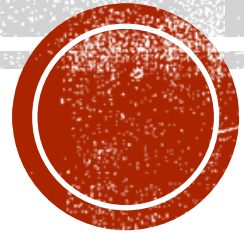
Indian Institute of Information Technology, Allahabad

Optimization & Regularization



By

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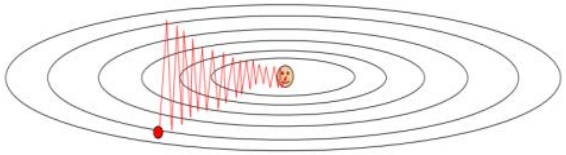
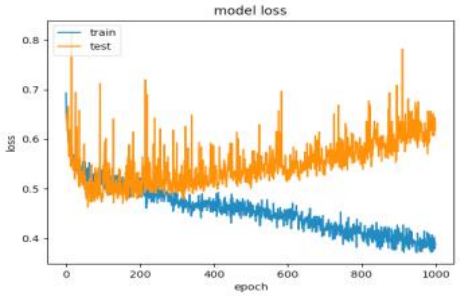
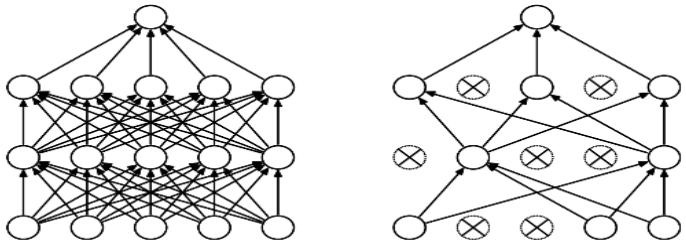
Training Aspects of CNN

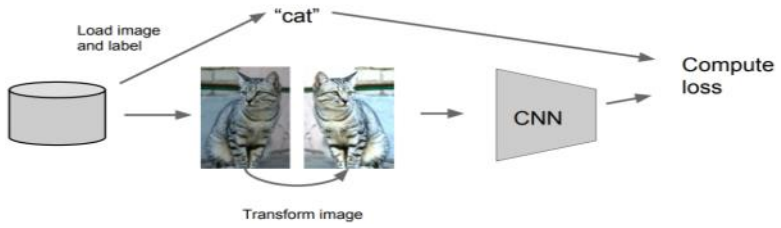
- Optimization
- Learning Rate
- Regularization
- Dropout
- Batch Normalization
- Data Augmentation
- Interpreting Loss Curve







(a) Standard Neural Net (b) After applying dropout.



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

Source: cs231n

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
```

Source: cs231n

SGD + MOMENTUM

SGD

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

```
while True:
    dx = compute_gradient(x)
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```

Source: cs231n

SGD + MOMENTUM

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SGD+Momentum

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

$$x_{t+1} = x_t - \alpha v_{t+1}$$

Source: cs231n

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

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

Source: cs231n

SGD + MOMENTUM

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  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

Source: cs231n

SGD + MOMENTUM

SGD

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

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while True:
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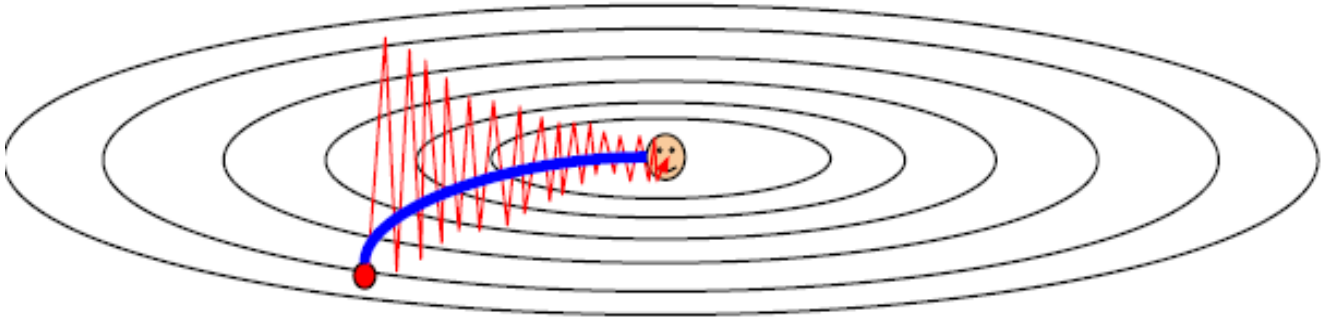

Source: cs231n

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

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

Source: cs231n

ADAGRAD

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What happens to the step size over long time?

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

Source: cs231n

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```

What happens to the step size over long time?

Effective learning rate diminishing problem

Duchi et al, "Adaptive subgradient methods for online learning and stochastic optimization", JMLR 2011

Source: cs231n

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)
```

Tieleman and Hinton, 2012

Source: cs231n

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))
```

