# Lecture 8:
# Training Neural Networks, Part 2

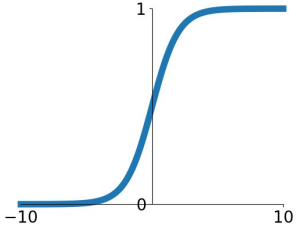
# Administrative:

- A1 grades will be released this weekend: Check Piazza for regrade policy
- Project proposal was due on monday
- A2 is due Wednesday April 30th, 11:59pm
- We didn't cover transfer learning last class. We will cover it next week.

# Last time: Activation Functions

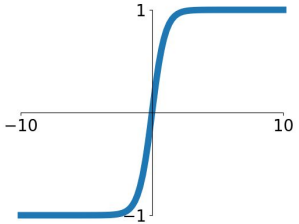
**Sigmoid**

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



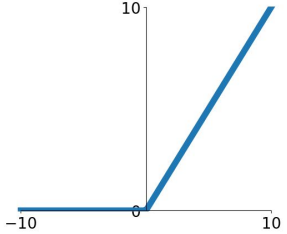

**tanh**

$$\tanh(x)$$



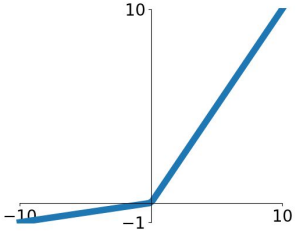

**ReLU**

$$\max(0, x)$$




**Leaky ReLU**

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

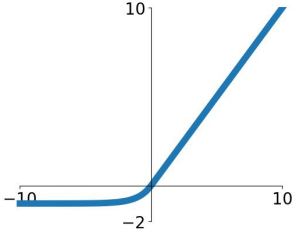



**Maxout**

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

**ELU**

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



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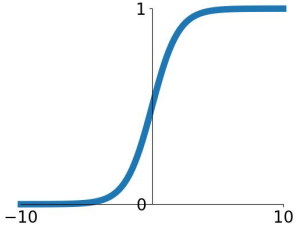


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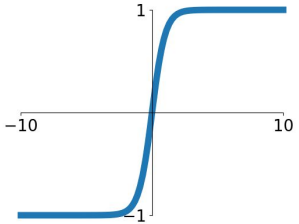
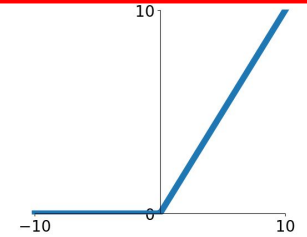



**ReLU**

$$\max(0, x)$$

Good default choice

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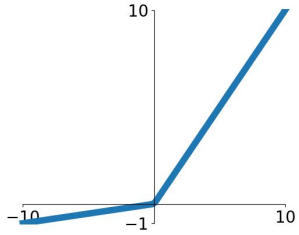


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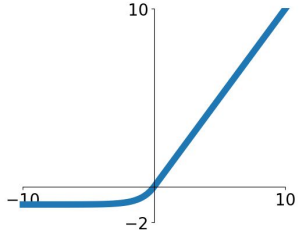
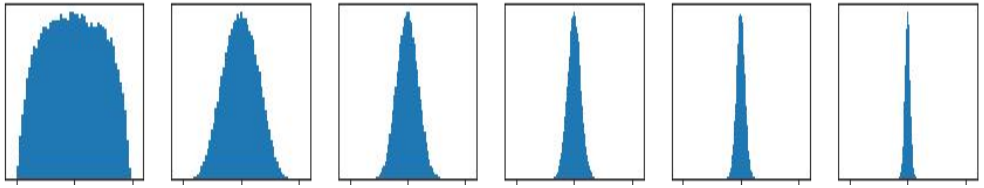
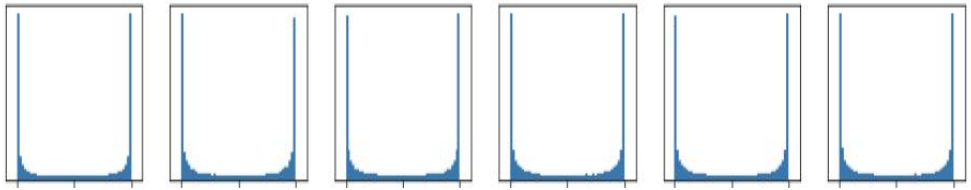


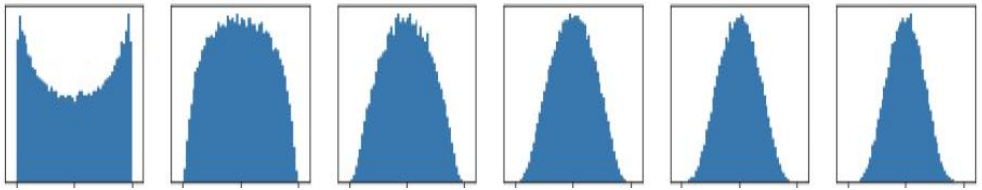
# Last time: Weight Initialization



**Initialization too small**:
Activations go to zero, gradients also zero,
No learning =(

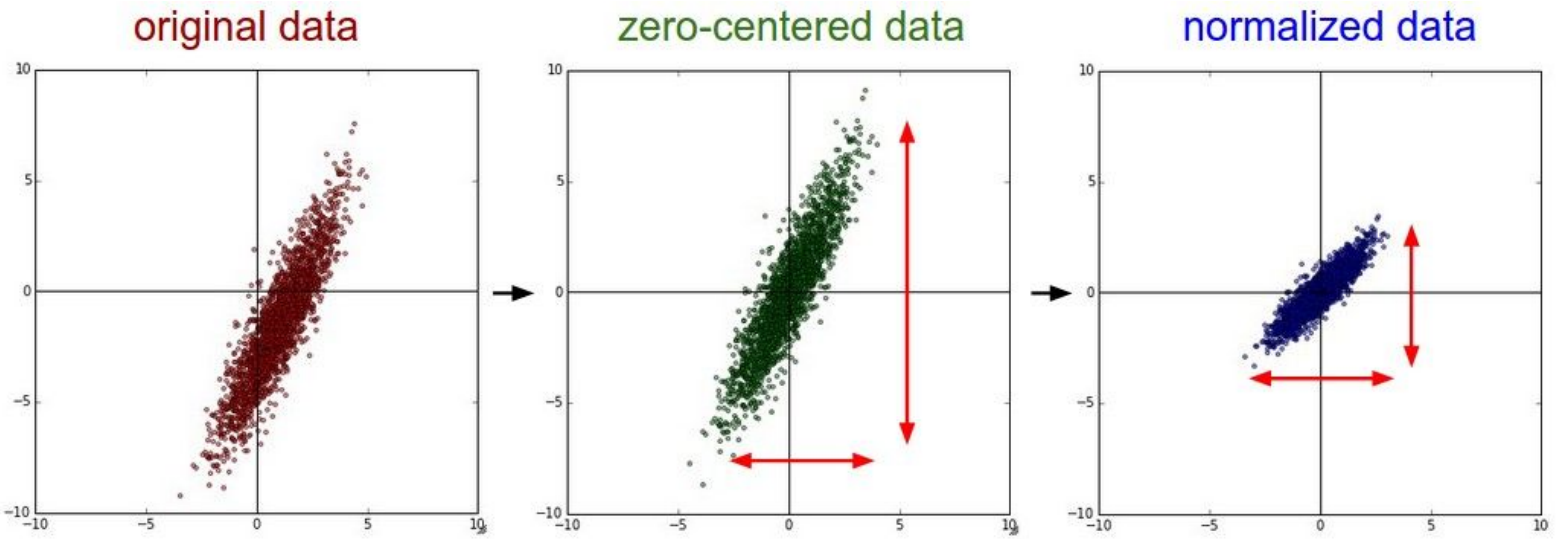


**Initialization too big**:
Activations saturate (for tanh),
Gradients zero, no learning =(



**Initialization just right**:
Nice distribution of activations at all layers,
Learning proceeds nicely =)

# Last time: Data Preprocessing



# Last Time: Batch Normalization

[Ioffe and Szegedy, 2015]

**Input:** $x : N \times D$

**Learnable scale and shift parameters:**

$$\gamma, \beta : D$$

Learning $\gamma = \sigma$, $\beta = \mu$ will recover the identity function!

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

Per-channel mean, shape is D

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

Per-channel var, shape is D

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

Normalized x, Shape is N x D

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

Output, Shape is N x D

# Today

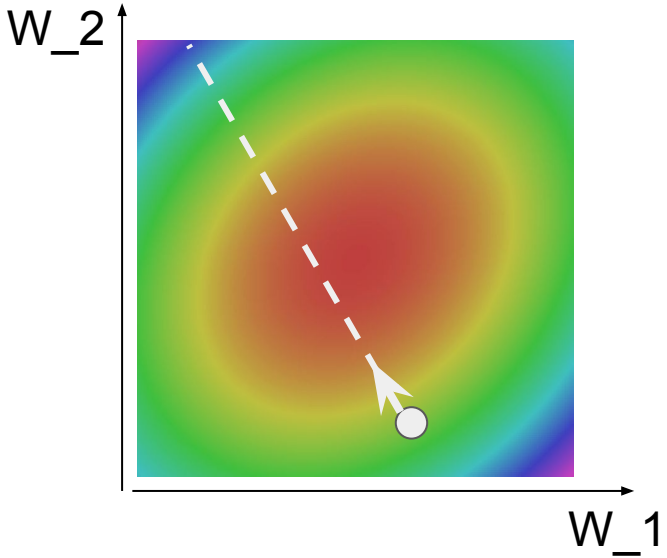
- Improve your training error:
  - (Fancier) Optimizers
  - Learning rate schedules
- Improve your test error:
  - Regularization
  - Choosing Hyperparameters

