CS 4644-DL / 7643-A: LECTURE 10
DANFEI XU

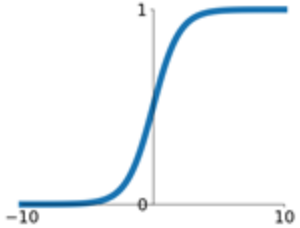
Topics:

- Training Neural Networks (Part 2)

Activation Functions

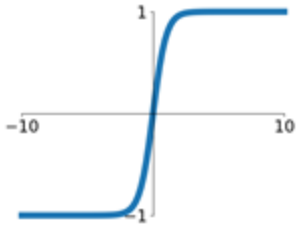
Sigmoid

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



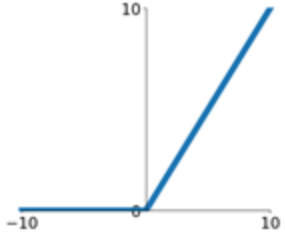
tanh

$$\tanh(x)$$



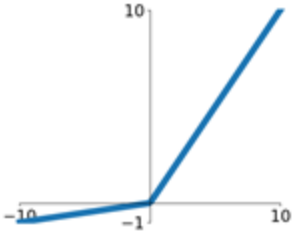
ReLU

$$\max(0, x)$$



Leaky ReLU

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

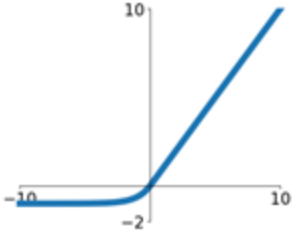


Maxout

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

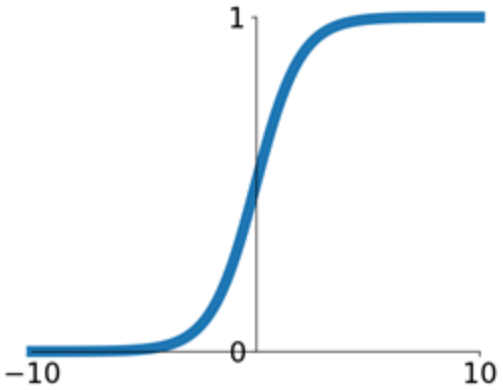
ELU

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



Activation Functions

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



Sigmoid

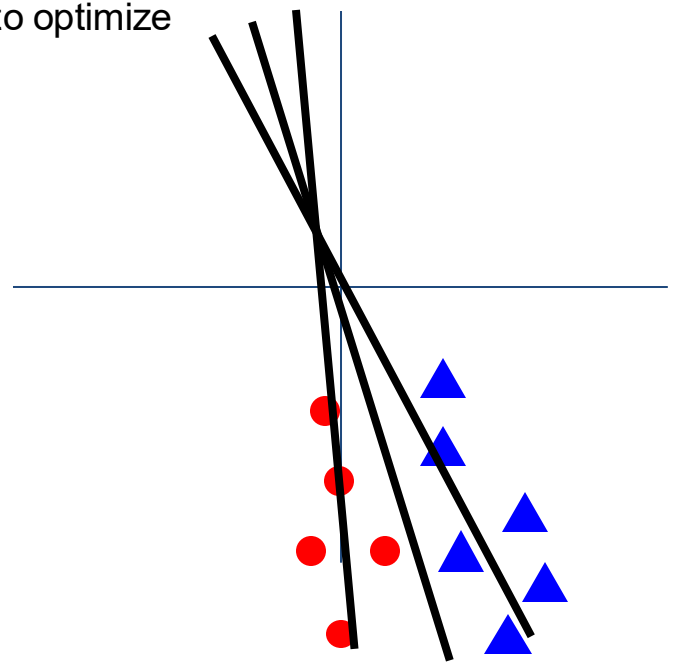
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

2 problems:

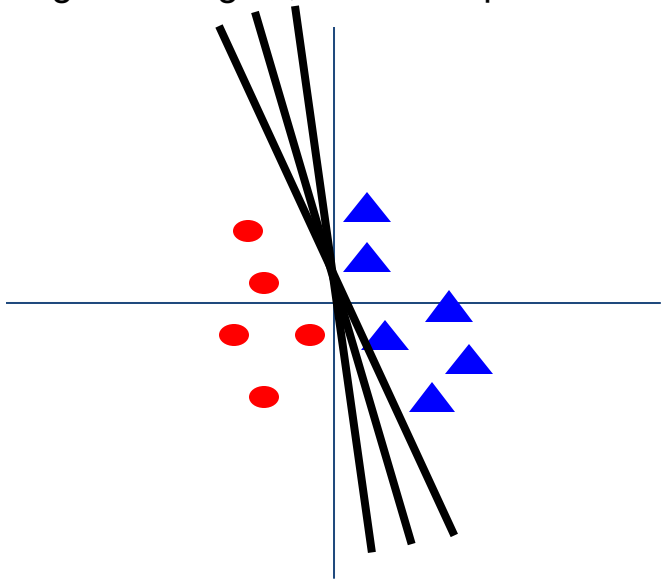
1. **Saturated neurons “kill” the gradients**
2. exp() is a bit compute expensive

Data Preprocessing

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize



After normalization: less sensitive to small changes in weights; easier to optimize



Batch Normalization

[Ioffe and Szegedy, 2015]

Input: $x : N \times D$

Learnable scale and shift parameters:

γ, β: $\mathbb{R}^D$

We want to give the model a chance to **adjust batchnorm** if the default is not optimal.

Learning $\gamma = \sigma$ and $\beta = \mu$ will recover the original input batch!

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

Per-batch mean, shape is D

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

Per-batch 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

Initialize $\gamma = 1, \beta = 0$

Batch Normalization: Test-Time

Input: $x : N \times D$

Learnable scale and shift parameters:

γ, β: $\mathbb{R}^D$

$$\mu_j = \text{(Moving) average of values seen during training}$$

Per-batch mean, shape is D

$$\sigma_j^2 = \text{(Moving) average of values seen during training}$$

Per-batch var, shape is D

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

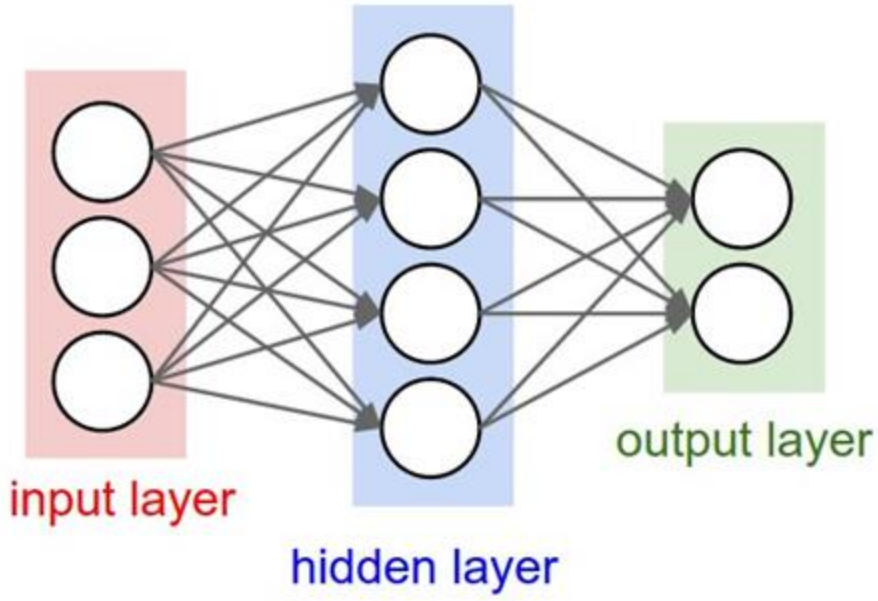
Normalized x, Shape is N x D

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

Output, Shape is N x D

During testing batchnorm becomes a linear operator!
Can be fused with the previous fully-connected or conv layer

Weight initialization: goal is to **maximize diversity with bounded variance** of layer output throughout the network, at least at the beginning of the training