Source: cs231n

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

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```

Sort of like RMSProp with Momentum

Source: cs231n

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```

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

```
first_moment = 0
second_moment = 0
for t in range(num_iterations):
  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
  second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

AdaGrad/ RMSProp

Bias Correction

Momentum

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

Source: cs231n

ADAM (WITH BIAS CORRECTION)

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  dx = compute_gradient(x)
  first_moment = beta1 * first_moment  + (1 - beta1) * dx
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  first_unbias = first_moment / (1 - beta1 ** t)
  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

AdaGrad/ RMSProp

Bias Correction

Momentum

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

Adam with **beta1 = 0.9**,
beta2 = 0.999, and **learning_rate = 1e-3 or 5e-4**
is a **great starting point** for many models!

Source: cs231n

OPTIMIZER

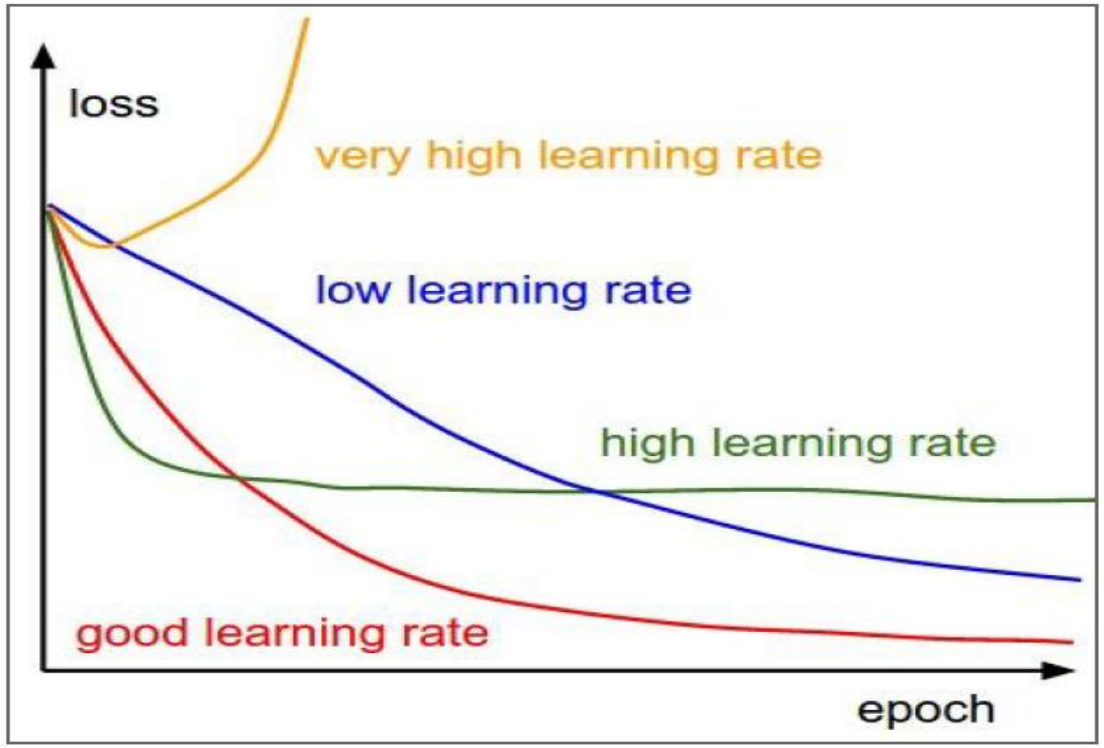
In Practice:

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

More Optimizer: **http://ruder.io/optimizing-gradient-descent/**

LEARNING RATE

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

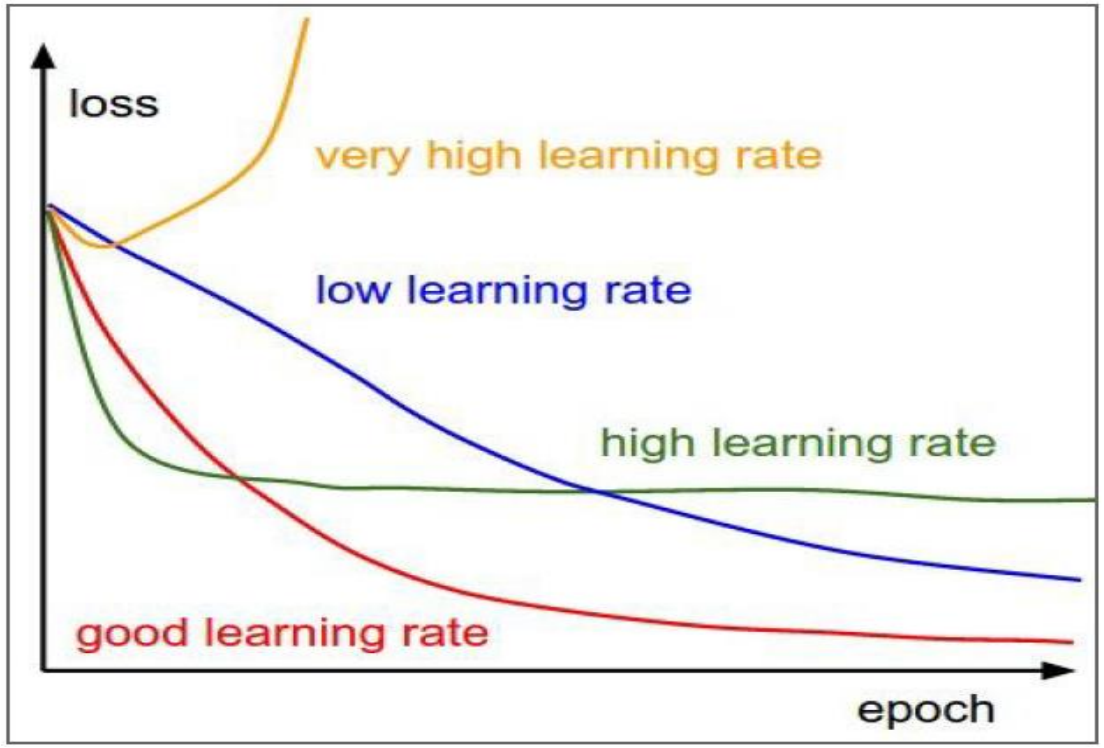


Q: Which one of these learning rates is best to use?

Source: cs231n

LEARNING RATE

