Lecture 7: Training Neural Networks, Part 2

Last time: Batch Normalization

Input: $x : N \times D$

Learnable params:

$\gamma, \beta : D$

Intermediates: $\mu, \sigma : D$

$\hat{x} : N \times D$

Output: $y : N \times D$

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

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

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

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

Last time: Batch Normalization

Estimate mean and variance from minibatch; Can't do this at test-time

Input: $x : N \times D$

Learnable params: $\gamma, \beta : D$

Intermediates: $\mu, \sigma : D$
$\hat{x} : N \times D$

Output: $y : N \times D$

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

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

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

Batch Normalization: Test Time

Input: $x : N \times D$

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

Learnable params:

$\gamma, \beta : D$

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

Intermediates: $\mu, \sigma : D$
$\hat{x} : N \times D$

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

Output: $y : N \times D$

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

Batch Normalization for ConvNets

Channel

Feature Size

Batch Normalization for **fully-connected** networks

Number of Samples

Number of Features

$\mathbf{x}$: N × D

Normalize

μ, σ: 1 × D

γ, β: 1 × D

$y = \gamma(x-\mu)/\sigma+\beta$

Batch Normalization for **convolutional** networks (Spatial Batchnorm, BatchNorm2D)

$\mathbf{x}$: N×C×H×W

Normalize

μ, σ: 1×C×1×1

γ, β: 1×C×1×1

$y = \gamma(x-\mu)/\sigma+\beta$

Layer Normalization

Batch Normalization for fully-connected networks

$$\mathbf{x}: N \times D$$

Normalize

$$\boldsymbol{\mu}, \boldsymbol{\sigma}: 1 \times D$$

$$\boldsymbol{\gamma}, \boldsymbol{\beta}: 1 \times D$$

$$\mathbf{y} = \gamma(\mathbf{x}-\boldsymbol{\mu})/\boldsymbol{\sigma}+\boldsymbol{\beta}$$

Layer Normalization for fully-connected networks

Same behavior at train and test!

Can be used in recurrent networks

$$\mathbf{x}: N \times D$$

Normalize

$$\boldsymbol{\mu}, \boldsymbol{\sigma}: N \times 1$$

$$\boldsymbol{\gamma}, \boldsymbol{\beta}: 1 \times D$$

$$\mathbf{y} = \gamma(\mathbf{x}-\boldsymbol{\mu})/\boldsymbol{\sigma}+\boldsymbol{\beta}$$

Ba, Kiros, and Hinton, “Layer Normalization”, arXiv 2016

Instance Normalization

Batch Normalization for convolutional networks

Normalize

$$x: N \times C \times H \times W$$

$$\mu, \sigma: 1 \times C \times 1 \times 1$$

$$\gamma, \beta: 1 \times C \times 1 \times 1$$

$$y = \gamma(x-\mu)/\sigma+\beta$$

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

Normalize

$$x: N \times C \times H \times W$$

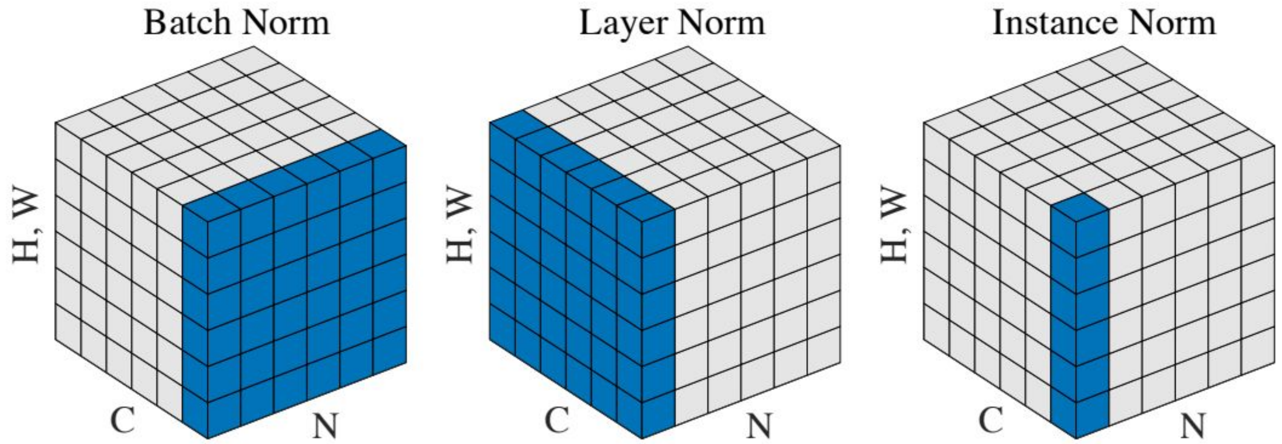
$$\mu, \sigma: N \times C \times 1 \times 1$$

$$\gamma, \beta: 1 \times C \times 1 \times 1$$

$$y = \gamma(x-\mu)/\sigma+\beta$$

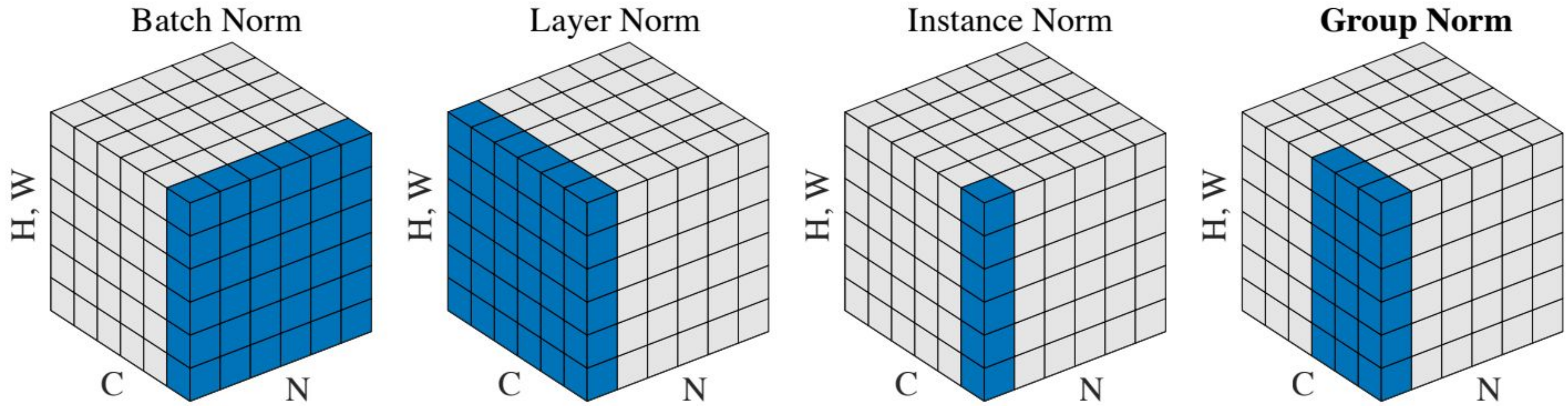
Ulyanov et al, Improved Texture Networks: Maximizing Quality and Diversity in Feed-forward Stylization and Texture Synthesis, CVPR 2017

Comparison of Normalization Layers



Wu and He, “Group Normalization”, arXiv 2018

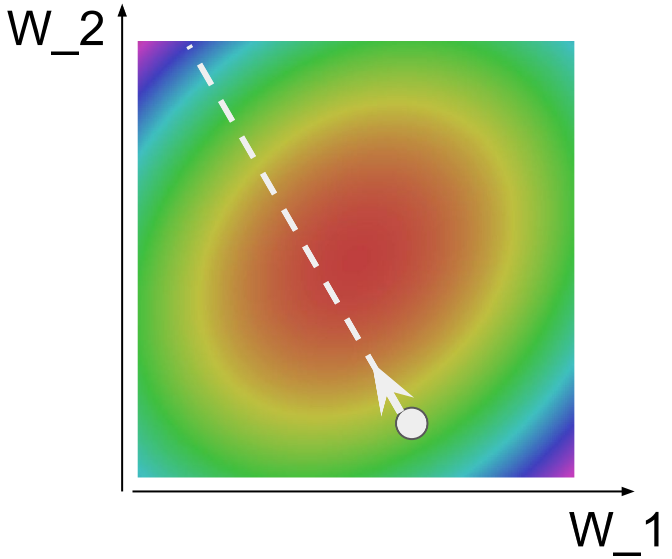
Group Normalization



Wu and He, “Group Normalization”, arXiv 2018 (Appeared 3/22/2018)

Optimization

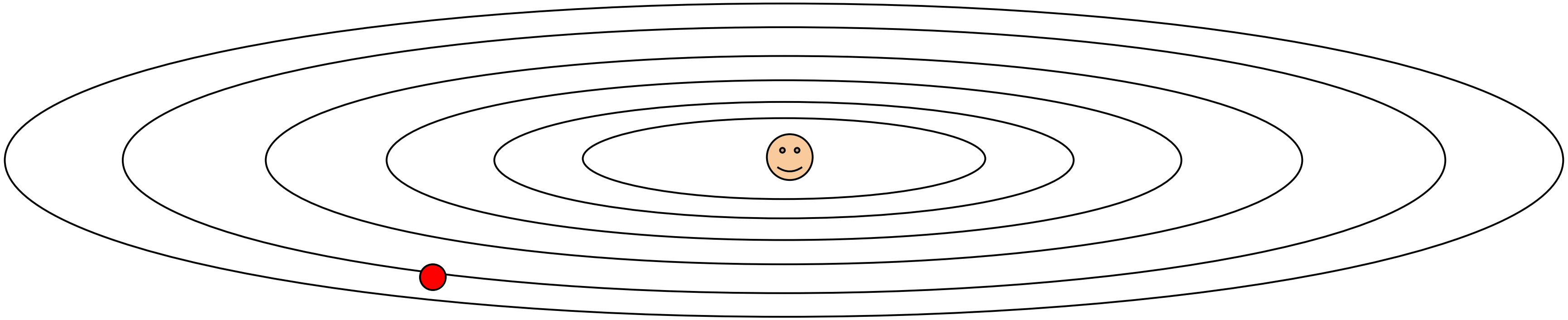
```
# Vanilla Gradient Descent

while True:
  weights_grad = evaluate_gradient(loss_fun, data, weights)
  weights += - step_size * weights_grad # perform parameter update
```