Weight Initialization: Activation statistics

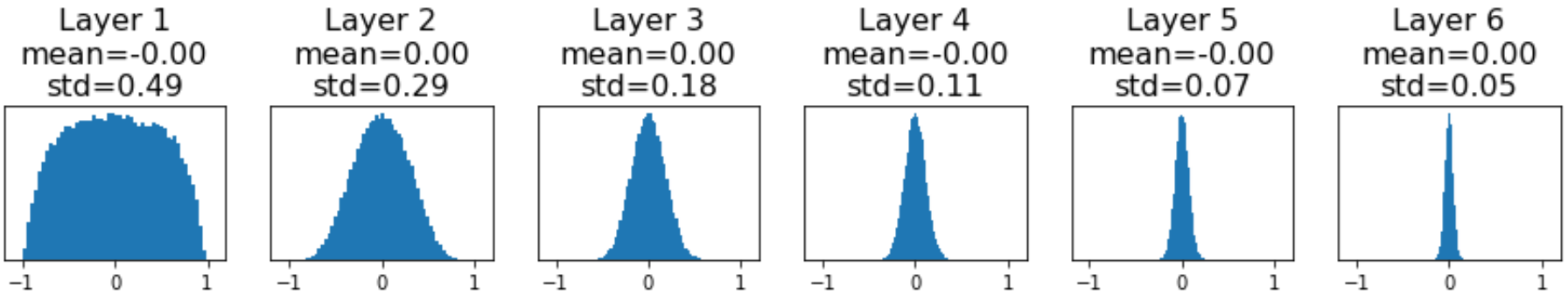
```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = 0.01 * np.random.randn(Din, Dout)
    x = np.tanh(x.dot(W))
    hs.append(x)
```

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

All activations tend to zero for deeper network layers

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

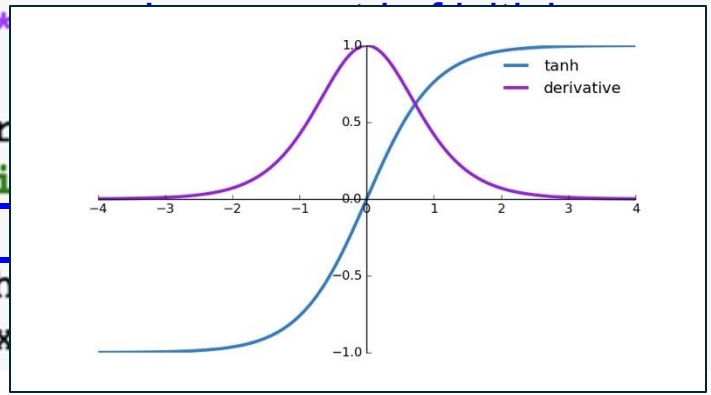
A: Very small, slow learning



Visualize distribution of activations

Weight Initialization: Activation statistics

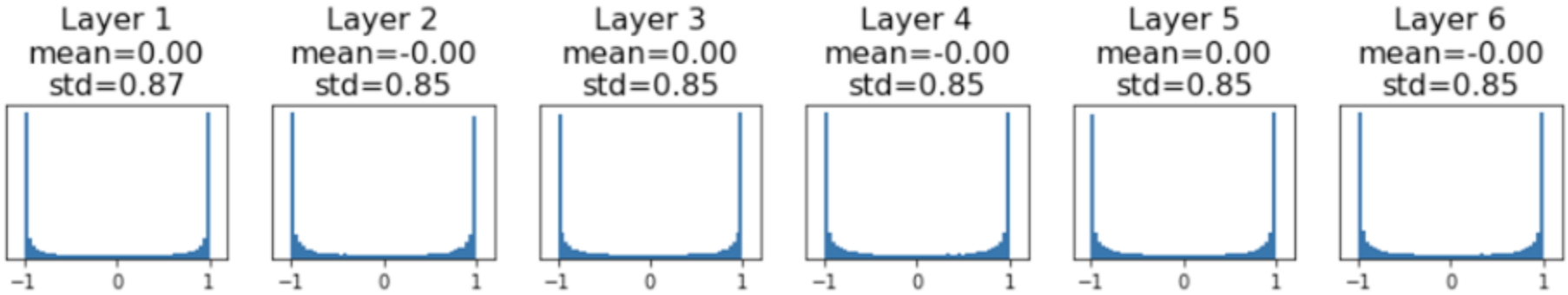
```
dims = [4096] *
hs = []
x = np.random.r
for Din, Dout i
    W = 0.05 *
    x = np.tanh
    hs.append(x
```



All activations saturate

Q: What do the gradients look like?

A: For tanh, large value -> small gradient



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Weight Initialization: Activation statistics

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

Increase std of initial weights from 0.01 to 0.05

All activations saturate

Q: What do the gradients look like?

More generally, *gradient explosion* (high w-> high output -> high gradient).

Visualize distribution of activations

Weight Initialization: “Xavier” Initialization

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

“Xavier” initialization:
std = 1/sqrt(Din)

Assume each input contribute similarly to output
more number of weights needs -> small weight multiplier

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

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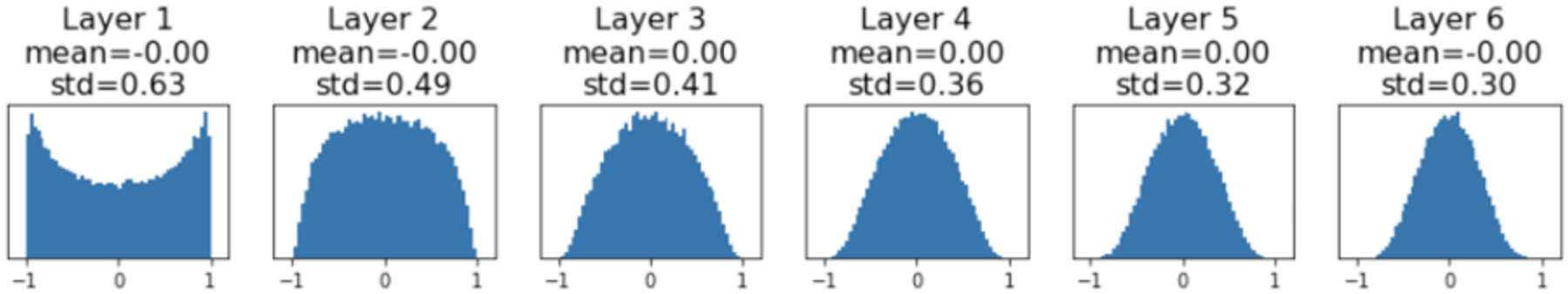
```

“Xavier” initialization:
std = 1/sqrt(Din)

“Just right”: Activations are nicely scaled for all layers!



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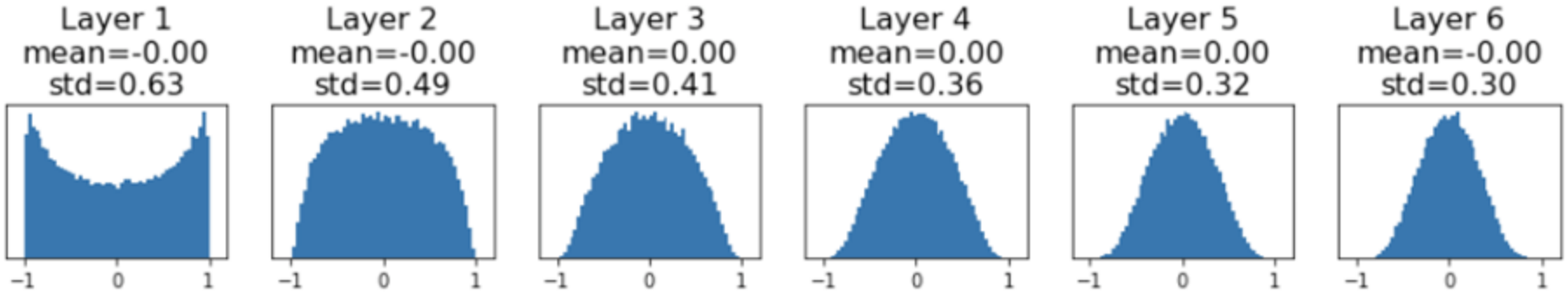
For conv layers, Din is filter_size^2 * input_channels



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Let: $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

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Assume: $Var(x_1) = Var(x_2)= ...=Var(x_{Din})$

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We want: $Var(y) = Var(x_i)$

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For conv layers, Din is filter_size^2 * input_channels

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Assume: $Var(x_1) = Var(x_2)= ...=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$
[substituting value of y]

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

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Assume: $Var(x_1) = Var(x_2)= ...=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$

$= \Sigma\, Var(x_iw_i) = Din\, Var(x_iw_i)$

[Assume all x_i, w_i are iid] $\sigma^2_{X+Y} = \sigma^2_X + \sigma^2_Y$

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

Weight Initialization: "Xavier" Initialization

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Let: $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= ...=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$

$= Din\ Var(x_iw_i)$

$= Din\ Var(x_i)\ Var(w_i)$

[Assume all x_i, w_i are zero mean]

$$Var(XY) = E(X^2Y^2) - (E(XY))^2 = Var(X)Var(Y) + Var(X)(E(Y))^2 + Var(Y)(E(X))^2$$

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

Weight Initialization: "Xavier" Initialization

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"Just right": Activations are nicely scaled for all layers!

For conv layers, Din is filter_size^2 * input_channels

Let: $y = x_1w_1+x_2w_2+...+x_{Din}w_{Din}$

Assume: $Var(x_1) = Var(x_2)= ...=Var(x_{Din})$

We want: $Var(y) = Var(x_i)$

$$Var(y) = Var(x_1w_1+x_2w_2+...+x_{Din}w_{Din})$$
$$= Din\ Var(x_iw_i)$$
$$= Din\ Var(x_i)\ Var(w_i)$$

[Assume all x_i, w_i are iid]

So, $Var(y) = Var(x_i)$ only when $Var(w_i) = 1/Din$

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

Weight Initialization: What about ReLU?

