Indian Institute of Information Technology, Allahabad





Optimization & Regularization

By

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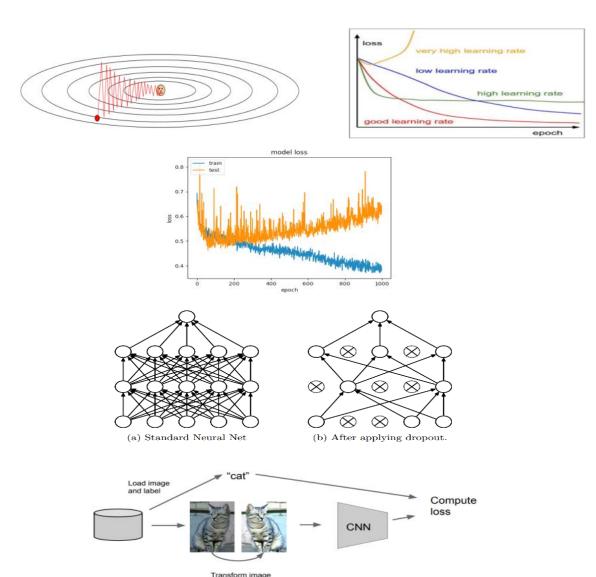
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Training Aspects of CNN

- Optimization
- Learning Rate
- Regularization
- Dropout
- Batch Normalization
- Data Augmentation
- Transfer Learning
- Interpreting Loss Curve





Optimization



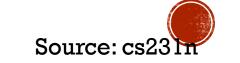


Source: cs231n

MINI-BATCH SGD

Loop:

- 1. Sample a batch of data
- 2. **Forward** prop it through the graph (network), get loss
- 3. Backprop to calculate the gradients
- 4. Update the parameters using the gradient

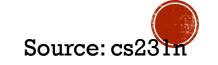


STOCHASTIC GRADIENT DESCENT (SGD)

The procedure of repeatedly evaluating the gradient of loss function and then performing a parameter update.

Vanilla (Original) Gradient Descent:

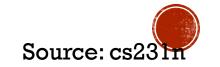
```
while True:
    dx = compute_gradient(x)
    x -= learning_rate * dx
```



SGD

```
x_{t+1} = x_t - \alpha \nabla f(x_t)
```

```
while True:
    dx = compute_gradient(x)
    x -= learning_rate * dx
```



SGD

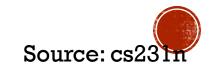
$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

while True:

$$dx = compute_gradient(x)$$

SGD+Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$



SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

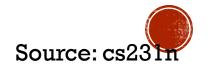
while True:

```
dx = compute\_gradient(x)
```

SGD+Momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x -= learning_rate * vx
```



SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

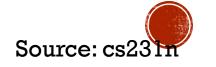
while True: dx = compute_gradient(x) x -= learning_rate * dx

SGD+Momentum

```
v_{t+1} = \rho v_t + \nabla f(x_t)x_{t+1} = x_t - \alpha v_{t+1}
```

```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x -= learning_rate * vx
```

- Build up "velocity" in any direction that has consistent gradient
- Rho gives "friction"; typically rho=0.9 or 0.99



SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

while True:

```
dx = compute\_gradient(x)
```

SGD+Momentum

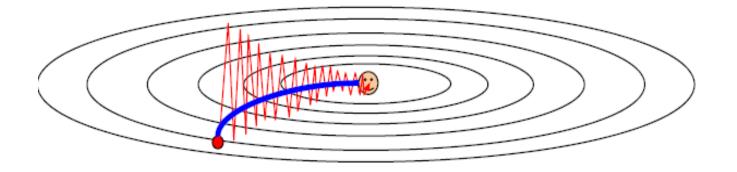
$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

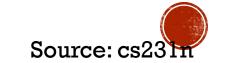
```
while True:
```

VX = 0

```
dx = compute_gradient(x)
```

$$vx = rho * vx + dx$$





ADAGRAD

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Added element-wise scaling of the gradient based on the historical sum of squares in each dimension



ADAGRAD

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

What happens to the step size over long time?



ADAGRAD

```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

What happens to the step size over long time?

Effective learning rate diminishing problem



RMSPROP

```
AdaGrad
grad_squared = 0
while True:
  dx = compute_gradient(x)
 grad_squared += dx * dx
 x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



```
RMSProp
```

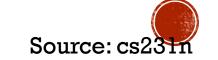
```
grad_squared = 0
while True:
  dx = compute\_gradient(x)
 grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
 x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



ADAM

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

```
first_moment = 0
second_moment = 0
while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```



ADAW

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

```
first_moment = 0
second_moment = 0
while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Sort of like RMSProp with Momentum





Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

```
first_moment = 0
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while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Sort of like RMSProp with Momentum

Problem:

Initially, second_moment=0 and beta2=0.999
After 1st iteration, second_moment -> close to zero
So, very large step for update of x

Source: cs231n

ADAM (WITH BIAS CORRECTION)

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

AdaGrad/ RMSProp

Bias Correction

Momentum

Bias correction for the fact that first and second moment estimates start at zero



ADAM (WITH BIAS CORRECTION)

Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

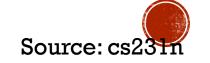
AdaGrad/ RMSProp

Bias Correction

Momentum

Bias correction for the fact that first and second moment estimates start at zero

Adam with betal = 0.9, beta2 = 0.999, and learning_rate = 1e-3 or 5e-4 is a great starting point for many models!



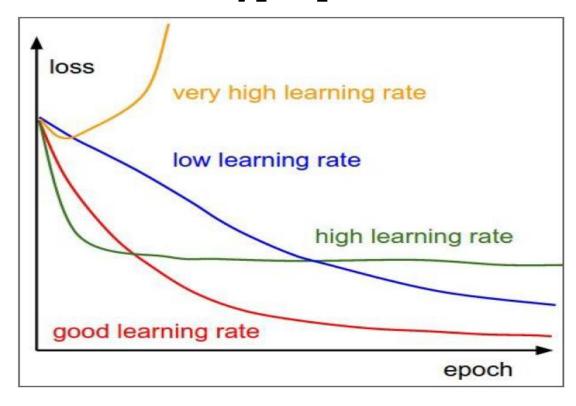
OPTIMIZER

In Practice:

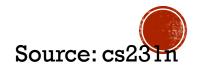
- Adam is a good default choice in most cases
 - Try out RADAM, diffGrad and AdaBelief



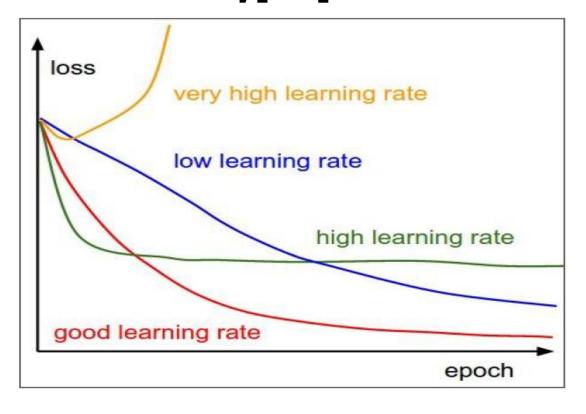
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning** rate as a hyperparameter.



Q: Which one of these learning rates is best to use?



SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning** rate as a hyperparameter.



=> Learning rate decay over time!

step decay:

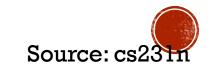
e.g. decay learning rate by half every few epochs.

exponential decay:

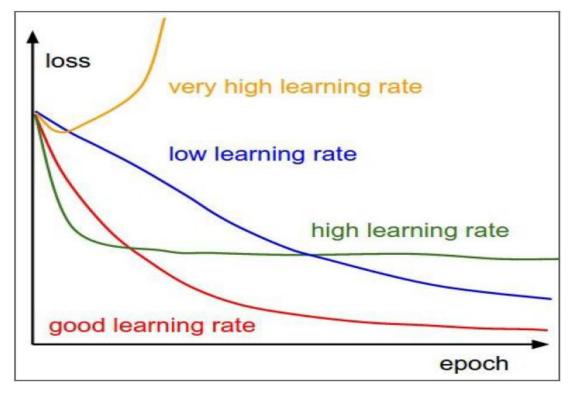
$$\alpha = \alpha_0 e^{-kt}$$

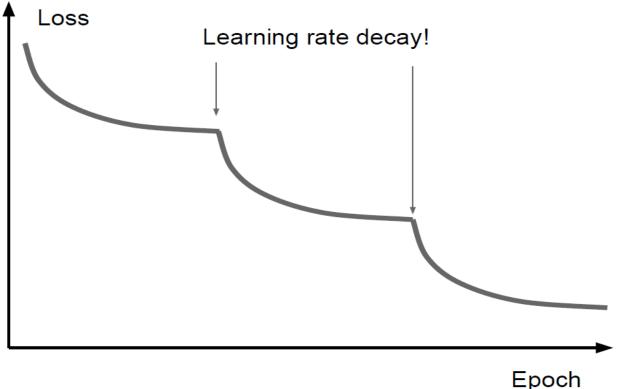
1/t decay:

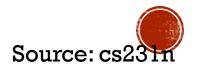
$$lpha=lpha_0/(1+kt)$$



SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning** rate as a hyperparameter.







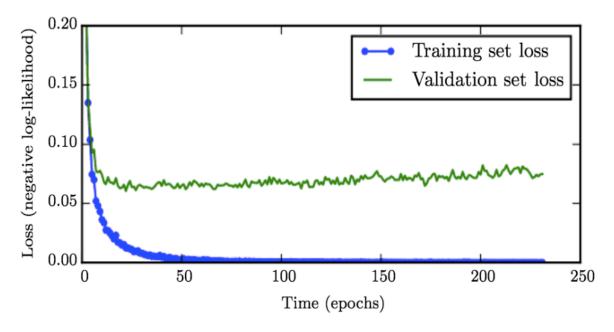
In Practice:

- Learning rate with step decay is commonly used
 - Step decay: reduce rate by a constant factor every few epochs, e.g., by 0.5 every 5 epochs, 0.1 every 20 epochs
 - Manual: watch validation error and reduce learning rate whenever it stops improving
 - "Patience" hyperparameter: number of epochs without improvement before reducing learning rate
- Warmup: train with a low learning rate for a first few epochs, or linearly increase learning rate before transitioning to normal decay schedule (<u>Goyal et al.</u>, 2018)

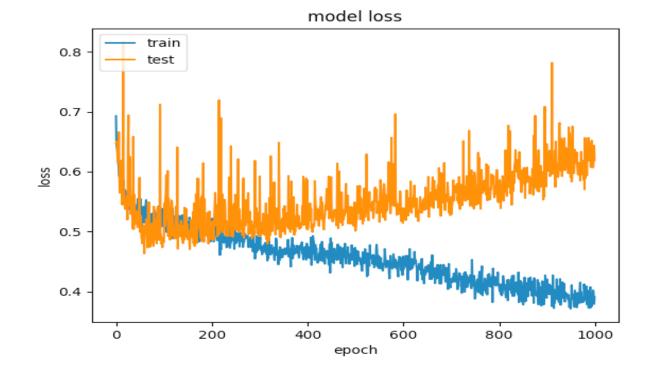


WHEN TO STOP TRAINING?

- Monitor validation error to decide when to stop
 - "Patience" hyperparameter: number of epochs without improvement before stopping
 - Early stopping can be viewed as a kind of regularization



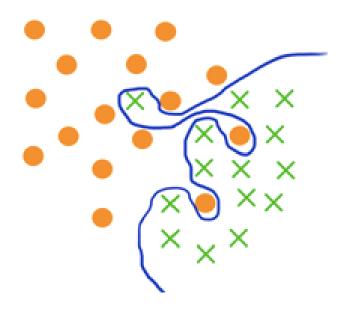


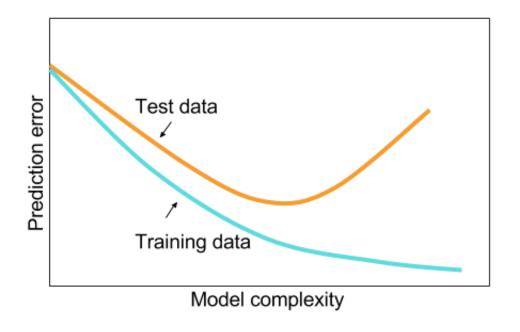


Regularization