Optimization: Problems with SGD

stochastic

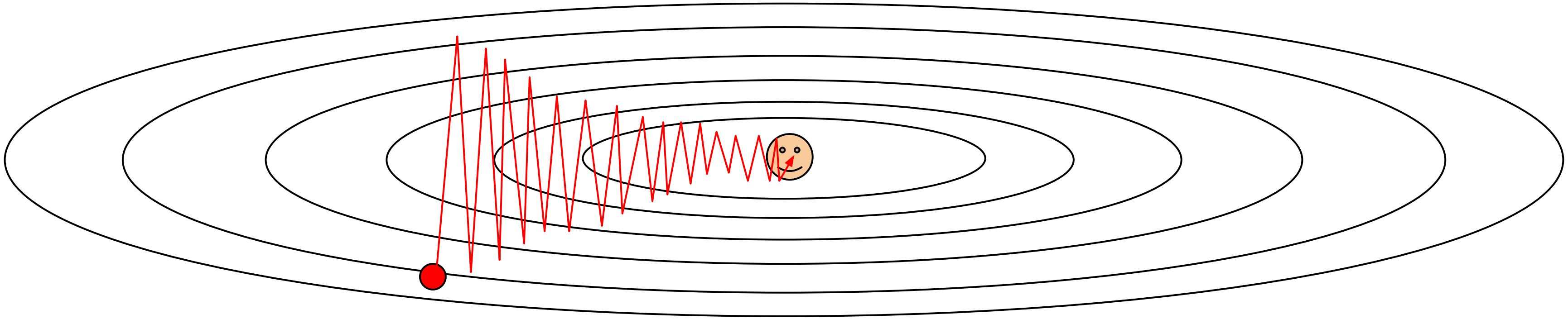
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Optimization: Problems with SGD

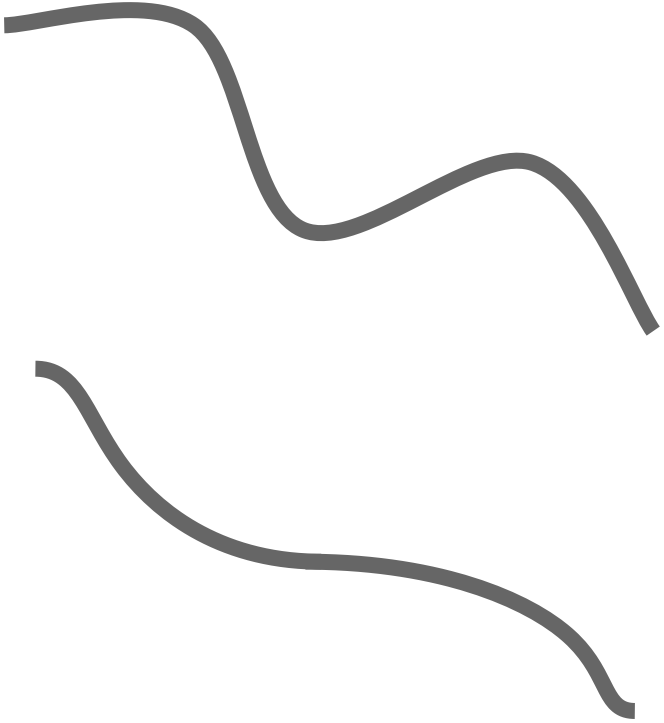
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction



Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Optimization: Problems with SGD

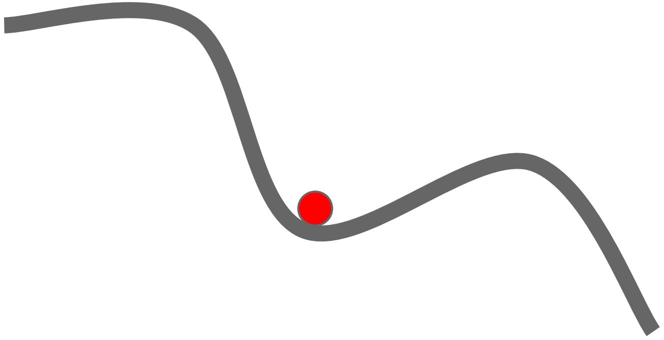
What if the loss function has a **local minima** or **saddle point**?

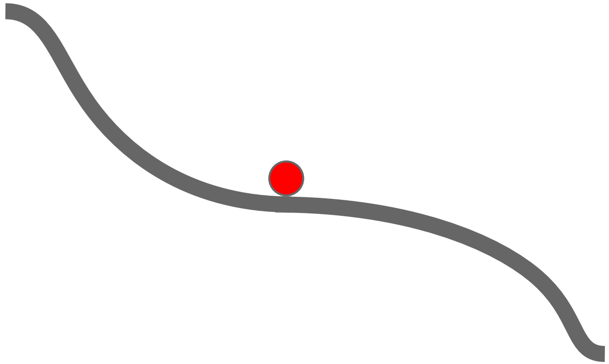


Optimization: Problems with SGD

What if the loss function has a **local minima** or **saddle point**?

Zero gradient, gradient descent gets stuck

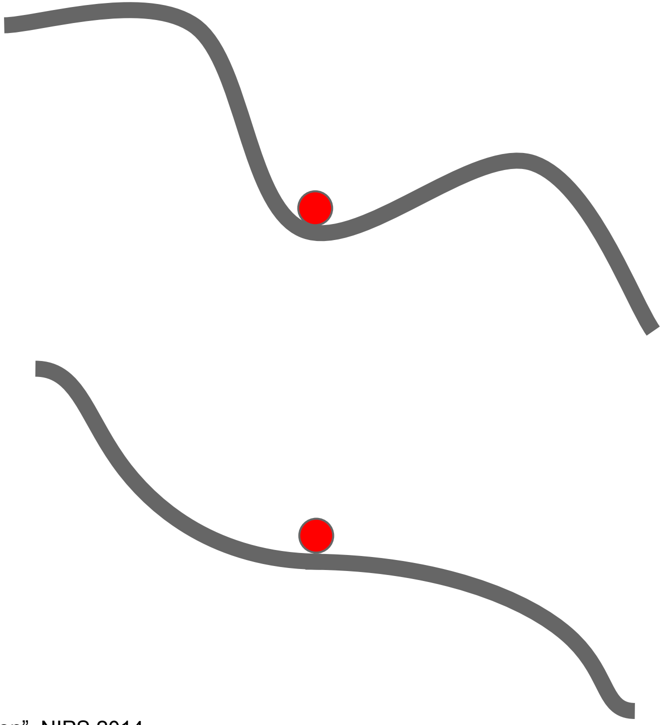




Optimization: Problems with SGD

What if the loss function has a **local minima** or **saddle point**?

Saddle points much more common in high dimension



Dauphin et al, “Identifying and attacking the saddle point problem in high-dimensional non-convex optimization”, NIPS 2014

Optimization: Problems with SGD

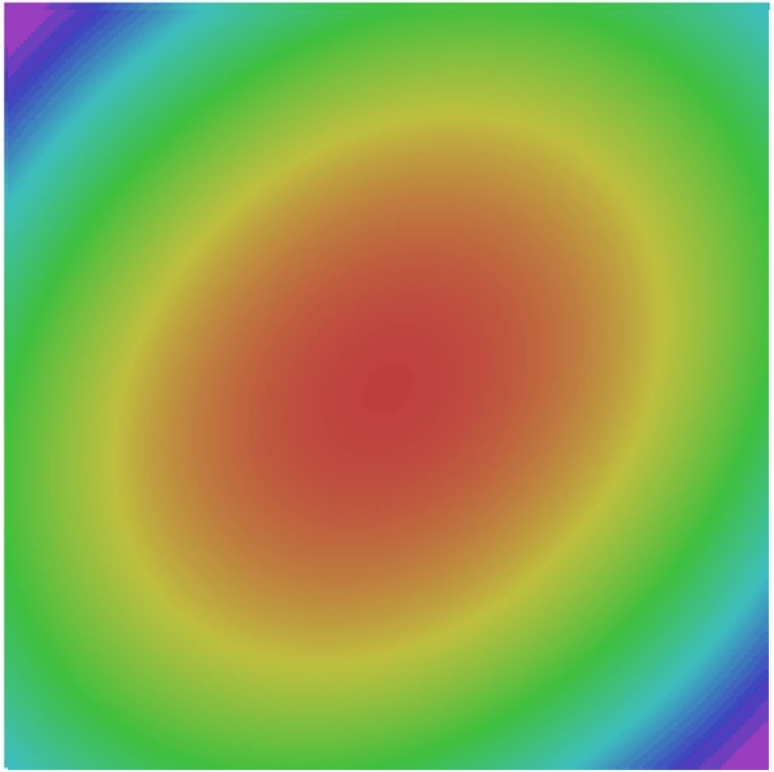
Our gradients come from minibatches so they can be noisy!