```
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hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) / np.sqrt(Din)
    x = np.maximum(0, x.dot(W))
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```

Change from tanh to ReLU

Weight Initialization: What about ReLU?

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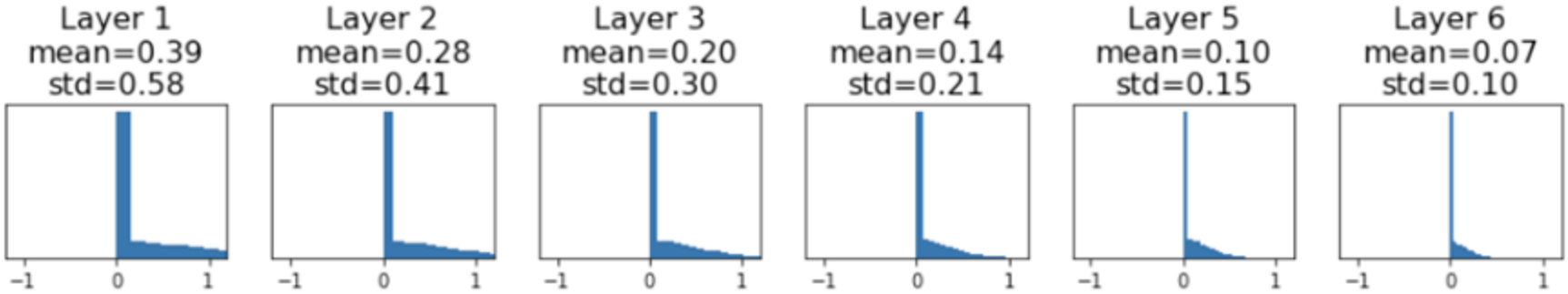
```

Change from tanh to ReLU

Xavier assumes zero centered activation function



Visualize distribution of activations

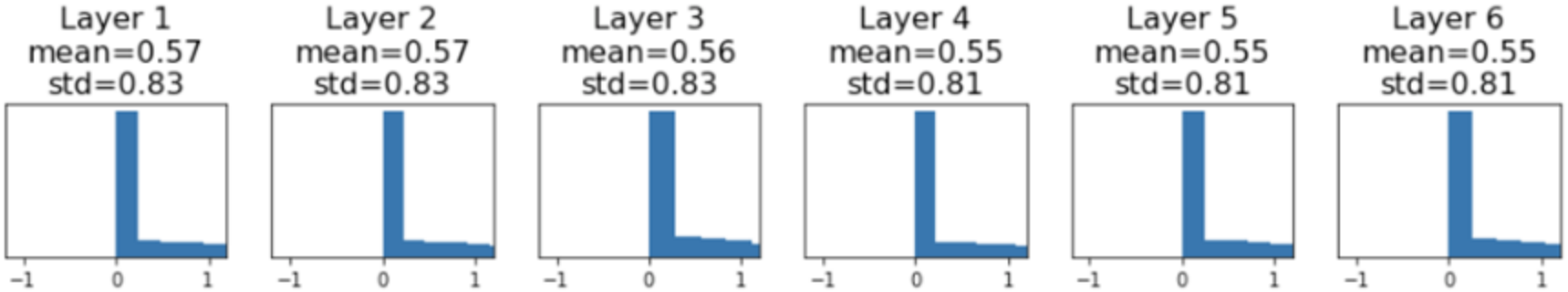
Weight Initialization: Kaiming / MSRA Initialization

```
dims = [4096] * 7
hs = []
x = np.random.randn(16, dims[0])
for Din, Dout in zip(dims[:-1], dims[1:]):
    W = np.random.randn(Din, Dout) * np.sqrt(2/Din)
    x = np.maximum(0, x.dot(W))
    hs.append(x)
```

ReLU correction: std = sqrt(2 / Din)

Issue: Half of the activation get killed.

Solution: make the non-zero output variance twice as large as input



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

Visualize distribution of activations

Proper initialization is still an active area of research…

Understanding the difficulty of training deep feedforward neural networks
by Glorot and Bengio, 2010

Exact solutions to the nonlinear dynamics of learning in deep linear neural networks by Saxe et al, 2013

Random walk initialization for training very deep feedforward networks by Sussillo and Abbott, 2014

Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification by He et al., 2015

Data-dependent Initializations of Convolutional Neural Networks by Krähenbühl et al., 2015

All you need is a good init, Mishkin and Matas, 2015

Fixup Initialization: Residual Learning Without Normalization, Zhang et al, 2019

The Lottery Ticket Hypothesis: Finding Sparse, Trainable Neural Networks, Frankle and Carbin, 2019

(Fancier) Optimizers

Optimization: (Stochastic) Gradient Descent

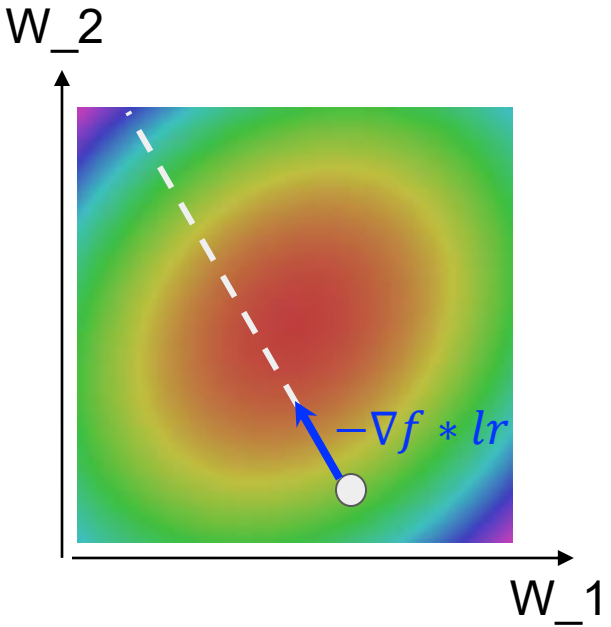
(Batch) Gradient Descent

```
While True:
    loss = model.compute_loss(dataset)
    loss.backward()
    model.weights -= model.weights.grad * lr
```

Dataset may be really large (millions of images)!

Minibatch (Stochastic) Gradient Descent