# (Fancier) Optimizers

# Optimization

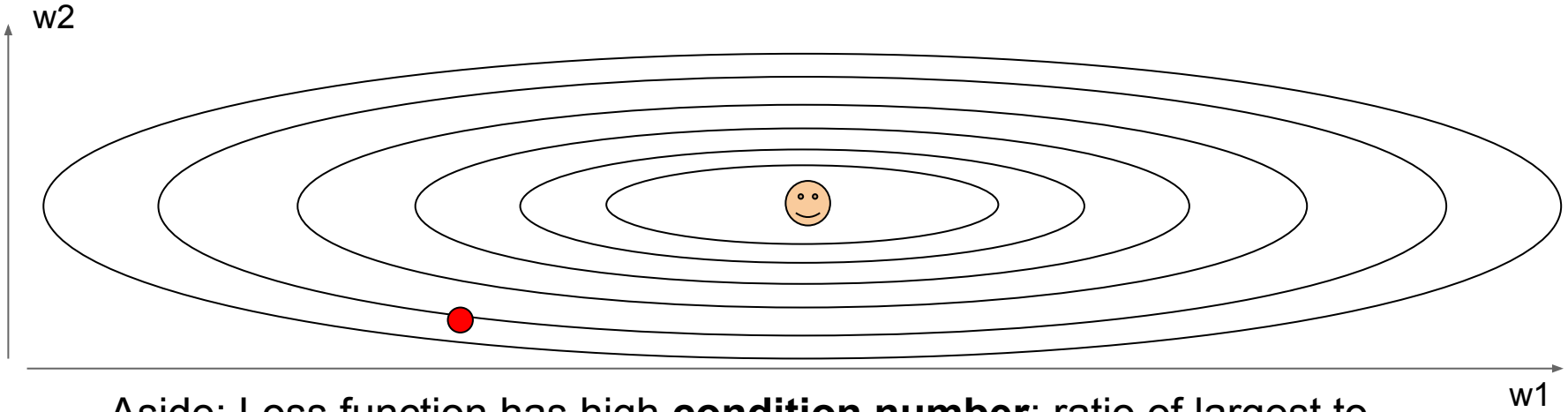
```
# Vanilla Gradient Descent

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



# Optimization: Problem #1 with SGD

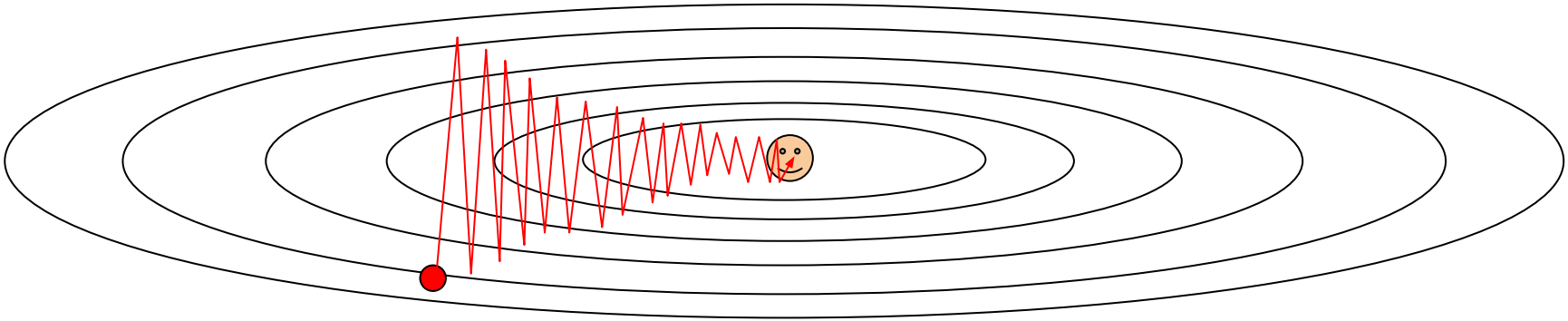
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?




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

# Optimization: Problem #1 with SGD

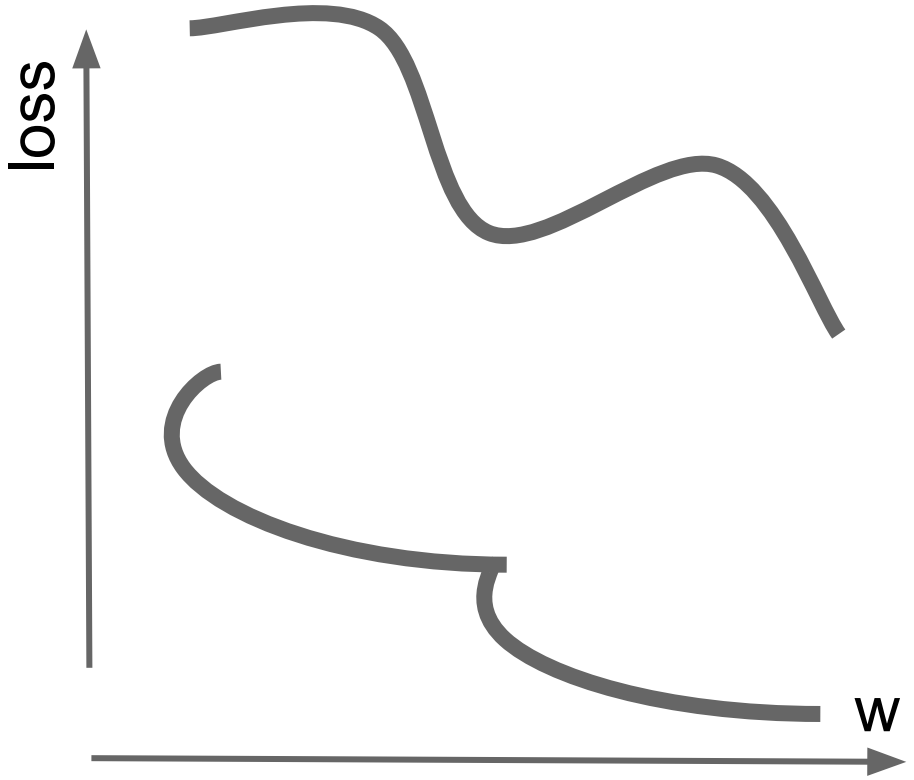
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction



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

# Optimization: Problem #2 with SGD

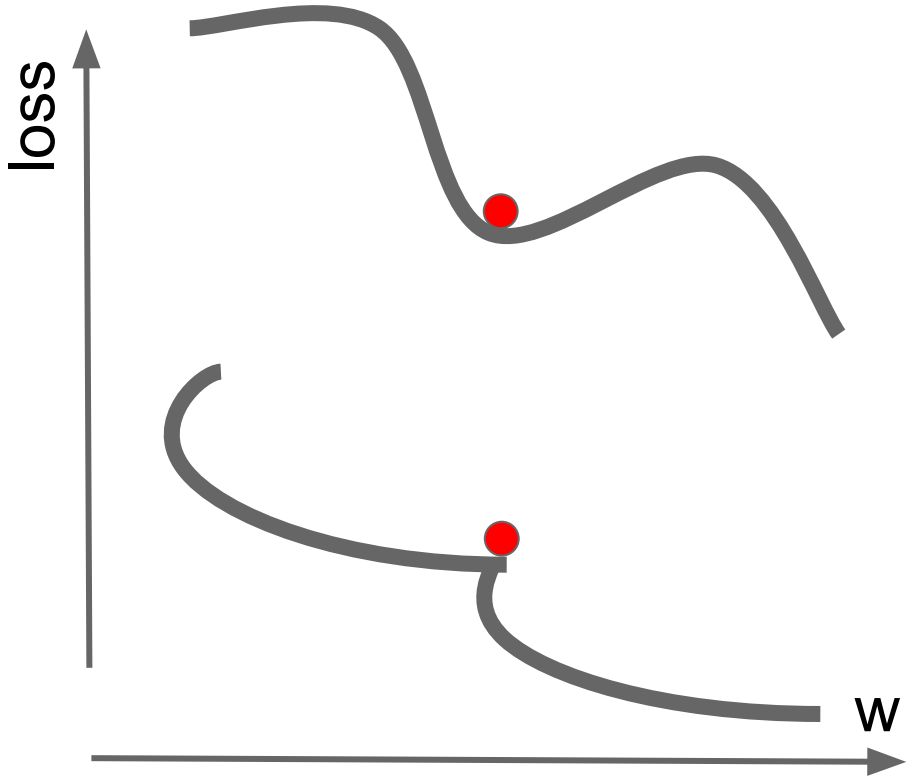
What if the loss function has a **local minima** or **saddle point**?



# Optimization: Problem #2 with SGD

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

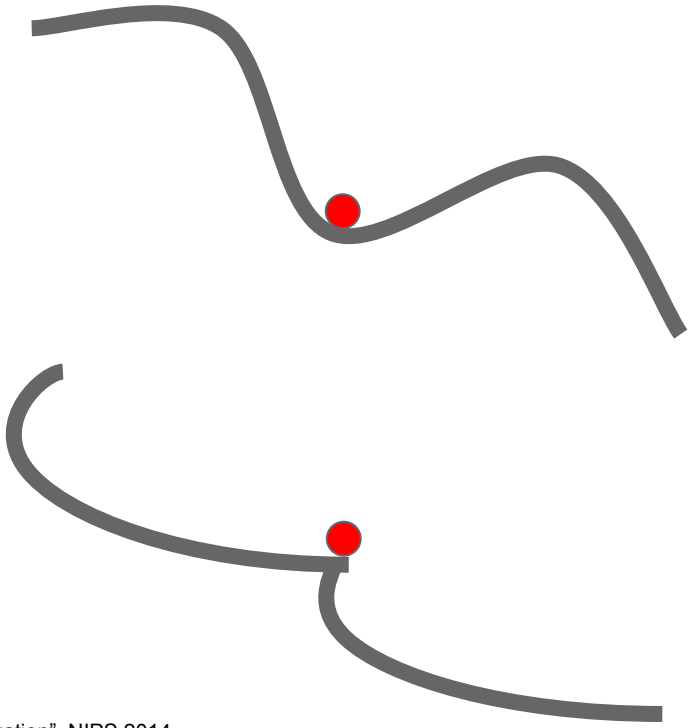
Zero gradient, gradient descent gets stuck



# Optimization: Problem #2 with SGD

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

Saddle points much more common in high dimension



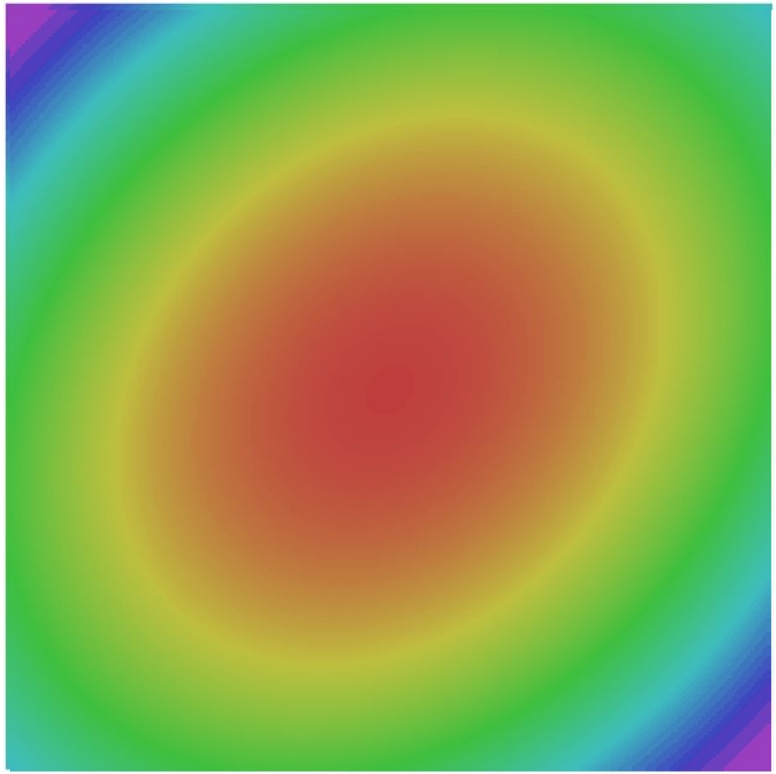
Dauphin et al, “Identifying and attacking the saddle point problem in high-dimensional non-convex optimization”, NIPS 2014

# Optimization: Problem #3 with SGD

Our gradients come from minibatches so they can be noisy!

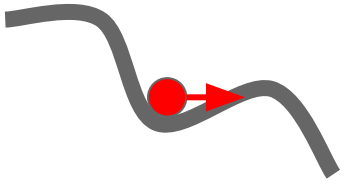
$$L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(x_i, y_i, W)$$

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

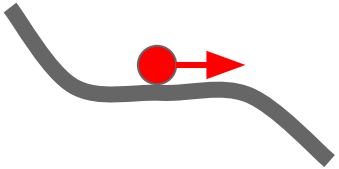


# SGD + Momentum

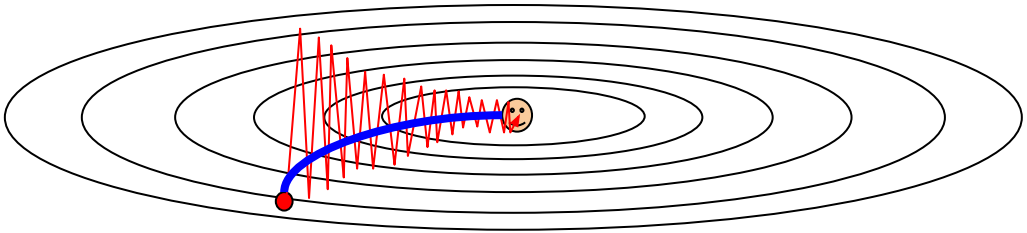
Local Minima



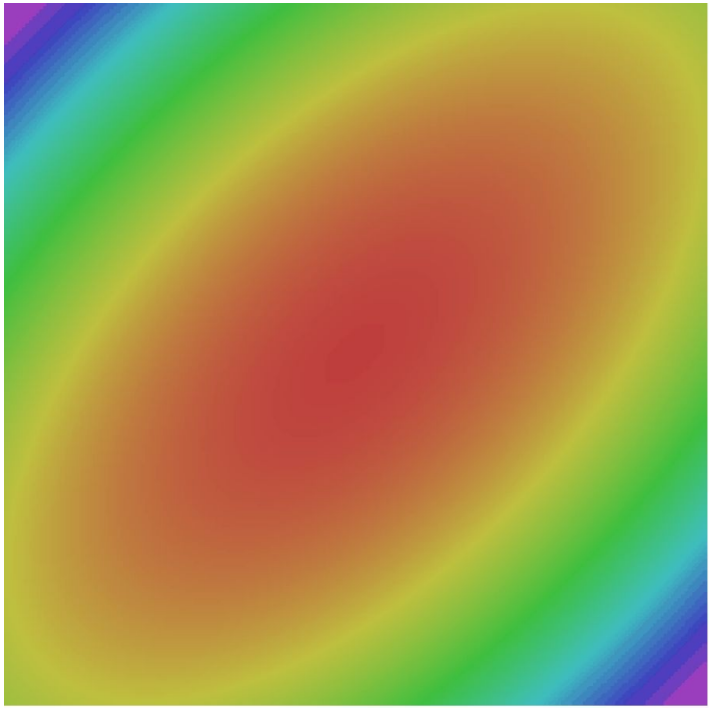
Saddle points



Poor Conditioning



Gradient Noise



SGD SGD+Momentum

# SGD: the simple two line update code

SGD

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

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

# SGD + Momentum:

continue moving in the general direction as the previous iterations

## SGD

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

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while True:
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## SGD+Momentum

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

- 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:

continue moving in the general direction as the previous iterations

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## SGD+Momentum

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

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

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

# SGD + Momentum:

## alternative equivalent formulation

### SGD+Momentum

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

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

### SGD+Momentum

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

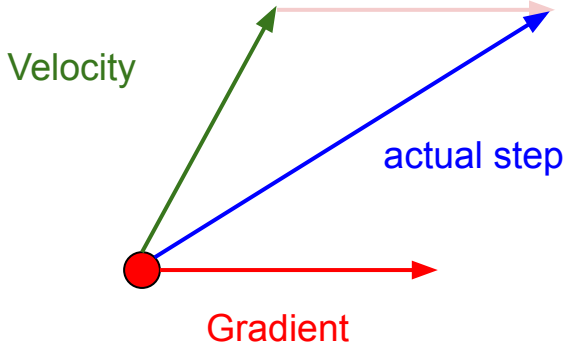
```
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x -= learning_rate * vx
```

You may see SGD+Momentum formulated different ways, but they are equivalent - give same sequence of x

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

# 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
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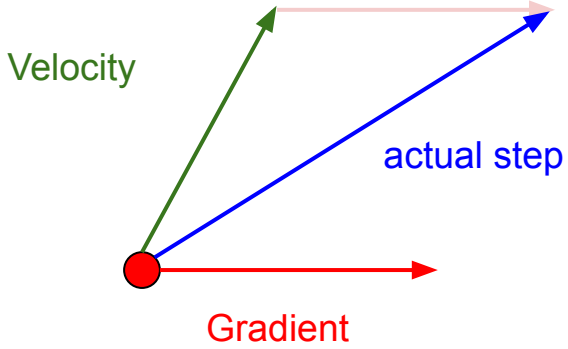
# Nesterov Momentum

## Momentum update:

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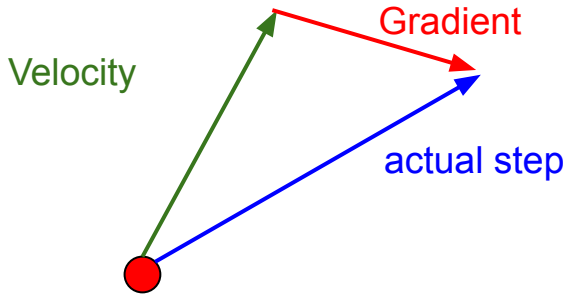


"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

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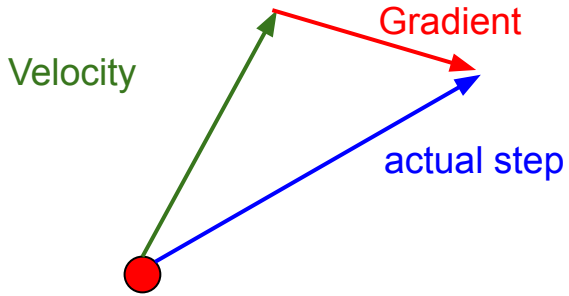


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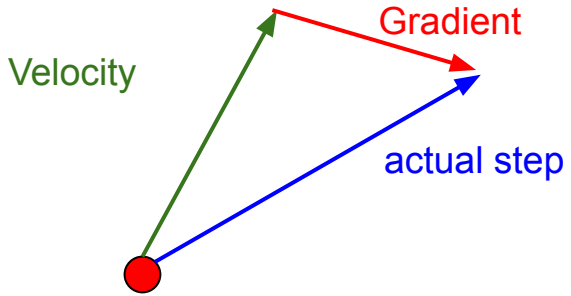
# Nesterov Momentum

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

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

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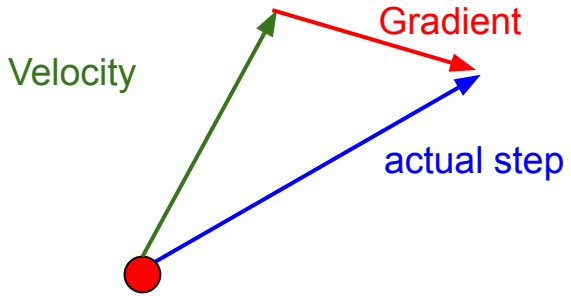
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$

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




"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

https://cs231n.github.io/neural-networks-3/

# Nesterov Momentum

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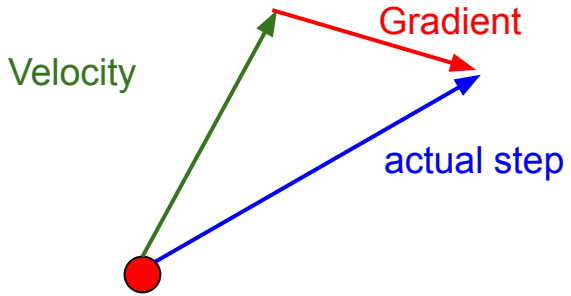
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$



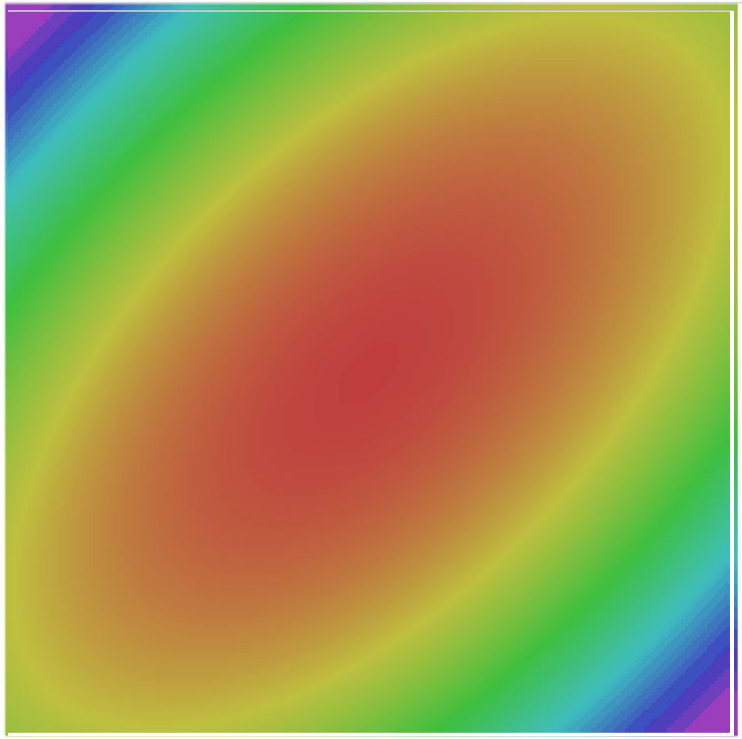

Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

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

"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

https://cs231n.github.io/neural-networks-3/

# Nesterov Momentum



SGD

SGD+Momentum

Nesterov

# AdaGrad

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

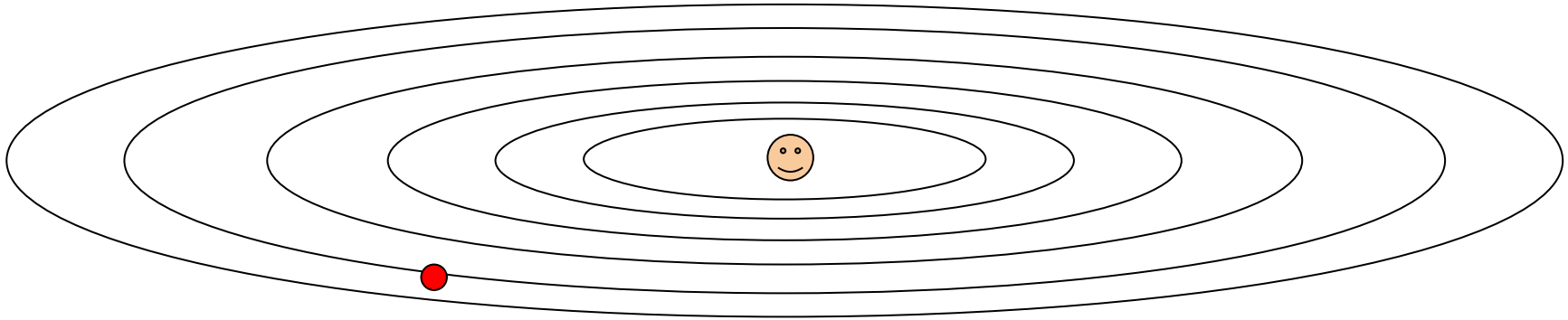
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

"Per-parameter learning rates"
or "adaptive learning rates"

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

# AdaGrad

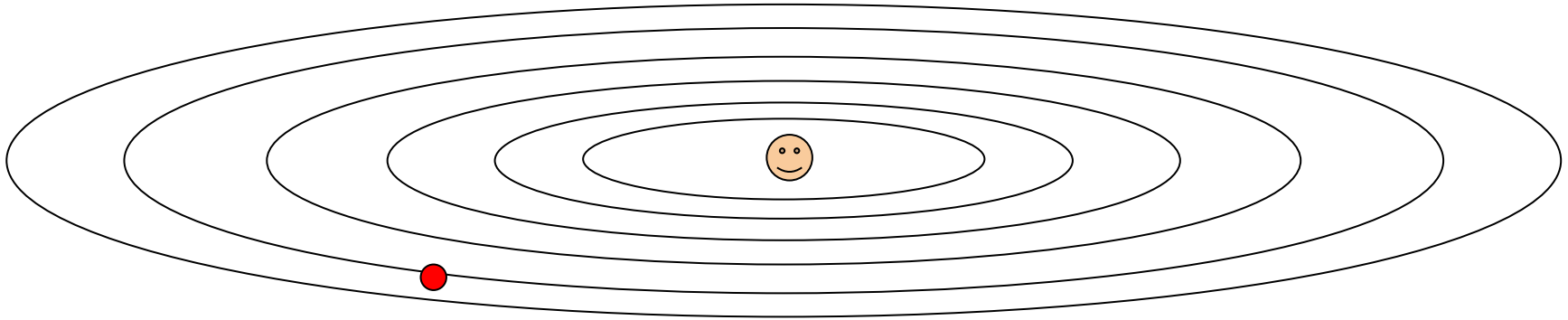
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q: What happens with AdaGrad?

# AdaGrad

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

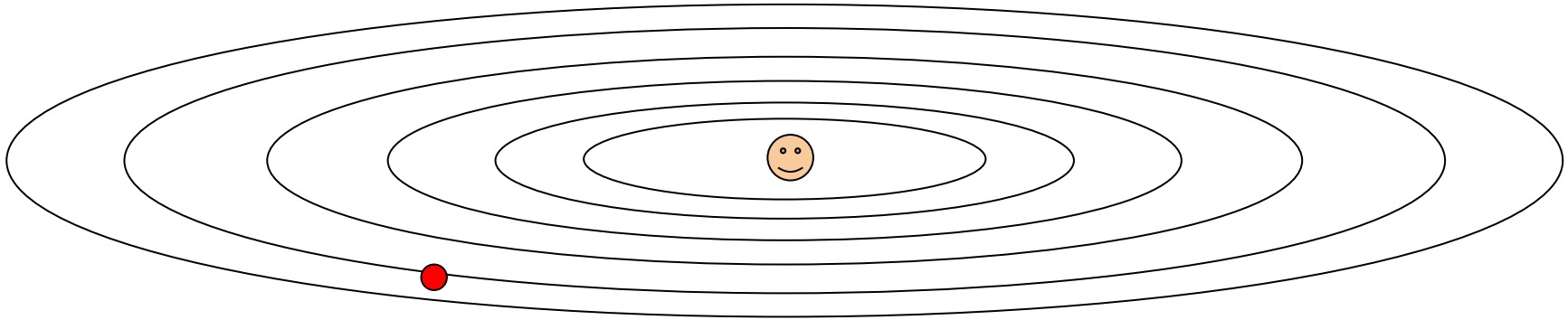


Q: What happens with AdaGrad?

Progress along “steep” directions is damped;
progress along “flat” directions is accelerated

# AdaGrad

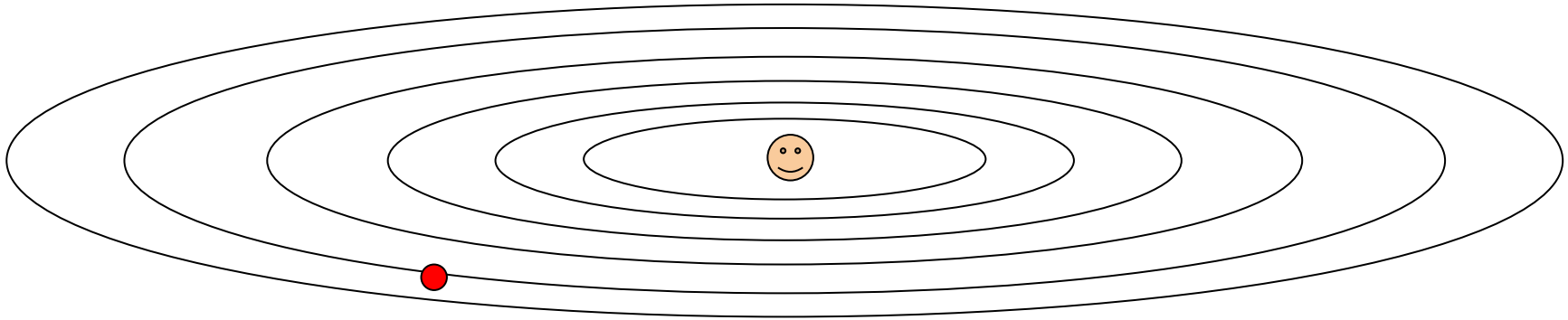
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q2: 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)
```