 Techniques for controlling the capacity of a neural network to prevent overfitting

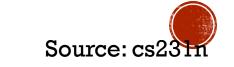






$$L(W) = \underbrace{\frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{i=1}$$

Data loss: Model predictions should match training data



 λ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data



 λ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

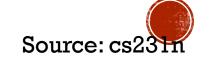
Regularization: Prevent the model from doing *too* well on training data

Simple examples

L2 regularization: $R(W) = \sum_{k} \sum_{l} W_{k,l}^2$

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

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



 λ = regularization strength (hyperparameter)

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(f(x_i, W), y_i) + \lambda R(W)$$

Data loss: Model predictions should match training data

Regularization: Prevent the model from doing *too* well on training data

Why regularize?

- Express preferences over weights
- Make the model simple so it works on test data
- Improve optimization by adding curvature



$$x = [1,1,1,1]$$

 $w_1 = [1,0,0,0]$
 $w_2 = [0.25,0.25,0.25,0.25]$



$$x = [1,1,1,1]$$

 $w_1 = [1,0,0,0]$
 $w_2 = [0.25,0.25,0.25,0.25]$

$$w_1 . x = w_2 . x = 1$$



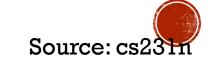
REGULARIZATION

$$x = [1,1,1,1]$$

 $w_1 = [1,0,0,0]$
 $w_2 = [0.25,0.25,0.25,0.25]$

$$w_1 . x = w_2 . x = 1$$

Which W to consider?



REGULARIZATION

$$x = [1,1,1,1]$$

 $w_1 = [1,0,0,0]$
 $w_2 = [0.25,0.25,0.25,0.25]$

$$w_1 . x = w_2 . x = 1$$

L2 Regularization

$$R(W) = \sum_{k} \sum_{l} W_{k,l}^2$$



REGULARIZATION

$$x = [1,1,1,1]$$

$$w_1 = [1,0,0,0]$$

$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

$$w_1 . x = w_2 . x = 1$$

L2 Regularization

$$R(W) = \sum_{k} \sum_{l} W_{k,l}^2$$

L2 regularization likes to "spread out" the weights



OTHER TYPES OF REGULARIZATION

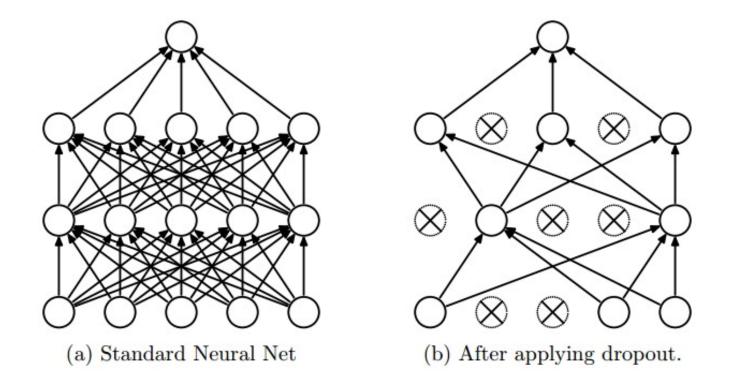
- Dropout
- Batch Normalization
- Data Augmentation
 - Adding noise to the inputs
 - Recall motivation of max margin criterion



Dropout

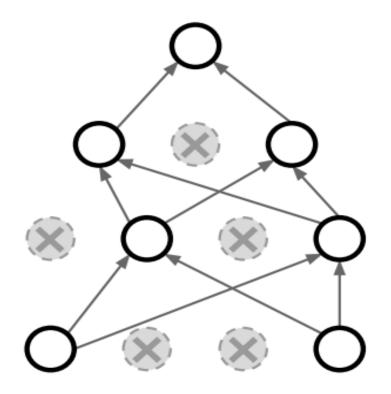


In each forward pass, randomly set some neurons to zero Probability of dropping is a hyperparameter; 0.5 is common

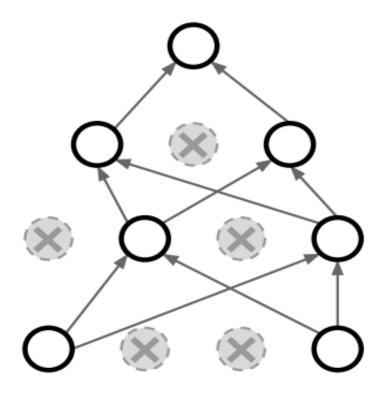




How can this possibly be a good idea?



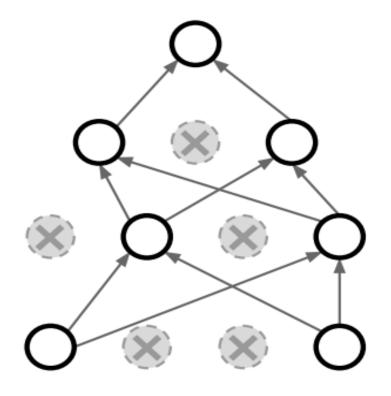
How can this possibly be a good idea?



Intuitions

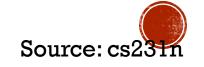
- Prevent "co-adaptation" of units, increase robustness to noise
- Train implicit ensemble

How can this possibly be a good idea?



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





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

More common: "Inverted dropout"



DROPOUT: MORE COMMON: "INVERTED DROPOUT"

We drop and scale at train time and don't do anything at test time.