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:

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

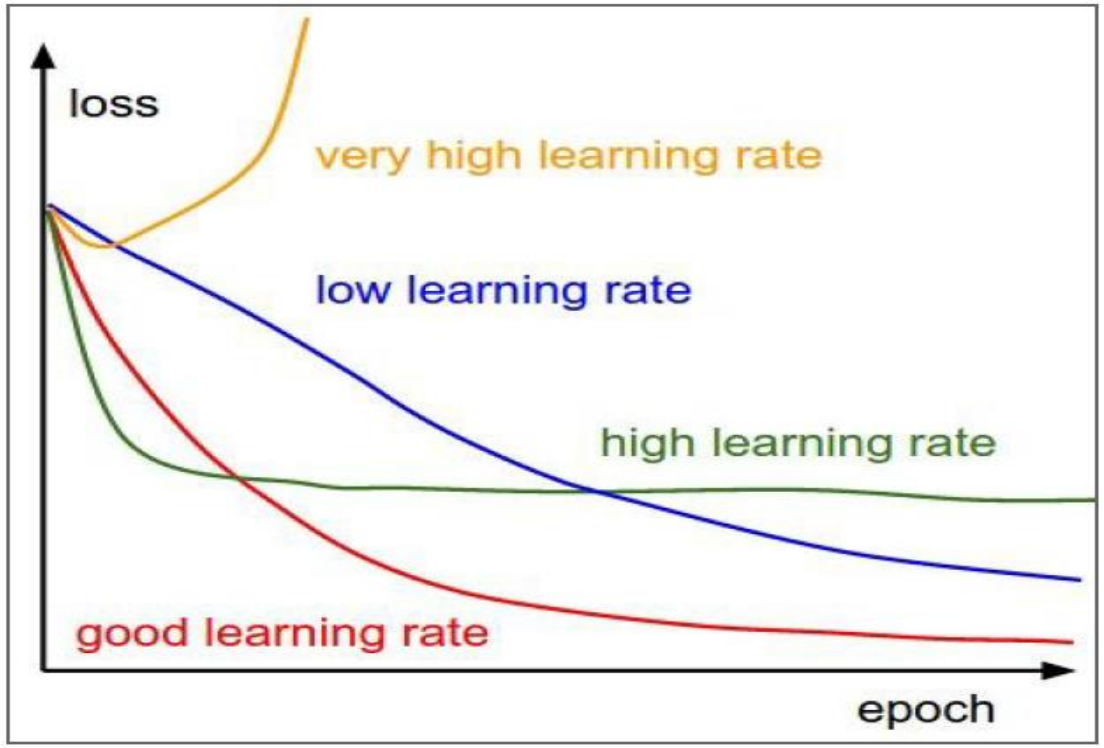
1/t decay:

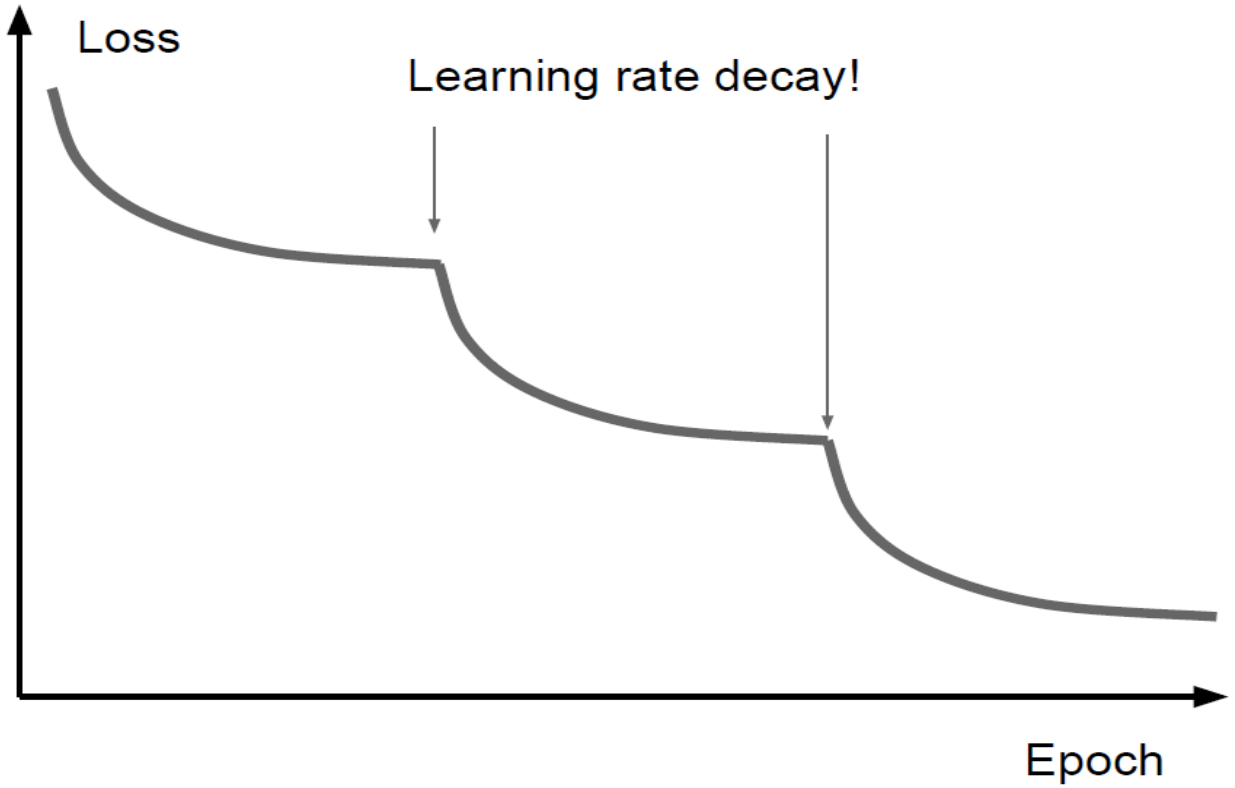
$$\alpha = \alpha_0 / (1 + kt)$$

Source: cs231n

LEARNING RATE

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





Source: cs231n

LEARNING RATE

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 (Goyal et al., 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

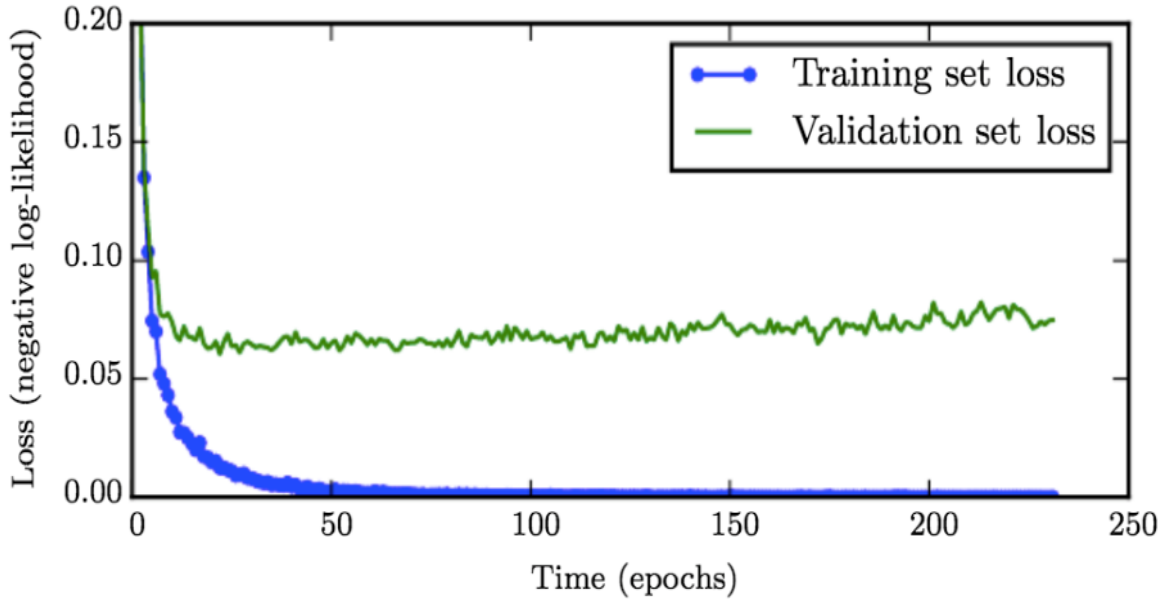


Figure from Deep Learning Book

Regularization

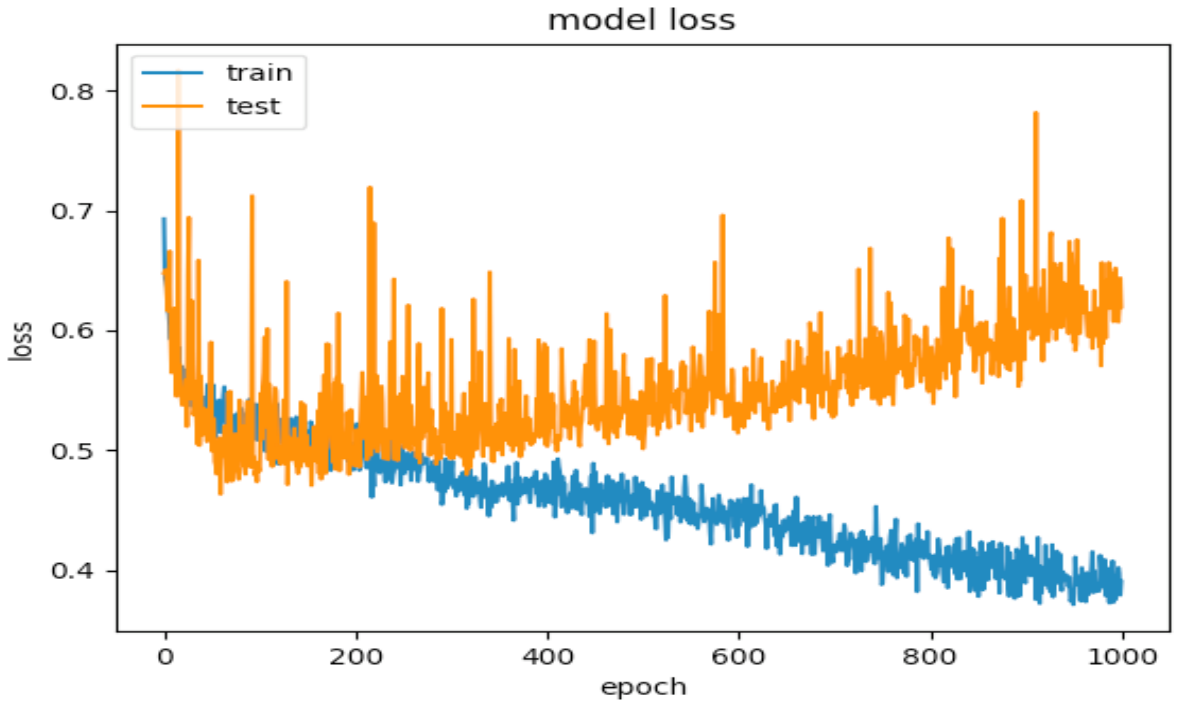
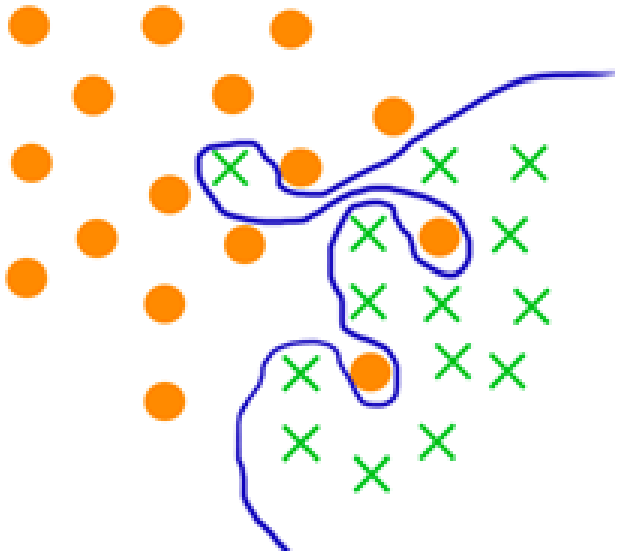
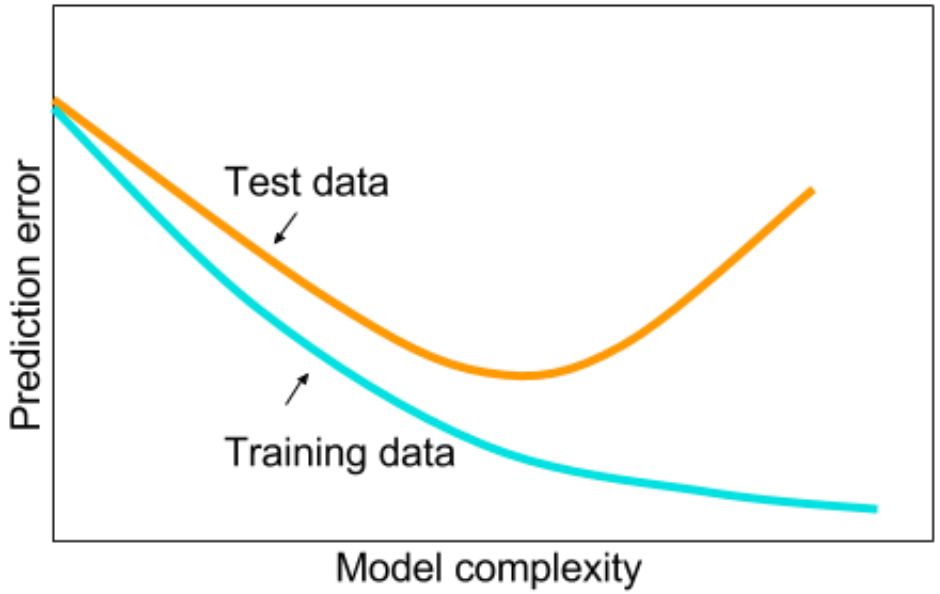


Image Source: https://stackoverflow.com/questions/44909134/how-to-avoid-overfitting-on-a-simple-feed-forward-network/44985765

REGULARIZATION

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





REGULARIZATION

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

Data loss: Model predictions should match training data

Source: cs231n

REGULARIZATION

λ = regularization strength (hyperparameter)

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

Data loss: Model predictions should match training data

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

Source: cs231n

REGULARIZATION

λ = regularization strength (hyperparameter)

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

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

Source: cs231n

REGULARIZATION

λ = regularization strength (hyperparameter)