Q2: What happens to the step size over long time? Decays to zero

# RMSProp: “Leaky AdaGrad”

AdaGrad

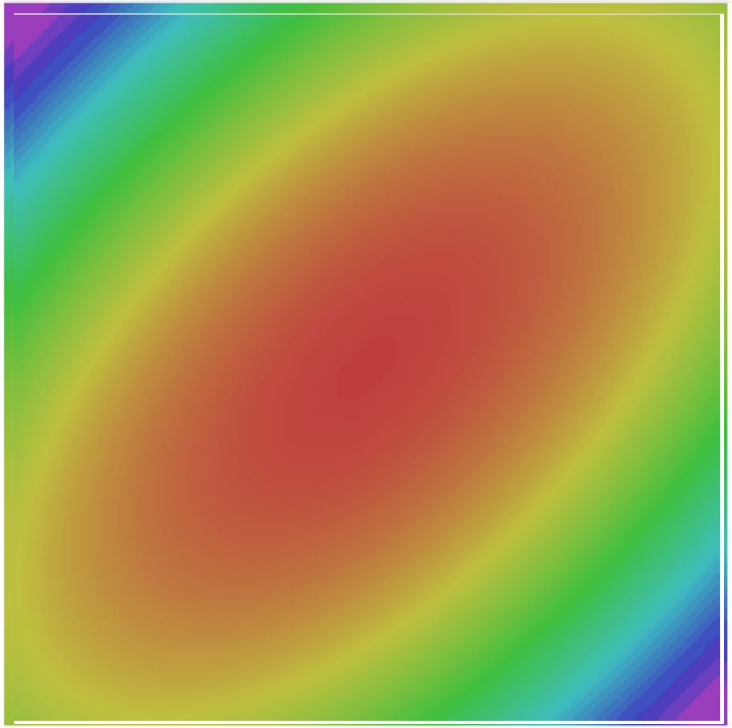
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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

# RMSProp



SGD

SGD+Momentum

RMSProp

AdaGrad

(stuck due to decaying lr)

# Adam (almost)

```
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))
```

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

# Adam (almost)

```
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))
```

Momentum

AdaGrad / RMSProp

Sort of like RMSProp with momentum

Q: What happens at first timestep?

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

# Adam (full form)

```
first_moment = 0
second_moment = 0
for t in range(1, 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))
```

Momentum

Bias correction

AdaGrad / RMSProp

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

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

# Adam (full form)

```
first_moment = 0
second_moment = 0
for t in range(1, 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))
```

Momentum

Bias correction

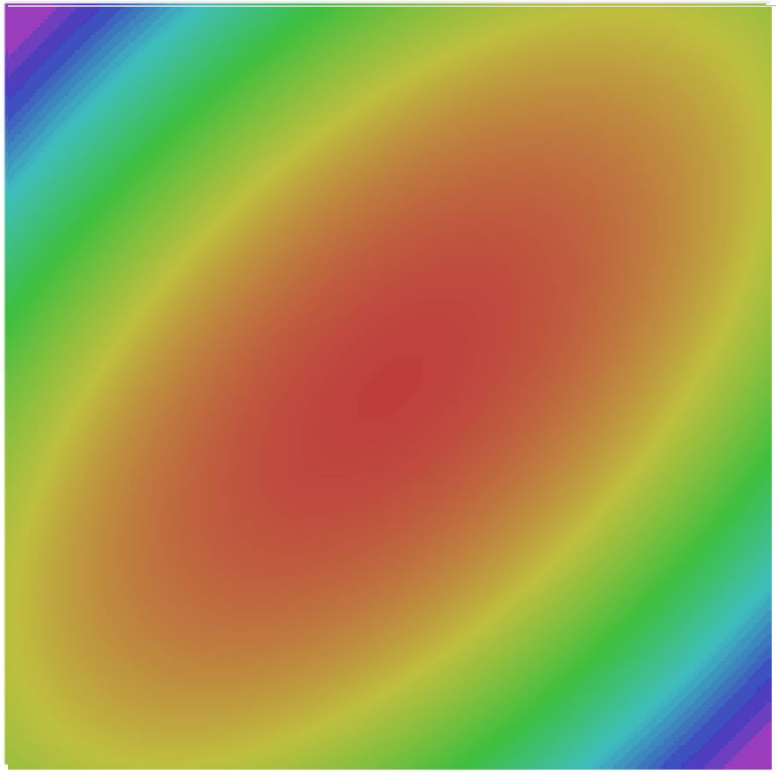
AdaGrad / RMSProp

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!

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

# Adam



SGD

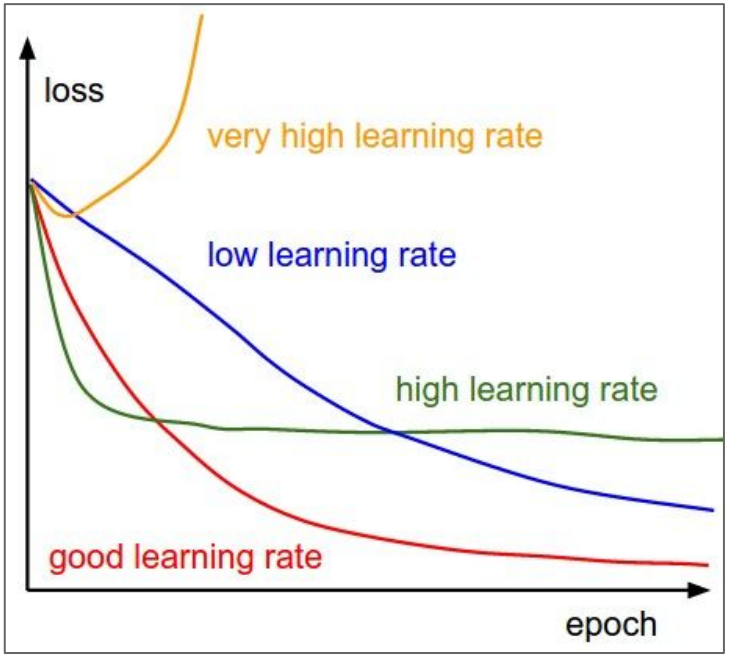
SGD+Momentum

RMSProp

Adam

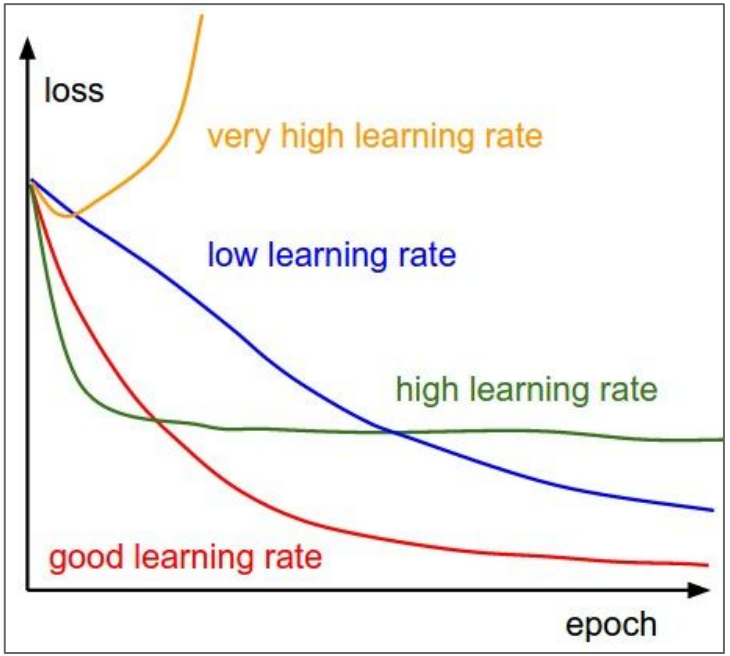
Learning rate schedules

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




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

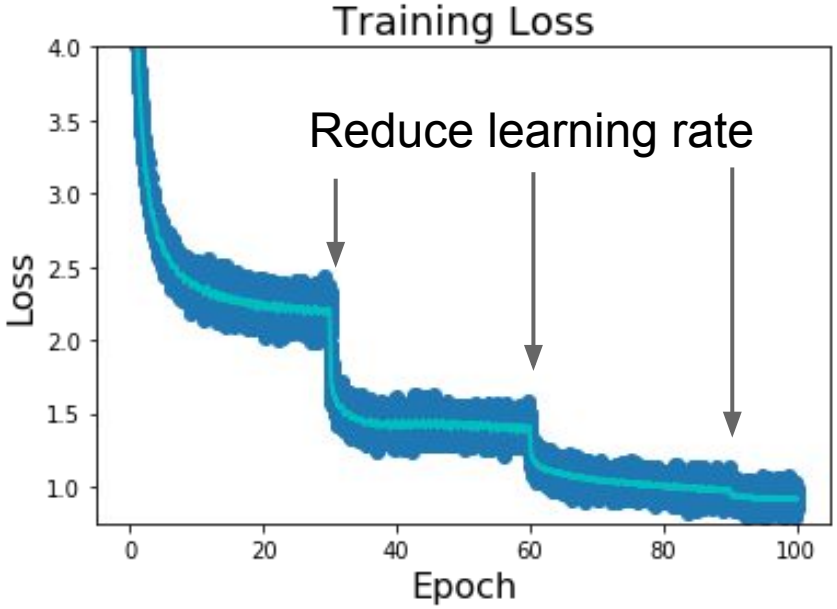
SGD, SGD+Momentum, Adagrad, RMSProp, Adam all have **learning rate** as a hyperparameter.




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

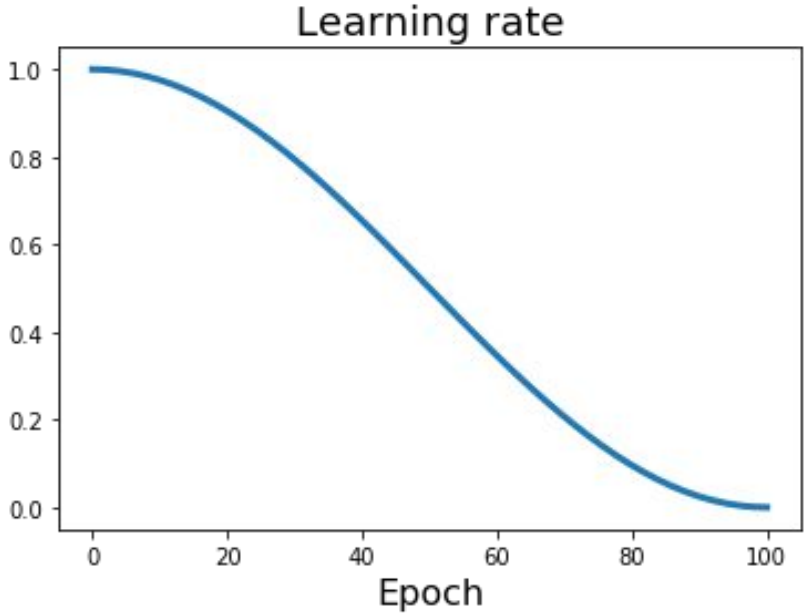
A: In reality, all of these are good learning rates.