```
While True:
    minibatch = sample(dataset, batch_size)
    loss = model.compute_loss(minibatch)
    loss.backward()
    model.weights -= model.weights.grad * lr
```



Optimization: (Stochastic) Gradient Descent

Minibatch (Stochastic) Gradient Descent

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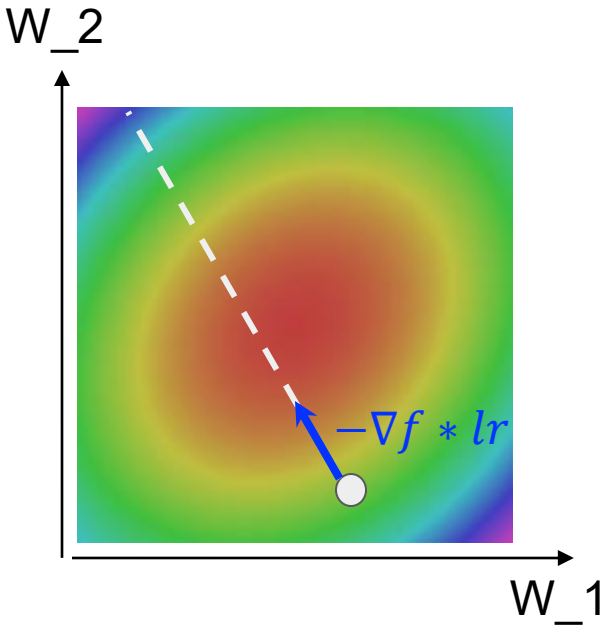
Reasons to prefer SGD over GD for Deep Learning:

- More computationally-tractable
- GD doesn't guarantee optimality for non-convex functions anyways



Optimization: (Stochastic) Gradient Descent

Minibatch (Stochastic) Gradient Descent

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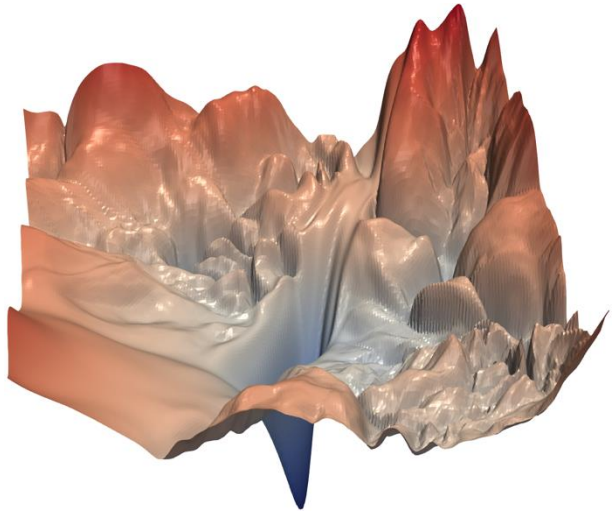
Reasons to prefer SGD over GD for Deep Learning:

- More computationally-tractable
- GD doesn't guarantee optimality for non-convex functions anyways
- SGD usually has faster convergence in wall-clock time, even if you can run GD



Loss landscape for DNN

https://www.cs.umd.edu/~tomg/projects/landscapes/

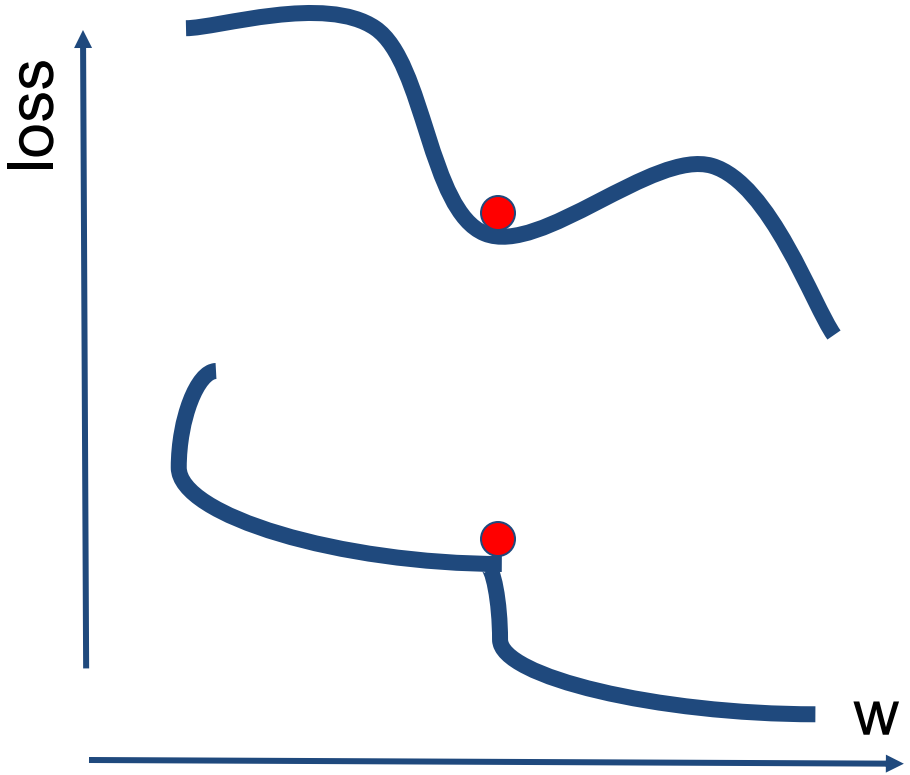
Optimization: Problem #1 with SGD

- Stochastic minibatch gives a **noisy estimate of the true gradient direction**. Approximates dataset gradient if batch is *large enough*.
- Very problematic when the batch size is small (e.g., due to compute resource limit).
- Poorly-selected learning rate makes the oscillation worse (overshoot)

http://web.cs.ucla.edu/~chohsieh/teaching/CS260_Winter2019/lecture4.pdf

Optimization: Problem #2 with SGD

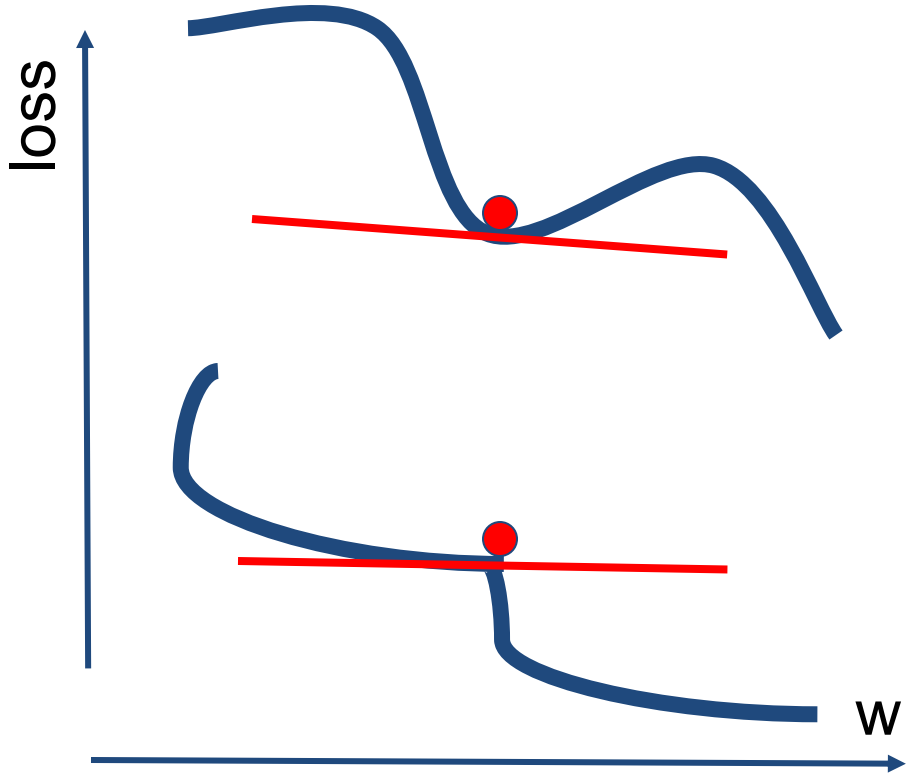
What if the loss function has a **local minima** or **saddle point**?



Optimization: Problem #2 with SGD

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

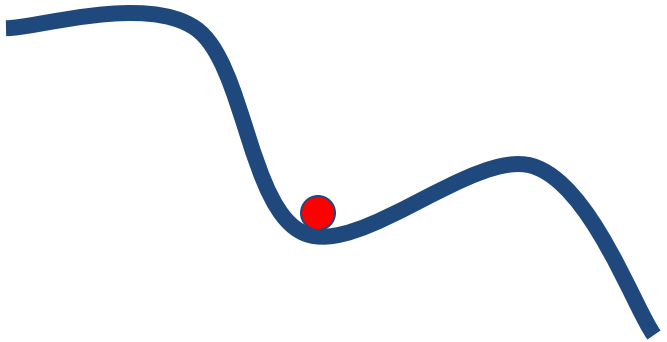
Zero gradient, gradient descent gets stuck

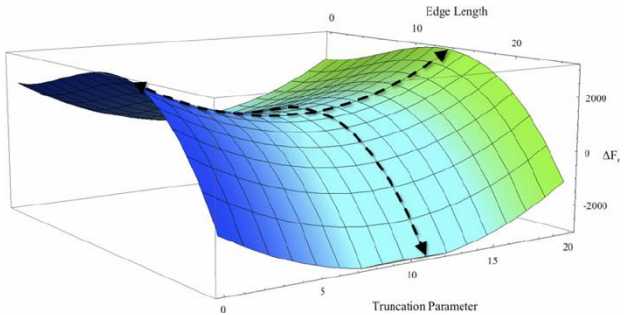


Optimization: Problem #2 with SGD

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

Saddle points are much more common in high dimension





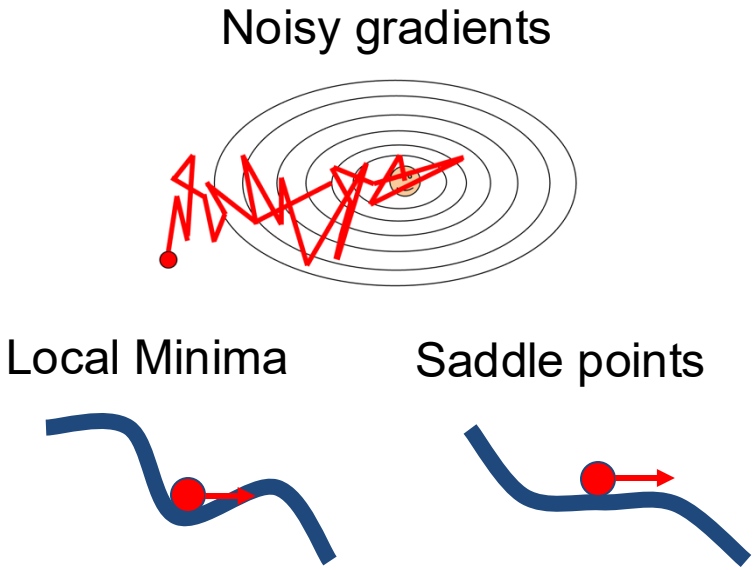
https://blog.paperspace.com/intro-to-optimization-in-deep-learning-gradient-descent/

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

SGD + Momentum

Intuitions:

- Think of a ball (set of parameters) moving in space (loss landscape), with momentum keeping it going in a direction.
- Individual gradient step may be noisy, the general trend accumulated over a few steps will point to the right direction.
- Momentum can “push” the ball over saddle points or local minima.



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

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

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

SGD+Momentum

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

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

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

- Build up “velocity/momentum” 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:

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

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

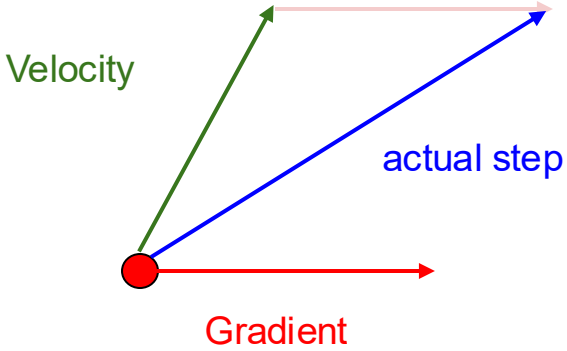
```
vx = 0
while True:
  dx = compute_gradient(x)
  vx = rho * vx + dx
  x -= learning_rate * vx
```

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:

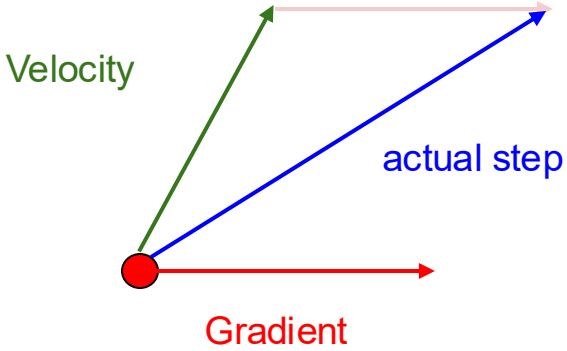


Combine gradient at current point with velocity to get step used to update weights