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

Loss Function

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

Gradient Decent



SGD + Momentum

SGD

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

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

SGD+Momentum

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

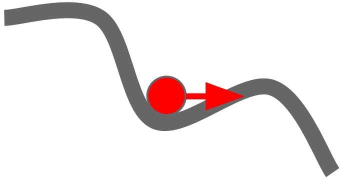
```python
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x -= learning_rate * vx
```

- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically rho=0.9 or 0.99

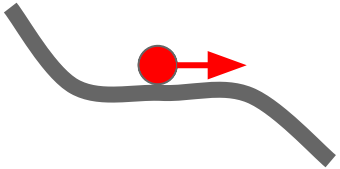
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

SGD + Momentum

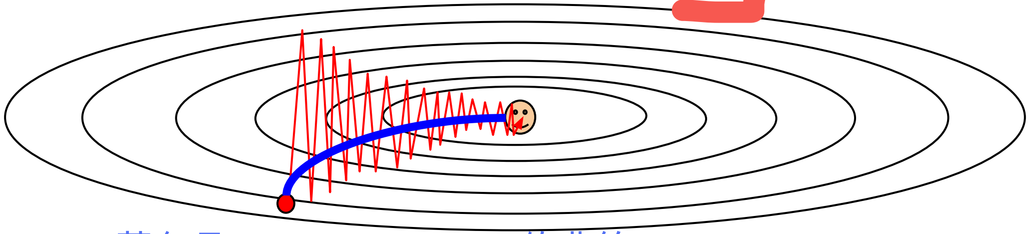
Local Minima



Saddle points

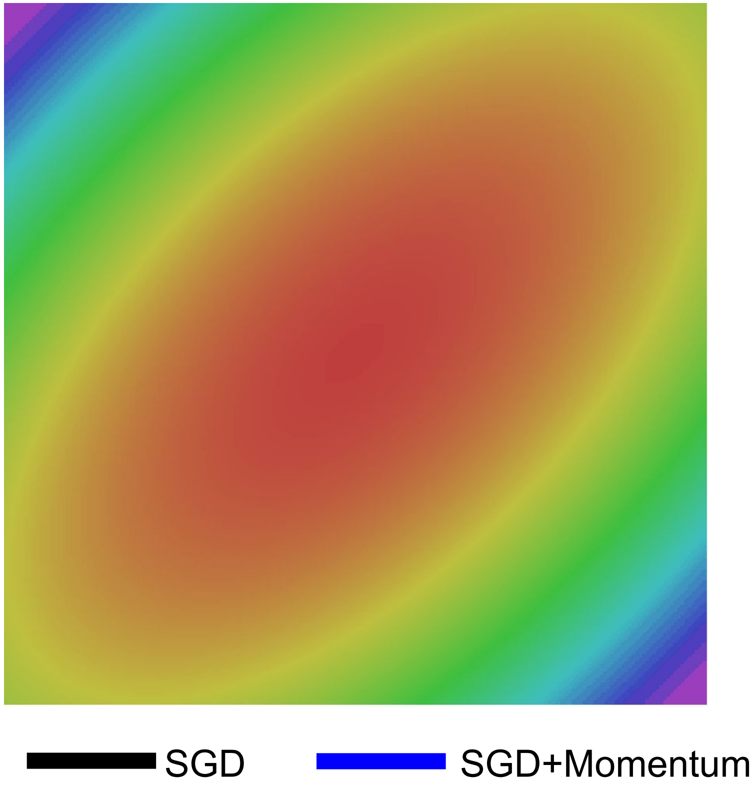


Poor Conditioning



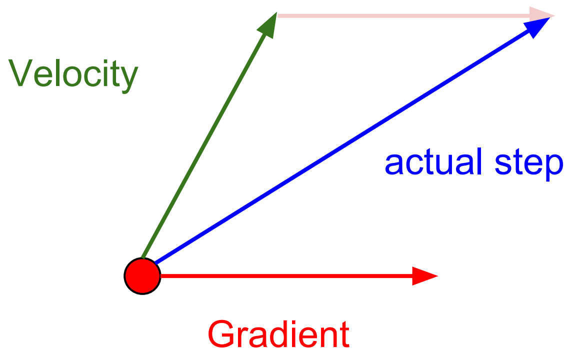
藍色是SGD+Momentum的曲線

Gradient Noise



SGD+Momentum

Momentum update:

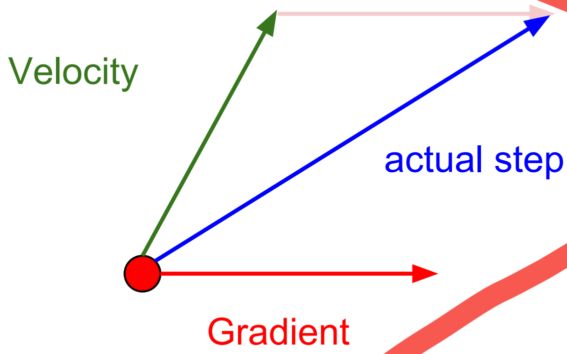


Combine gradient at current point with velocity to get step used to update weights

Nesterov, “A method of solving a convex programming problem with convergence rate O(1/k^2)”, 1983
Nesterov, “Introductory lectures on convex optimization: a basic course”, 2004
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

Nesterov Momentum

Momentum update:



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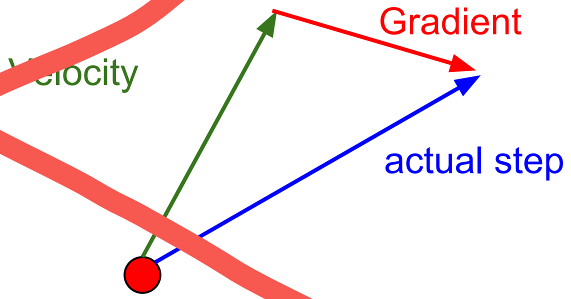
Nesterov Momentum



?

"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov, "A method of solving a convex programming problem with convergence rate O(1/k^2)", 1983
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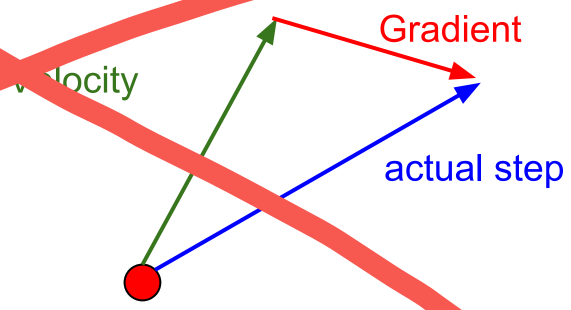
Nesterov Momentum

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



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$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
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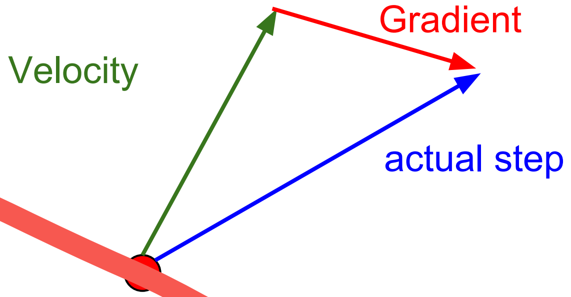
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



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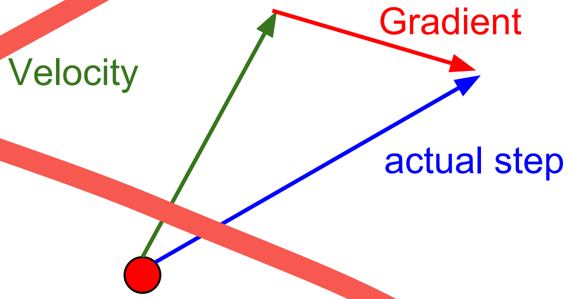
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$

Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

$$\begin{aligned} v_{t+1} &= \rho v_t - \alpha \nabla f(\tilde{x}_t) \\ \tilde{x}_{t+1} &= \tilde{x}_t - \rho v_t + (1 + \rho) v_{t+1} \\ &= \tilde{x}_t + v_{t+1} + \rho(v_{t+1} - v_t) \end{aligned}$$



“Look ahead” to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

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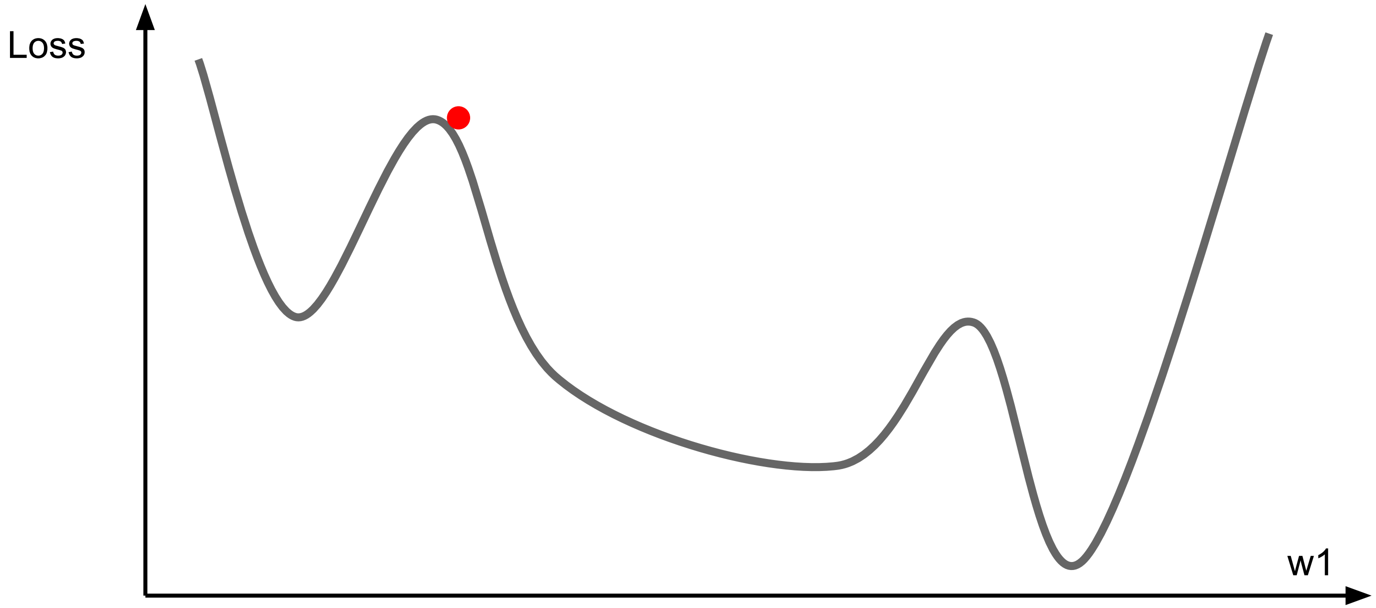
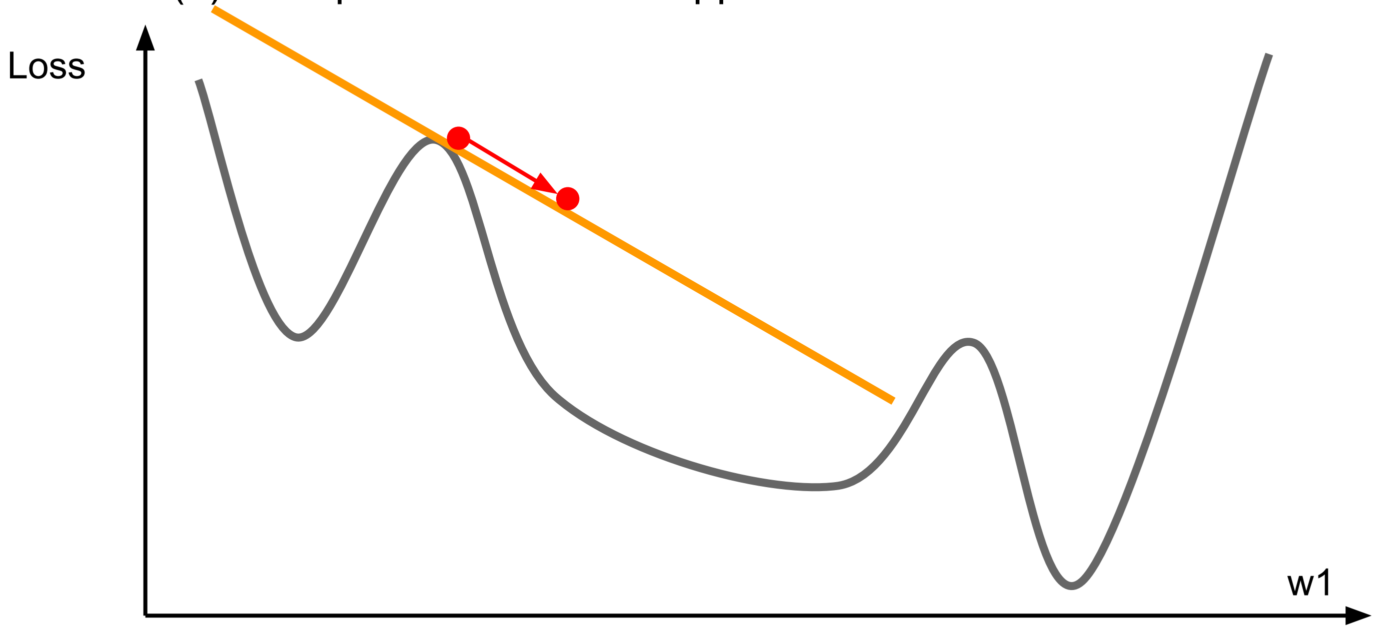
```
dx = compute_gradient(x)
old_v = v
v = rho * v - learning_rate * dx
x += -rho * old_v + (1 + rho) * v
```