```
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)
                                                                      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
```



Batch Normalization

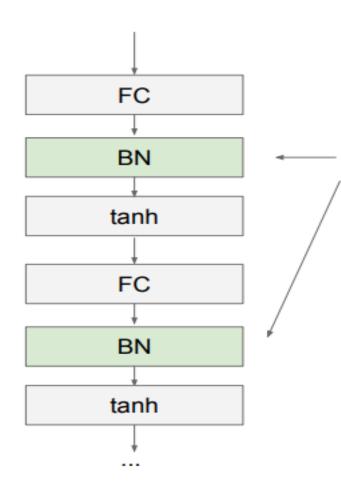


"We want zero-mean unit-variance activations? lets make them so."

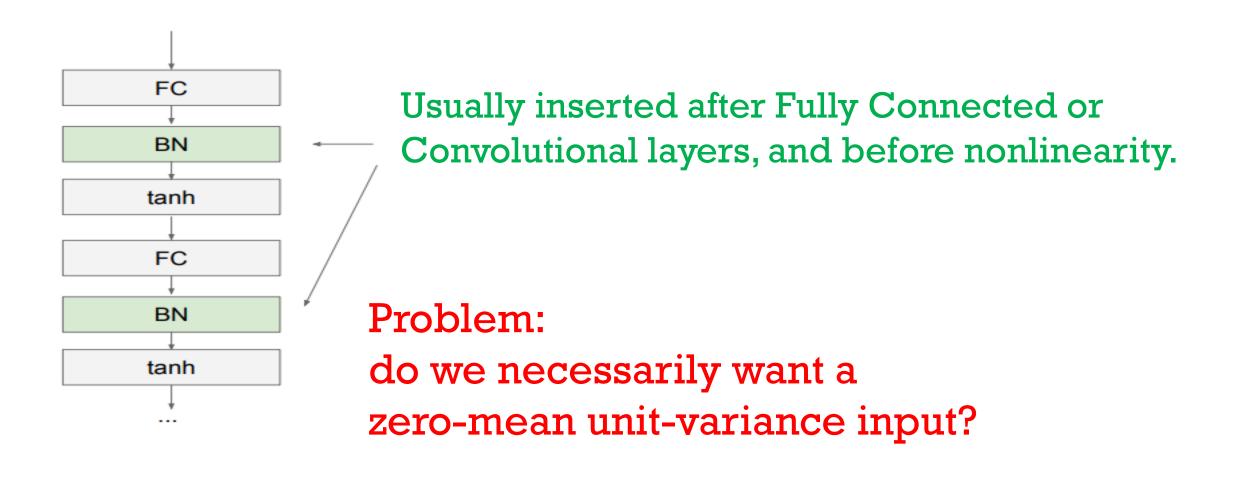
"We want zero-mean unit-variance activations? lets make them so."

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

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



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



Normalize:

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

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

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

Normalize:

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

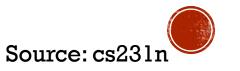
And then allow the network to squash the range if it wants to:

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

Note, the network can learn:

$$\gamma^{(k)} = \sqrt{\operatorname{Var}[x^{(k)}]}$$
$$\beta^{(k)} = \operatorname{E}[x^{(k)}]$$

to recover the identity mapping.



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

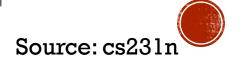
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

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

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

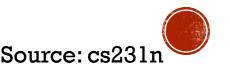


Note: at test time BatchNorm layer functions differently:

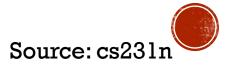
The mean/std are not computed based on the batch.

Instead, a single fixed empirical mean of activations during training is used.

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



Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1...m}\}$; Parameters to be learned: γ , β Output: $\{y_i = BN_{\gamma,\beta}(x_i)\}$ At test time (usually): // mini batch mean training set // mini-bateh variance training set // normalize



// scale and shift

 $y_i \leftarrow \gamma \hat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)$

Benefits

- Improves gradient flow through the network
- Allows higher learning rates and Accelerates convergence of training
- Reduces the strong dependence on initialization
- Acts as a form of regularization

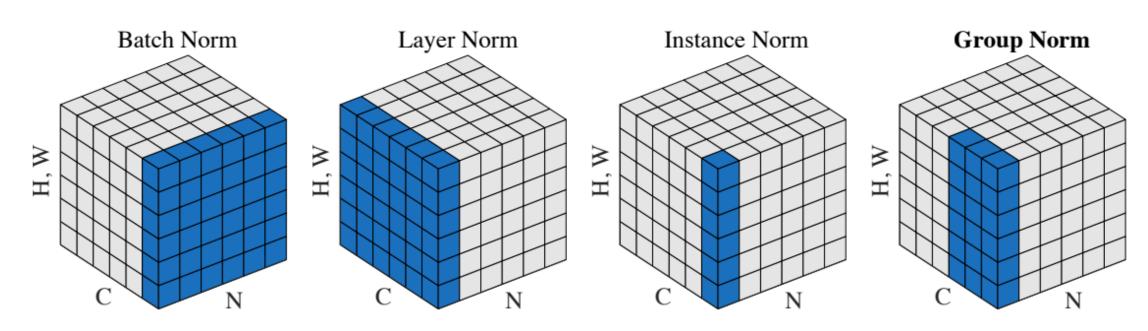
Pitfalls

- Behavior depends on composition of mini-batches, can lead to hard-to-catch bugs if there is a mismatch between training and test regime (example)
- Doesn't work well for small mini-batch sizes
- Cannot be used in recurrent models



OTHER TYPES OF NORMALIZATION

- <u>Layer normalization</u> (Ba et al., 2016)
- <u>Instance normalization</u> (Ulyanov et al., 2017)
- Group normalization (Wu and He, 2018)
- Weight normalization (Salimans et al., 2016)



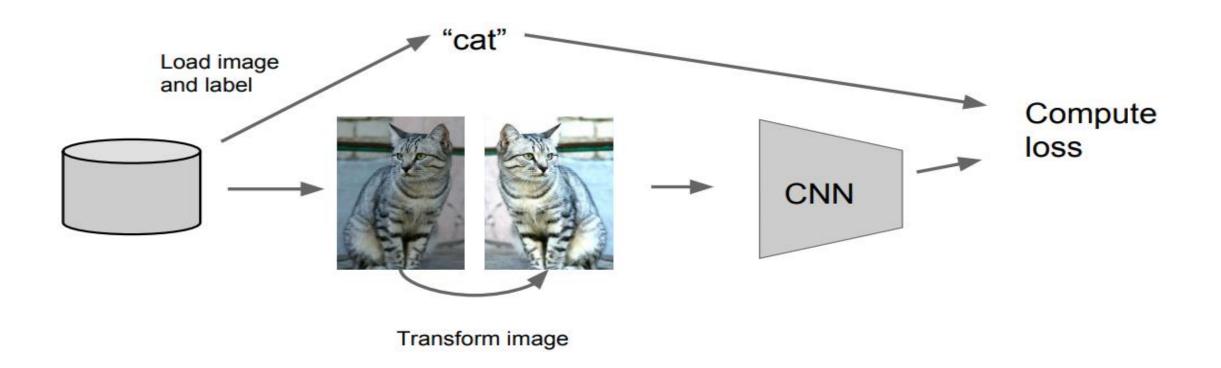
Y. Wu and K. He, Group Normalization, ECCV 2018

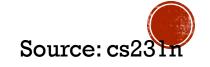


Data Augmentation



DATA AUGMENTATION (ITTERING)





DATA AUGMENTATION (JITTERING)

Horizontal Flips

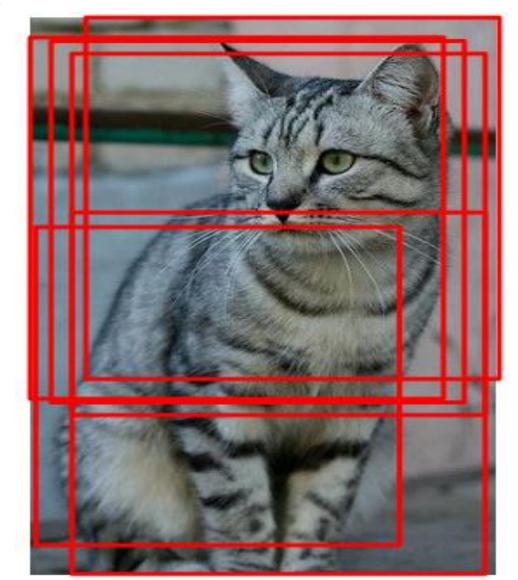




Source: cs231n

DATA AUGMENTATION (JITTERING)

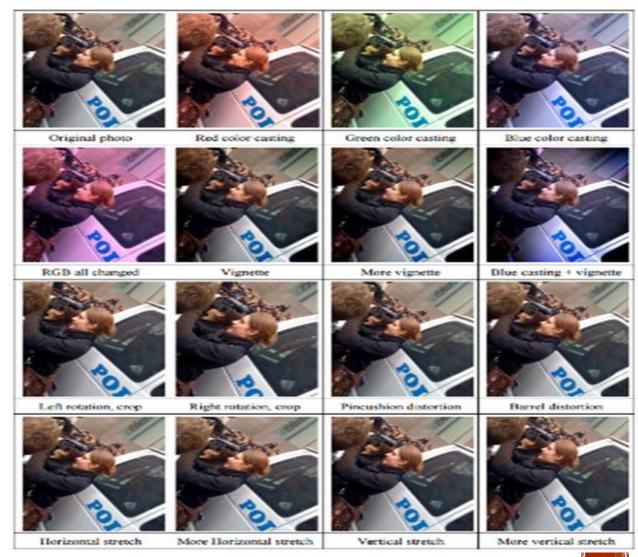
Random crops and scales





DATA AUGMENTATION (ITTERING)

- Create virtual training samples
- Get creative for your problem!
 - Horizontal flip
 - Random crop
 - Color casting
 - Randomize contrast
 - Randomize brightness
 - Geometric distortion
 - Rotation
 - Photometric changes





Transfer Learning