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

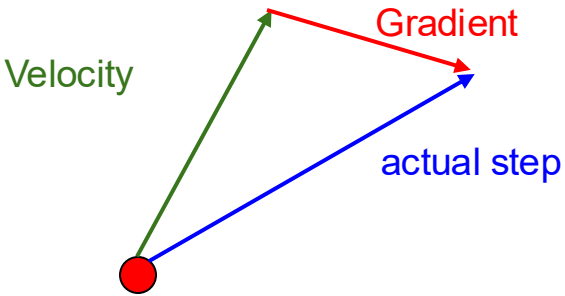
Nesterov Momentum

Momentum update:



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

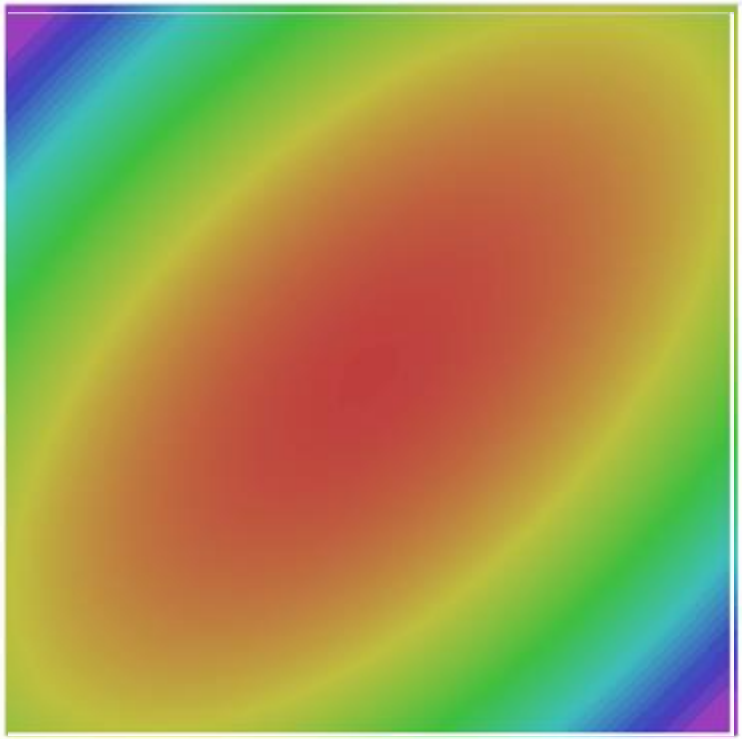
Nesterov Momentum



"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
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



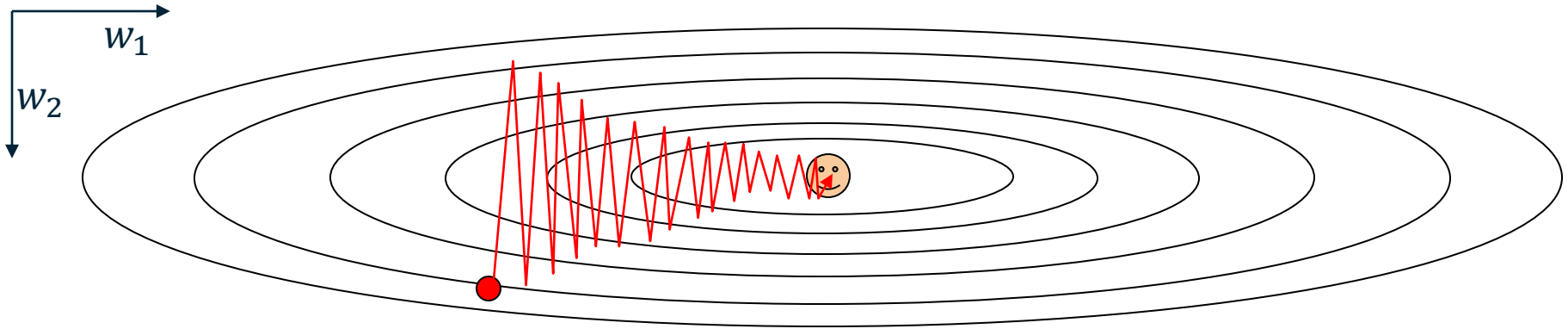
SGD

SGD+Momentum

Nesterov

Optimization: Problem #3 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



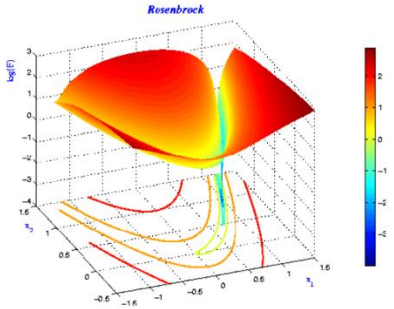
Assume each contour line has the same loss
(iso-loss contour)

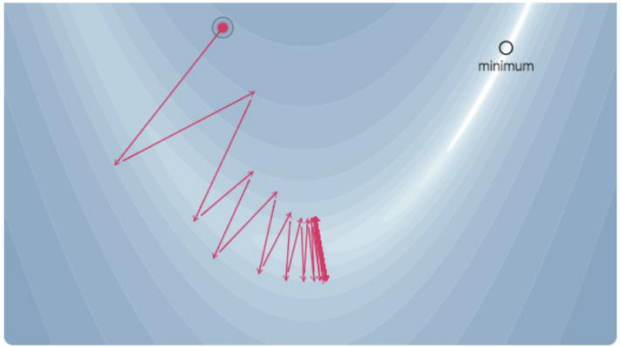
Optimization: Problem #3 with SGD

What if loss changes quickly in one direction and slowly in another?

Very slow progress along shallow dimension, jitter along steep direction

Long, narrow ravines:





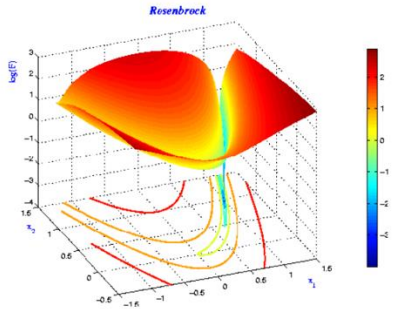
https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec07.pdf

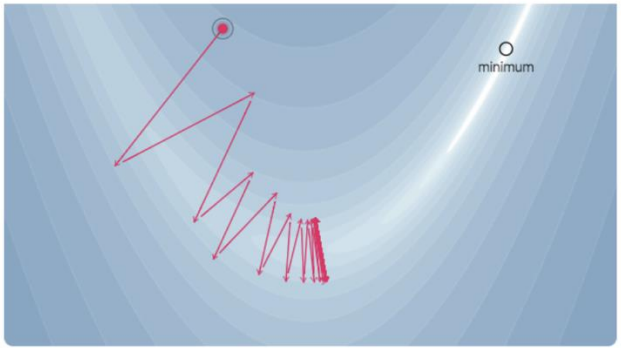
Optimization: Problem #3 with SGD

What if loss changes quickly in one direction and slowly in another?

Very slow progress along shallow dimension, jitter along steep direction

Long, narrow ravines:





https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec07.pdf

Loss function has high **condition number**: ratio of largest to smallest eigen value ($\lambda_{max}/\lambda_{min}$) of the Hessian matrix of a loss function is large

Small condition number in loss Hessian -> circular contour

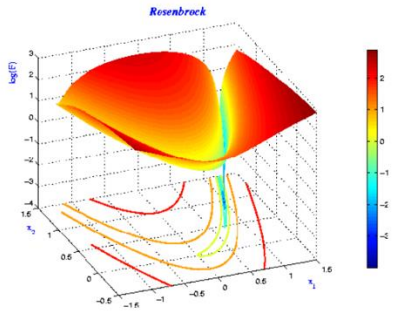
Large condition number in loss Hessian -> skewed contour

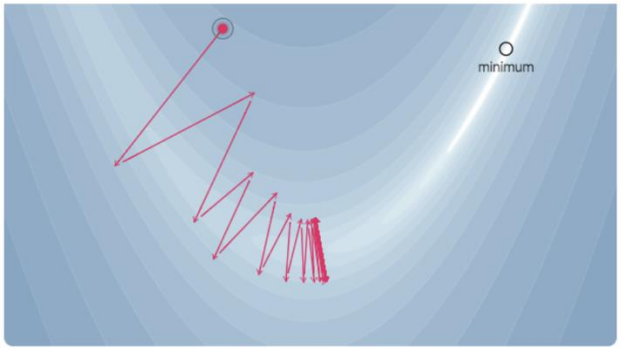
Optimization: Problem #3 with SGD

What if loss changes quickly in one direction and slowly in another?

Very slow progress along shallow dimension, jitter along steep direction

Long, narrow ravines:





https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec07.pdf

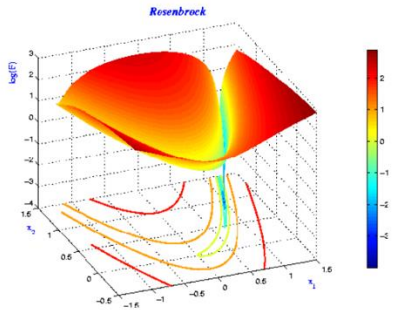
Q: What's the simplest solution to this problem?

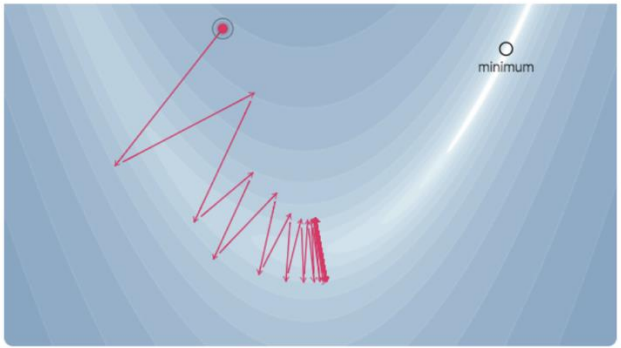
Optimization: Problem #3 with SGD

What if loss changes quickly in one direction and slowly in another?

Very slow progress along shallow dimension, jitter along steep direction

Long, narrow ravines:





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Q: What's the simplest solution to this problem?

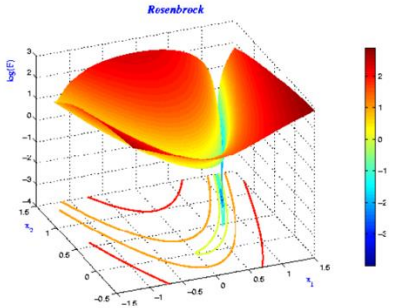
A: Pick a different learning rate for each direction! E.g., lower the learning rate for fast-changing directions

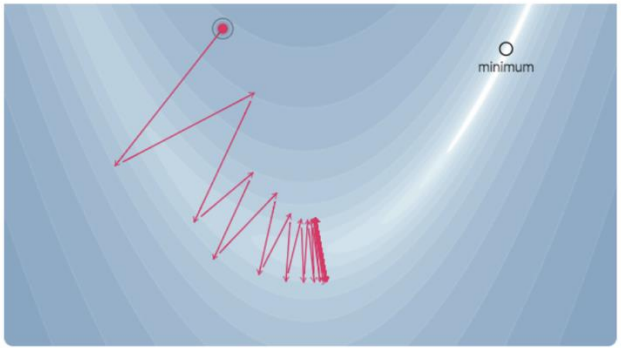
Optimization: Problem #3 with SGD

What if loss changes quickly in one direction and slowly in another?

Very slow progress along shallow dimension, jitter along steep direction

Long, narrow ravines:





https://www.cs.toronto.edu/~rgrosse/courses/csc421_2019/slides/lec07.pdf

Q: What's the simplest solution to this problem?

A: Pick a different learning rate for each direction! E.g., lower the learning rate for fast-changing directions

But manually picking an optimal LR for each weight dimension seems hard …

AdaGrad

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

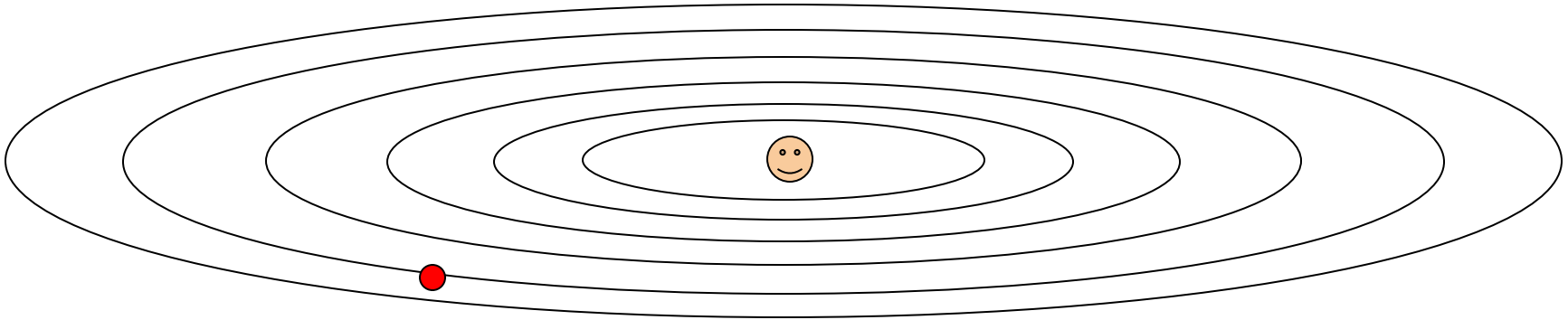
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

“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)
```