$$L(W) = \underbrace{\frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

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

Source: cs231n

REGULARIZATION

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

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

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

Source: cs231n

REGULARIZATION

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

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

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$$w_1 \,.x = w_2 \,.x = 1$$

Source: cs231n

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$$w_1 \,.x = w_2 \,.x = 1$$

Which W to consider?

Source: cs231n

REGULARIZATION

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

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

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

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L2 Regularization

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

Source: cs231n

REGULARIZATION

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

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

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

$w_1 \cdot x = w_2 \cdot x = 1$

L2 regularization likes to "spread out" the weights

L2 Regularization

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

Source: cs231n

OTHER TYPES OF REGULARIZATION

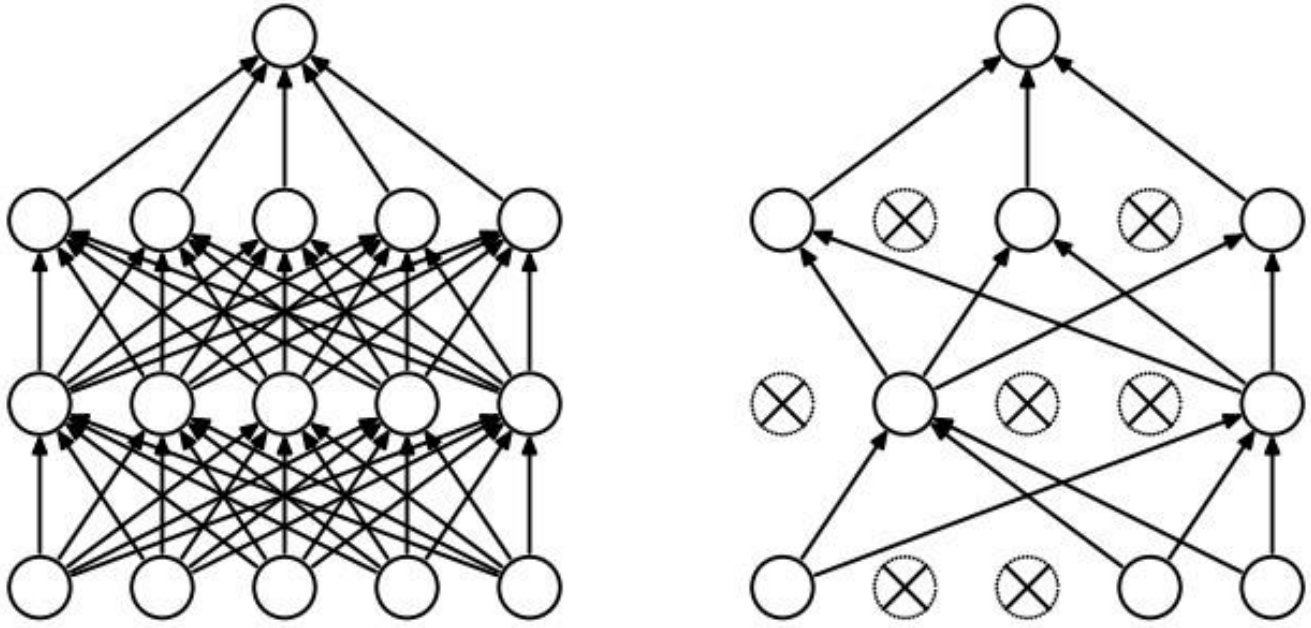
- Dropout
- Batch Normalization
- Data Augmentation
  - Adding noise to the inputs