1. Train on Imagenet



Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014

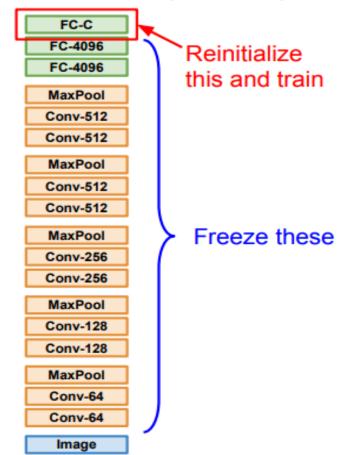
Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

Source: cs231:

1. Train on Imagenet

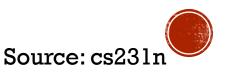
FC-1000 FC-4096 FC-4096 MaxPool Conv-512 Conv-512 MaxPool Conv-512 Conv-512 MaxPool Conv-256 Conv-256 MaxPool Conv-128 Conv-128 MaxPool Conv-64 Conv-64 **Image**

2. Small Dataset (C classes)



Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014

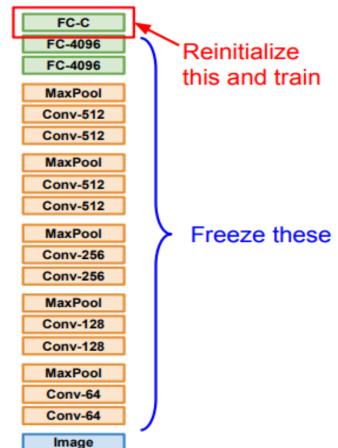
Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014



1. Train on Imagenet

FC-1000 FC-4096 FC-4096 MaxPool Conv-512 Conv-512 MaxPool Conv-512 Conv-512 MaxPool Conv-256 Conv-256 MaxPool Conv-128 Conv-128 MaxPool Conv-64 Conv-64 **Image**

2. Small Dataset (C classes)



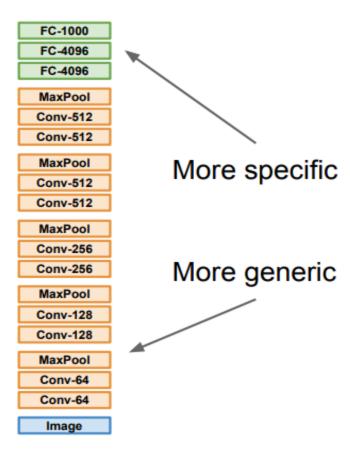
3. Bigger dataset FC-C FC-4096 Train these FC-4096 MaxPool Conv-512 With bigger Conv-512 dataset, train MaxPool more layers Conv-512 Conv-512 MaxPool Conv-256 Freeze these Conv-256 MaxPool Lower learning rate Conv-128 when finetuning; Conv-128 1/10 of original LR MaxPool Conv-64 is good starting Conv-64 point

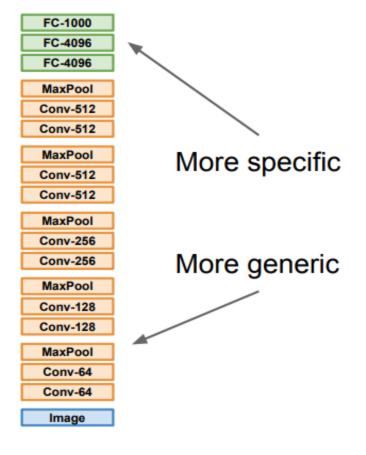
Source: cs231:

Image

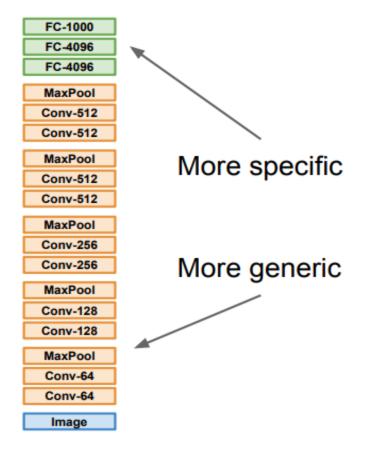
Donahue et al, "DeCAF: A Deep Convolutional Activation Feature for Generic Visual Recognition", ICML 2014

Razavian et al, "CNN Features Off-the-Shelf: An Astounding Baseline for Recognition", CVPR Workshops 2014

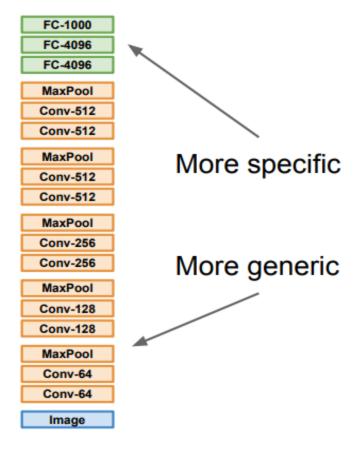




	very similar dataset	very different dataset
very little data		
quite a lot of data		

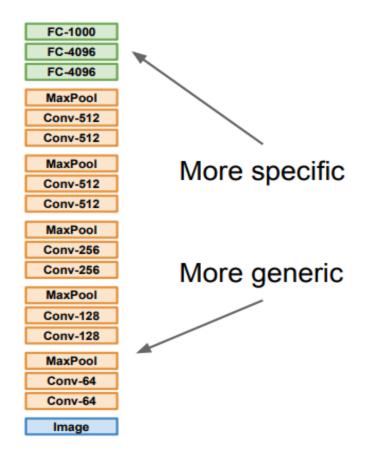


	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	
quite a lot of data		