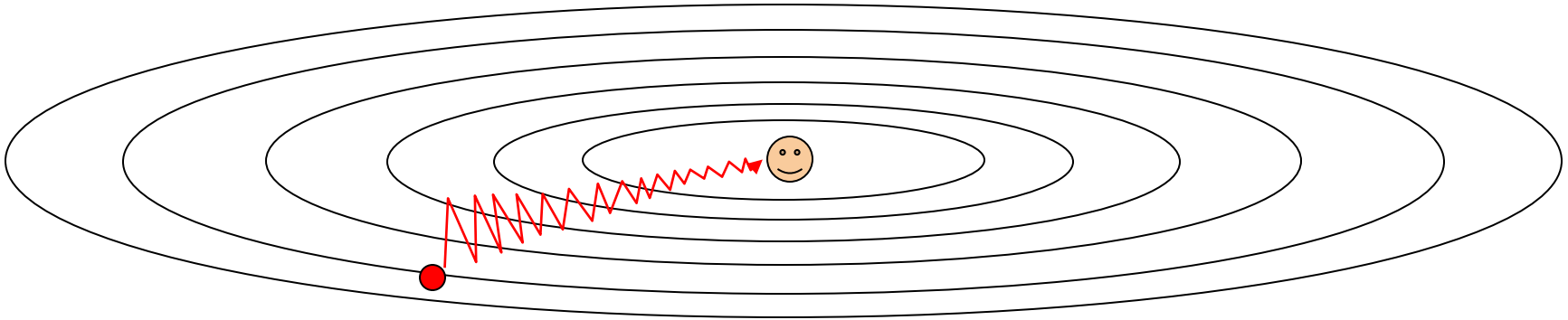


Q: What happens with AdaGrad?