  - Recall motivation of max margin criterion

Dropout

DROPOUT

In each forward pass, randomly set some neurons to zero

Probability of dropping is a hyperparameter; 0.5 is common



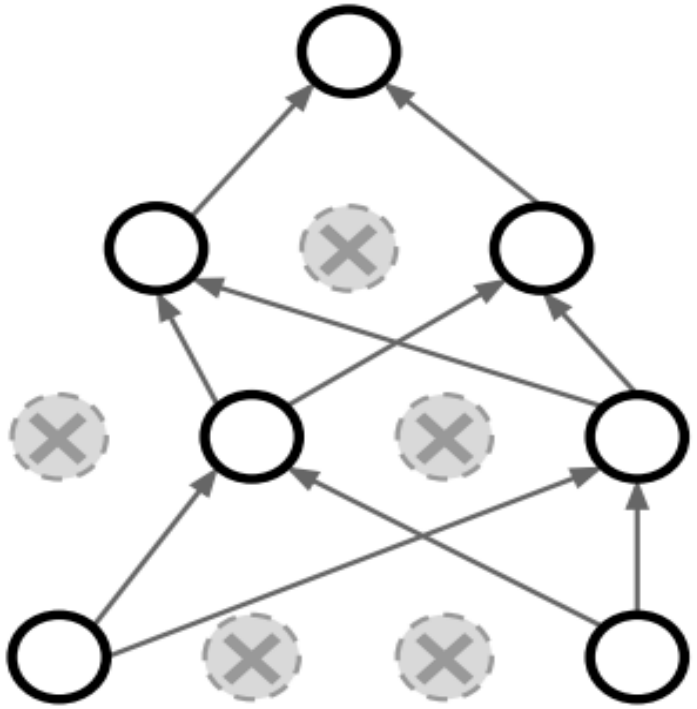
(a) Standard Neural Net

(b) After applying dropout.

Dropout: A simple way to prevent neural networks from overfitting [Srivastava JMLR 2014]

DROPOUT

How can this possibly be a good idea?



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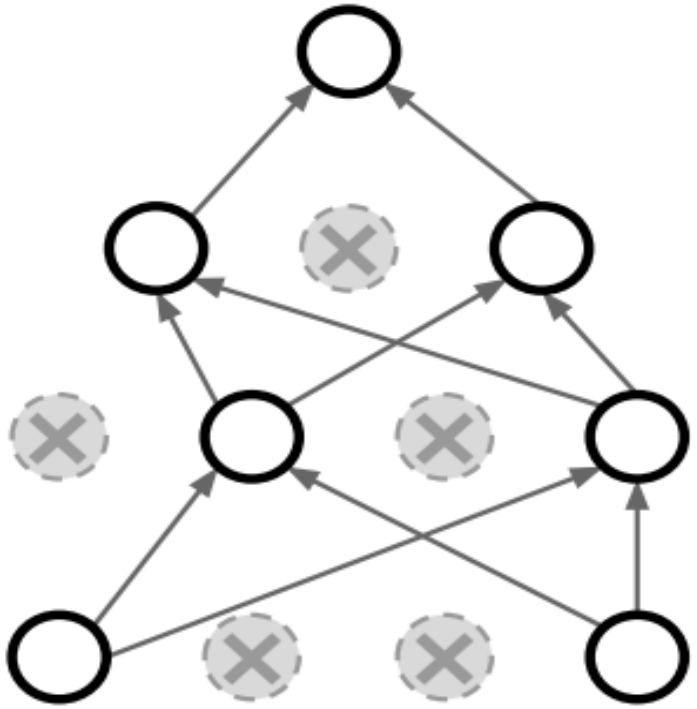
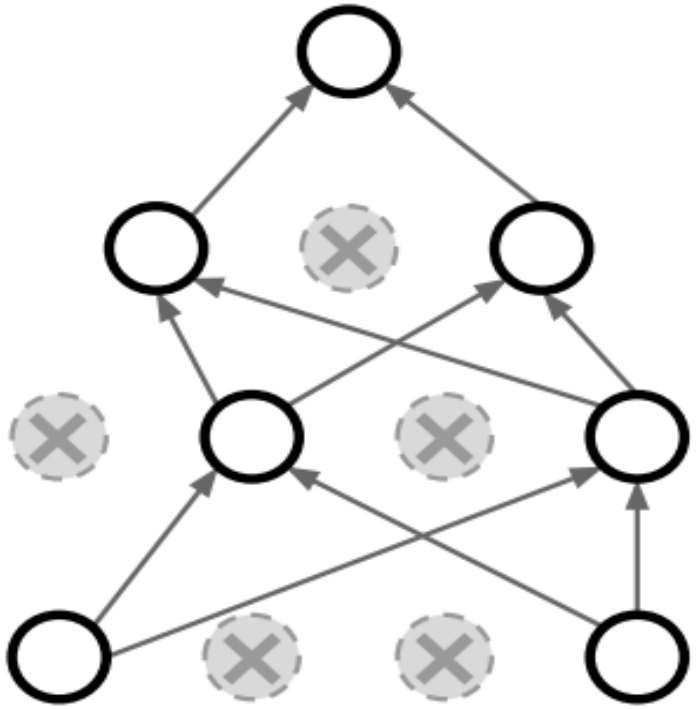


- Intuitions
  - Prevent "co-adaptation" of units, increase robustness to noise
  - Train *implicit ensemble*

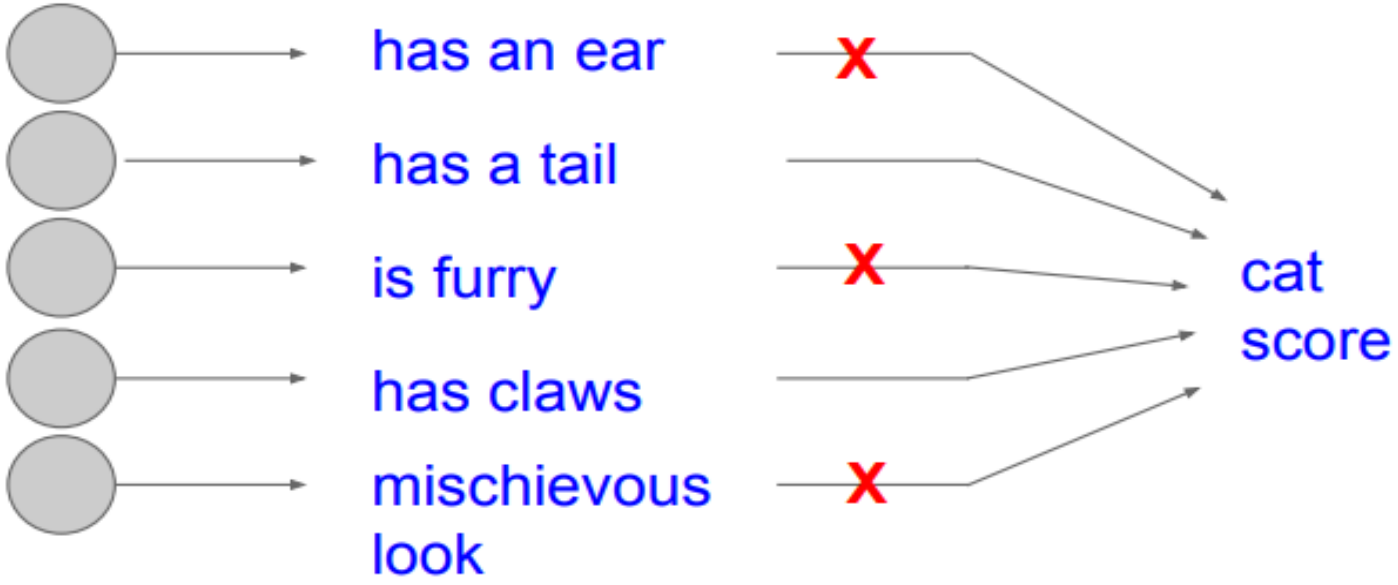
Source: cs231n

DROPOUT

How can this possibly be a good idea?



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



Source: cs231n

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"

Source: cs231n

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)

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!

Source: cs231n

Batch Normalization

BATCH NORMALIZATION

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

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

Source: cs231n

BATCH NORMALIZATION

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

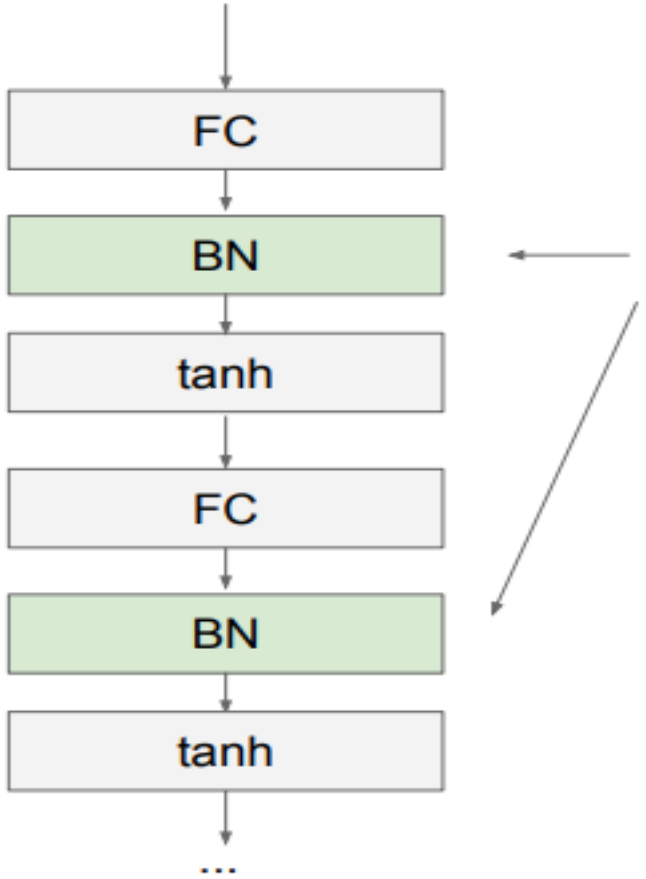
consider a batch of activations at some layer. To make each dimension zero-mean unit-variance, apply:

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

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

Source: cs231n

