize over the noise

Examples:

Dropout

Batch Normalization

Data Augmentation

Regularization: DropConnect

Training: Drop connections between neurons (set weights to 0)

Testing: Use all the connections

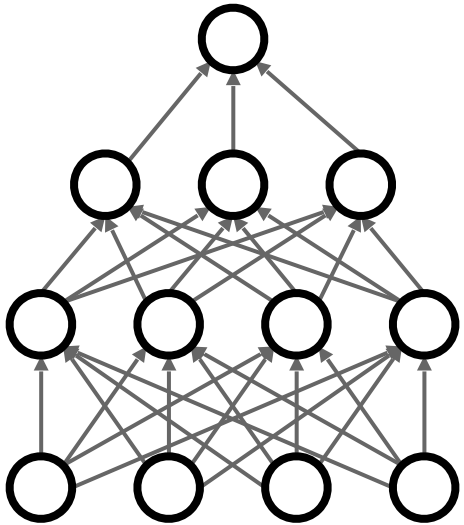
Examples:

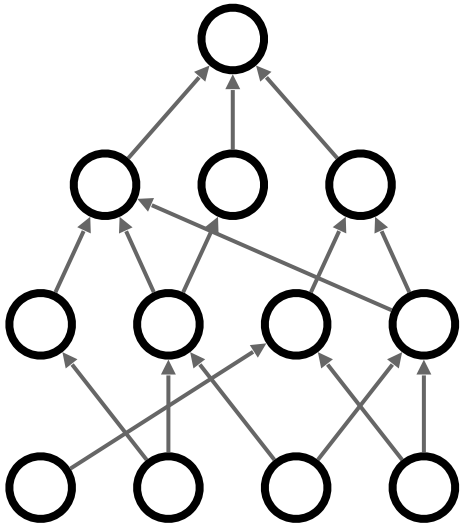
Dropout

Batch Normalization

Data Augmentation

DropConnect





Wan et al, “Regularization of Neural Networks using DropConnect”, ICML 2013

Regularization: Stochastic Depth

Training: Skip some layers in the network

Testing: Use all the layer

Examples:

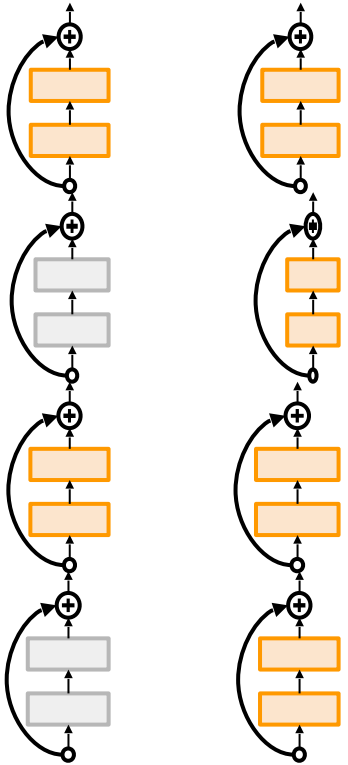
Dropout

Batch Normalization

Data Augmentation

DropConnect

Stochastic Depth



Huang et al, “Deep Networks with Stochastic Depth”, ECCV 2016

Regularization: Cutout

Training: Set random image regions to zero

Testing: Use full image

Examples:

Dropout

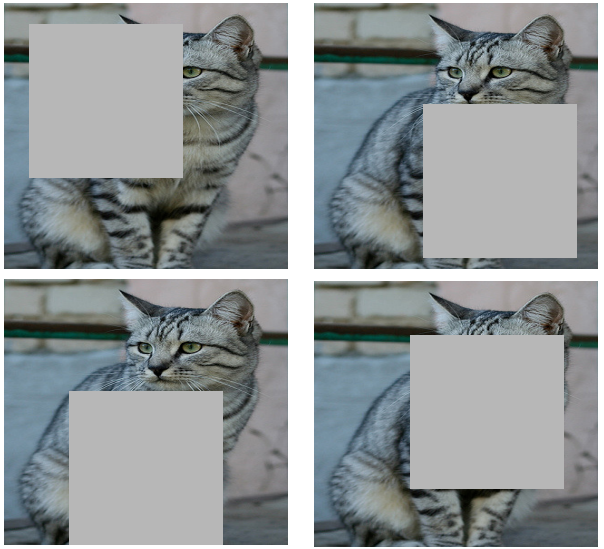
Batch Normalization

Data Augmentation

DropConnect

Stochastic Depth

Cutout / Random Crop



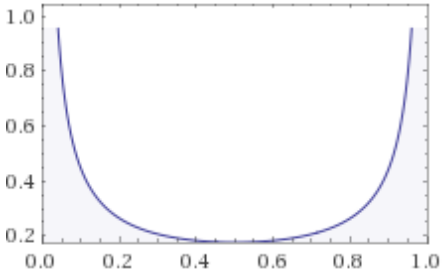
Works very well for small datasets like CIFAR, less common for large datasets like ImageNet