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)
```



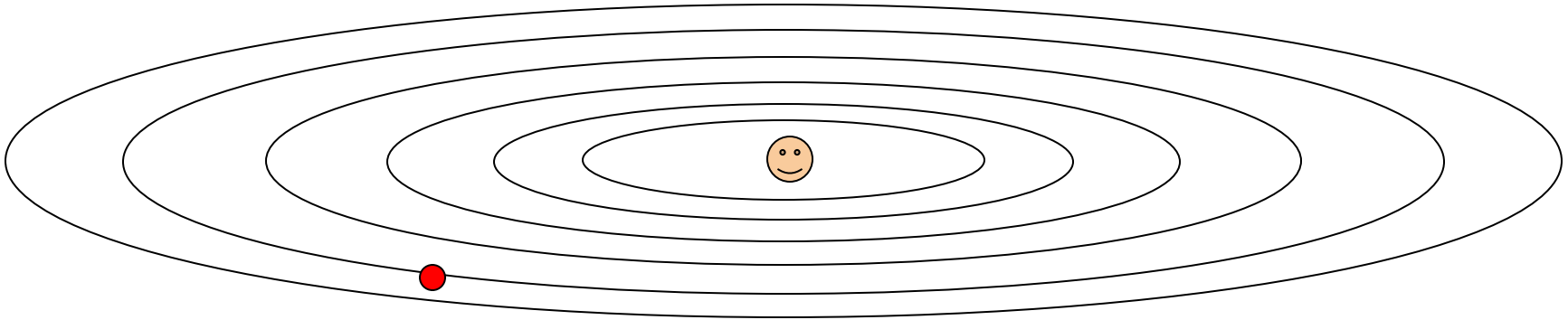
Q: What happens with AdaGrad?

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

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)
```

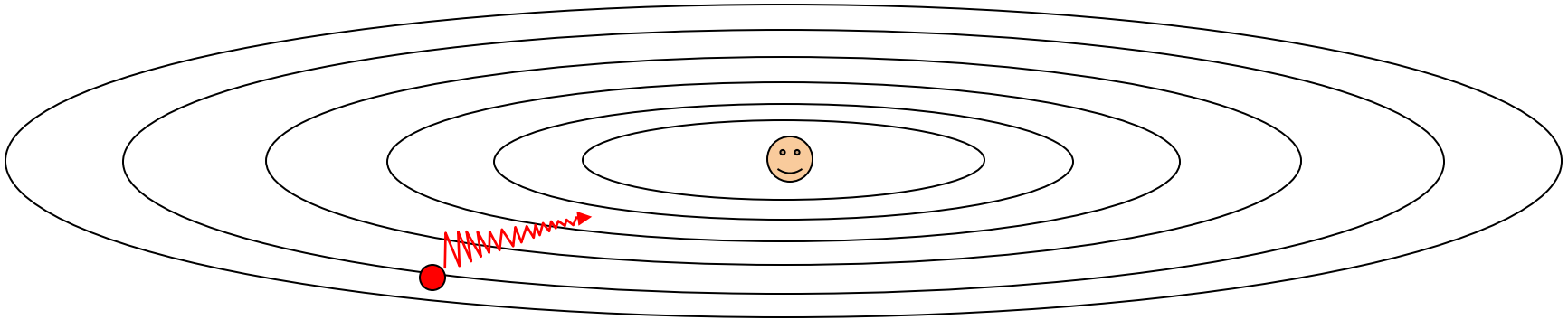


Q2: What happens to the step size over long time?

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)
```



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

Reduces to zero ☹

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

RMSProp: “Leaky AdaGrad”

AdaGrad

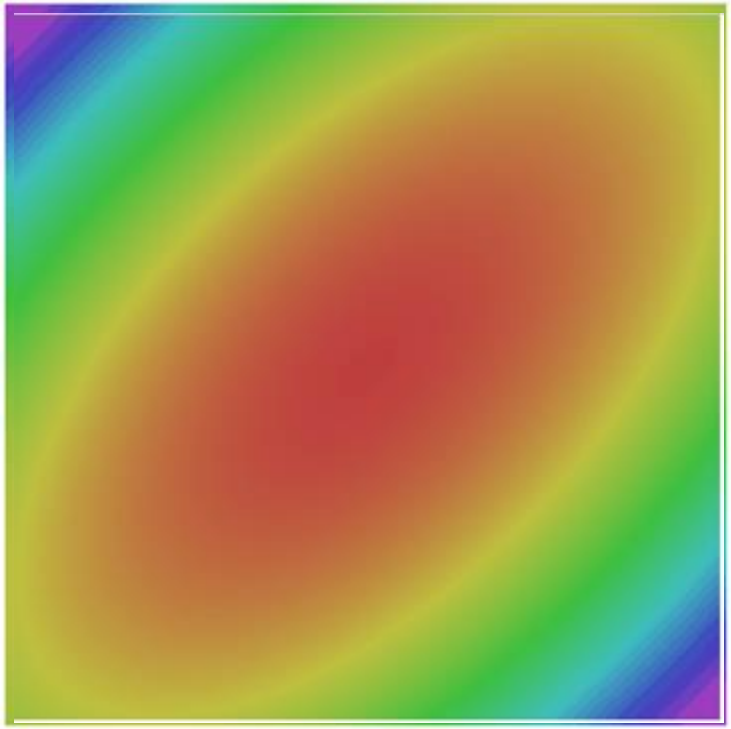
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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))
```

Typical hyperparams: beta1=0.9, beta2=0.999

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

Typical hyperparams: beta1=0.9, beta2=0.999

Sort of like RMSProp with momentum

Q: What happens at first timestep?

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

Typical hyperparams: beta1=0.9, beta2=0.999

Small -> divide by small number -> bad initial step

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

Typical hyperparams: beta1=0.9, beta2=0.999

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

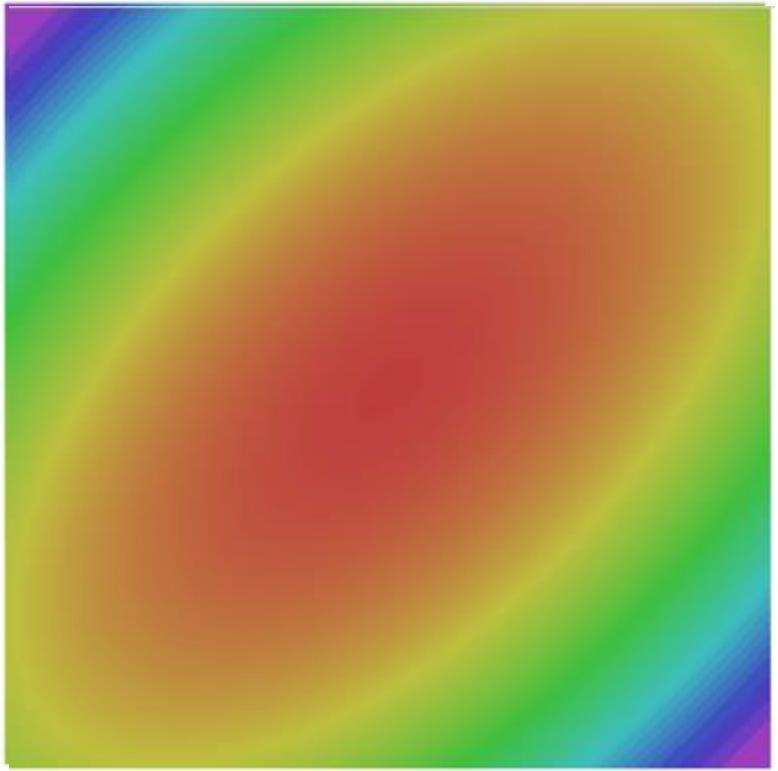
Typical hyperparams: beta1=0.9, beta2=0.999