BATCH NORMALIZATION



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

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

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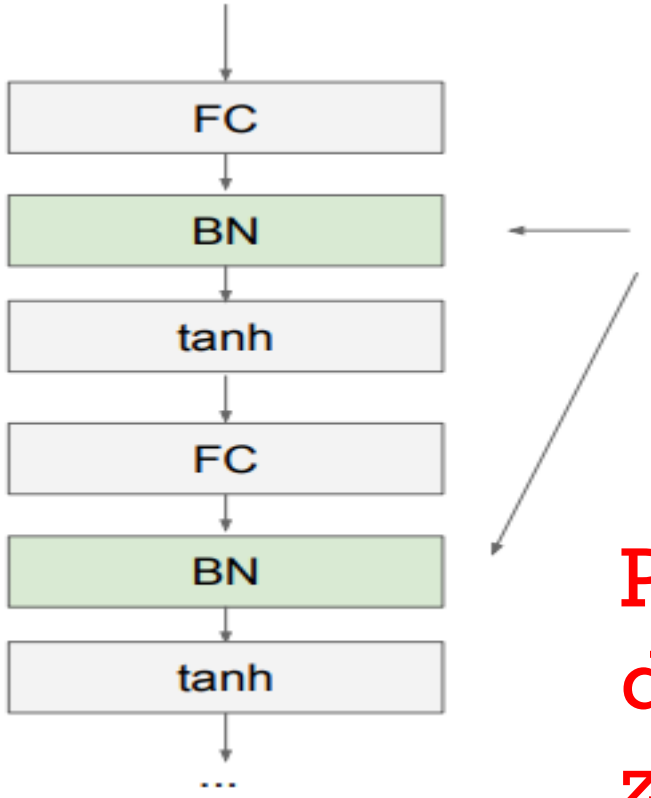
BATCH NORMALIZATION



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

Problem:
do we necessarily want a
zero-mean unit-variance input?

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

Source: cs231n

BATCH NORMALIZATION

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:

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

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Note, the network can learn:

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

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

to recover the identity mapping.

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BATCH NORMALIZATION

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

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

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

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

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

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

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

Source: cs231n

BATCH NORMALIZATION

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: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

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BATCH NORMALIZATION

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