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

Regularization: Mixup

Training: Train on random blends of images

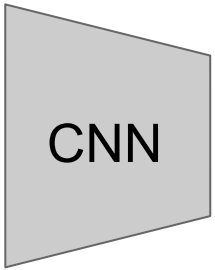
Testing: Use original images



Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Stochastic Depth
Cutout / Random Crop
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

Regularization - In practice

Training: Add random noise

Testing: Marginalize over the noise

Examples:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Stochastic Depth
Cutout / Random Crop
Mixup

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

Choosing Hyperparameters

(without tons of GPUs)

Choosing Hyperparameters

Step 1: Check initial loss

Turn off weight decay, sanity check loss at initialization
e.g. log(C) for softmax with C classes

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample

Try to train to 100% training accuracy on a small sample of training data (~5-10 minibatches); fiddle with architecture, learning rate, weight initialization

Loss not going down? LR too low, bad initialization
Loss explodes to Inf or NaN? LR too high, bad initialization

Choosing Hyperparameters

Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down

Use the architecture from the previous step, use all training data, turn on small weight decay, find a learning rate that makes the loss drop significantly within ~100 iterations

Good learning rates to try: 1e-1, 1e-2, 1e-3, 1e-4

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

Choose a few values of learning rate and weight decay around what worked from Step 3, train a few models for ~1-5 epochs.