# Learning rate decays over time




**Step:** Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

# Learning Rate Decay



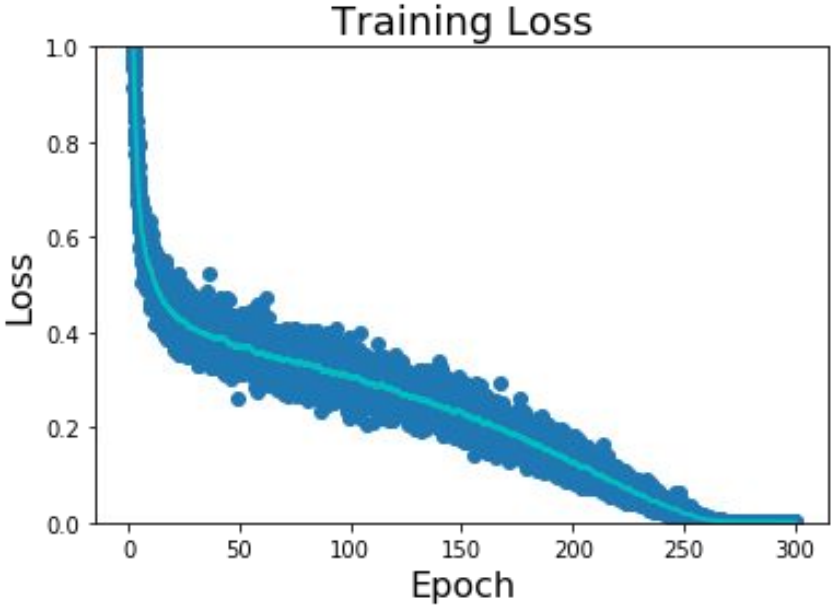

**Step:** Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

**Cosine**: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$

$\alpha_0$ : Initial learning rate
$\alpha_t$ : Learning rate at epoch t
$T$ : Total number of epochs

Loshchilov and Hutter, "SGDR: Stochastic Gradient Descent with Warm Restarts", ICLR 2017
Radford et al, "Improving Language Understanding by Generative Pre-Training", 2018
Feichtenhofer et al, "SlowFast Networks for Video Recognition", arXiv 2018
Child at al, "Generating Long Sequences with Sparse Transformers", arXiv 2019

# Learning Rate Decay

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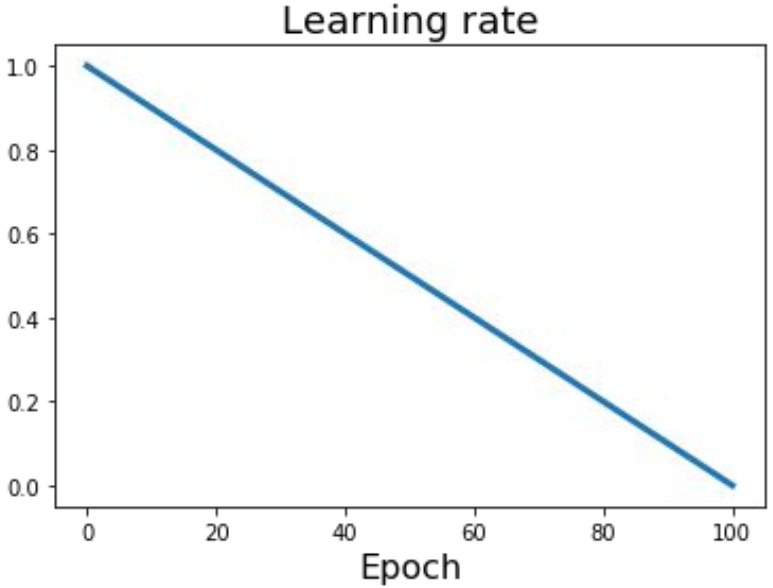
# Learning Rate Decay

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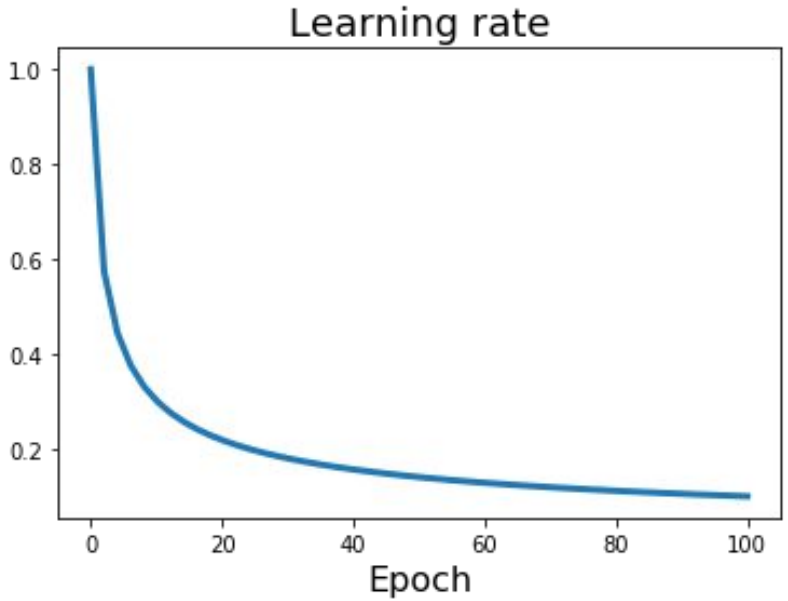
**Linear:** $\alpha_t = \alpha_0(1 - t/T)$

$\alpha_0$ : Initial learning rate
$\alpha_t$ : Learning rate at epoch t
$T$ : Total number of epochs

Devlin et al, “BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding”, 2018

# Learning Rate Decay

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**Cosine**: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$

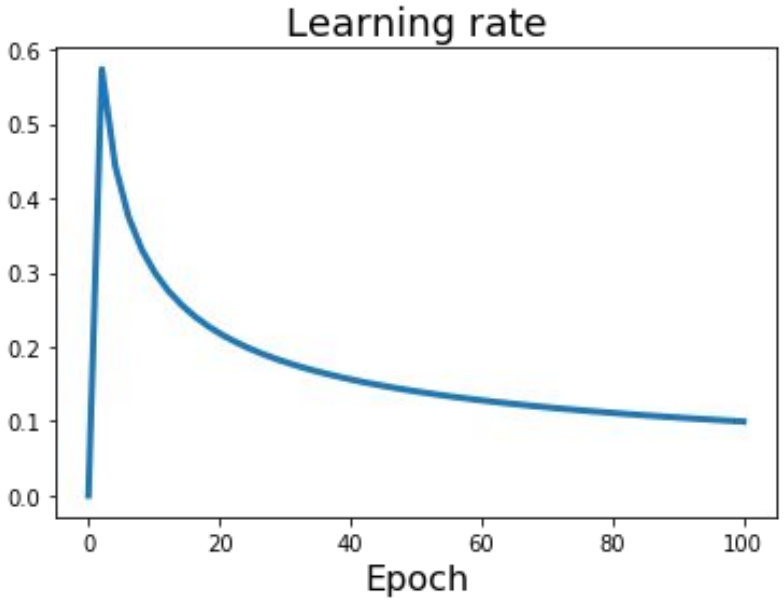
**Linear:** $\alpha_t = \alpha_0(1 - t/T)$

**Inverse sqrt:** $\alpha_t = \alpha_0/\sqrt{t}$

$\alpha_0$ : Initial learning rate
$\alpha_t$ : Learning rate at epoch t
$T$ : Total number of epochs

Vaswani et al, “Attention is all you need”, NIPS 2017

# Learning Rate Decay: Linear Warmup

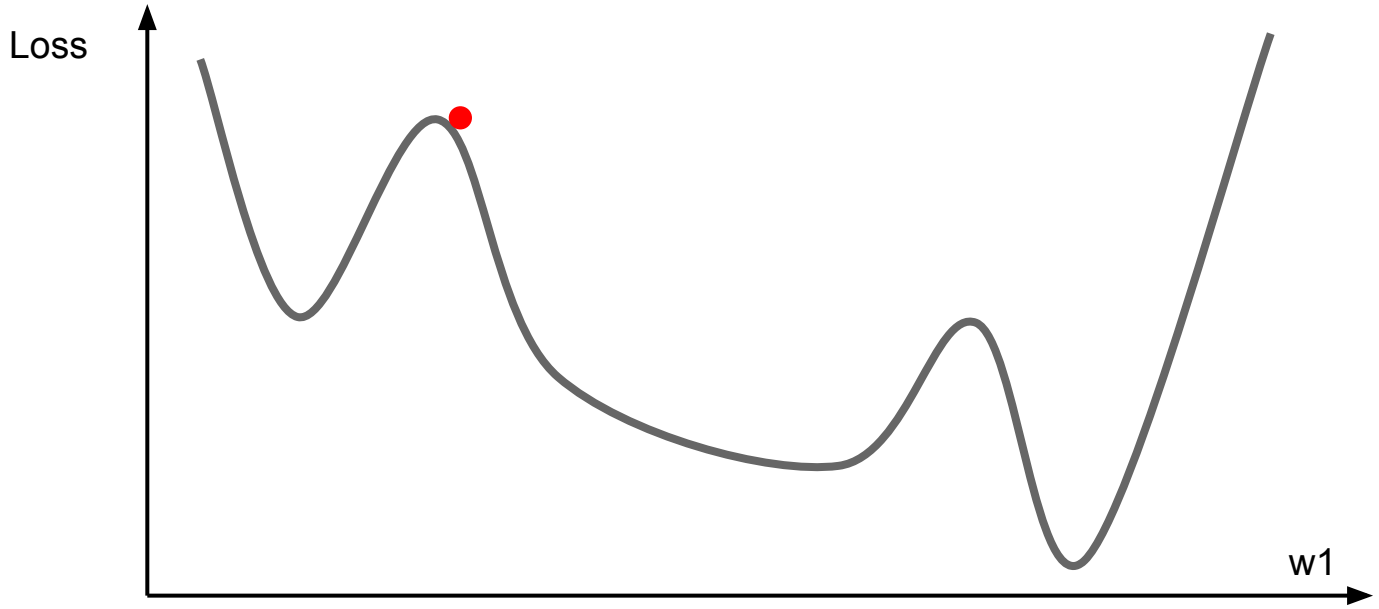



High initial learning rates can make loss explode; linearly increasing learning rate from 0 over the first ~5000 iterations can prevent this

Empirical rule of thumb: If you increase the batch size by N, also scale the initial learning rate by N

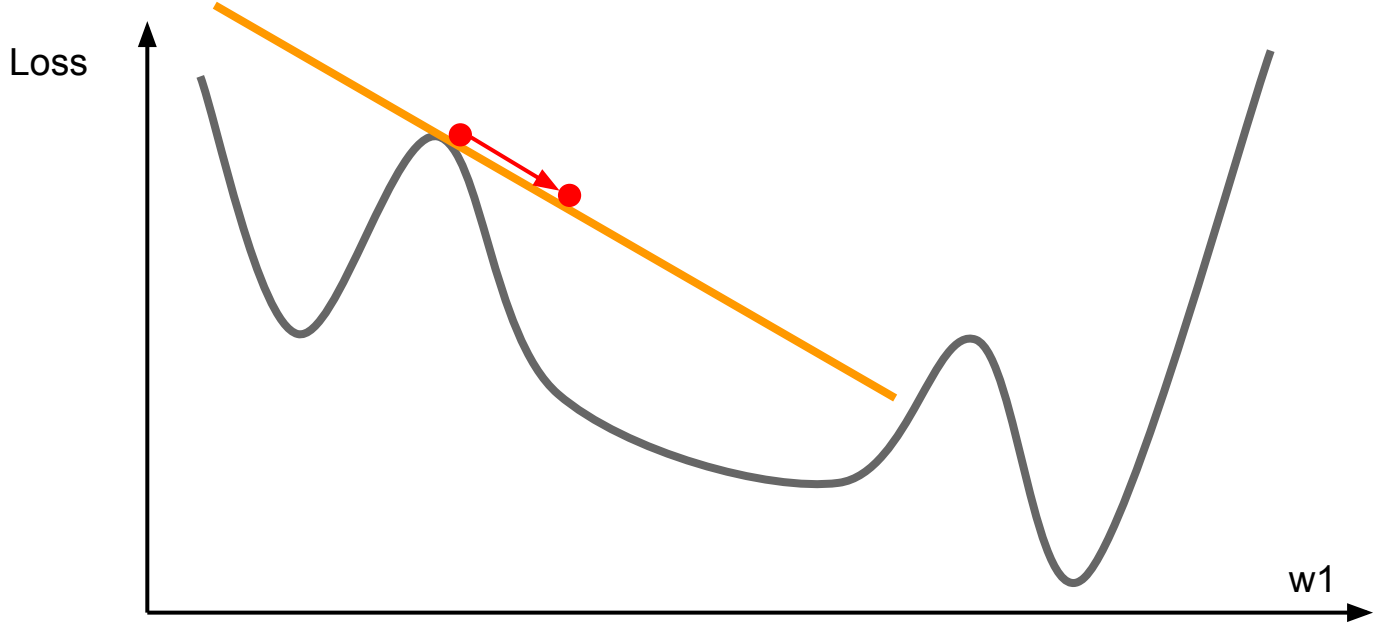
Goyal et al, “Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour”, arXiv 2017

# First-Order Optimization



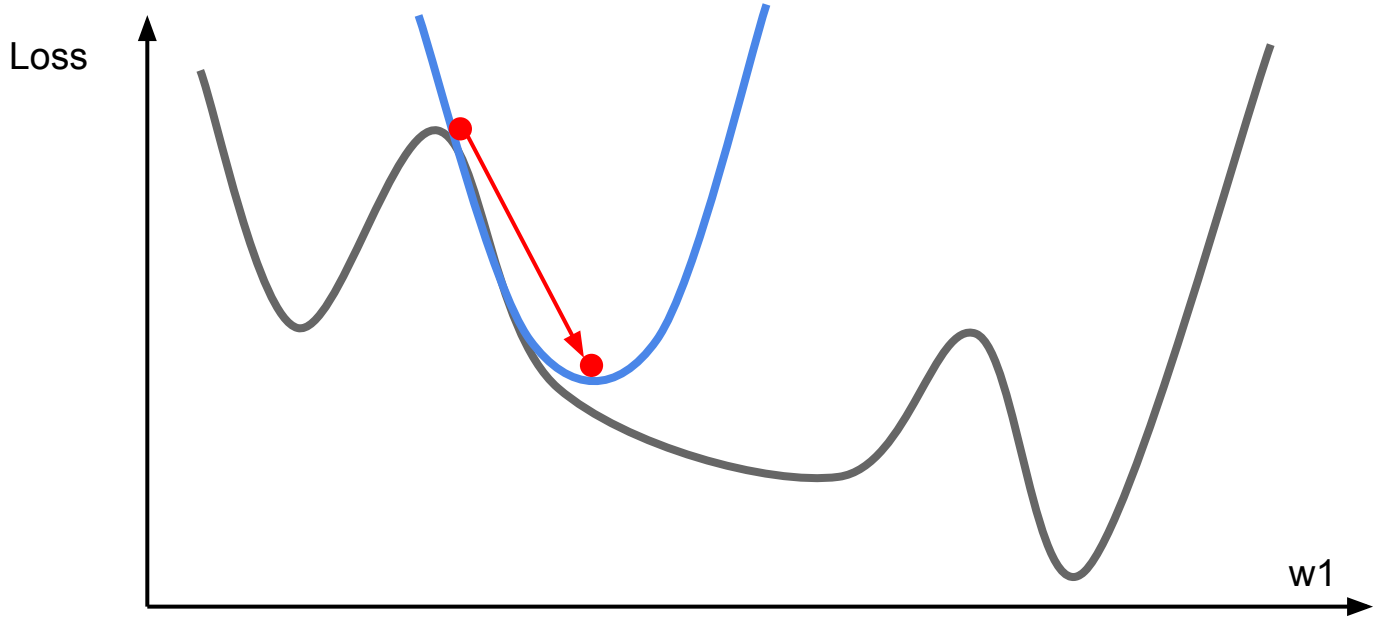
# First-Order Optimization

(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: Why is this bad for deep learning?

# Second-Order Optimization

second-order Taylor expansion:

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

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

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

Q: Why is this bad for deep learning?

# Second-Order Optimization

$$\theta^* = \theta_0 - \boldsymbol{H}^{-1} \nabla_\theta J(\theta_0)$$

- 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

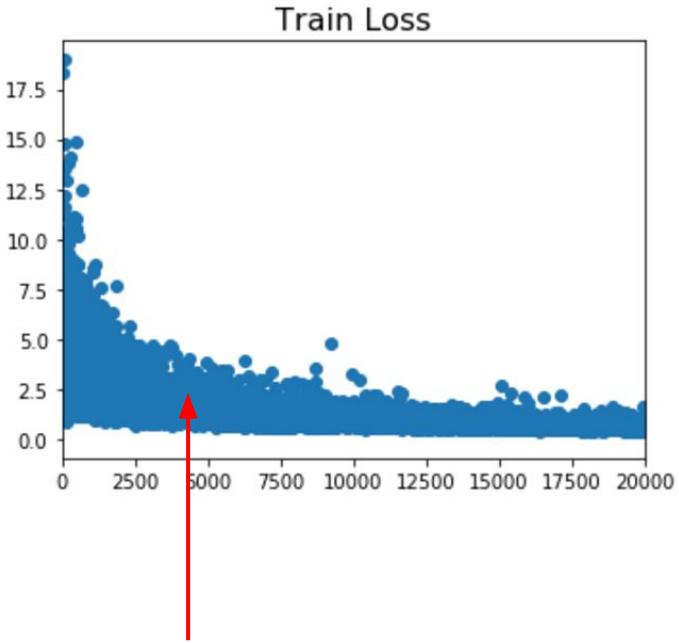
# In practice:

- **Adam** is a good default choice in many cases; it often works ok even with constant learning rate
- **SGD+Momentum** can outperform Adam but may require more tuning of LR and schedule
  - Try cosine schedule, very few hyperparameters!