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

At test time (usually):

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

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

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

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

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

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BATCH NORMALIZATION

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

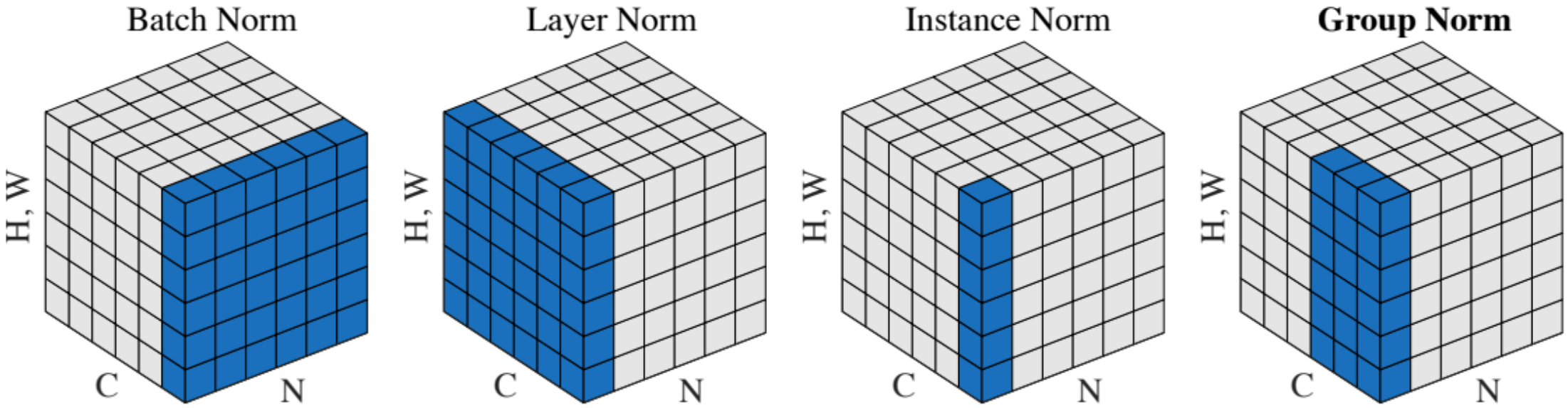
- Behavior depends on composition of mini-batches, can lead to hard-to-catch bugs if there is a mismatch between training and test regime (example)
- Doesn't work well for small mini-batch sizes
- Cannot be used in recurrent models

Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift [Ioffe and Szegedy 2015]

Source: cs231n

OTHER TYPES OF NORMALIZATION

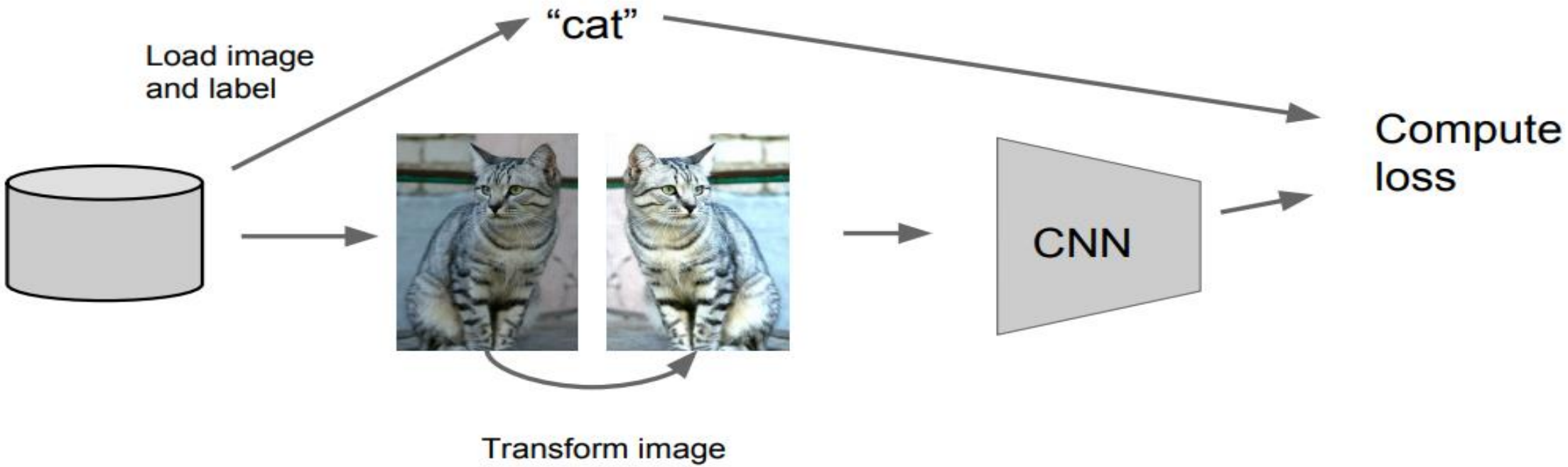
- Layer normalization (Ba et al., 2016)
- Instance normalization (Ulyanov et al., 2017)
- Group normalization (Wu and He, 2018)
- Weight normalization (Salimans et al., 2016)



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

Data Augmentation

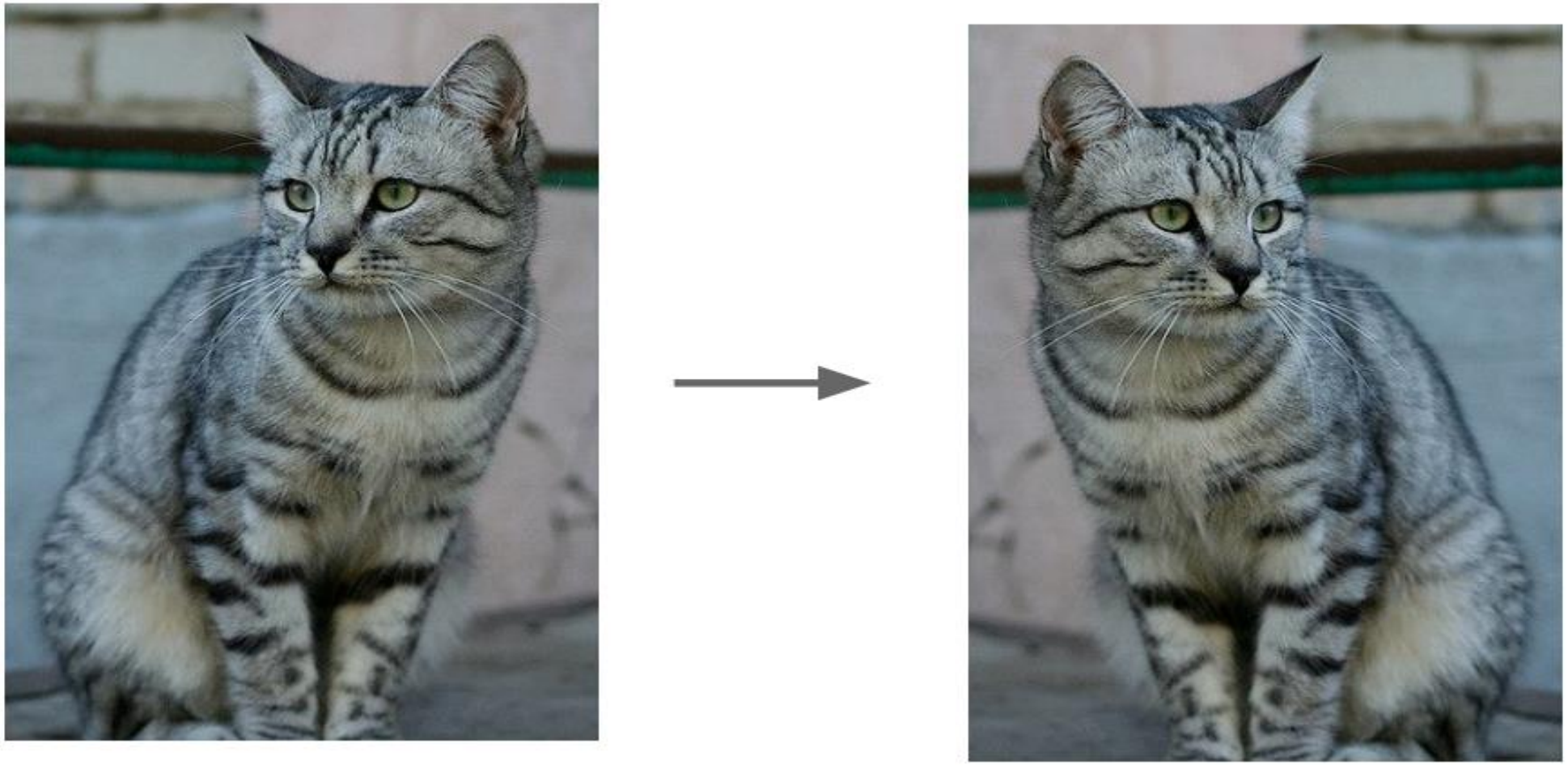
DATA AUGMENTATION (JITTERING)



Source: cs231n

DATA AUGMENTATION (JITTERING)

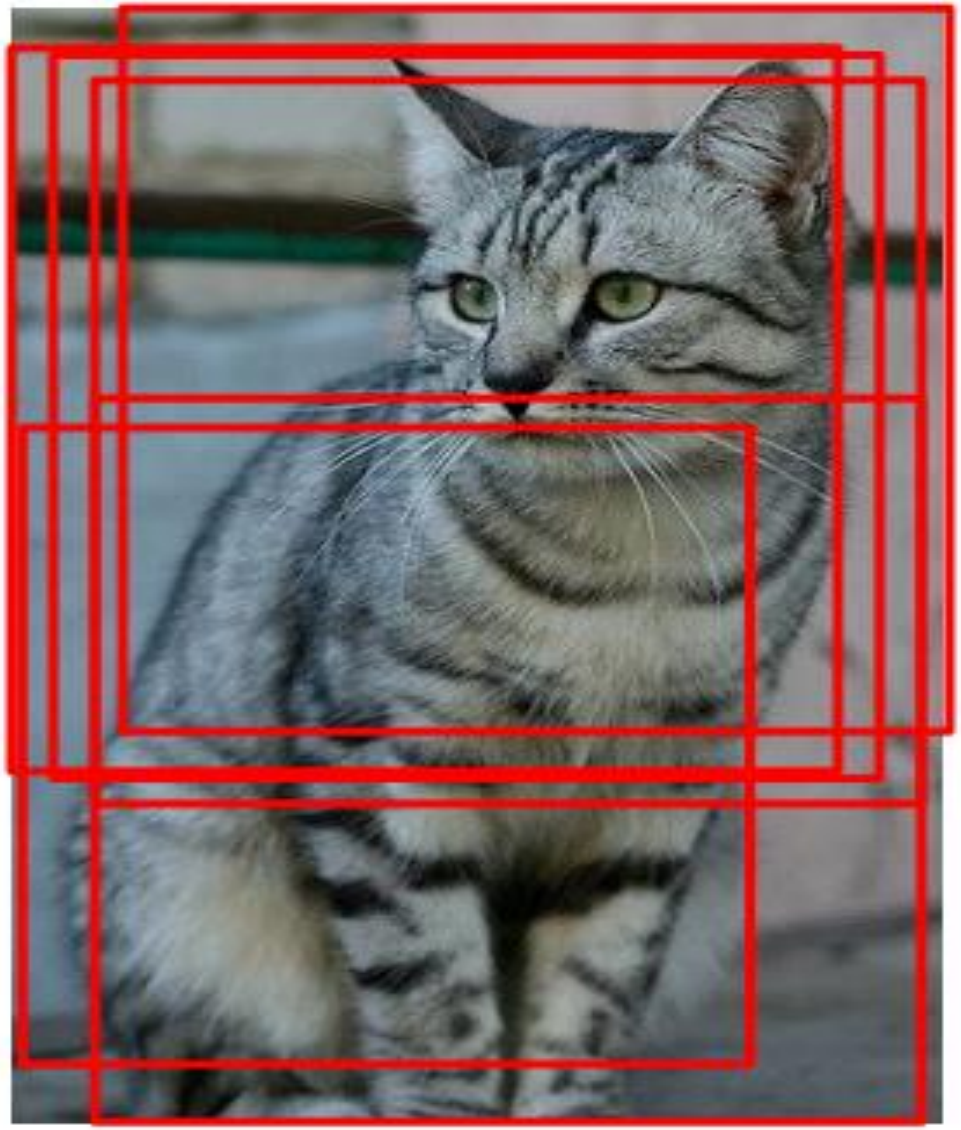
Horizontal Flips



Source: cs231n

DATA AUGMENTATION (JITTERING)

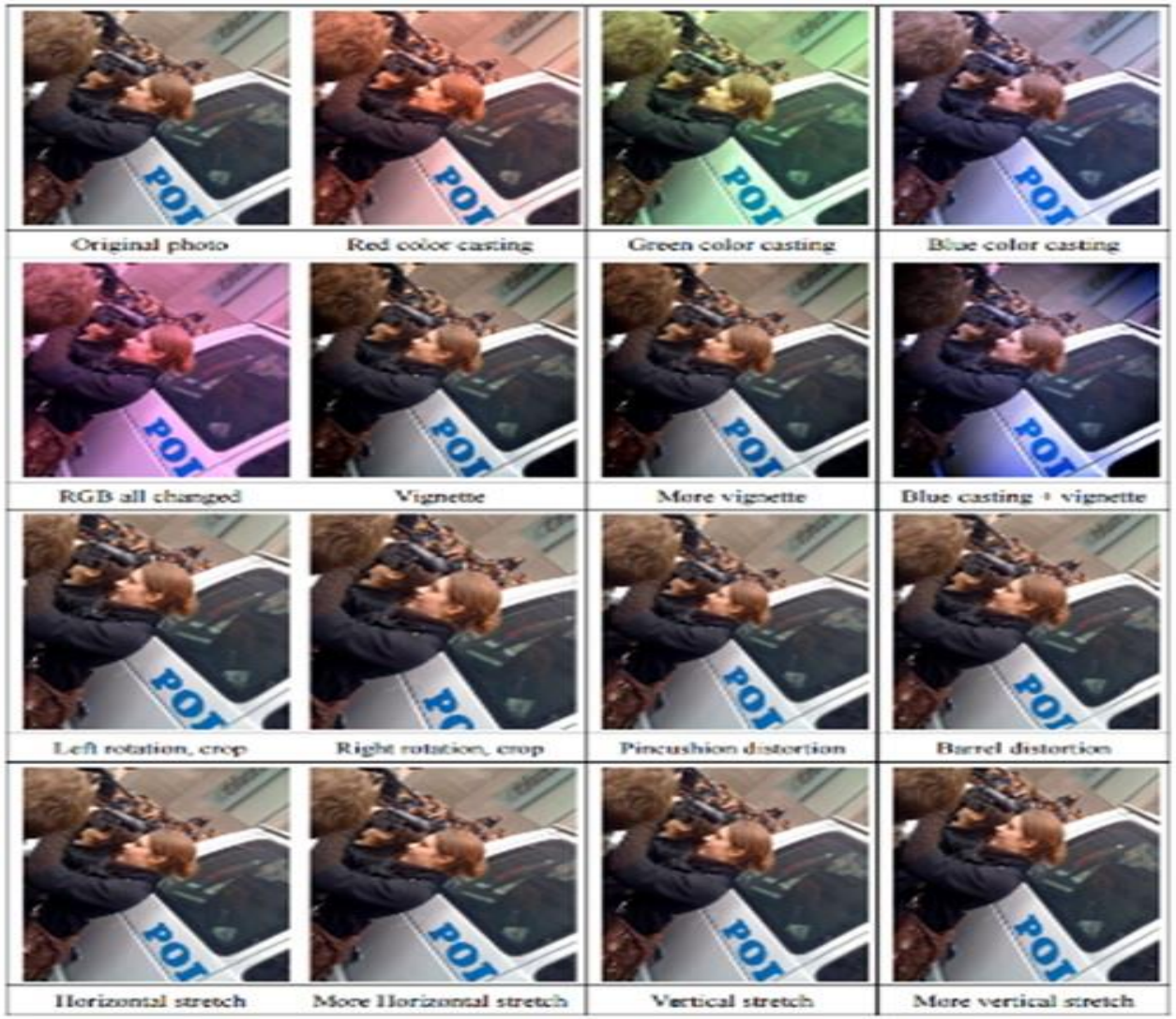
Random crops and scales



Source: cs231n

DATA AUGMENTATION (JITTERING)

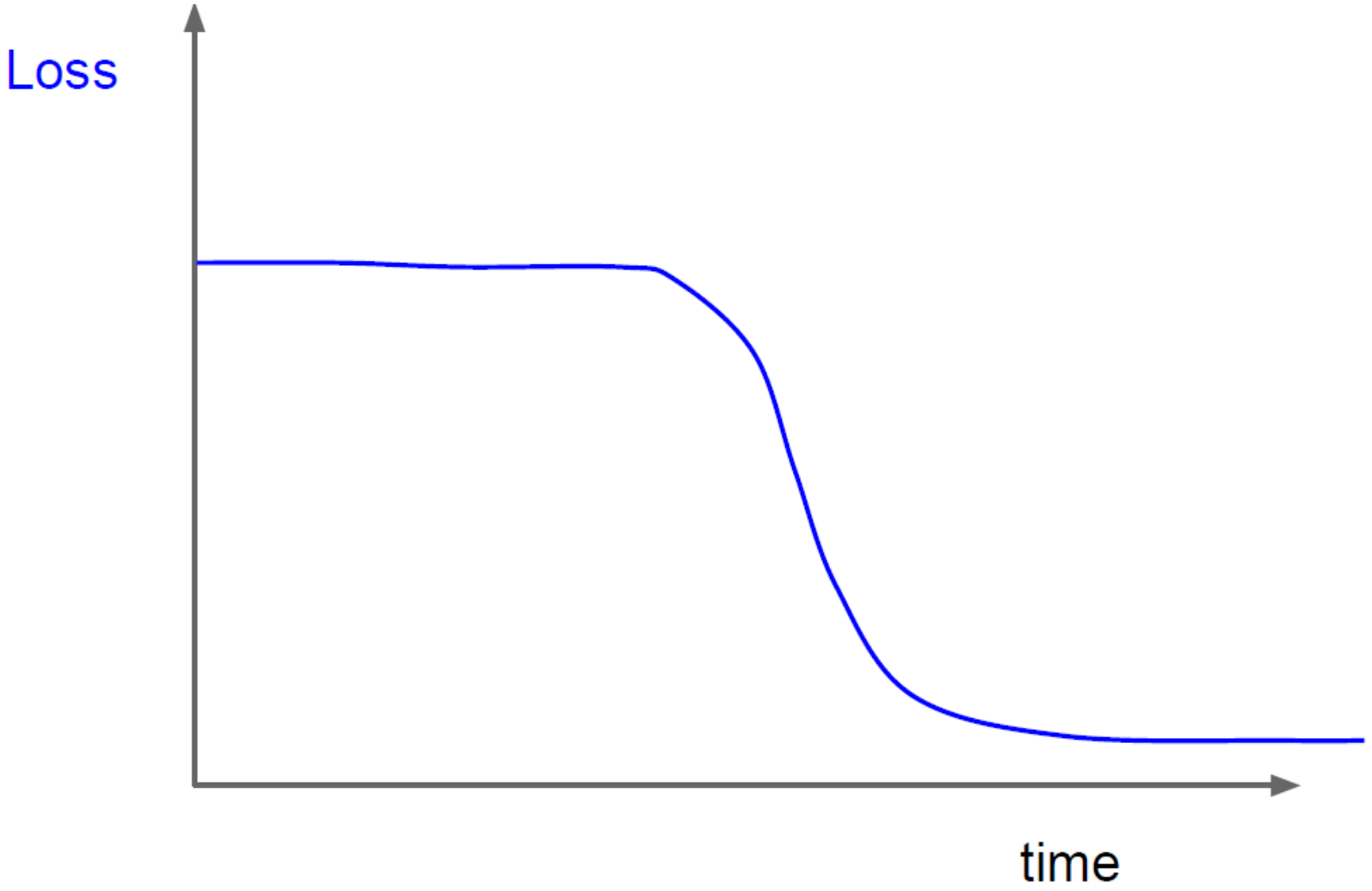