First-Order Optimization



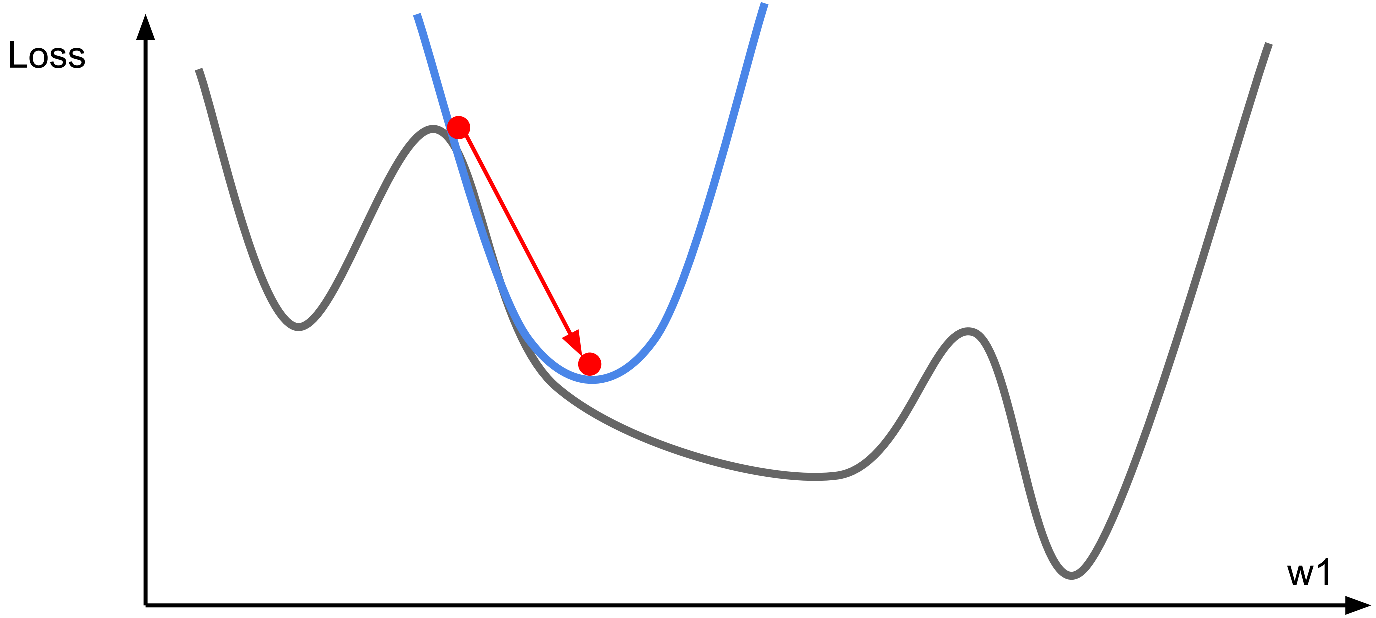
First-Order Optimization

(1) Use gradient form linear approximation
(2) Step to minimize the approximation



Second-Order Optimization

(1) Use gradient **and Hessian** to form **quadratic** approximation
(2) Step to the **minima** of the approximation



Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Q: What is nice about this update?

Second-Order Optimization

second-order Taylor expansion:

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Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

No hyperparameters!
No learning rate!
(Though you might use one in practice)

Q: What is nice about this update?

Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Q2: Why is this bad for deep learning?

Second-Order Optimization

second-order Taylor expansion:

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \boldsymbol{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

Solving for the critical point we obtain the Newton parameter update:

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Hessian has O(N^2) elements
Inverting takes O(N^3)
N = (Tens or Hundreds of) Millions

Q2: Why is this bad for deep learning?

Second-Order Optimization

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \boldsymbol{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

- Quasi-Newton methods (**BGFS** most popular):
  instead of inverting the Hessian (O(n^3)), approximate inverse Hessian with rank 1 updates over time (O(n^2) each).

- **L-BFGS** (Limited memory BFGS):
  Does not form/store the full inverse Hessian.

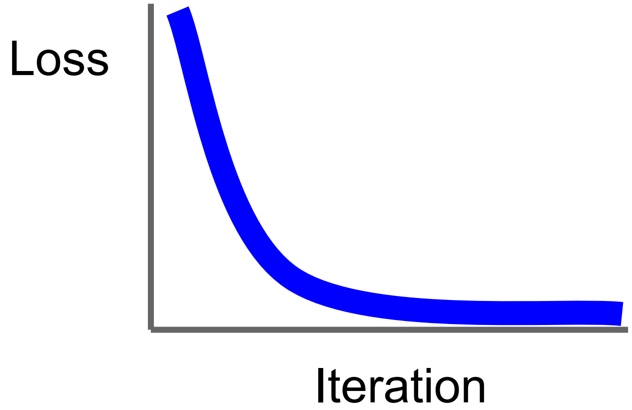
L-BFGS

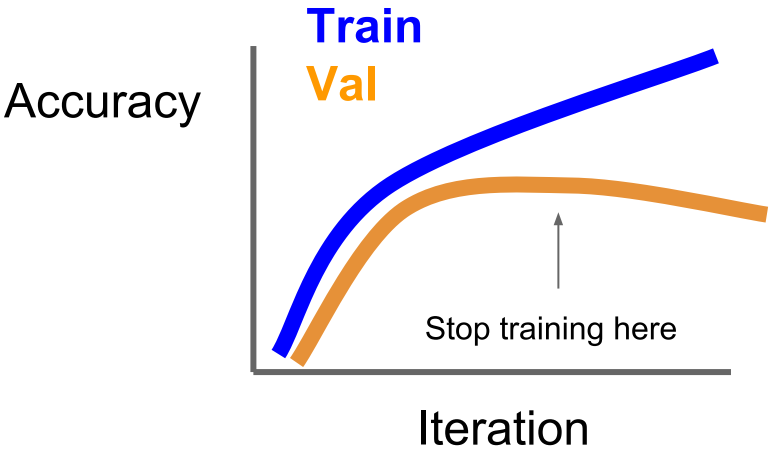
- **Usually works very well in full batch, deterministic mode** i.e. if you have a single, deterministic f(x) then L-BFGS will probably work very nicely

- **Does not transfer very well to mini-batch setting**. Gives bad results. Adapting second-order methods to large-scale, stochastic setting is an active area of research.

Le et al, "On optimization methods for deep learning, ICML 2011"
Ba et al, "Distributed second-order optimization using Kronecker-factored approximations", ICLR 2017

Early Stopping





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

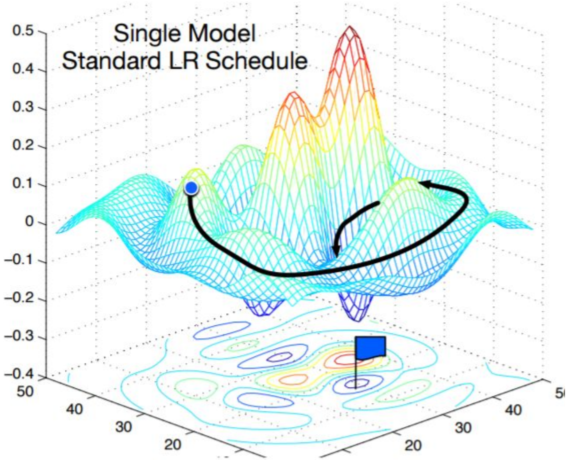
1. Train multiple independent models
2. At test time average their results

   (Take average of predicted probability distributions, then choose argmax)

Enjoy 2% extra performance

Model Ensembles: Tips and Tricks

Instead of training independent models, use multiple snapshots of a single model during training!



Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016
Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017

Model Ensembles: Tips and Tricks

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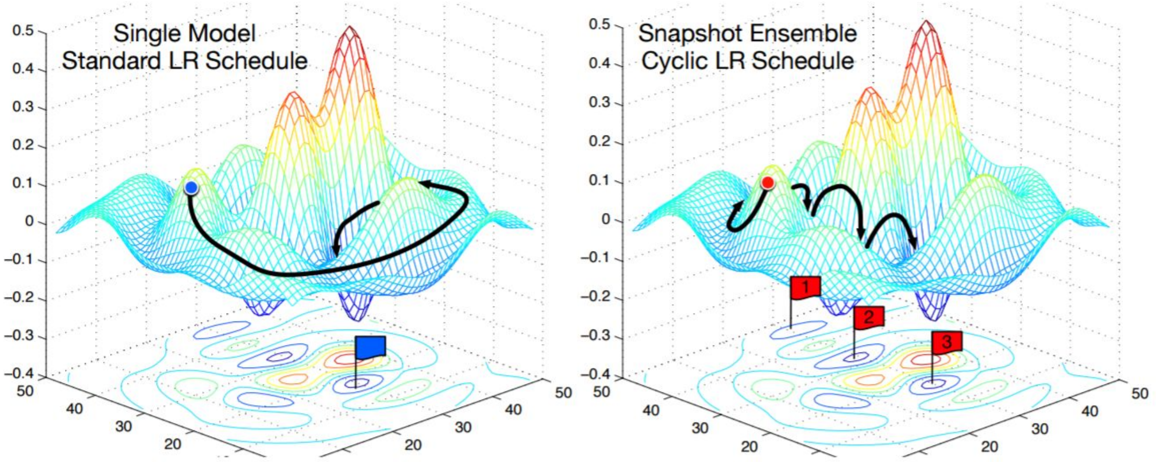
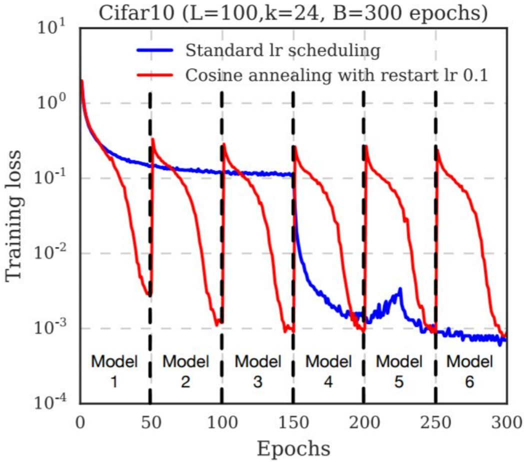




Loshchilov and Hutter, "SGDR: Stochastic gradient descent with restarts", arXiv 2016
Huang et al, "Snapshot ensembles: train 1, get M for free", ICLR 2017

Cyclic learning rate schedules can make this work even better!