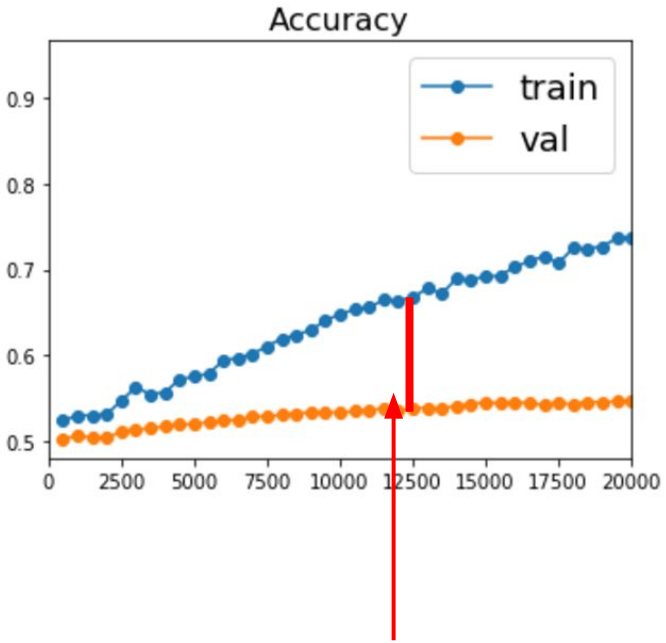
- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)

Improve test error

# Beyond Training Error

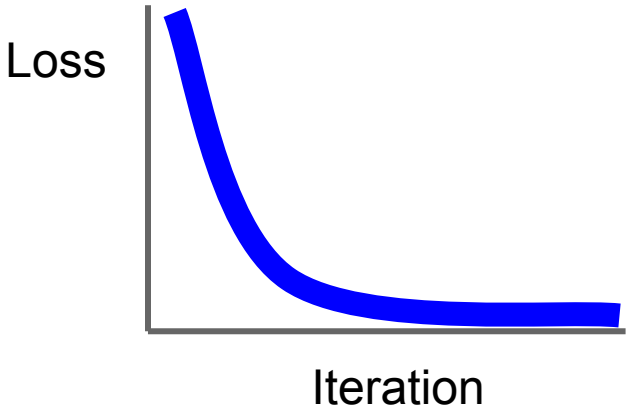


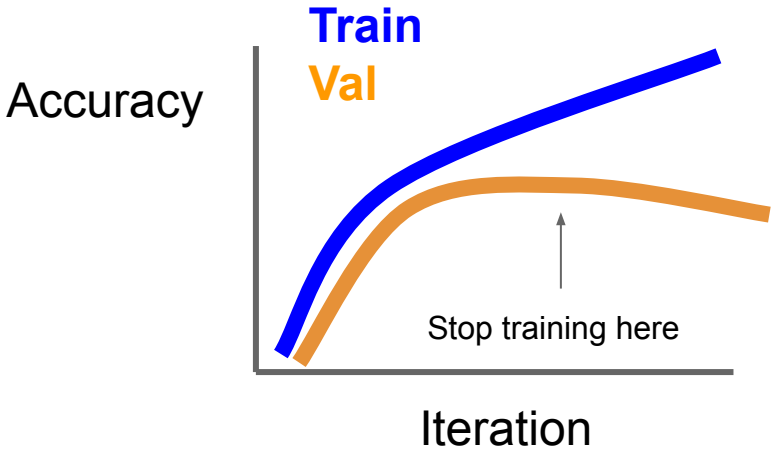

Better optimization algorithms help reduce training loss




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

# Early Stopping: Always do this



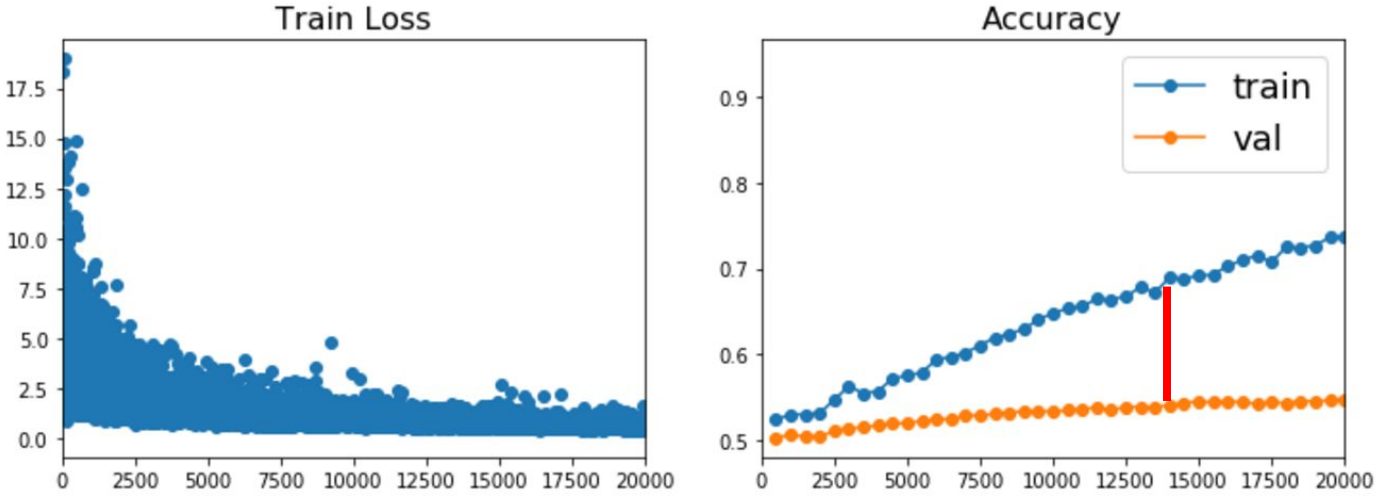

Stop training the model when accuracy on the validation set decreases
Or train for a long time, but always keep track of the model snapshot that worked best on val

# 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:

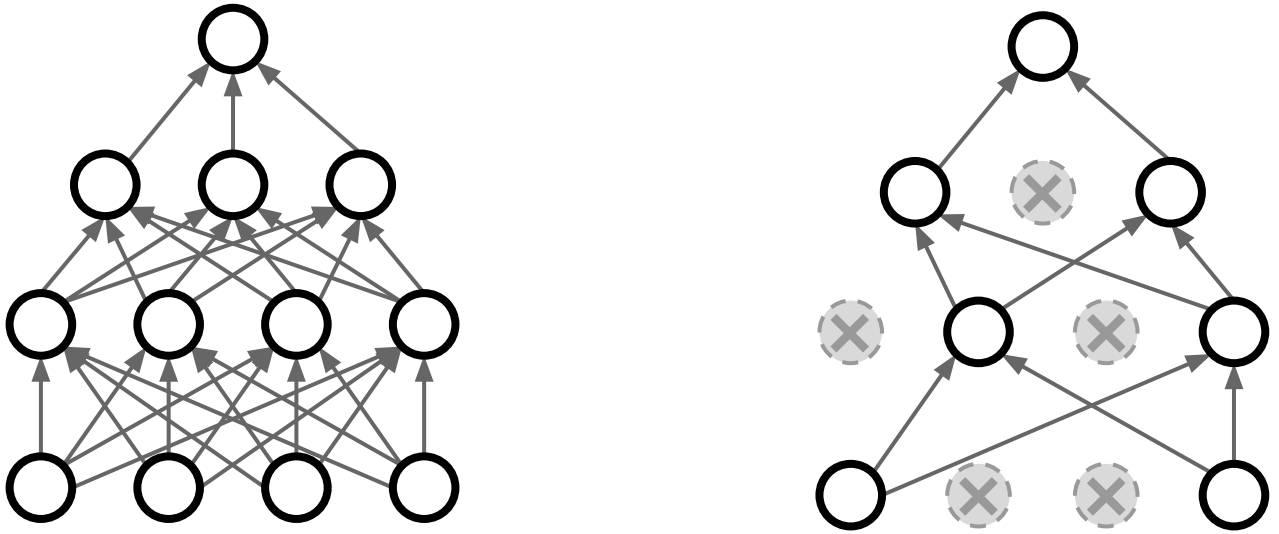
L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ (Weight decay)

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

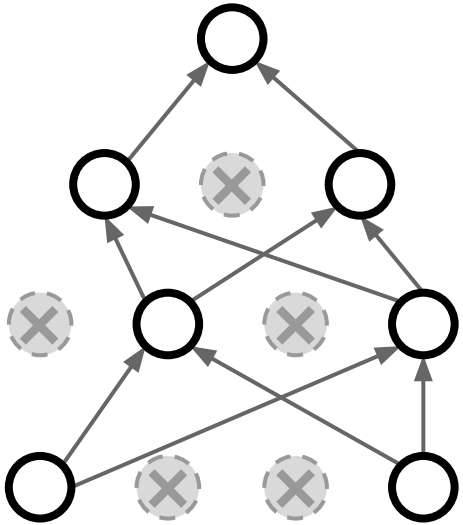


Srivastava et al, “Dropout: A simple way to prevent neural networks from overfitting”, JMLR 2014