- Create *virtual* training samples
- Get creative for your problem!
  - Horizontal flip
  - Random crop
  - Color casting
  - Randomize contrast
  - Randomize brightness
  - Geometric distortion
  - Rotation
  - Photometric changes



Deep Image [Wu et al. 2015]

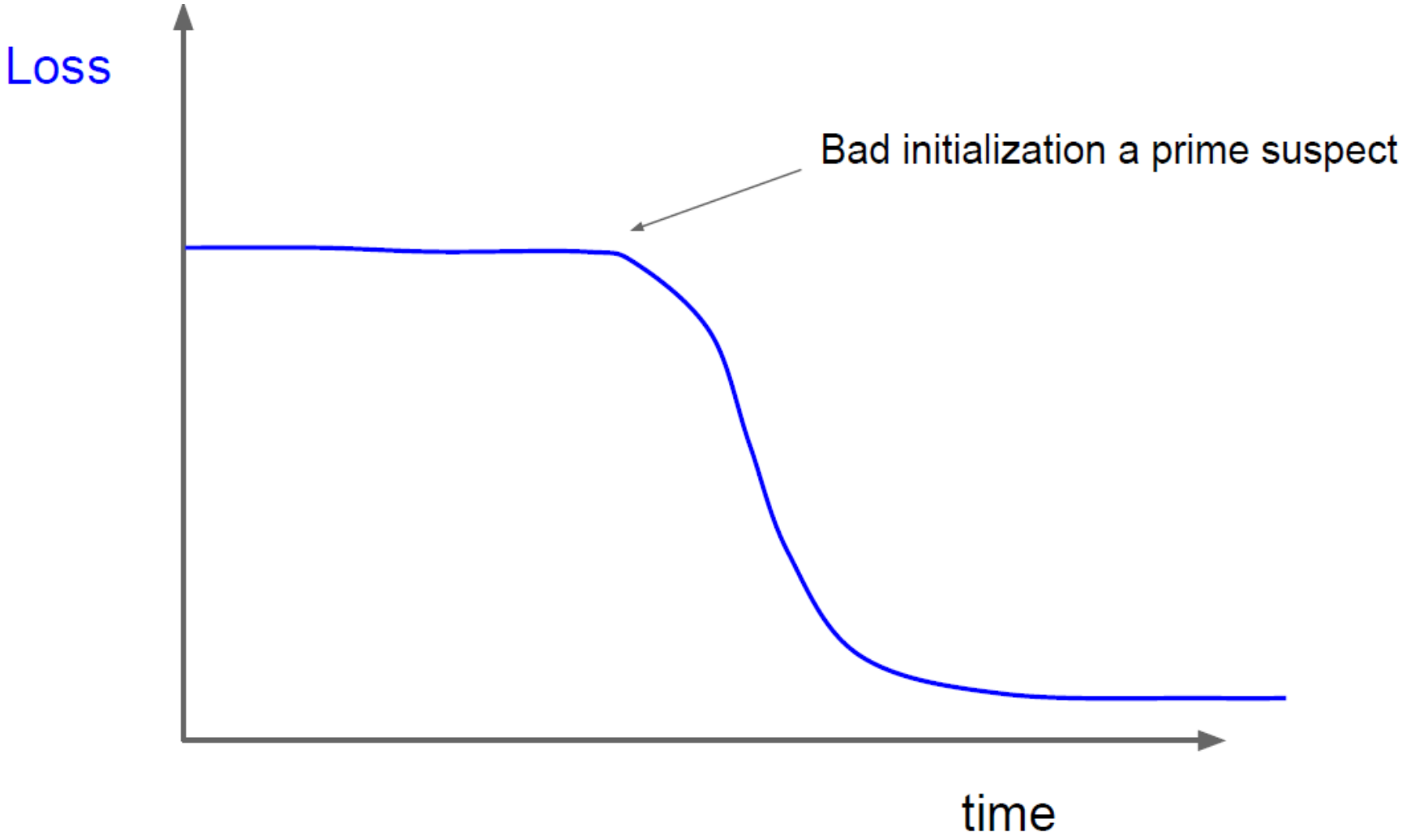
MONITOR AND VISUALIZE THE LOSS CURVE

MONITOR AND VISUALIZE THE LOSS CURVE



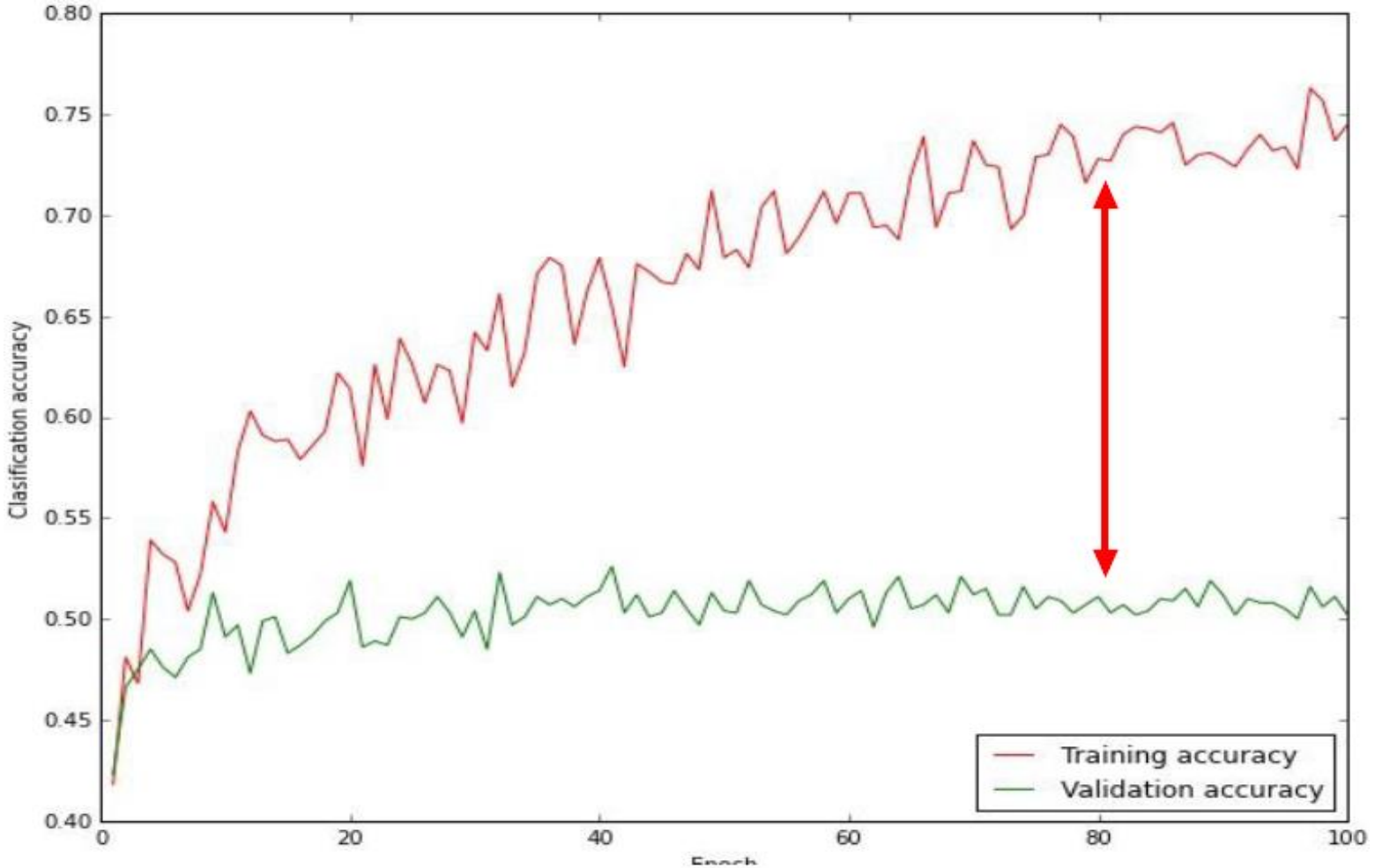
Source: cs231n

MONITOR AND VISUALIZE THE LOSS CURVE



Source: cs231n

MONITOR AND VISUALIZE THE LOSS CURVE

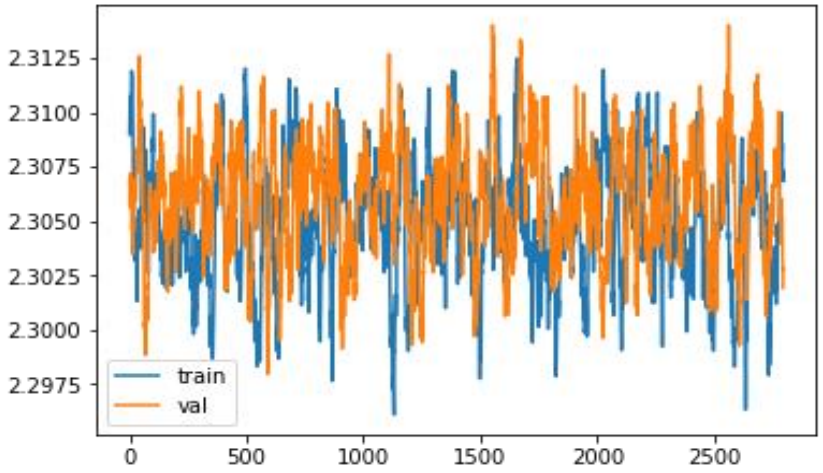


big gap = overfitting
=> increase regularization strength?

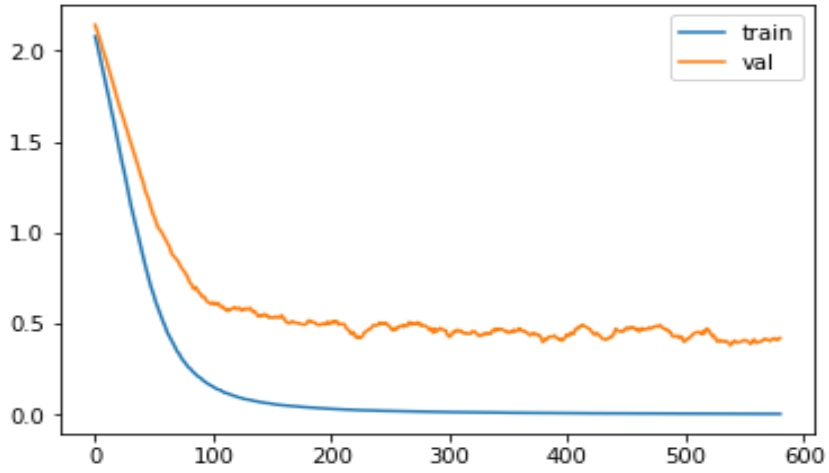
no gap
=> increase model capacity?

Source: cs231n

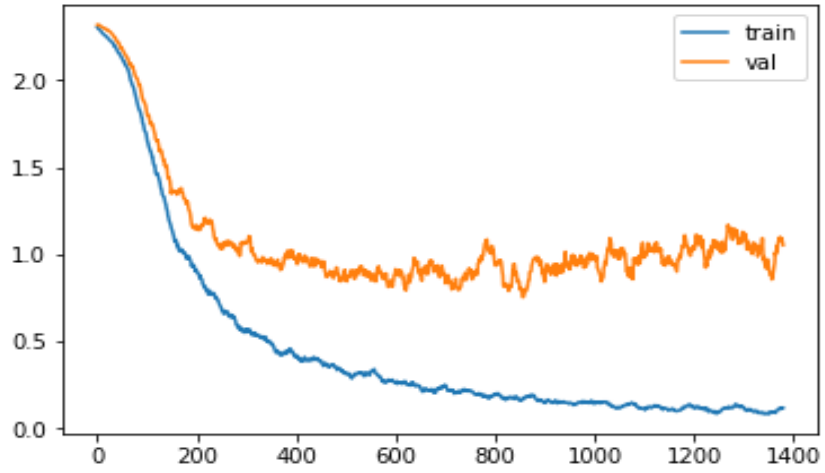
MONITOR AND VISUALIZE THE LOSS CURVE



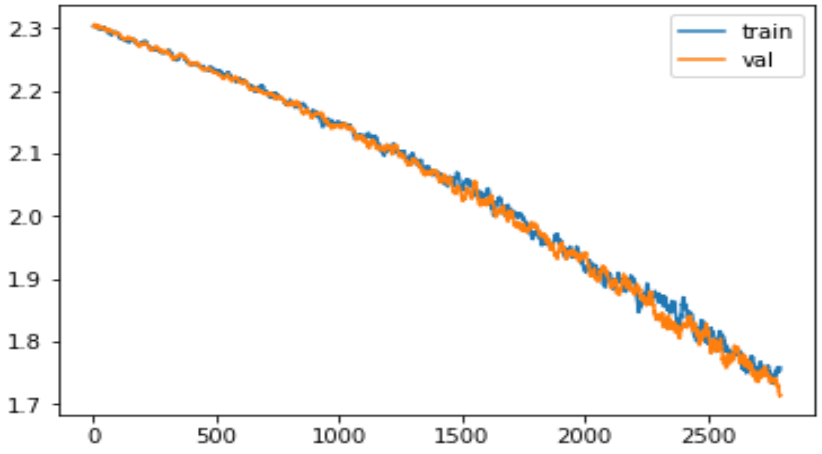
Not learning: gradients not applied to weights



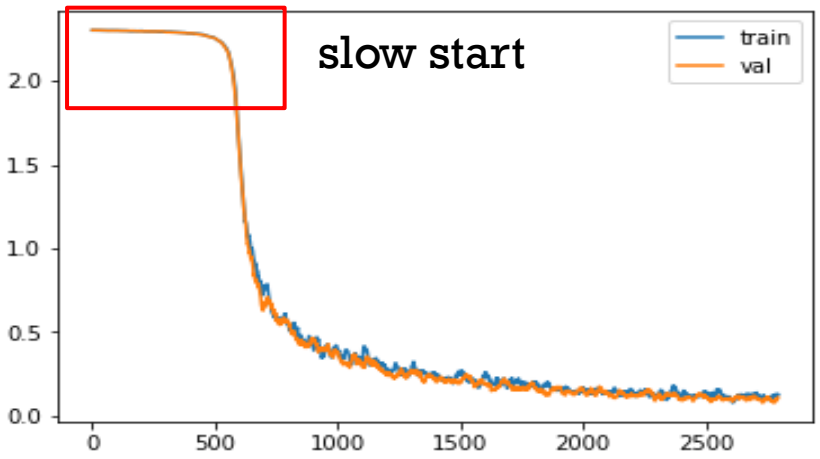
Overfit: model too large/dataset too small



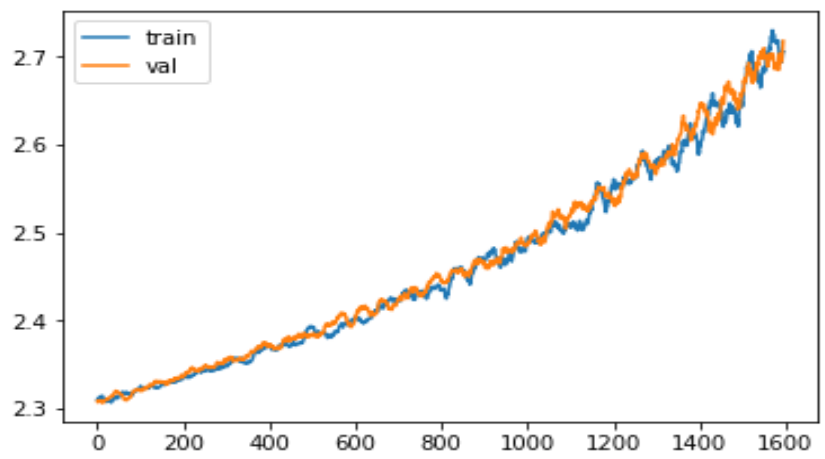
More extreme case of overfitting



Not converged yet: need longer training



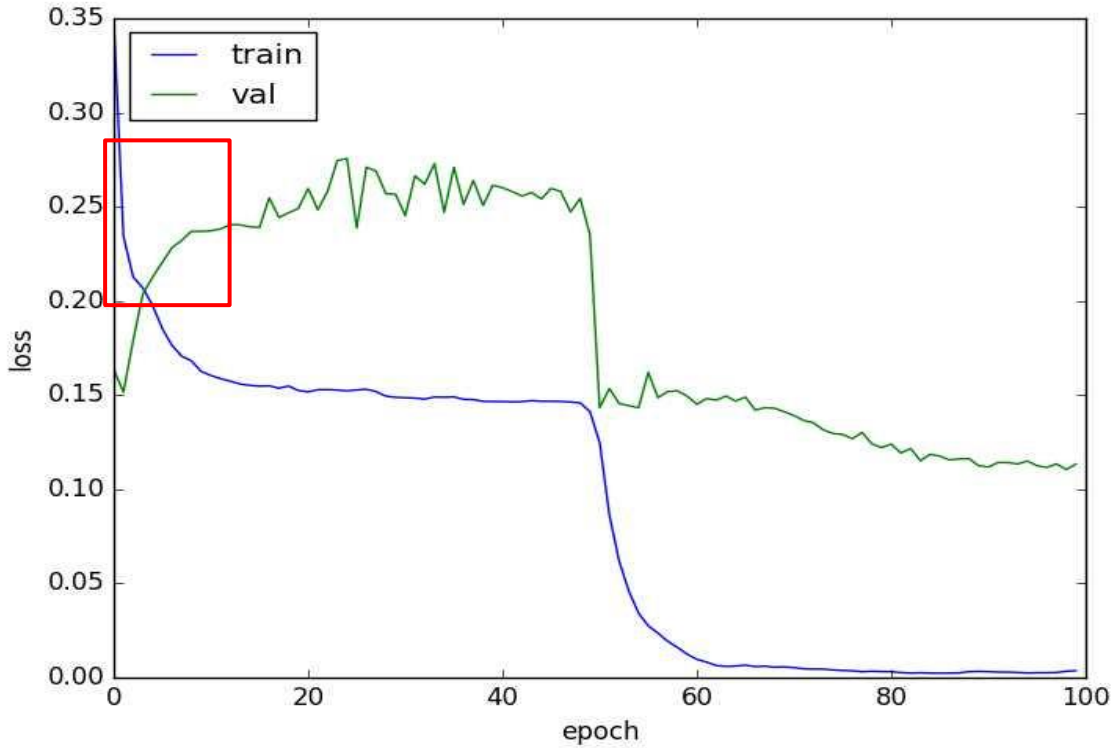
Slow start: initialization weights too small



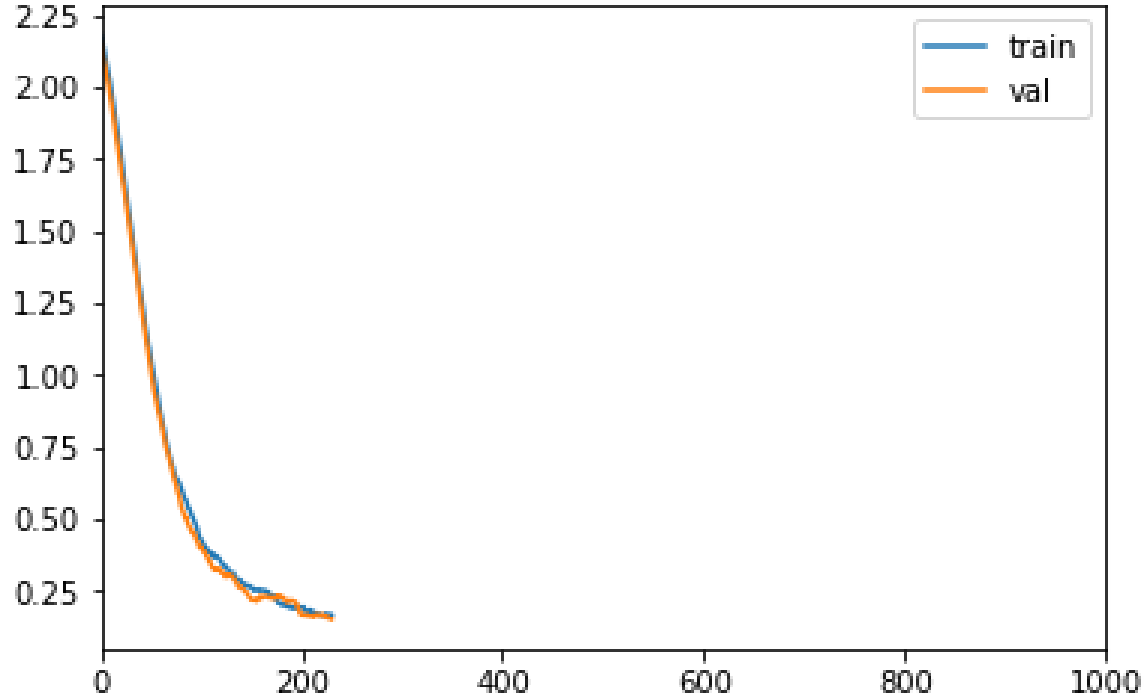
Applied the negative of gradients

Source: cs231n

MONITOR AND VISUALIZE THE LOSS CURVE



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

Source: cs231n

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

THINGS TO REMEMBER

- 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

Questions?