Good weight decay to try: 1e-4, 1e-5, 0

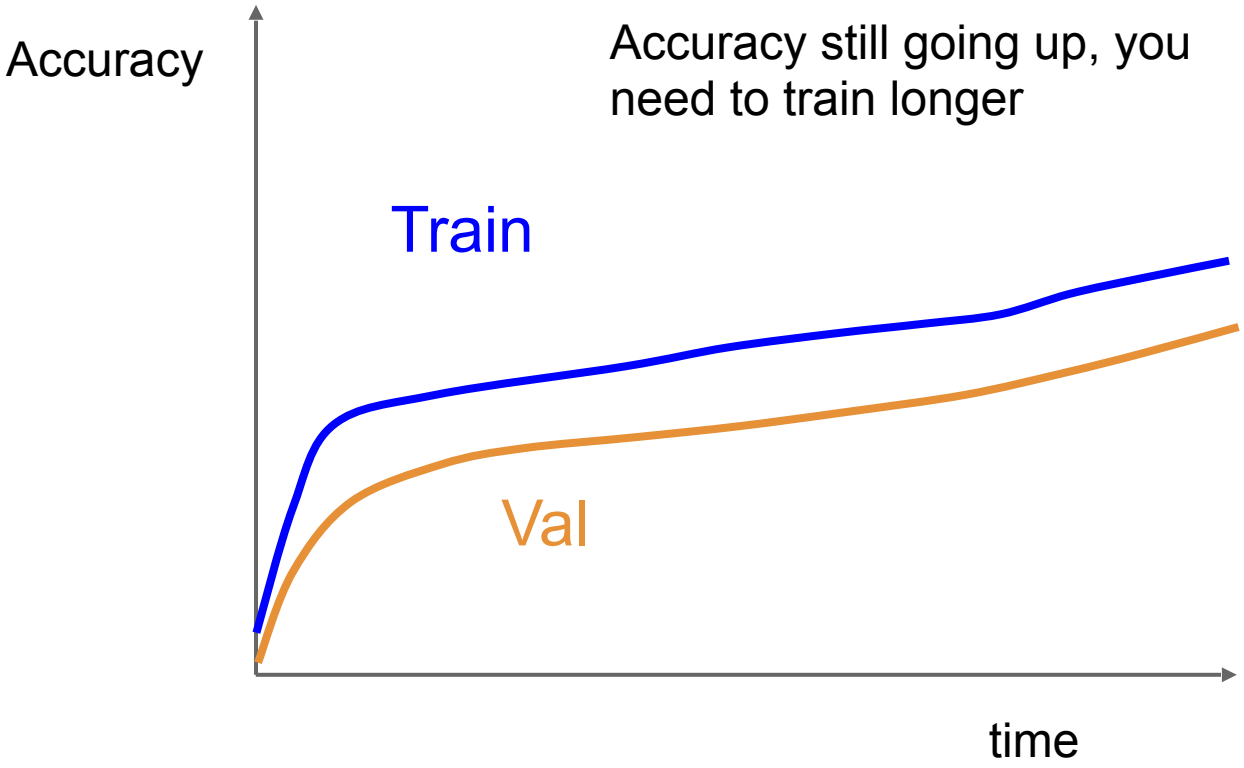
Choosing Hyperparameters

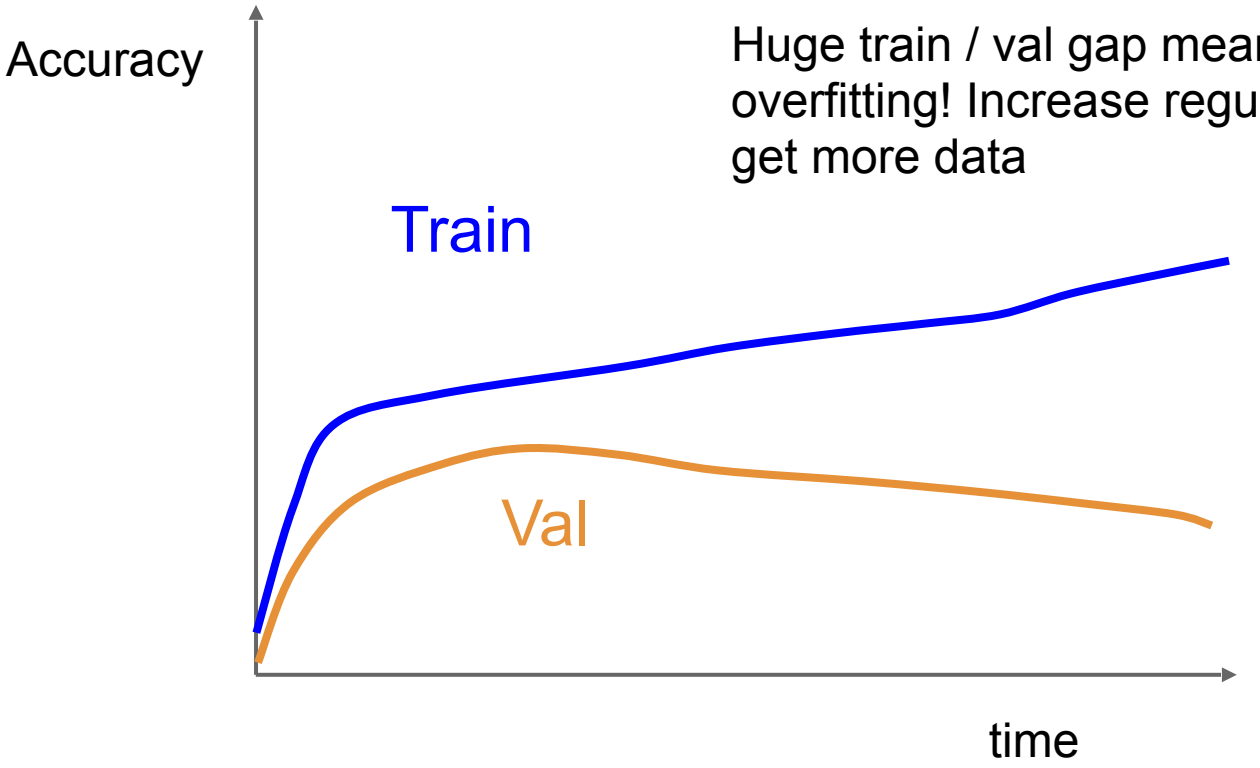
Step 1: Check initial loss
Step 2: Overfit a small sample
Step 3: Find LR that makes loss go down
Step 4: Coarse grid, train for ~1-5 epochs
Step 5: Refine grid, train longer

Pick best models from Step 4, train them for longer (~10-20 epochs) without learning rate decay