# Regularization: Dropout

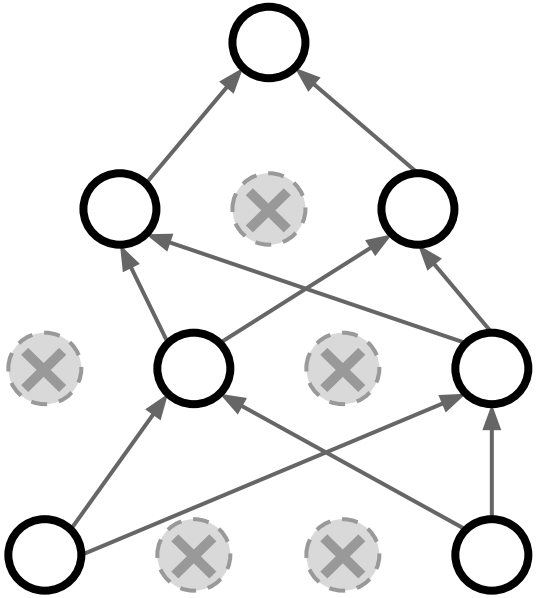
```python
p = 0.5 # probability of keeping a unit active. higher = less dropout

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

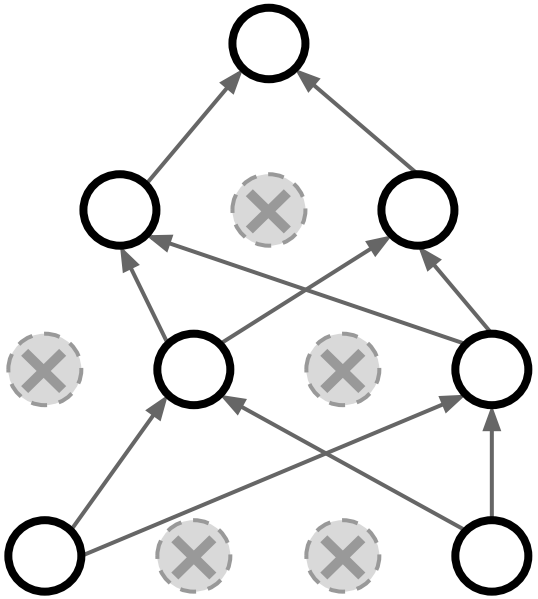
How can this possibly be a good idea?



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

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

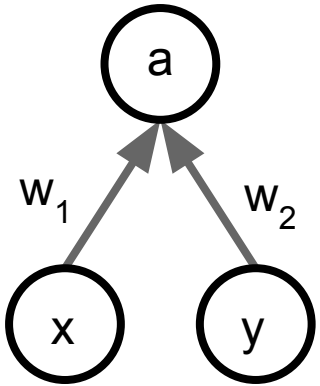
But this integral seems hard …

# Dropout: Test time

Want to approximate the integral

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

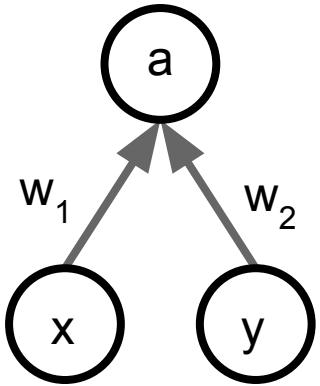
Consider a single neuron.



# Dropout: Test time

Want to approximate the integral

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



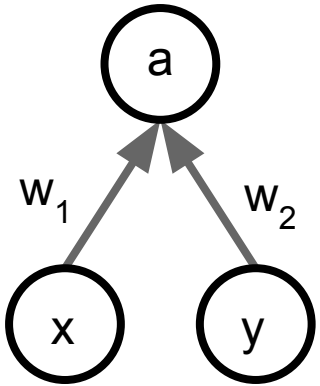

Consider a single neuron.

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

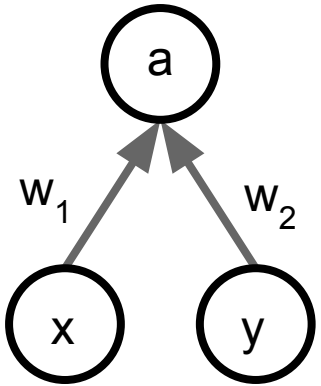
During training we have:

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

# 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.

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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:
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)

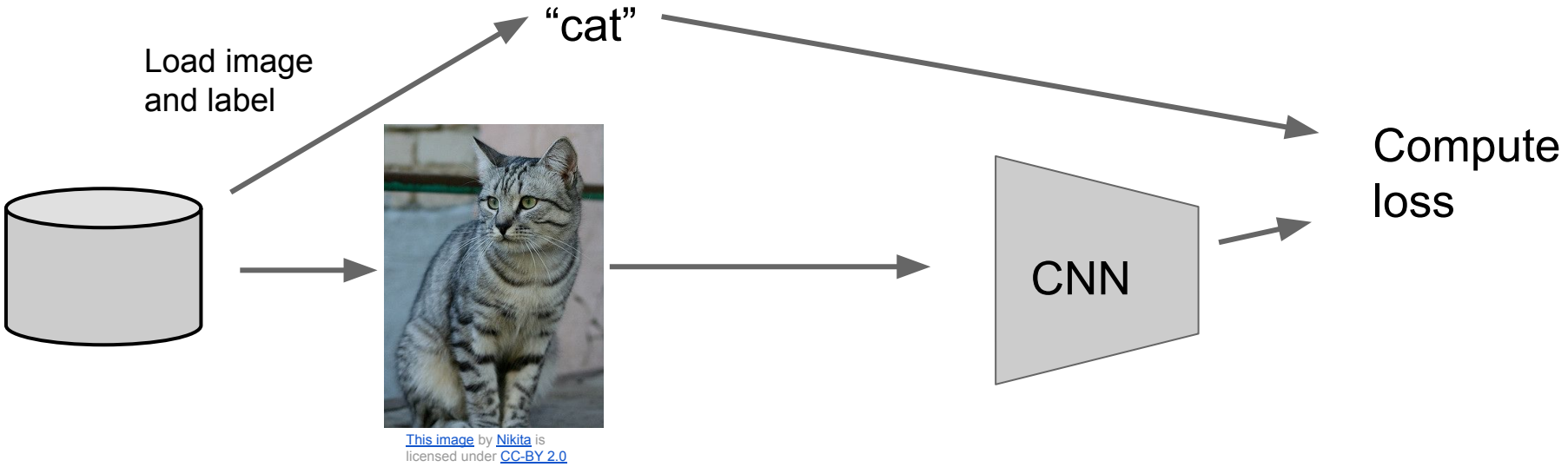
$$y = f(x) = E_z\big[f(x, z)\big] = \int p(z) f(x, z) dz$$

**Example**: Batch Normalization

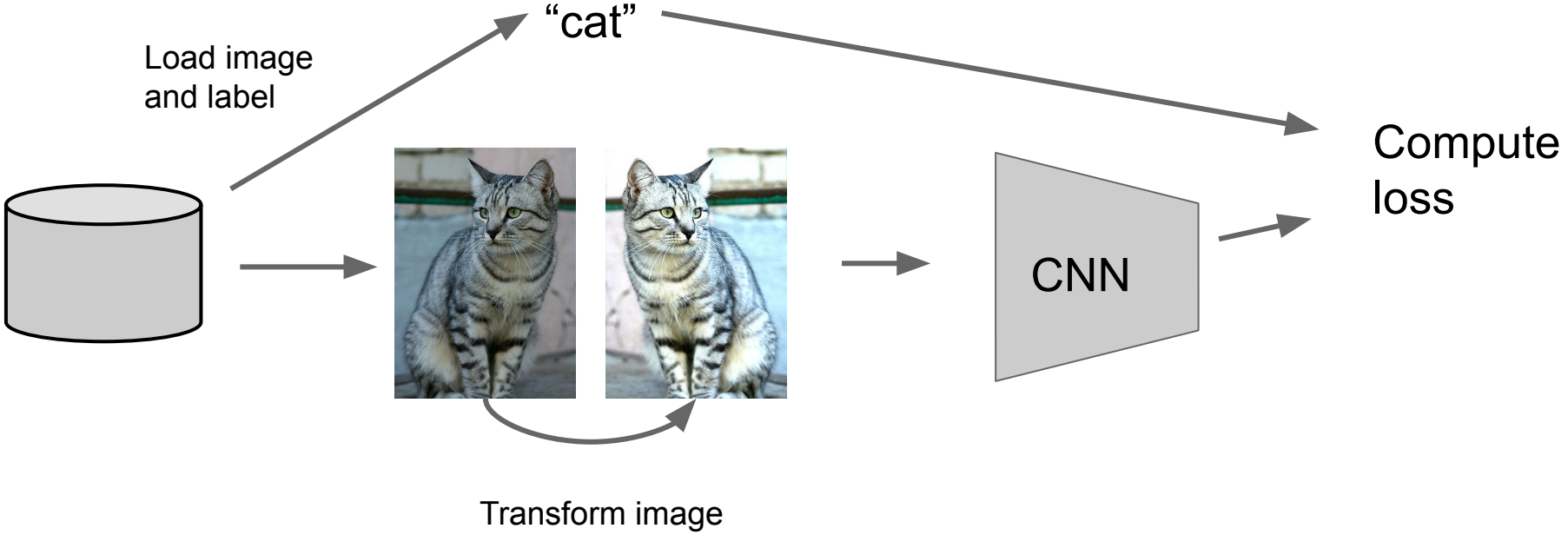
**Training**: Normalize using stats from random minibatches

**Testing**: Use fixed stats to normalize

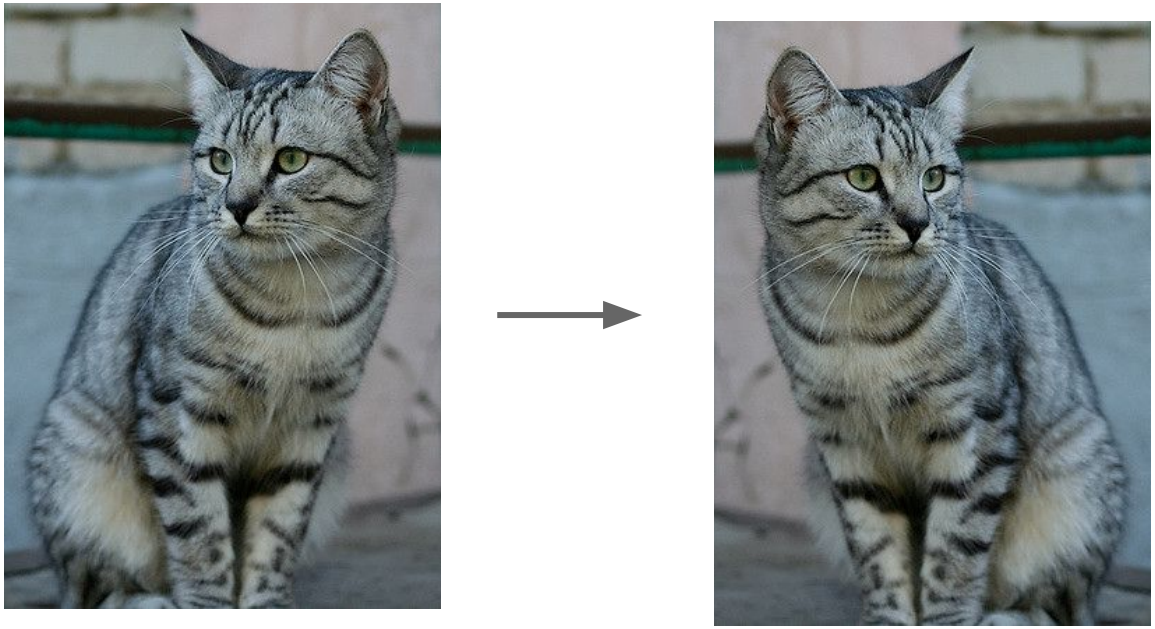
# Regularization: Data Augmentation



# Regularization: Data Augmentation



# Data Augmentation
## Horizontal Flips



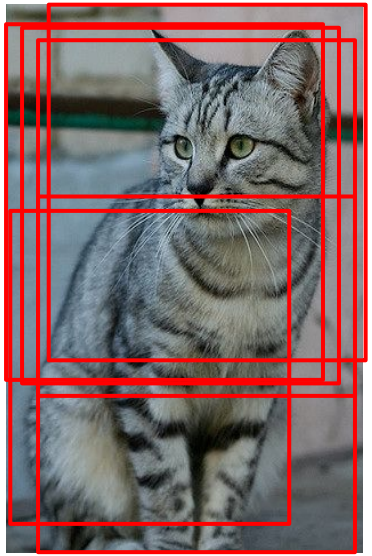
# Data Augmentation

## Random crops and scales

**Training**: sample random crops / scales

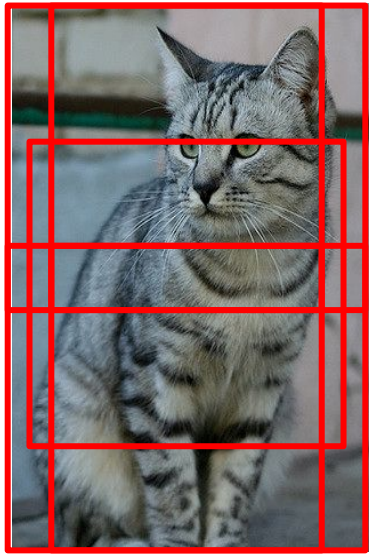
ResNet:

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

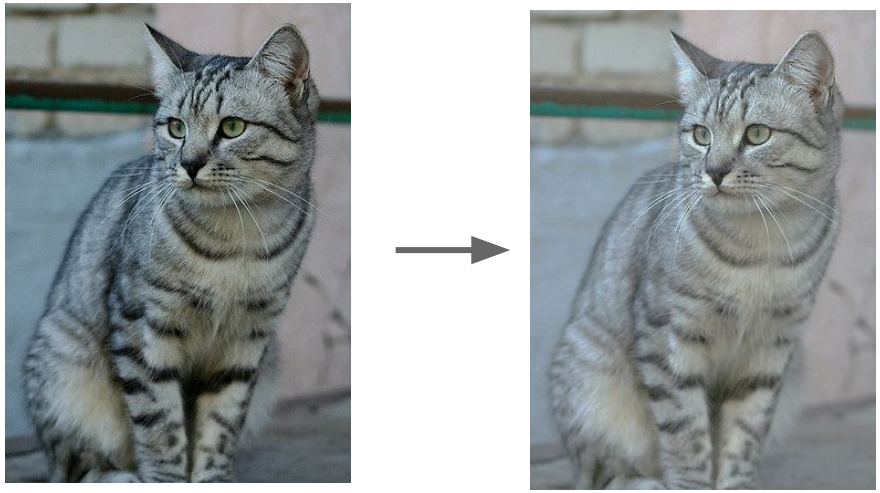
**Testing**: average a fixed set of crops

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

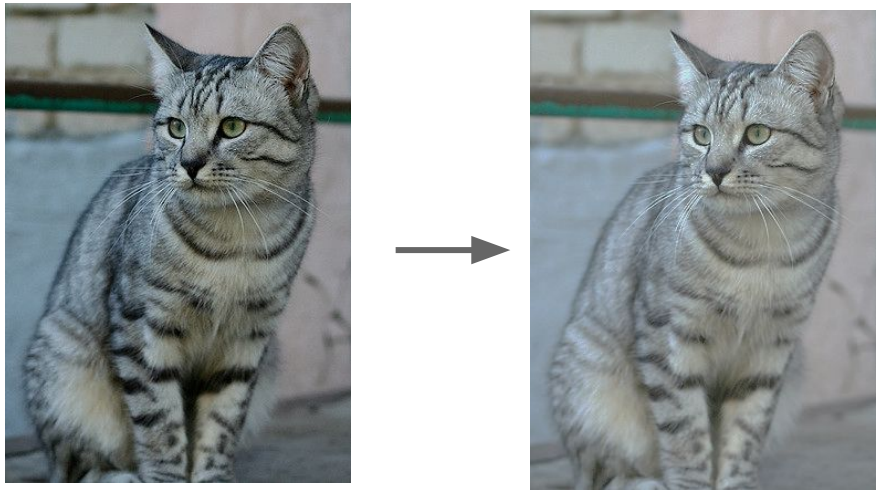
# Data Augmentation
## Color Jitter

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
1. Add offset to all pixels of a training image

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

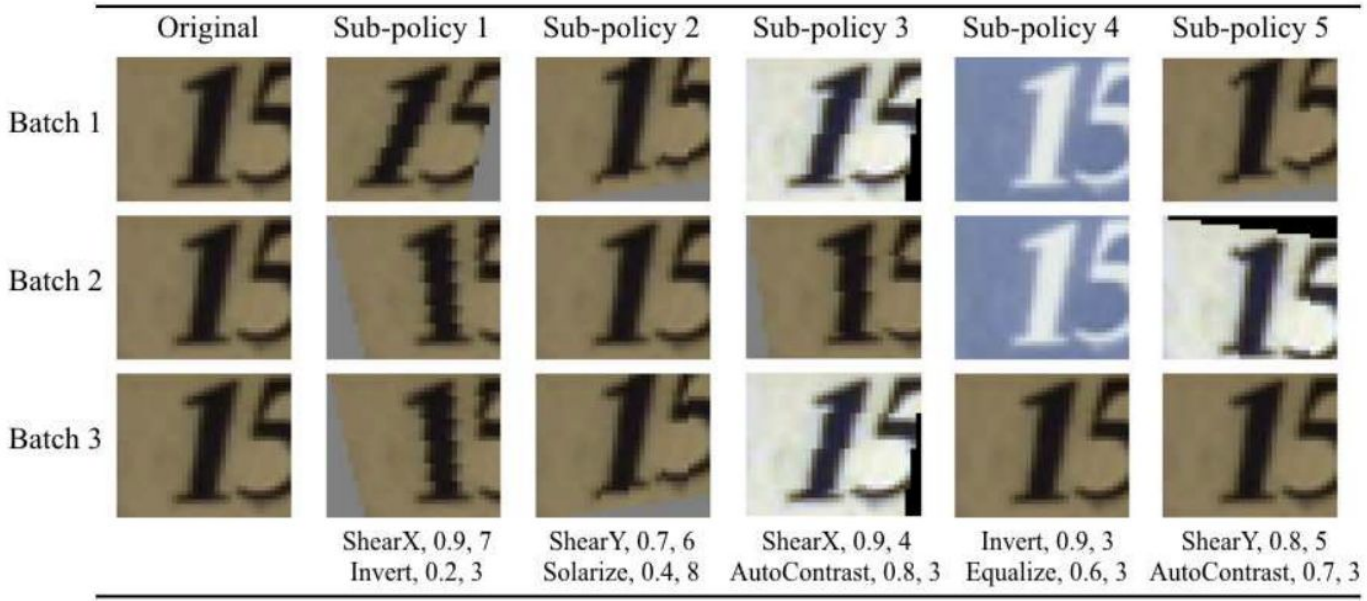