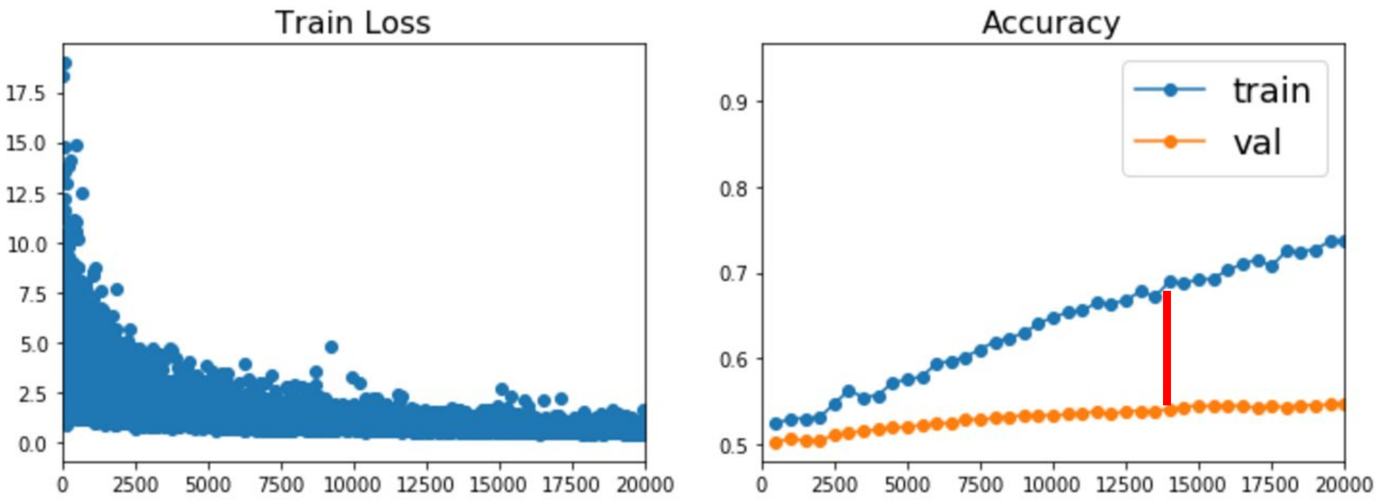
Model Ensembles: Tips and Tricks

Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
while True:
  data_batch = dataset.sample_data_batch()
  loss = network.forward(data_batch)
  dx = network.backward()
  x += - learning_rate * dx
  x_test = 0.995*x_test + 0.005*x # use for test set
```

Polyak and Juditsky, “Acceleration of stochastic approximation by averaging”, SIAM Journal on Control and Optimization, 1992.

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:

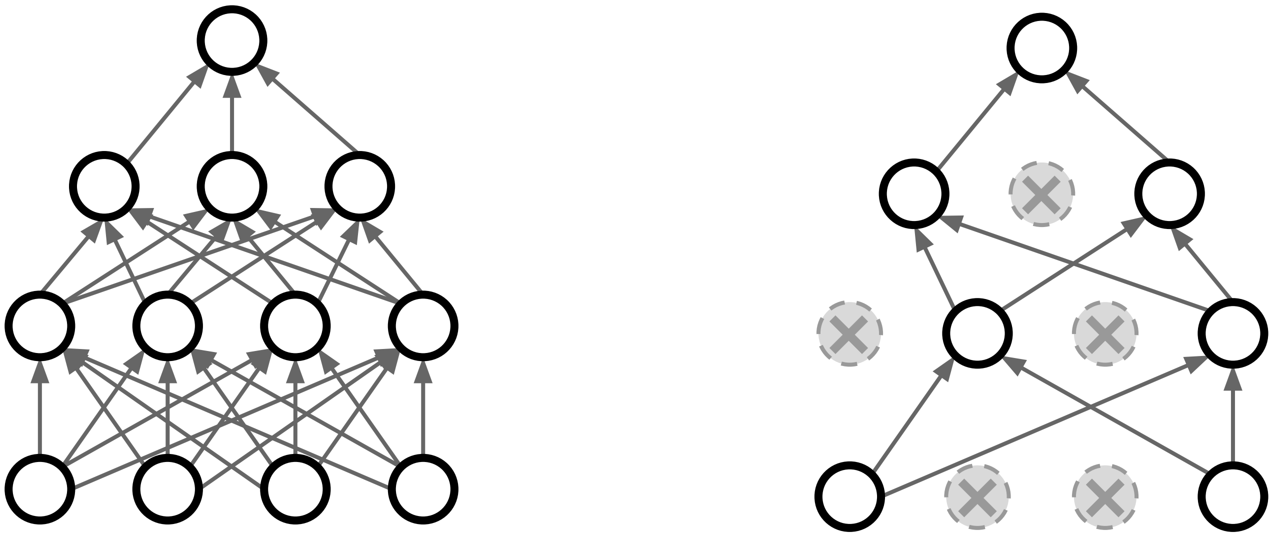
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

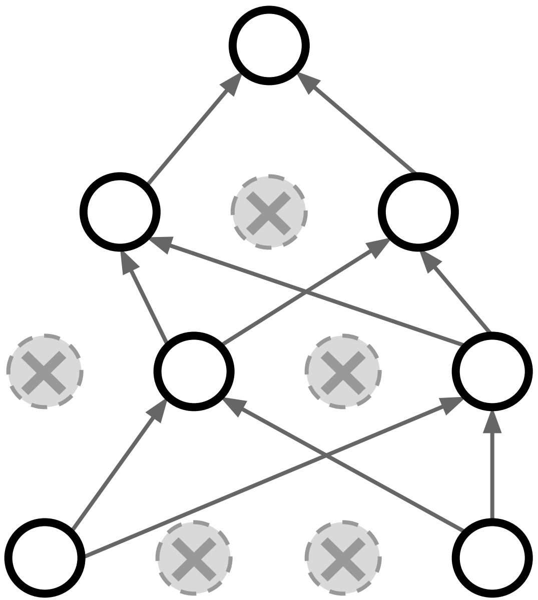
In each forward pass, randomly set some neurons to zero
Probability of dropping is a hyperparameter; 0.5 is common



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

Regularization: Dropout

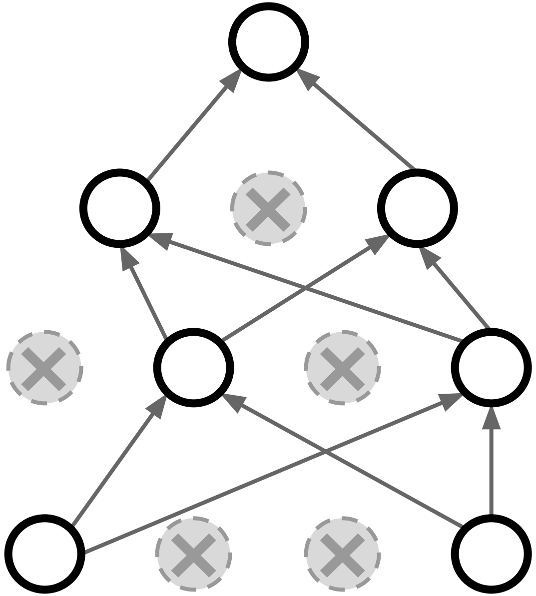
How can this possibly be a good idea?



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!

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

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

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

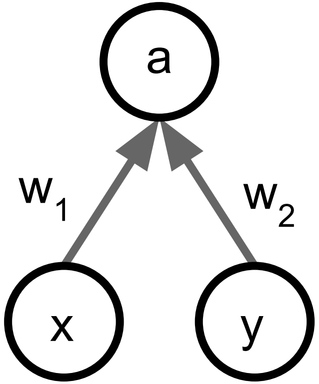
But this integral seems hard …

Dropout: Test time

Want to approximate the integral

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

Consider a single neuron.



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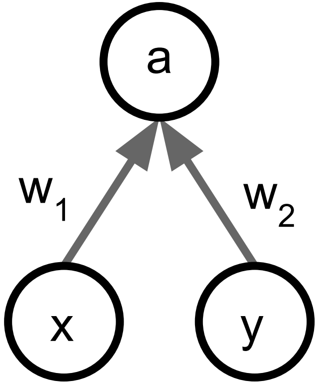

Consider a single neuron.

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

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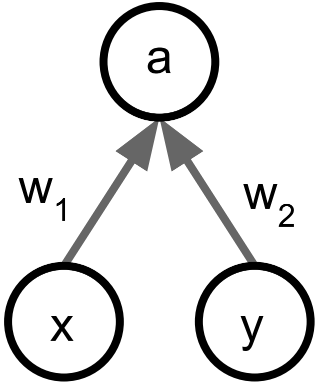


Consider a single neuron.

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

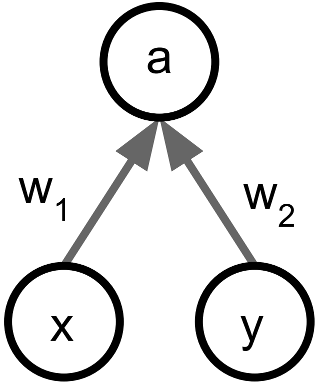
During training we have:

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