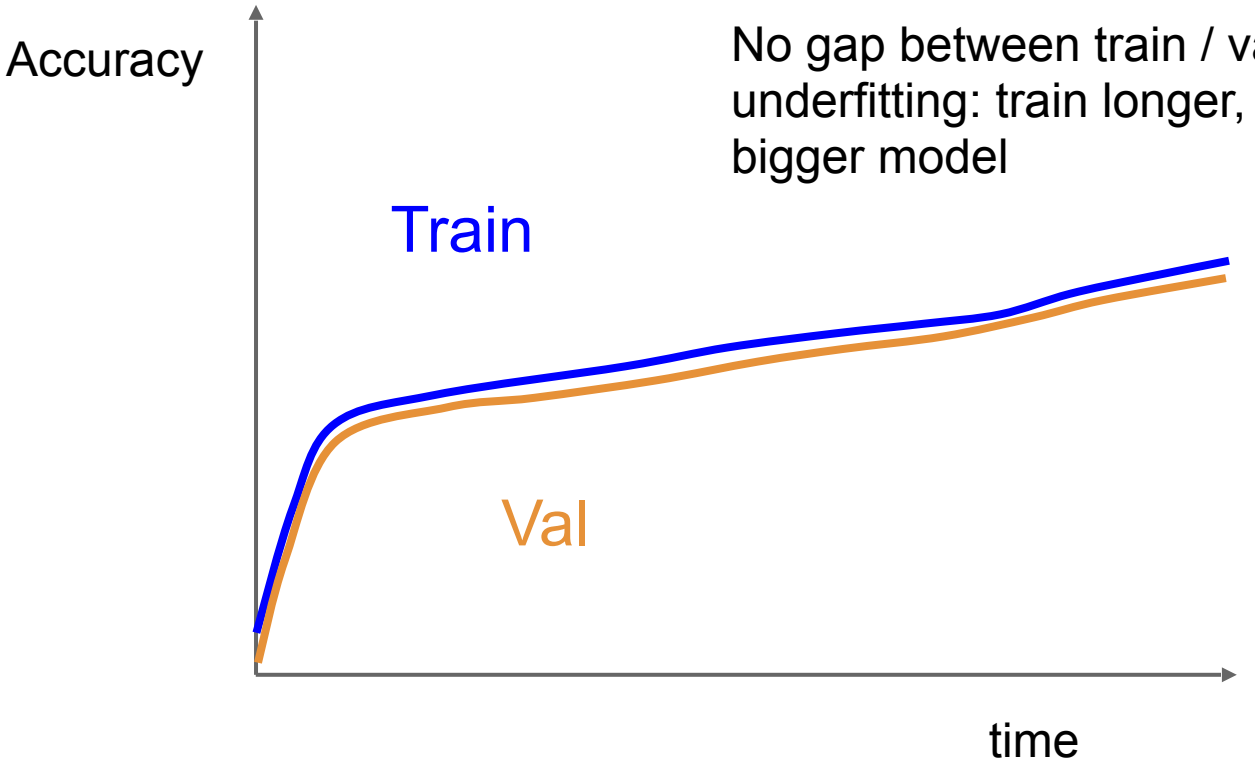
Choosing Hyperparameters

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 and accuracy curves


Accuracy
Accuracy still going up, you need to train longer
Train
Val
time

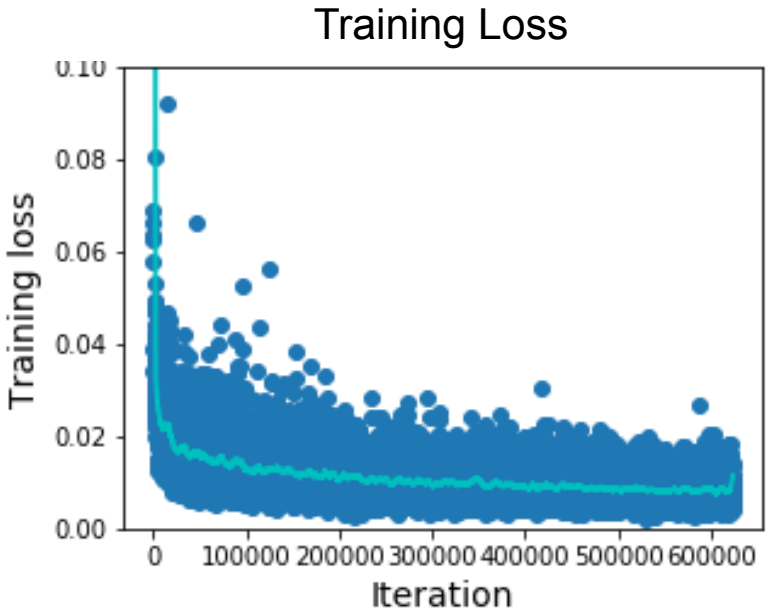


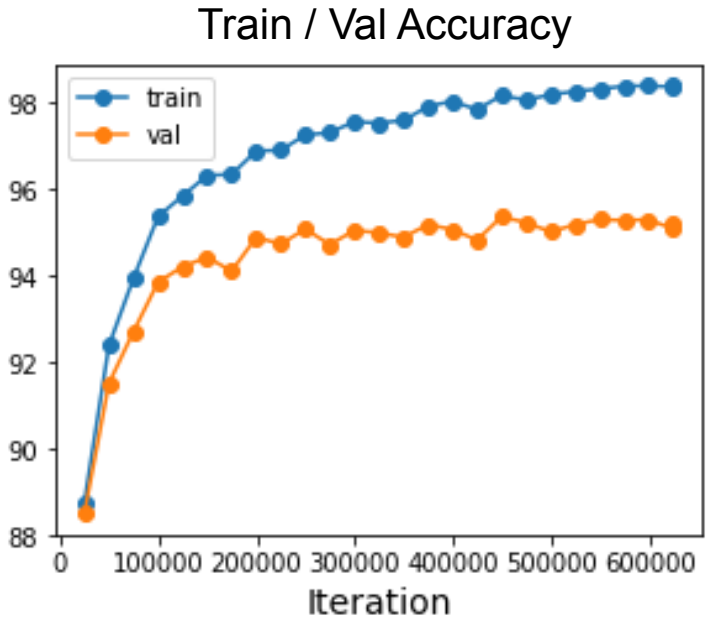
Huge train / val gap means overfitting! Increase regularization, get more data



No gap between train / val means underfitting: train longer, use a bigger model

Look at learning curves!