# Data Augmentation

## 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

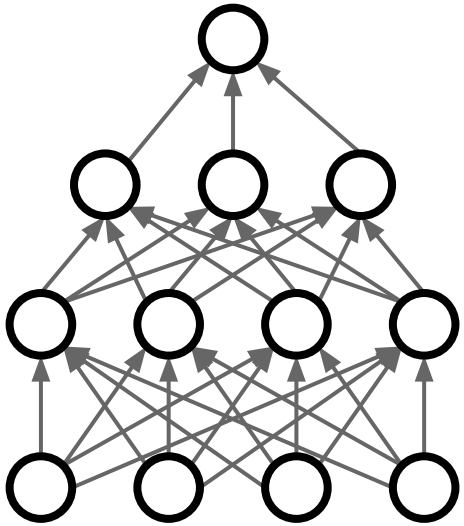
**Examples**:

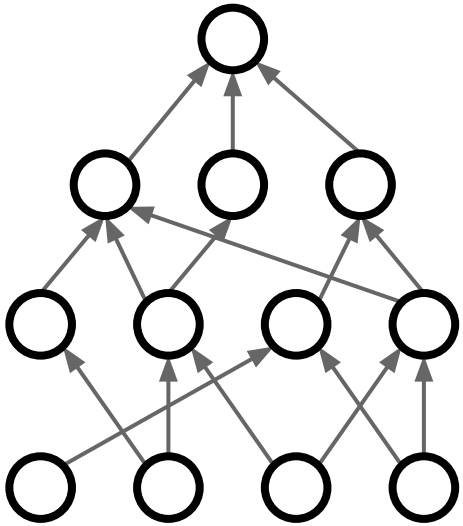
Dropout

Batch Normalization

Data Augmentation

DropConnect





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

# Regularization: Fractional Pooling

**Training**: Use randomized pooling regions

**Testing**: Average predictions from several regions

**Examples**:

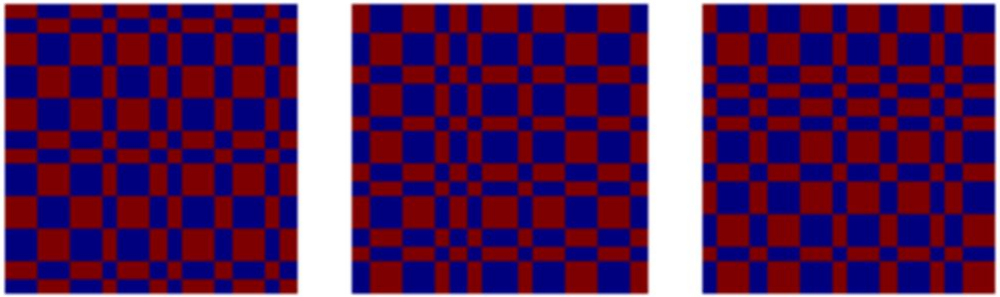
Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

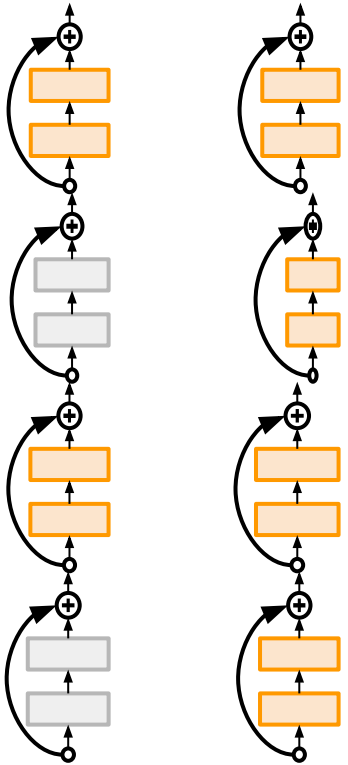


Graham, “Fractional Max Pooling”, arXiv 2014

# Regularization: Stochastic Depth

**Training**: Skip some layers in the network

**Testing**: Use all the layer



**Examples**:

Dropout

Batch Normalization

Data Augmentation

DropConnect

Fractional Max Pooling

Stochastic Depth (will become more clear in next week's lecture)

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

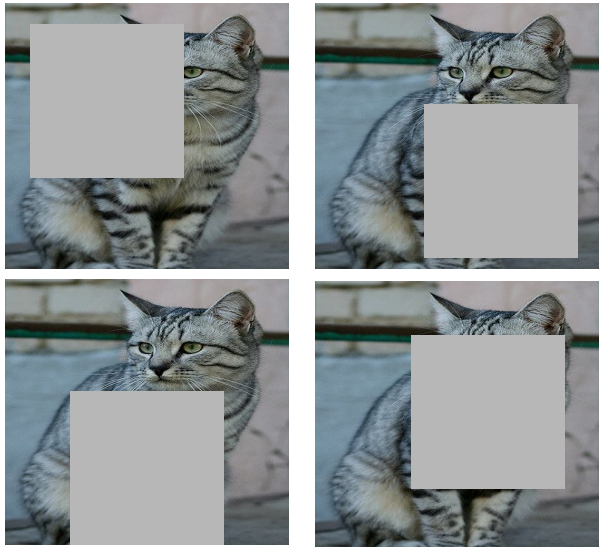
# Regularization: Cutout

**Training**: Set random image regions to zero

**Testing**: Use full image

**Examples**:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
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

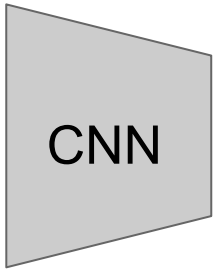
**Training**: Train on random blends of images

**Testing**: Use original images

**Examples**:

Dropout
Batch Normalization
Data Augmentation
DropConnect
Fractional Max Pooling
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
Fractional Max Pooling
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

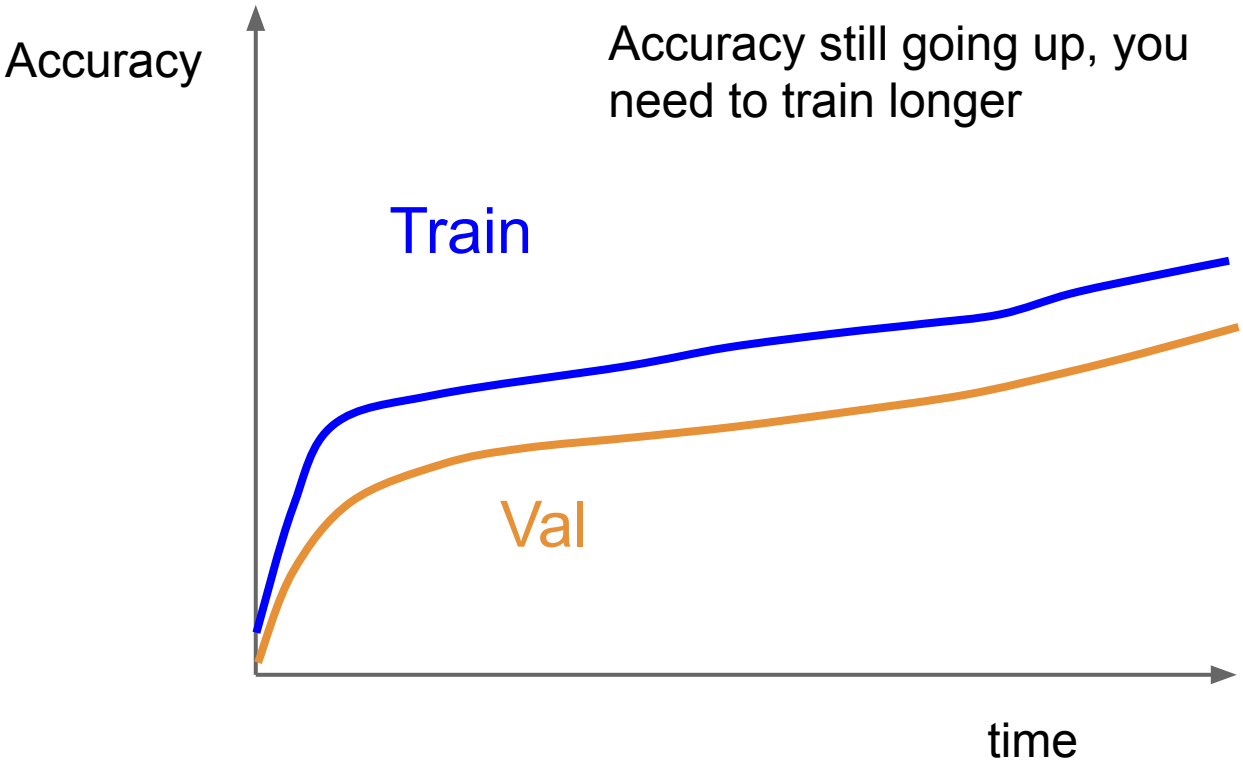
# Choosing Hyperparameters

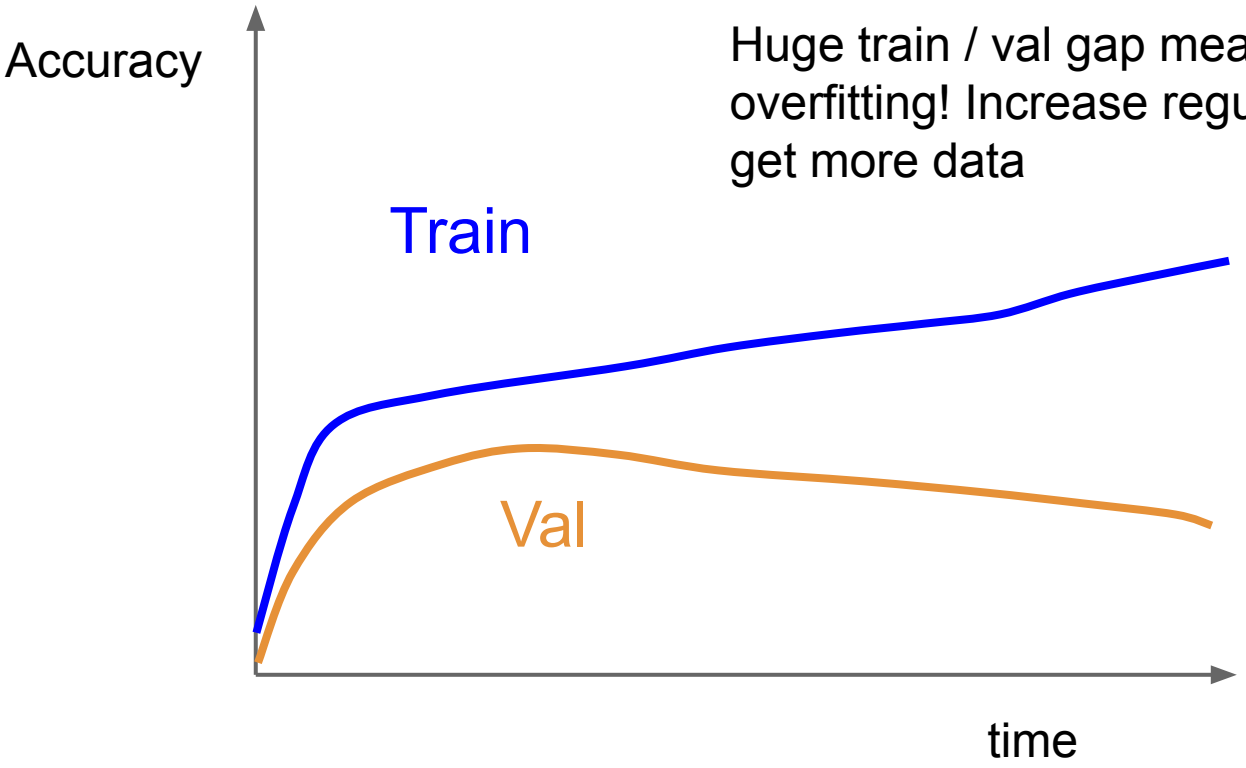
**Step 1**: Check initial loss
**Step 2**: Overfit a small sample
**Step 3**: Find LR that makes loss go down
**Step 4**: Coarse grid, train for ~1-5 epochs
**Step 5**: Refine grid, train longer

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

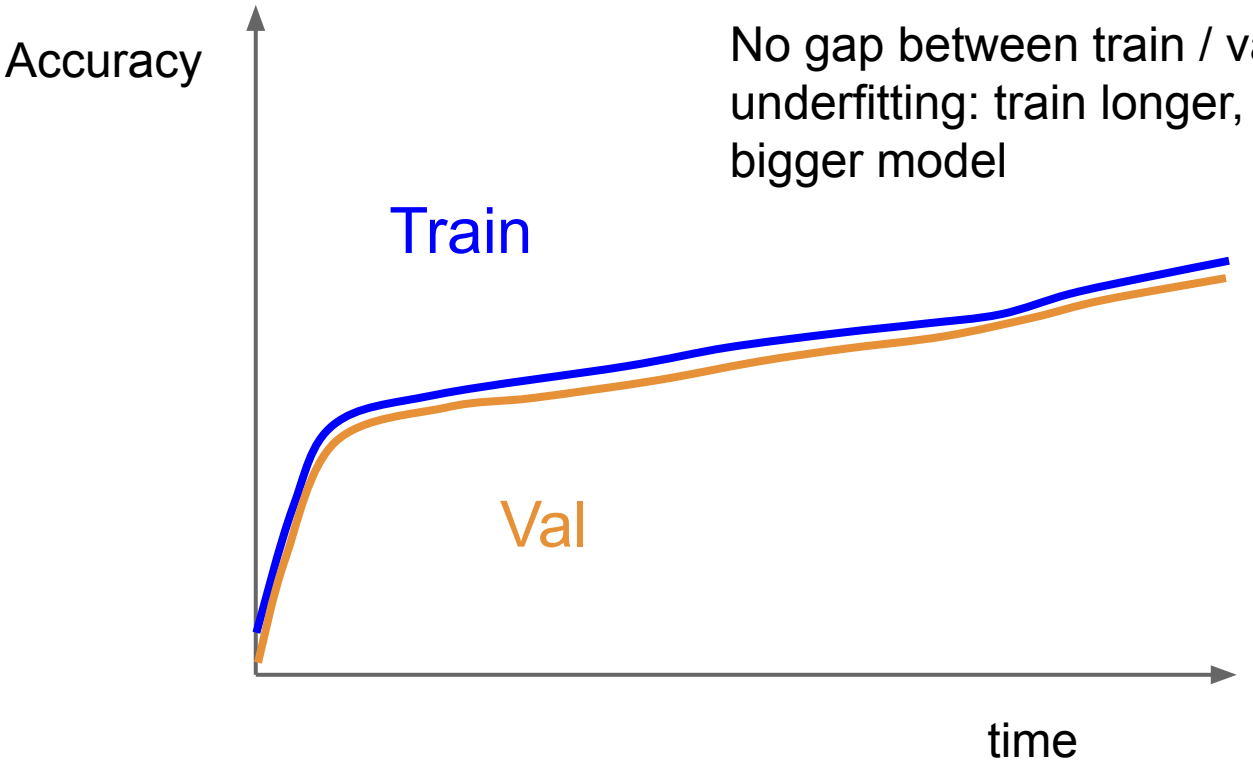
# Choosing Hyperparameters

**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



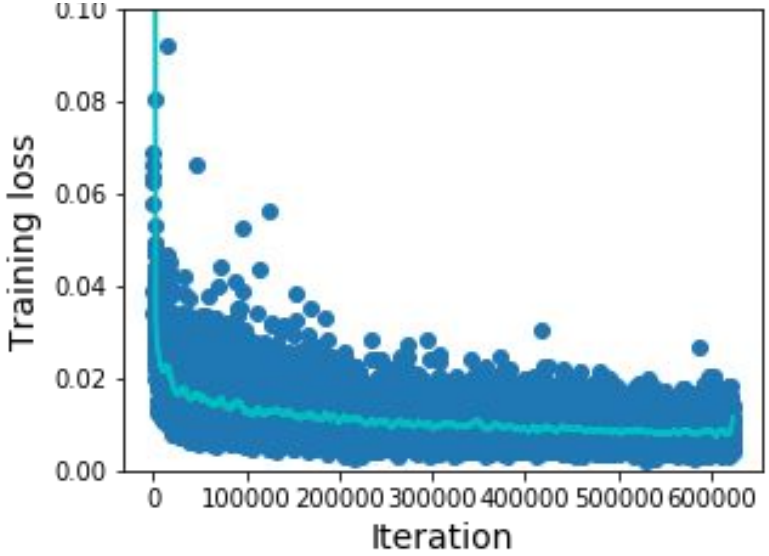

Huge train / val gap means overfitting! Increase regularization, get more data



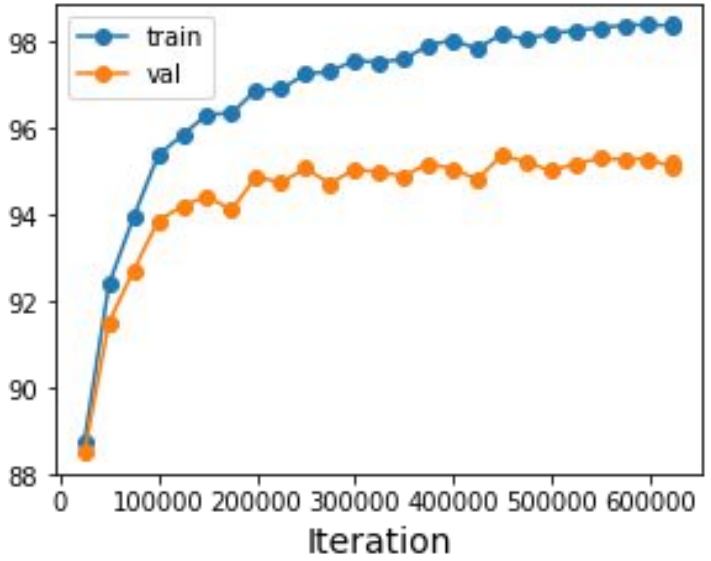

No gap between train / val means underfitting: train longer, use a bigger model

# Look at learning curves!

Training Loss




Train / Val Accuracy

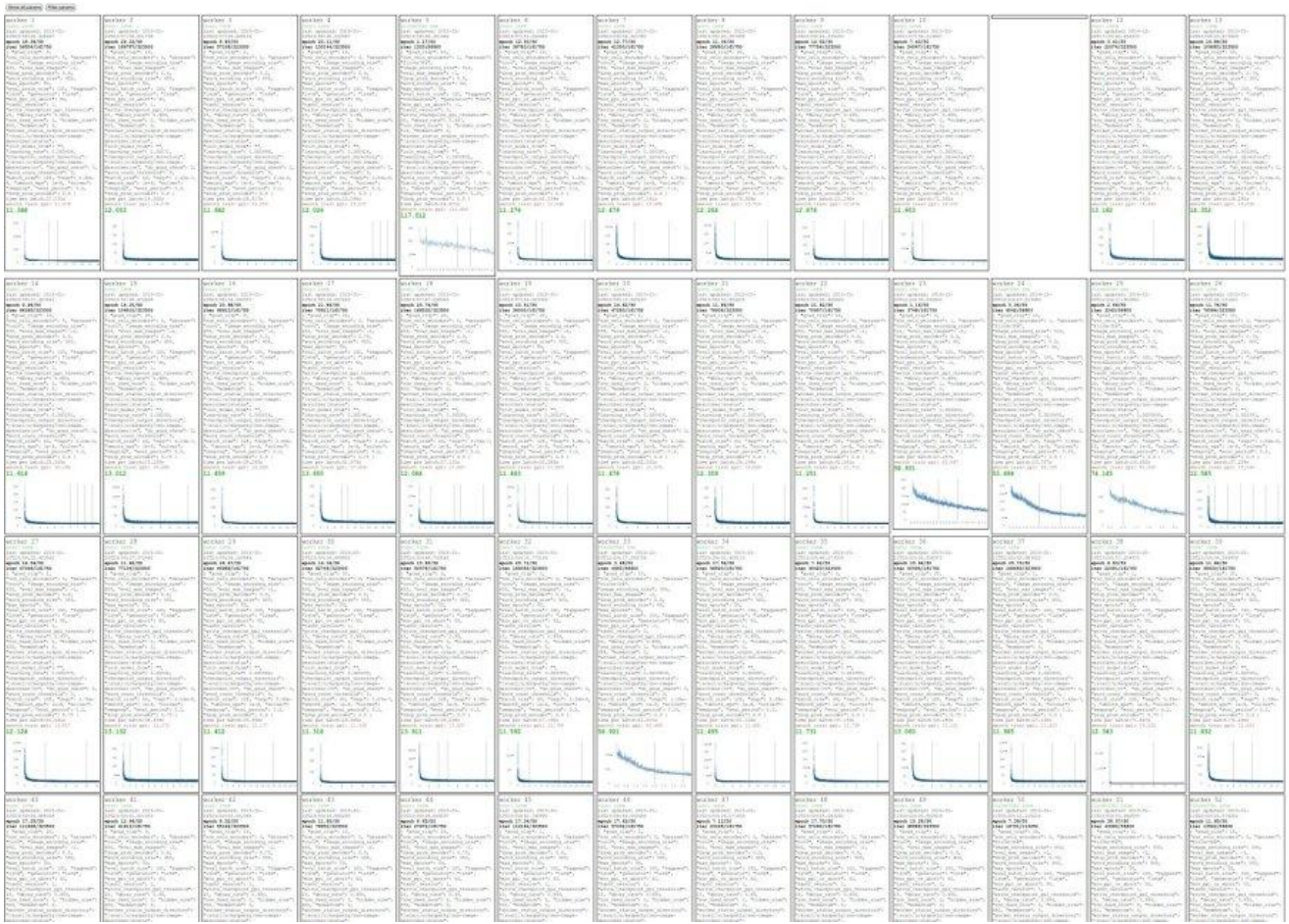