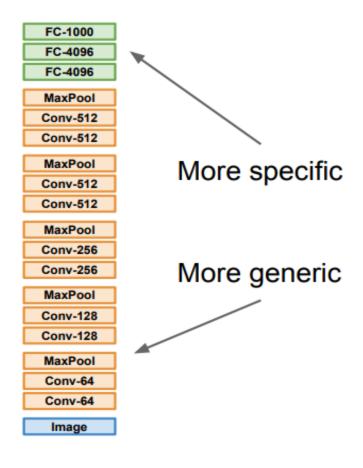
	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	
quite a lot of data	Finetune a few layers	

TRANSFER LEARNING WITH CNNS

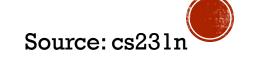


	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	
quite a lot of data	Finetune a few layers	Finetune a larger number of layers

TRANSFER LEARNING WITH CNNS



	very similar dataset	very different dataset
very little data	Use Linear Classifier on top layer	You're in trouble Try linear classifier from different stages
quite a lot of data	Finetune a few layers	Finetune a larger number of layers



TRANSFER LEARNING WITH CNNS

Takeaway for your projects and beyond:

Have some dataset of interest but it has $< \sim 1M$ images?

- 1. Find a very large dataset that has similar data, train a big ConvNet there
- 2. Transfer learn to your dataset

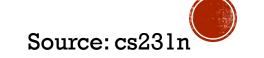
Deep learning frameworks provide a "Model Zoo" of pretrained models so you don't need to train your own

Caffe: https://github.com/BVLC/caffe/wiki/Model-Zoo

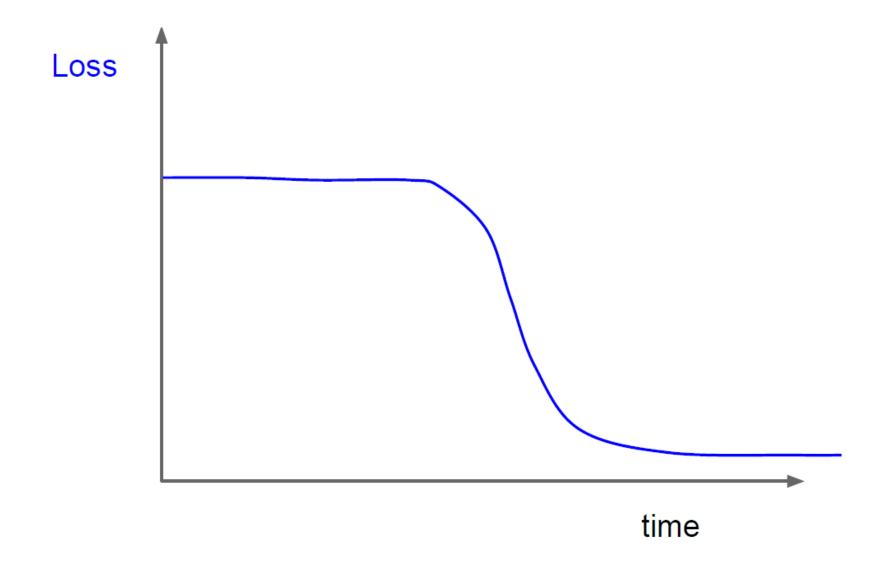
TensorFlow: https://github.com/tensorflow/models

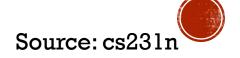
PyTorch: https://github.com/pytorch/vision

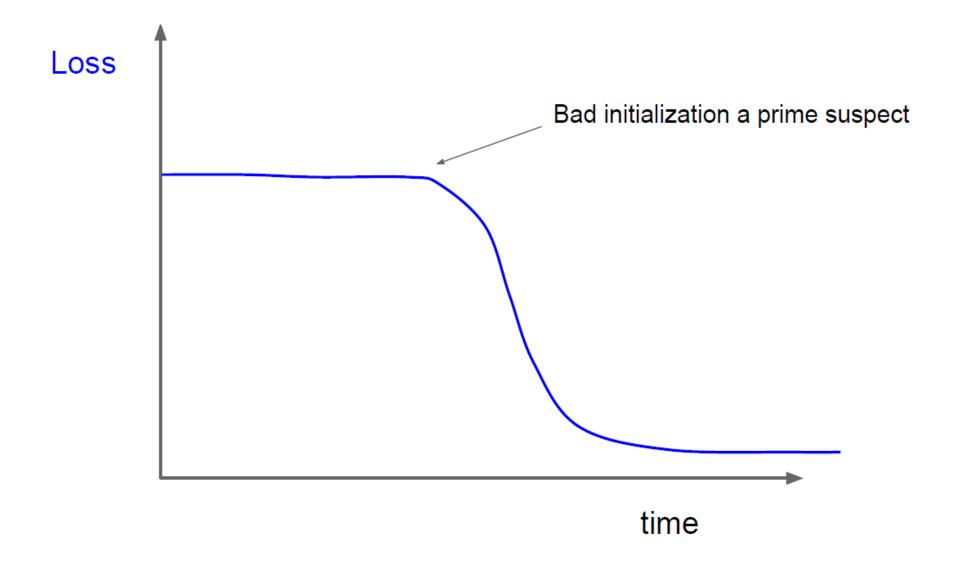
Matconvnet: http://www.vlfeat.org/matconvnet/pretrained/

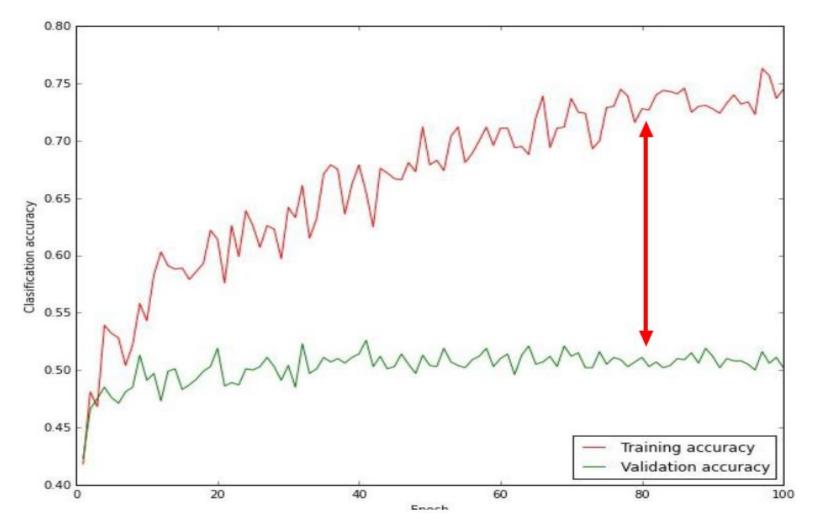






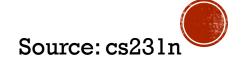


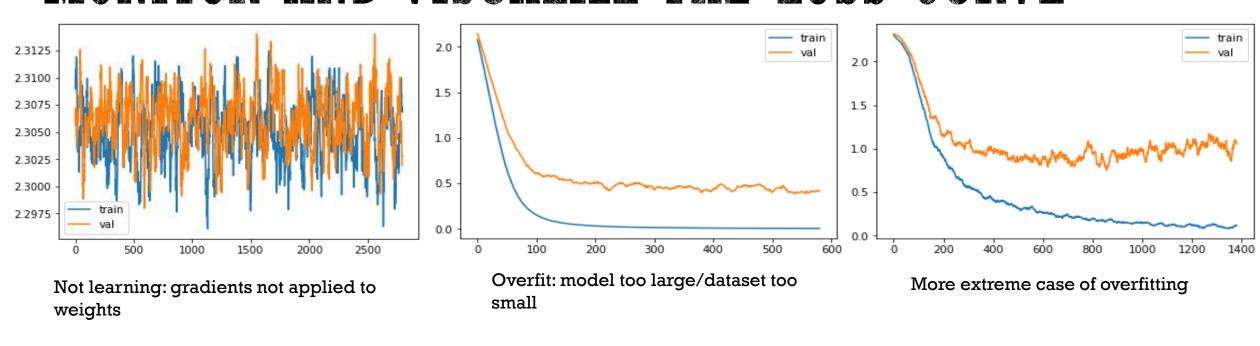




big gap = overfitting
=> increase
regularization strength?

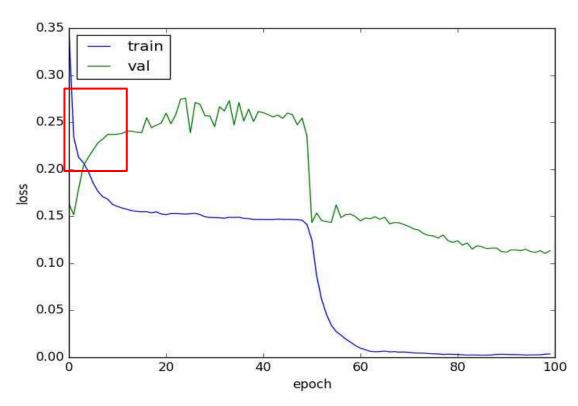
no gap
=> increase model
capacity?



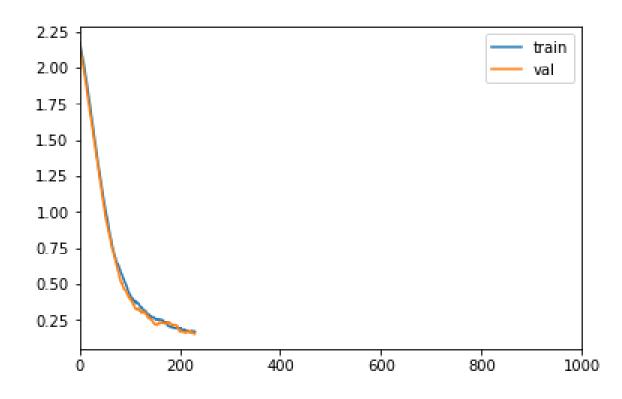