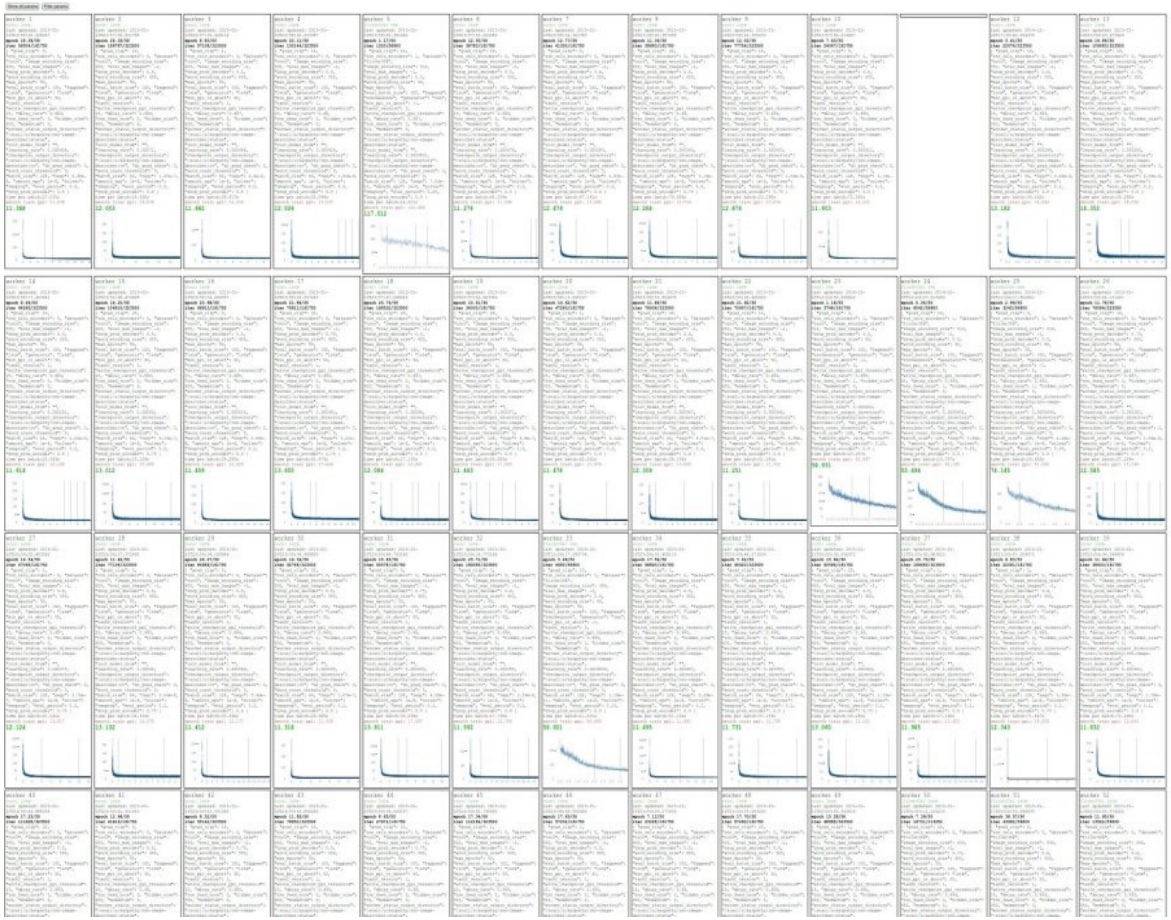


Losses may be noisy, use a scatter plot and also plot moving average to see trends better