Losses may be noisy, use a scatter plot and also plot moving average to see trends better

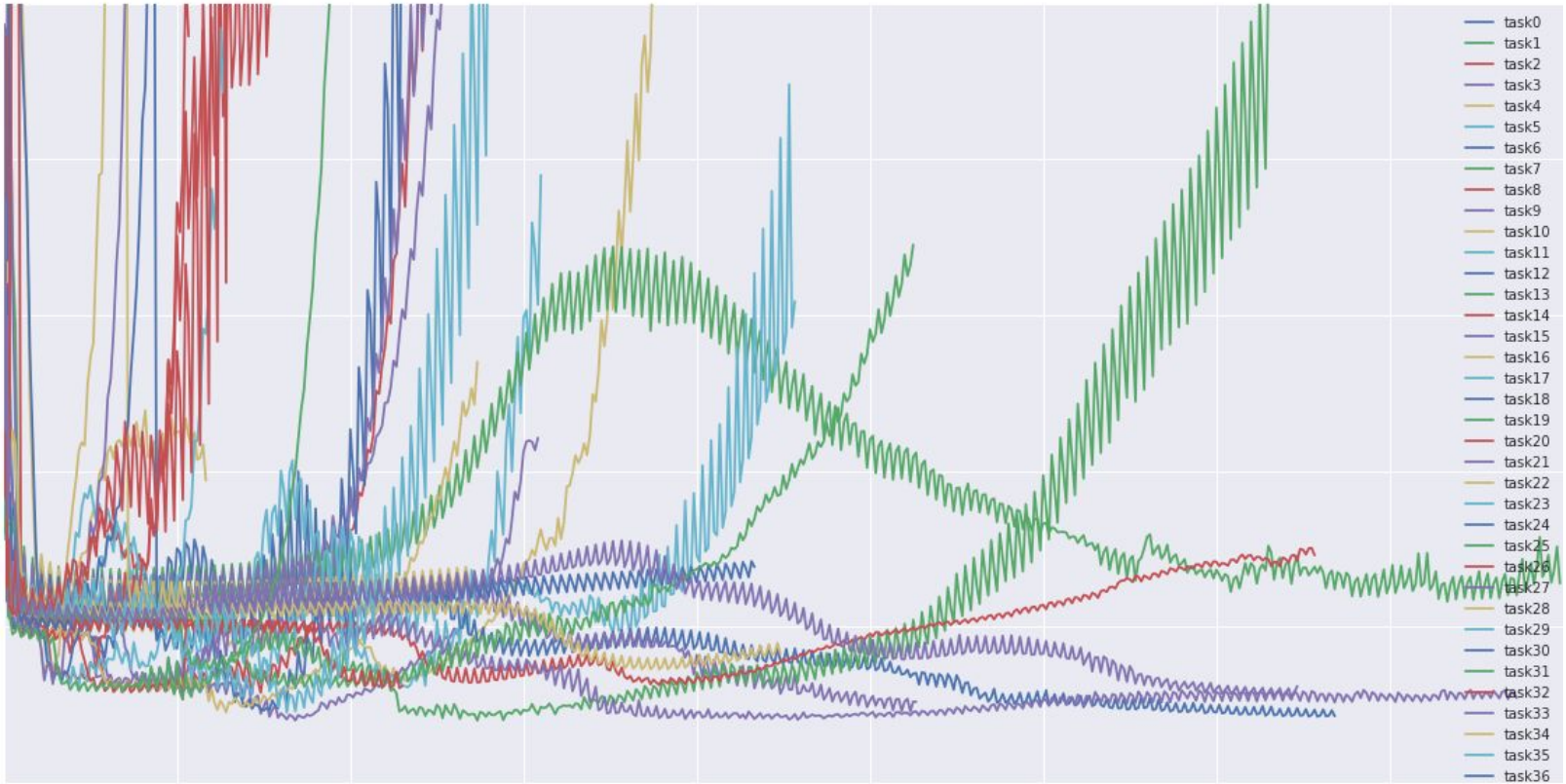
Cross-validation

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

# Hyperparameters to play with:

- network architecture
- learning rate, its decay schedule, update type
- regularization (L2/Dropout strength)

# Random Search vs. Grid Search

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

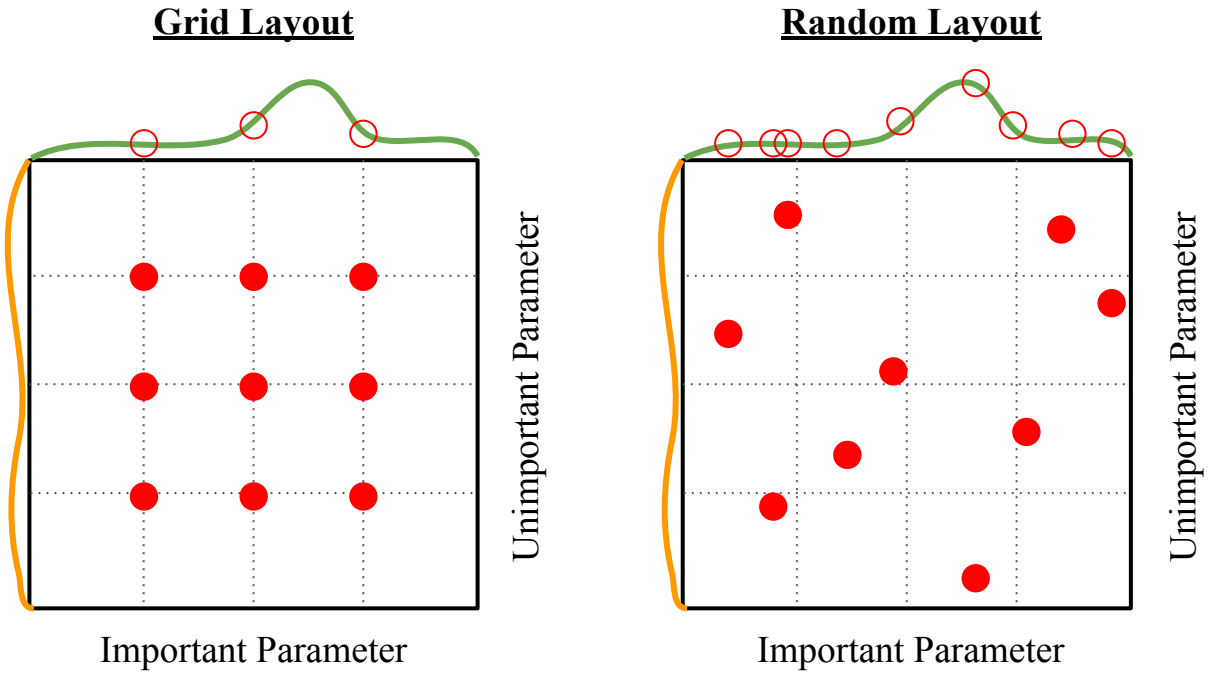



Illustration of Bergstra et al., 2012 by Shayne Longpre, copyright CS231n 2017

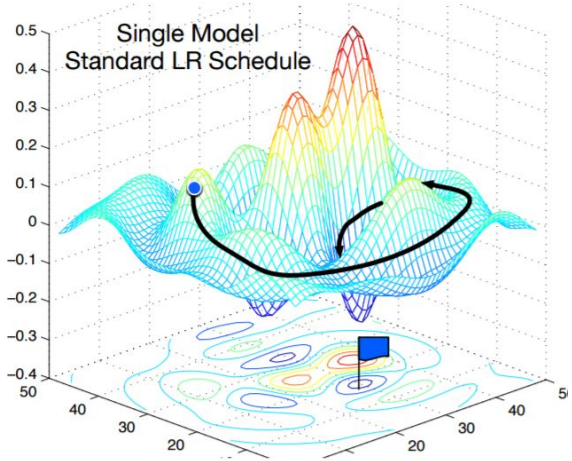
# Summary

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

# Next time: CNN Architecture Design

# Model Ensembles: Tips and Tricks

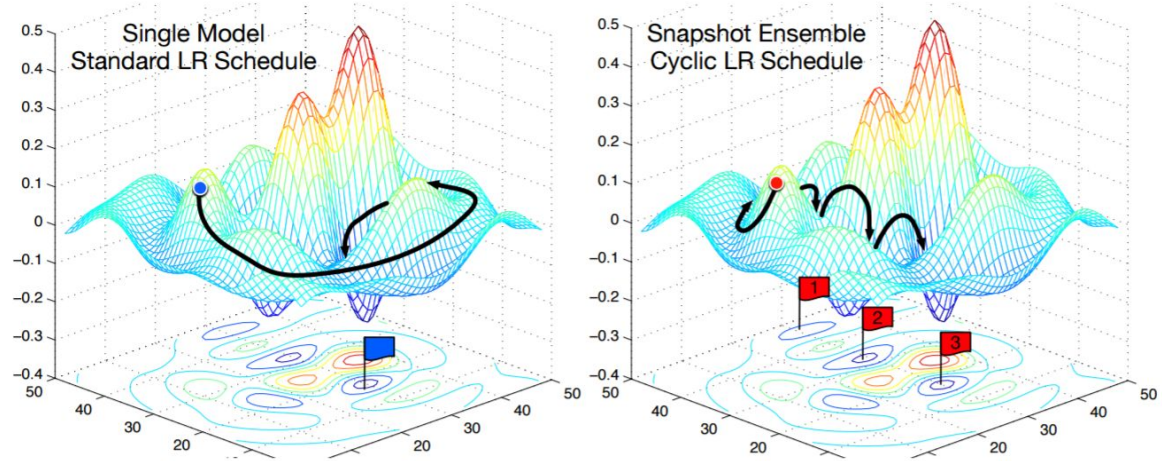
Instead of training independent models, use multiple snapshots of a single model during training!

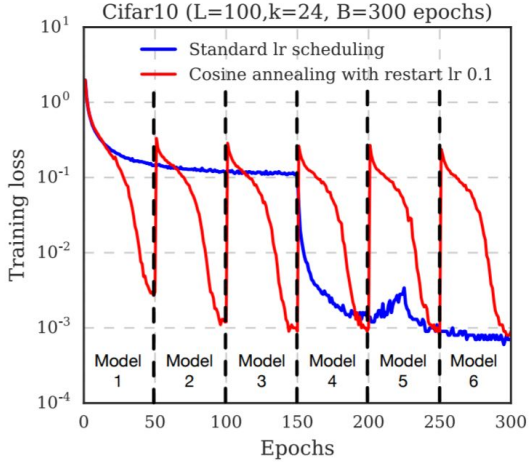



Loshchilov and Hutter, “SGDR: Stochastic gradient descent with restarts”, arXiv 2016
Huang et al, “Snapshot ensembles: train 1, get M for free”, ICLR 2017
Figures copyright Yixuan Li and Geoff Pleiss, 2017. Reproduced with permission.

# 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
Figures copyright Yixuan Li and Geoff Pleiss, 2017. Reproduced with permission.

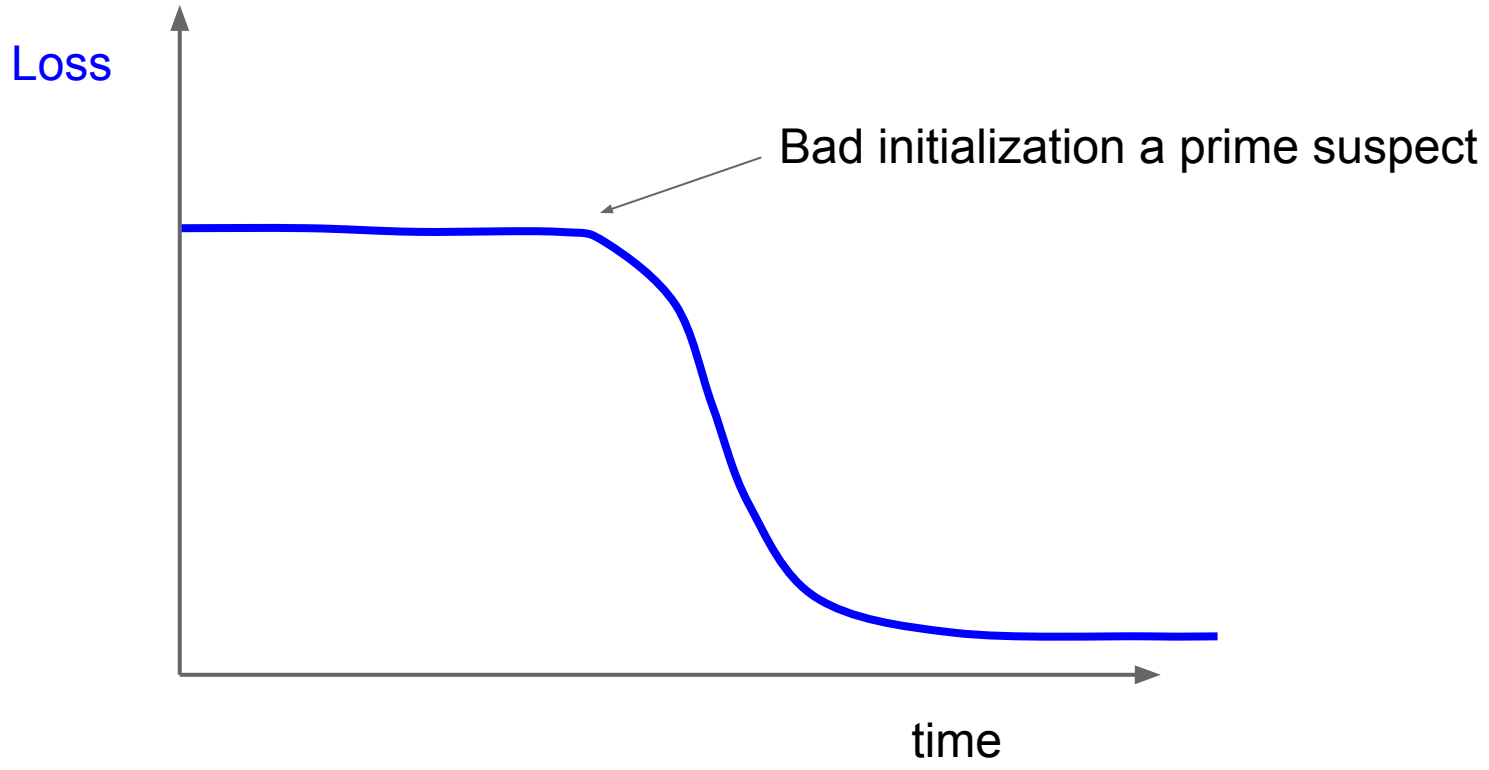
Cyclic learning rate schedules can make this work even better!

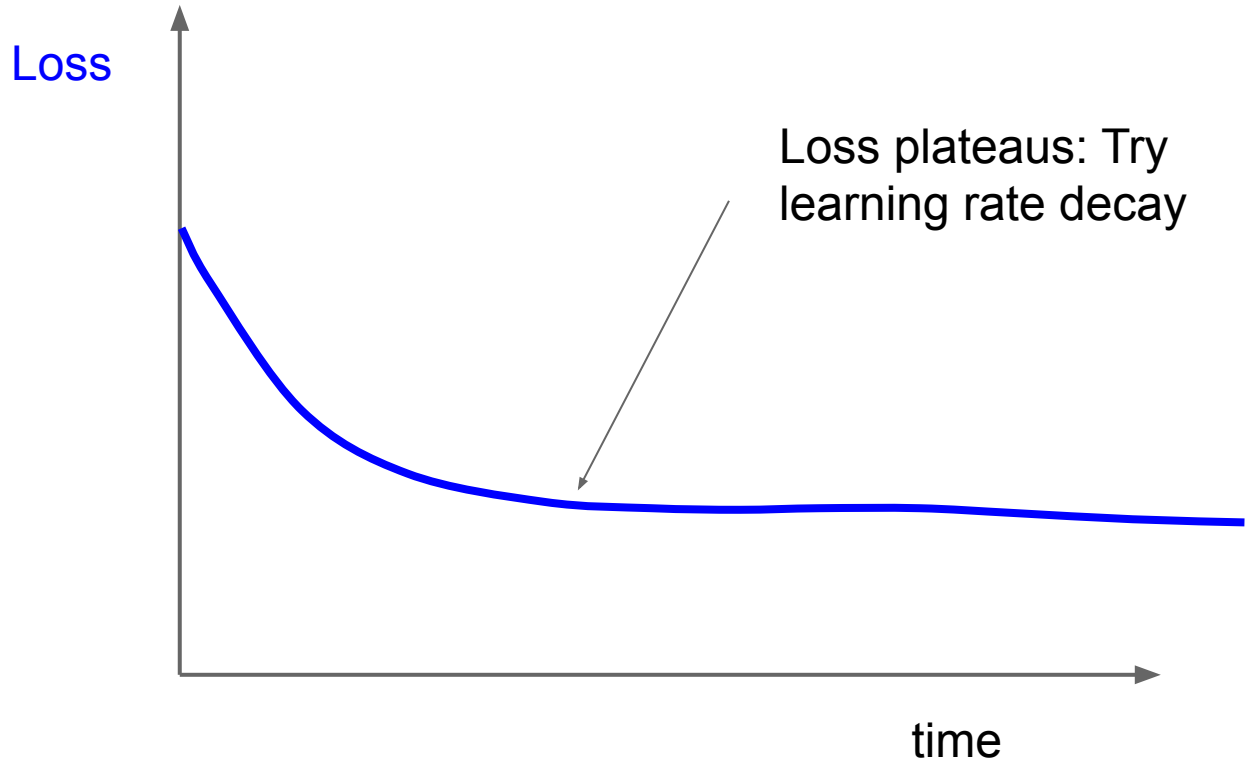
# Model Ensembles: Tips and Tricks

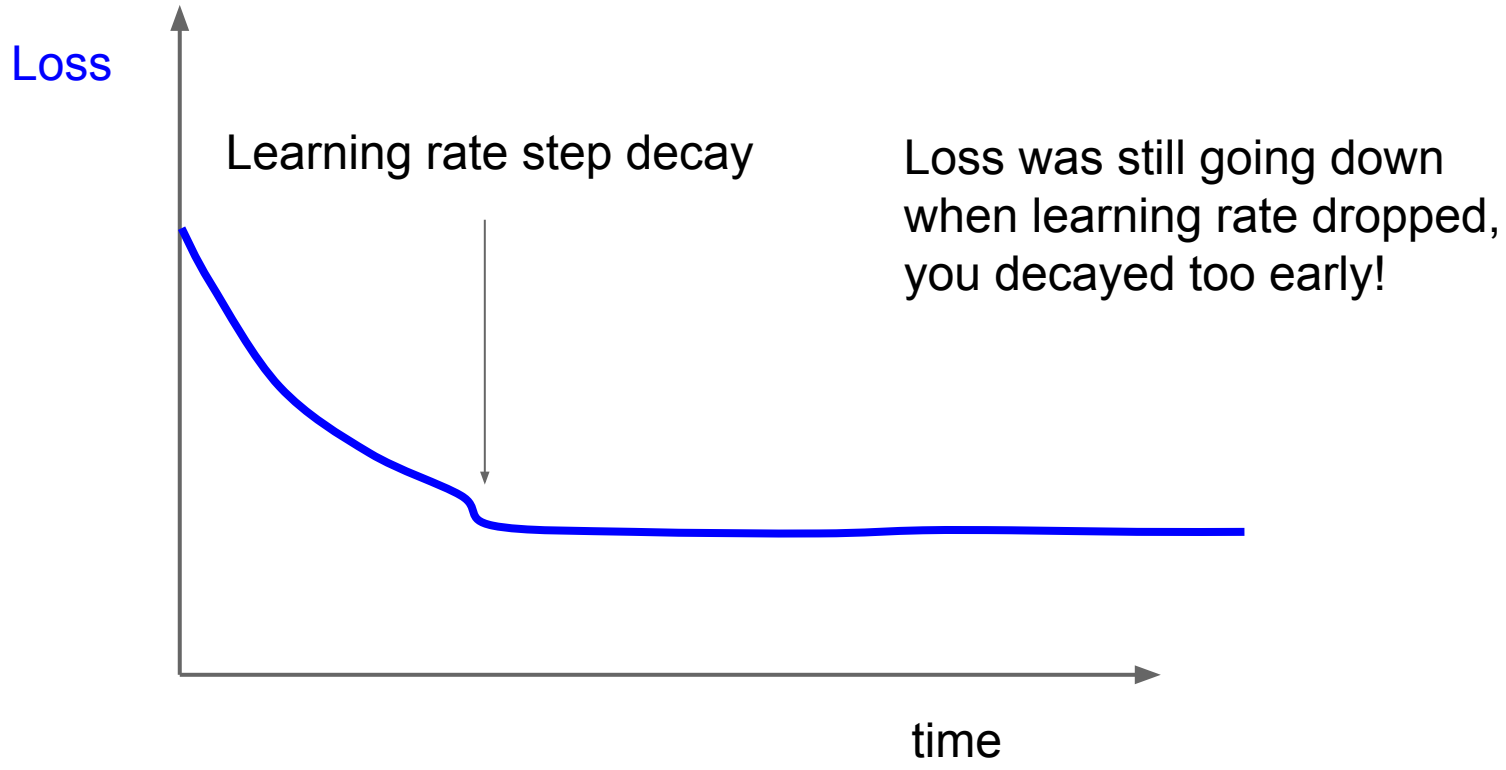
Instead of using actual parameter vector, keep a moving average of the parameter vector and use that at test time (Polyak averaging)

```
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.


Loss
Bad initialization a prime suspect
time


Loss
Loss plateaus: Try
learning rate decay
time


Loss
Learning rate step decay
Loss was still going down
when learning rate dropped,
you decayed too early!
time

# Track the ratio of weight updates / weight magnitudes:

```
# assume parameter vector W and its gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW # simple SGD update
update_scale = np.linalg.norm(update.ravel())
W += update # the actual update
print update_scale / param_scale # want ~1e-3
```

ratio between the updates and values: ~ 0.0002 / 0.02 = 0.01 (about okay)
**want this to be somewhere around 0.001 or so**