Dropout: Test time

Want to approximate the integral

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



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

Dropout: Test time

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

At test time all neurons are active always

=> We must scale the activations so that for each neuron:

<u>output at test time</u> = <u>expected output at training time</u>

Regularization: A common pattern

Training: Add some kind of randomness

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

Testing: Average out randomness (sometimes approximate)

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

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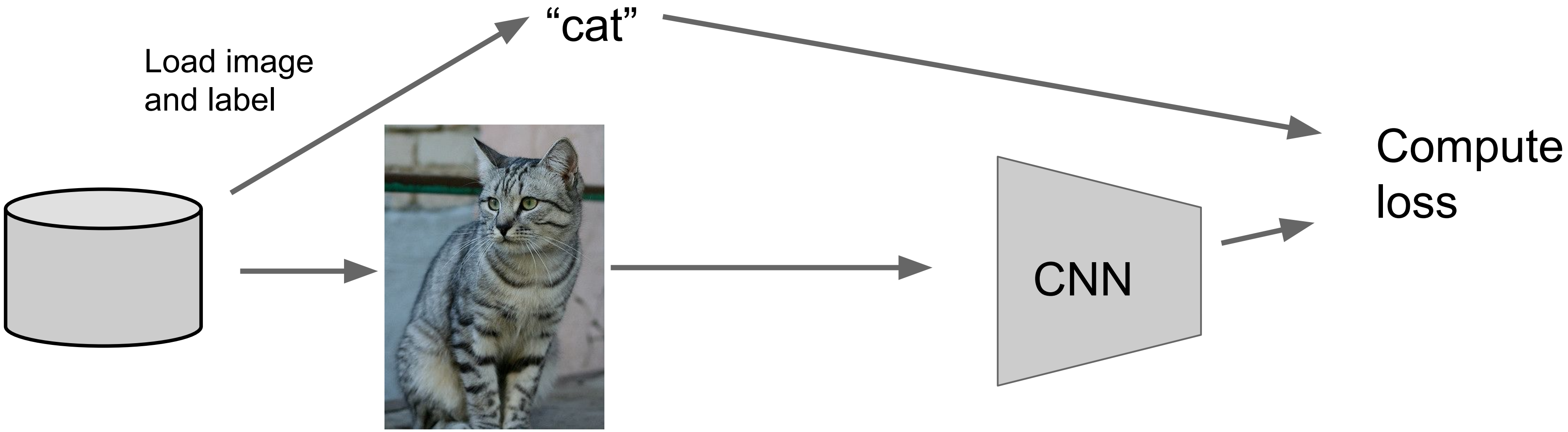
Example: Batch Normalization

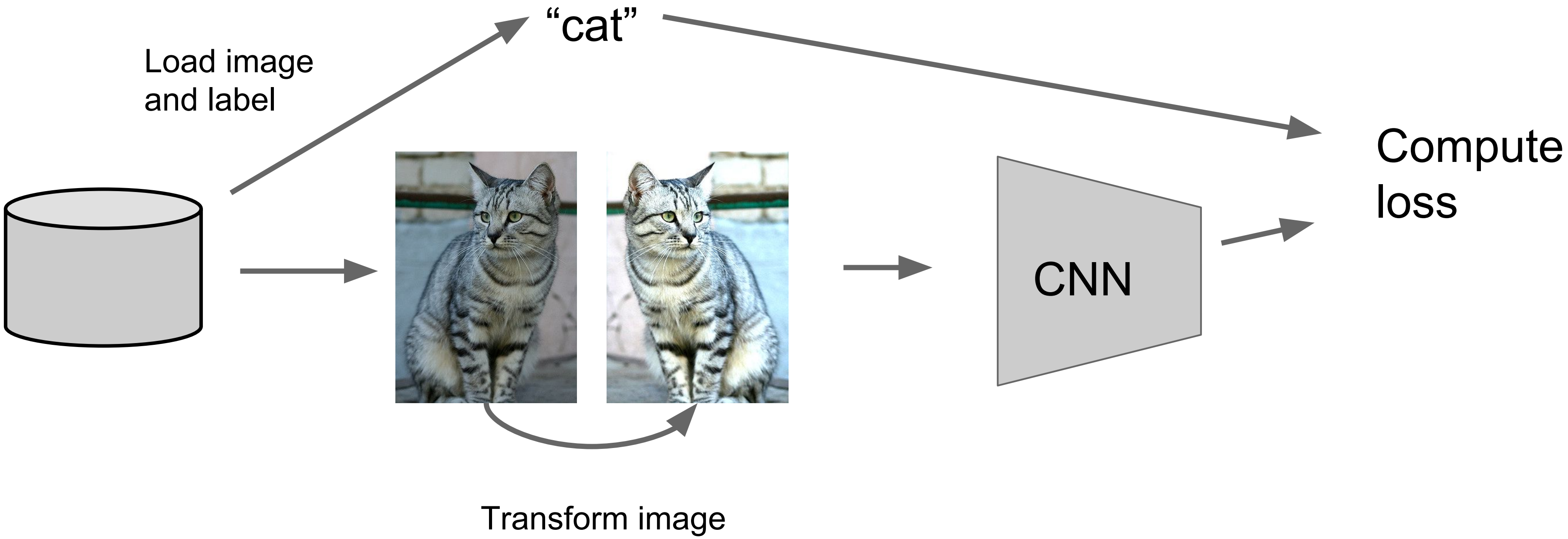
Training: Normalize using stats from random minibatches

Testing: Use fixed stats to normalize

Regularization: Data Augmentation



Regularization: Data Augmentation



Data Augmentation
Horizontal Flips

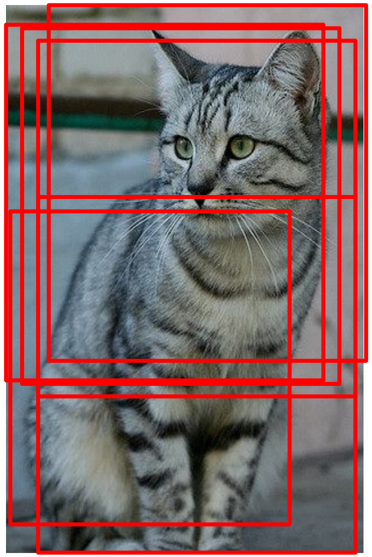
Data Augmentation

Random crops and scales

Training: sample random crops / scales

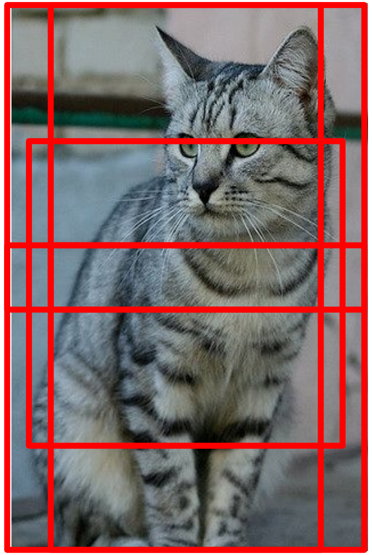
ResNet:

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

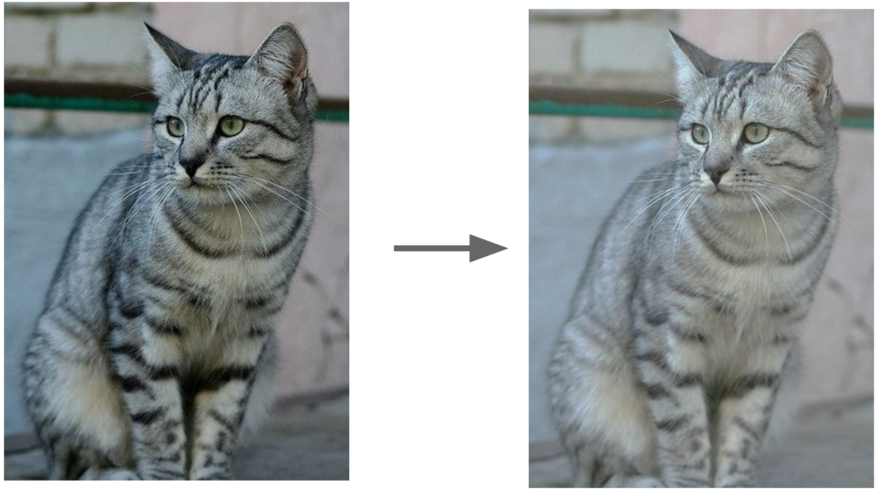
Testing: average a fixed set of crops

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



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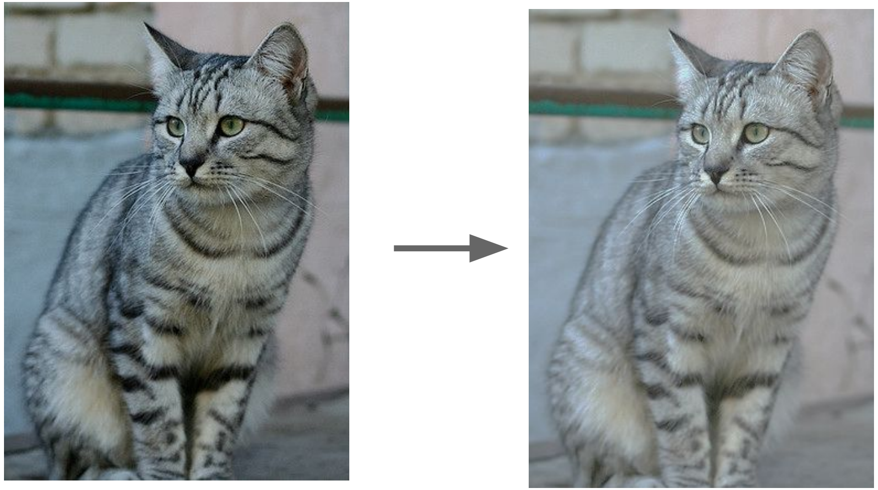
Color Jitter

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!

Random mix/combinations of :

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

Regularization: A common pattern

Training: Add random noise

Testing: Marginalize over the noise

Examples:

Dropout

Batch Normalization

Data Augmentation

Regularization: A common pattern