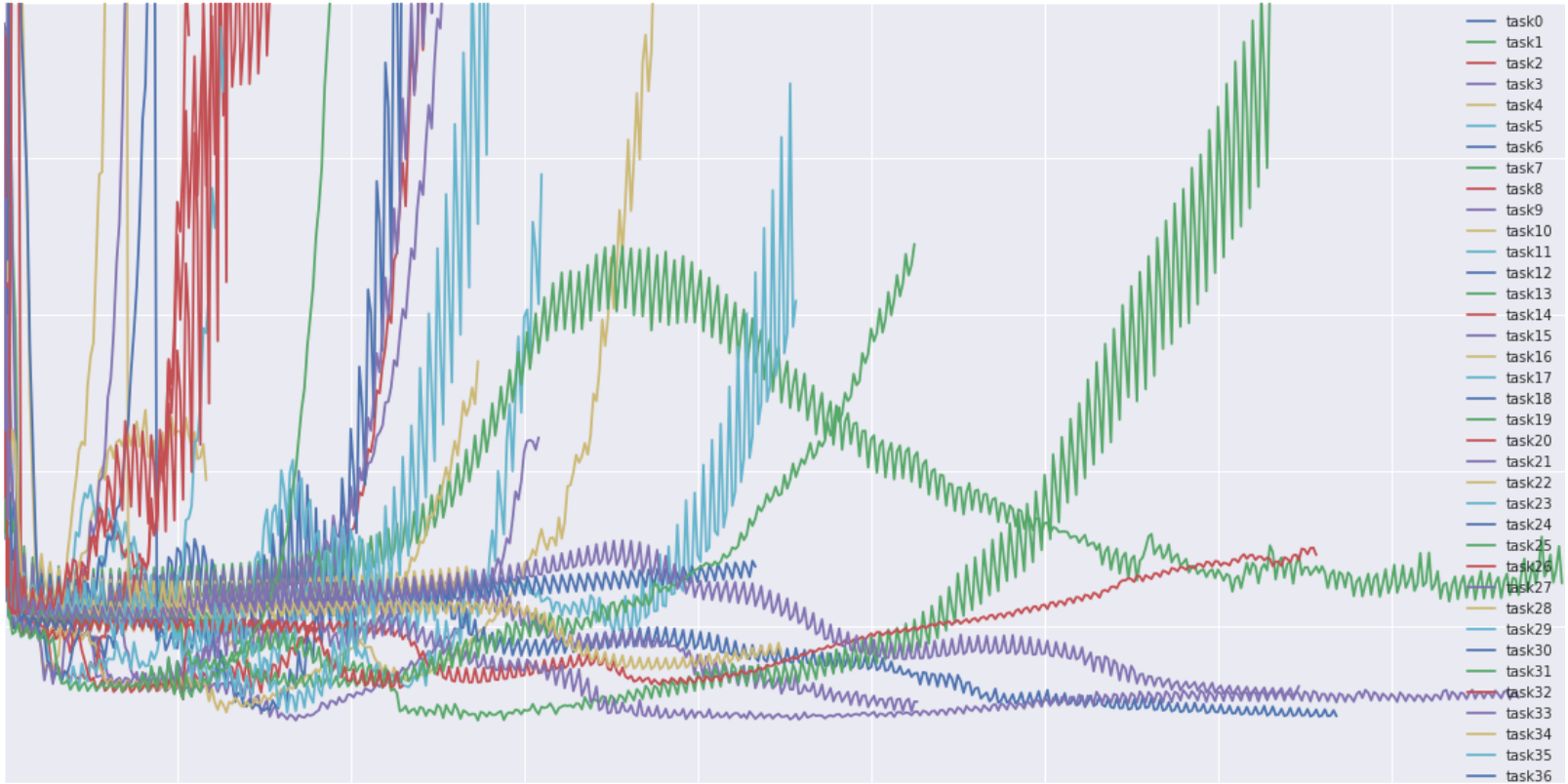
Cross-validation

We develop "command centers" to visualize all our models training with different hyperparameters

check out [weights and biases]



You can plot all your loss curves for different hyperparameters on a single plot



Don't look at accuracy or loss curves for too long!

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 and accuracy curves
Step 7: GOTO step 5

Random Search vs. Grid Search

Random Search for Hyper-Parameter Optimization
Bergstra and Bengio, 2012