2.3 train train train slow start 2.0 2.2 2.6 2.1 1.5 2.0 2.5 1.0 1.9 2.4 1.8 1.7 500 1000 1500 2000 2500 2000 500 1000 1500 2500 1000 1200 1400 Applied the negative of gradients Not converged yet: need longer training Slow start: initialization weights too small

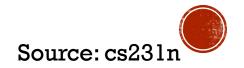
Source: cs231n



Problem: val set too small, statistics not meaningful

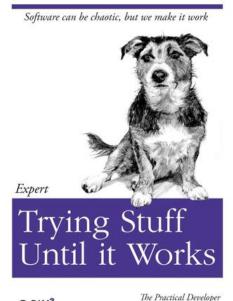


Get nans in the loss after a number of iterations: caused by high learning rate and numerical instability in models

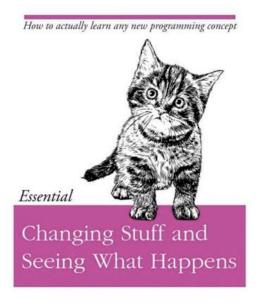


ATTEMPT AT A CONCLUSION

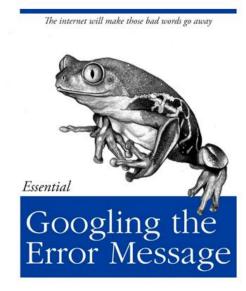
- Training neural networks is still a black art
- Process requires close "babysitting"
- For many techniques, the reasons why, when, and whether they work are in active dispute - read everything but don't trust anything
- It all comes down to (principled) trial and error
- Further reading: A. Karpathy, A recipe for training neural networks



@ThePracticalDev



@ThePracticalDev



The Practical Developer

@ThePracticalDev



THINGS TO REWEMBER

Training CNN

- Adam is common (AMSGrad can be tried)
- Learning rate: Step decay, Cyclic learning rate
- Transfer learning, Fine tuning

Regularization

- L2/L1/Elastic regularization
- Dropout and Dropconnect
- Batch Norm
- Data Augmentation: Flip, Crop, Contrast, etc.

Interpreting Loss

- Bad initialization
- Overfitting
- Slow/High learning rates
- Update in wrong direction
- Etc.



ACKNOWLEDGEMENT

- Deep Learning, Stanford University
- Introduction to Deep Learning, University of Illinois at Urbana-Champaign
- Introduction to Deep Learning, Carnegie Mellon University
- Convolutional Neural Networks for Visual Recognition, Stanford University
- Natural Language Processing with Deep Learning, Stanford University
- NVDIEA Deep Learning Teaching Kit