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Testing: Marginalize over the noise

Examples:

Dropout

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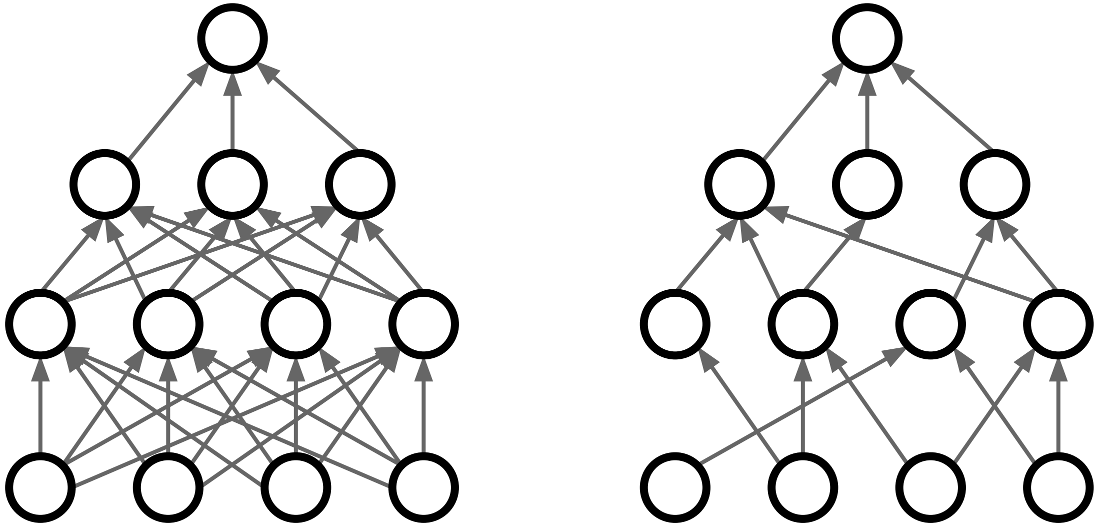
DropConnect



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

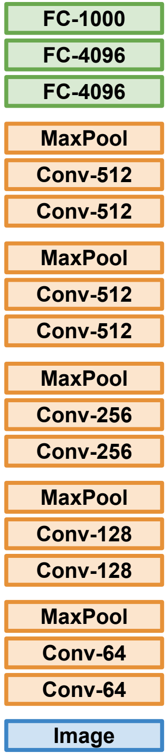
Transfer Learning

"You need a lot of a data if you want to train/use CNNs"

Transfer Learning with CNNs

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



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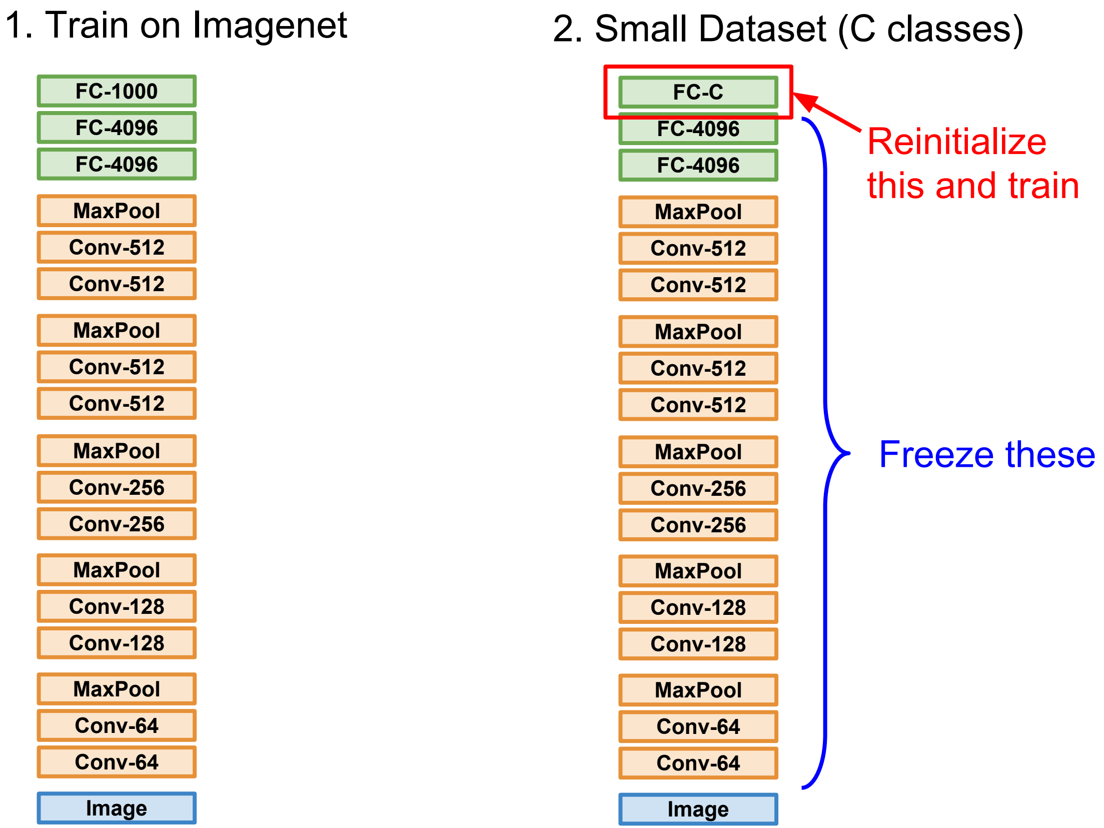

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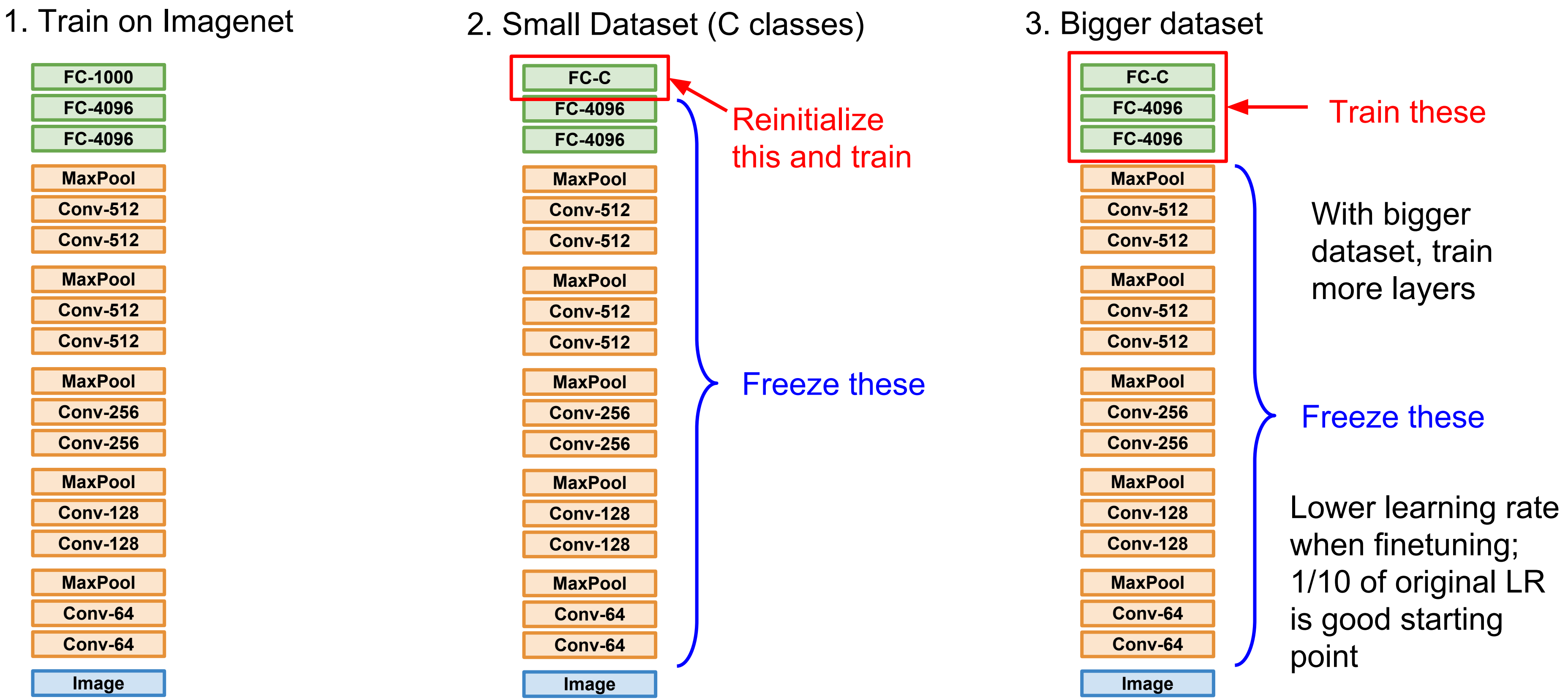
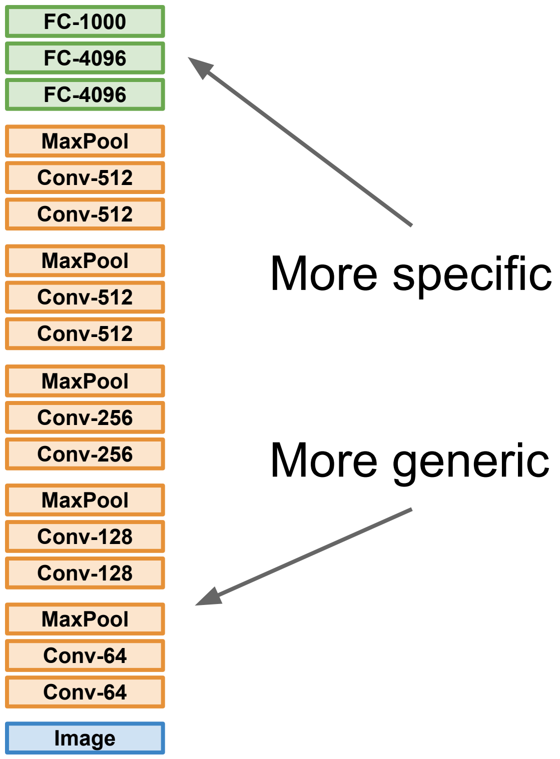
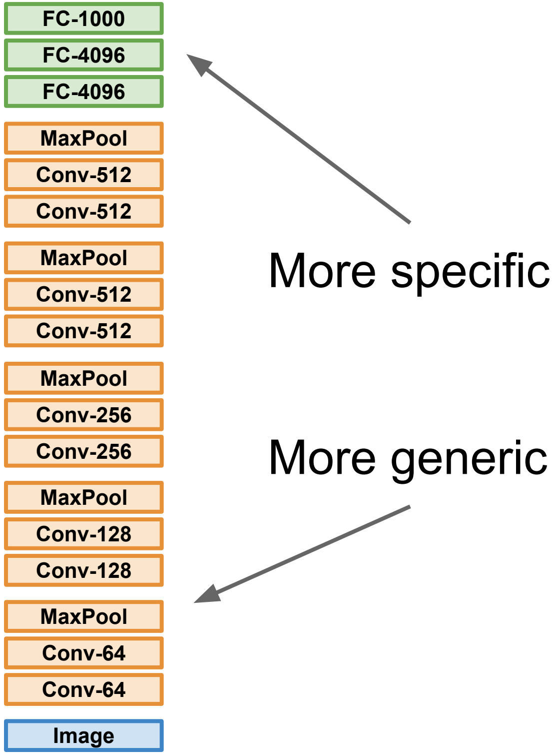
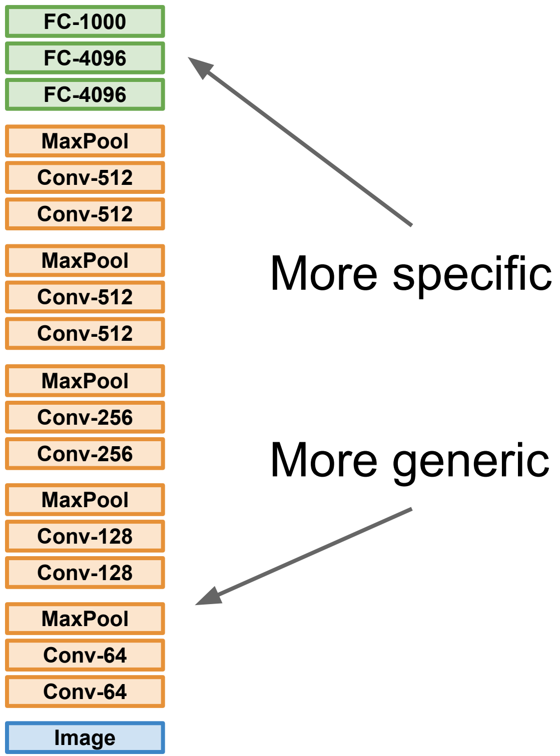




	very similar dataset	**very different dataset**
very little data	?	?
quite a lot of data	?	?



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



	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 is pervasive…
(it's the norm, not an exception)

Object Detection
(Fast R-CNN)

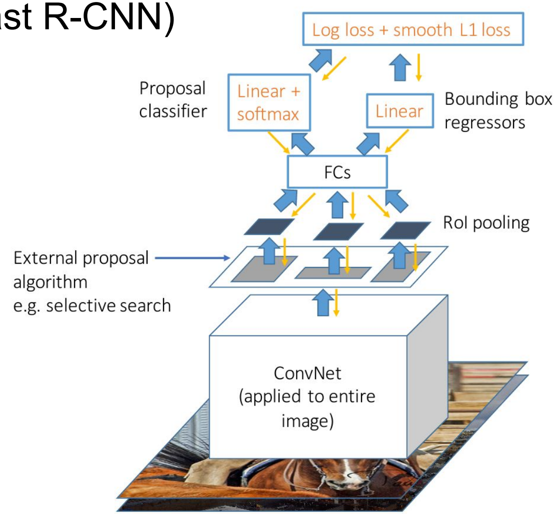
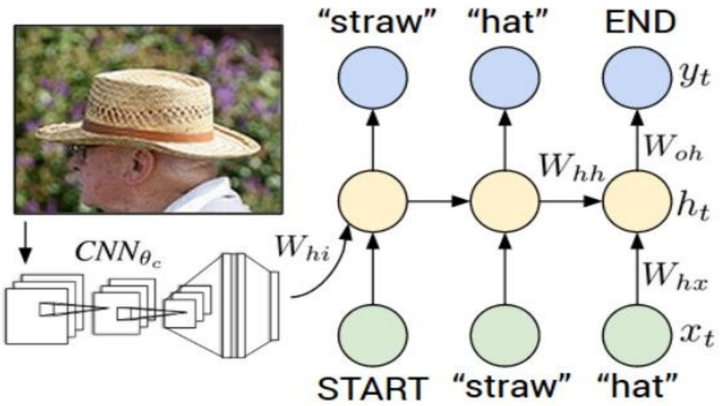


Image Captioning: CNN + RNN



Girshick, "Fast R-CNN", ICCV 2015

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015

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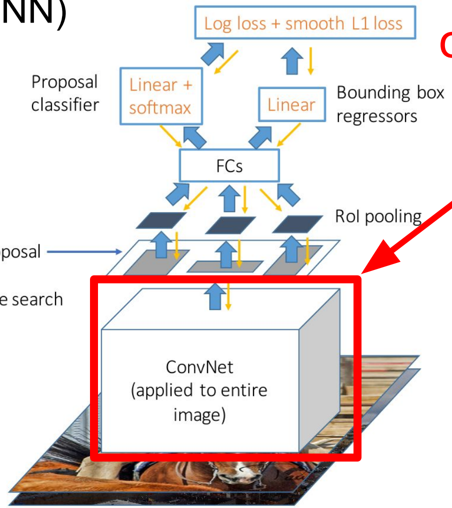
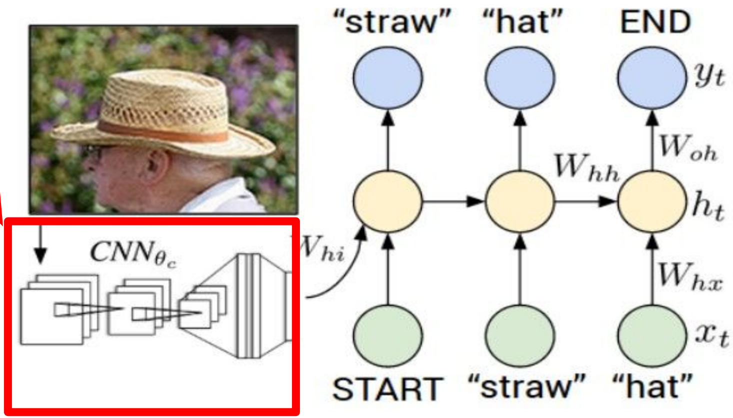


CNN pretrained on ImageNet

Image Captioning: CNN + RNN



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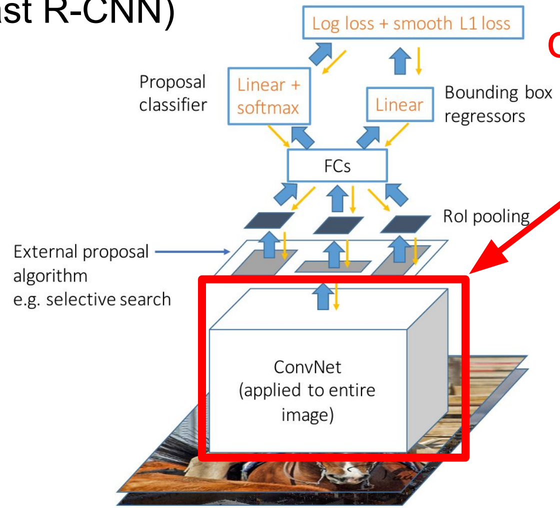

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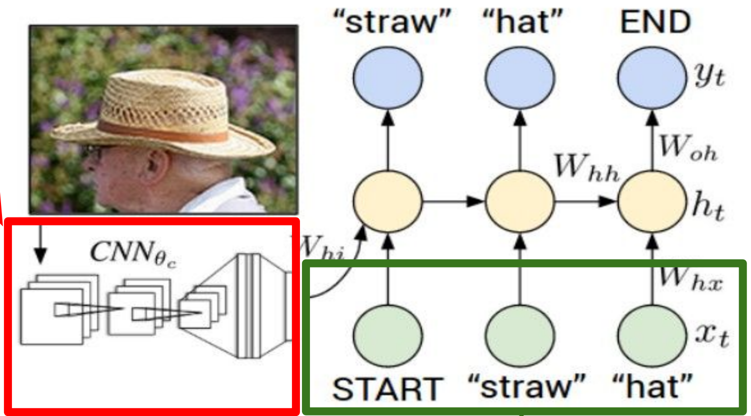

Word vectors pretrained with word2vec

Girshick, "Fast R-CNN", ICCV 2015

Karpathy and Fei-Fei, "Deep Visual-Semantic Alignments for Generating Image Descriptions", CVPR 2015