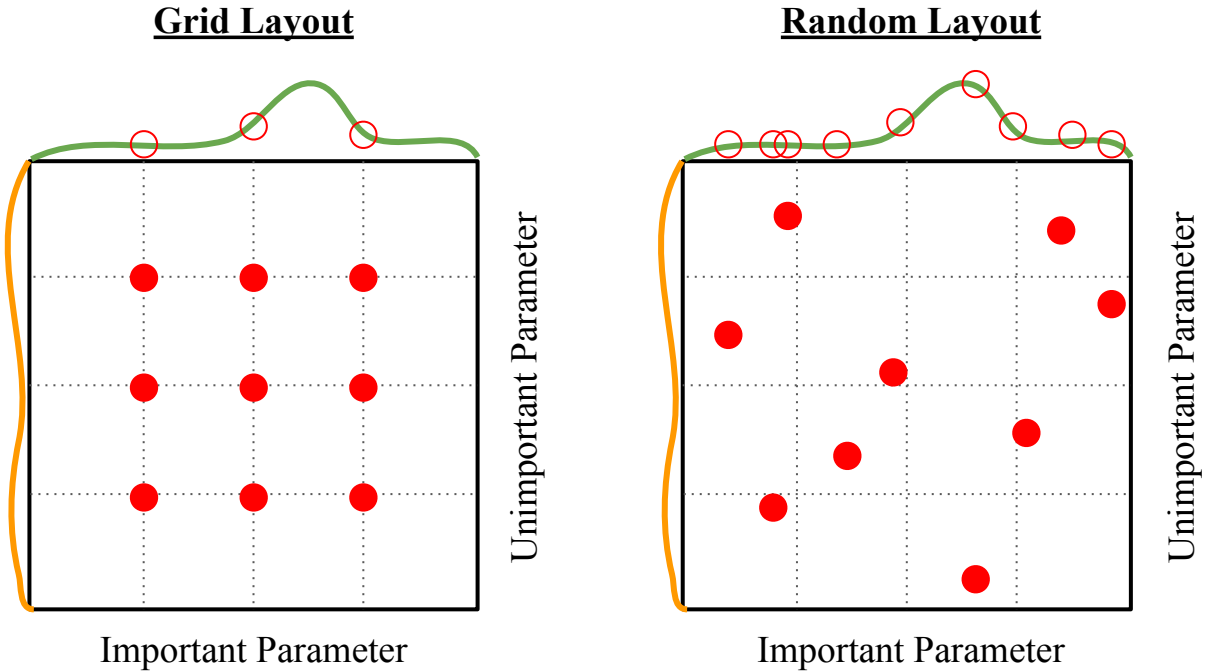


Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

Summary

- Improve your training error:
  - Optimizers
  - Learning rate schedules
- Improve your test error:
  - Regularization
  - Choosing Hyperparameters

Summary

TLDRs

We looked in detail at:

- Activation Functions (use ReLU)
- Data Preprocessing (images: subtract mean)
- Weight Initialization (use Xavier/Kaiming init)
- Batch Normalization (use this!)
- Transfer learning (use this if you can!)

Next time: Convolutional Networks