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

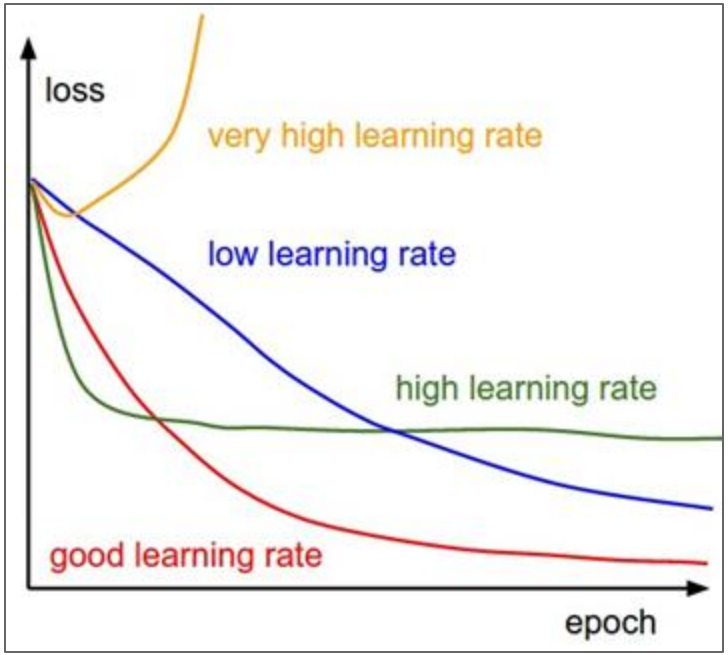
SGD+Momentum

RMSProp

Adam

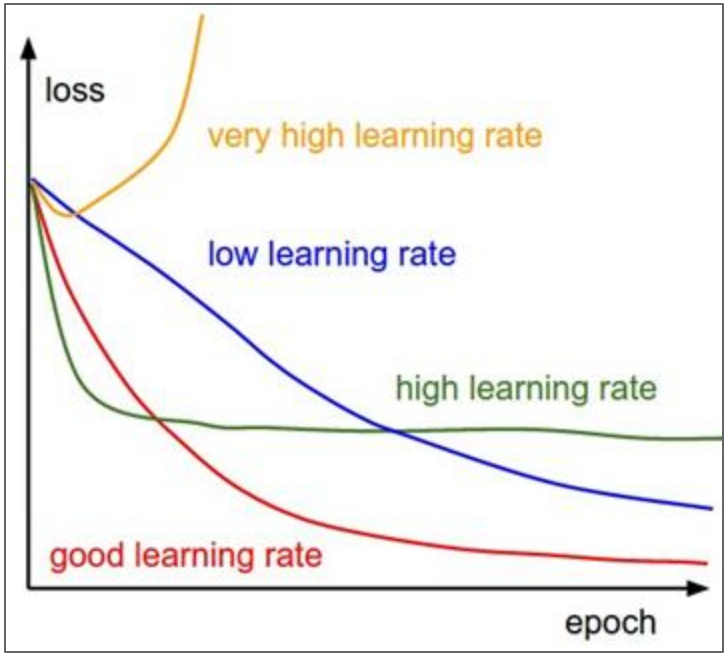
Learning rate schedules

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.

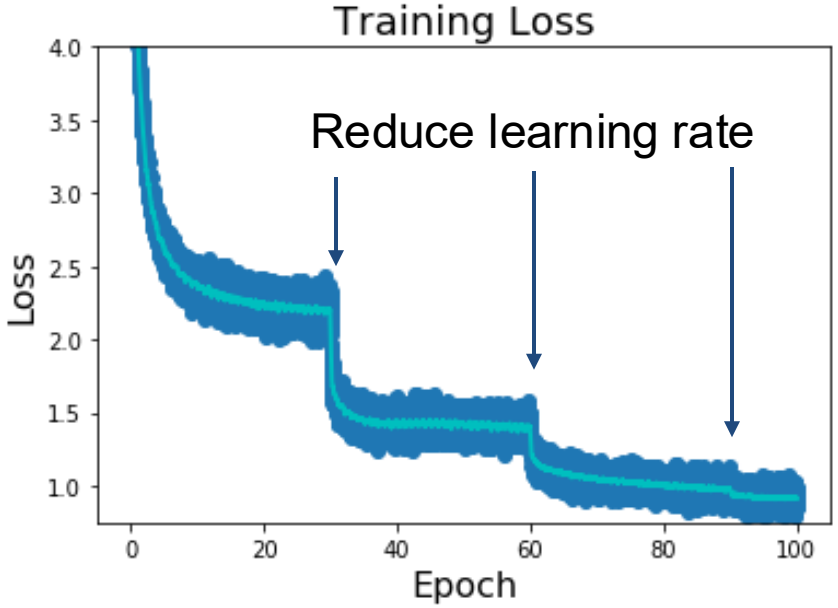


Q: Which one of these learning rates is best to use?

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

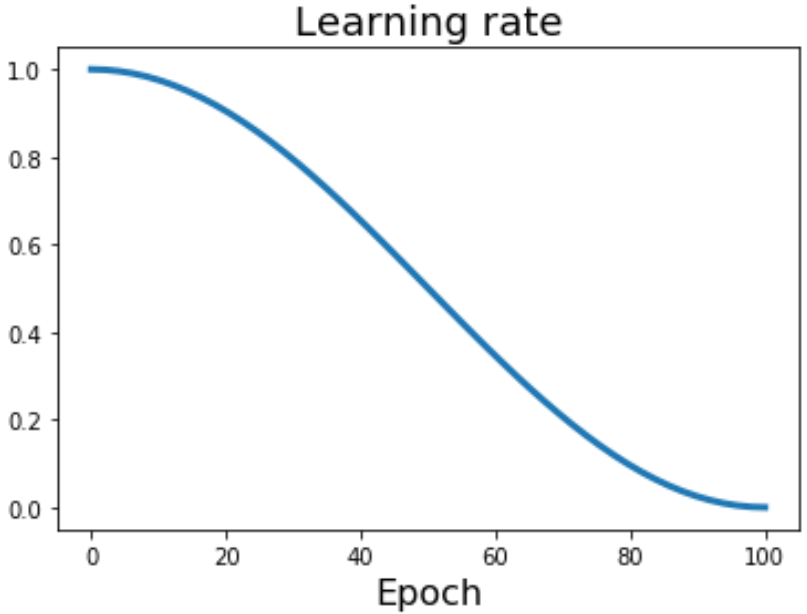
Need finer adjustment closer to convergence, so we want to reduce learning rate over time to keep making progress.

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



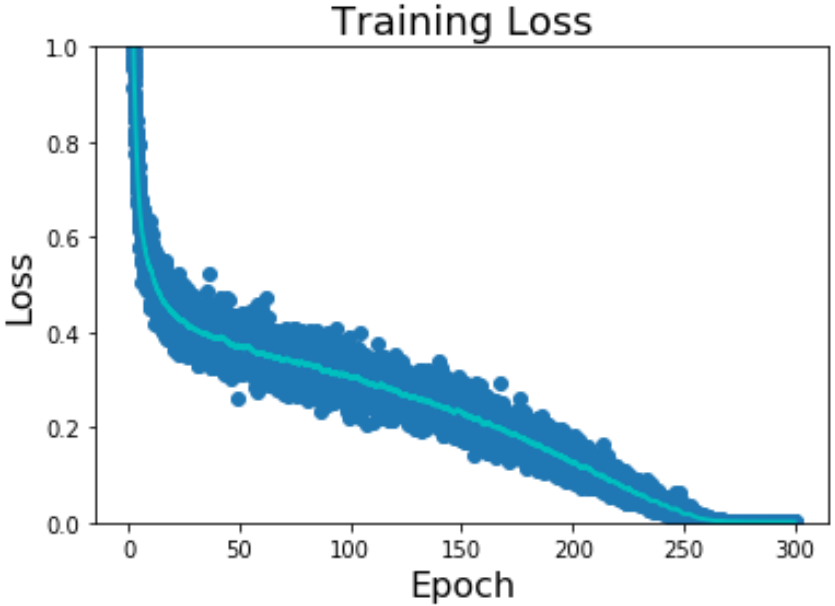
Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

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

α_0 : Initial learning rate
α_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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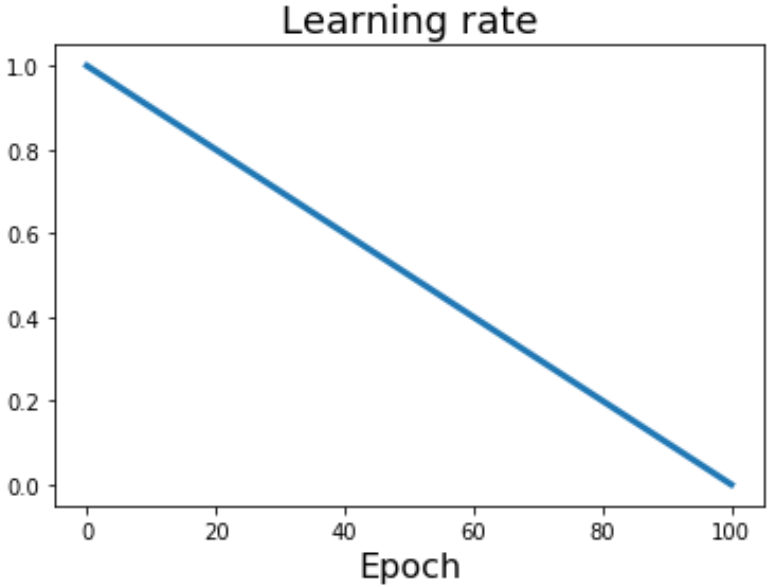
Child at al, “Generating Long Sequences with Sparse Transformers”, arXiv 2019

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.

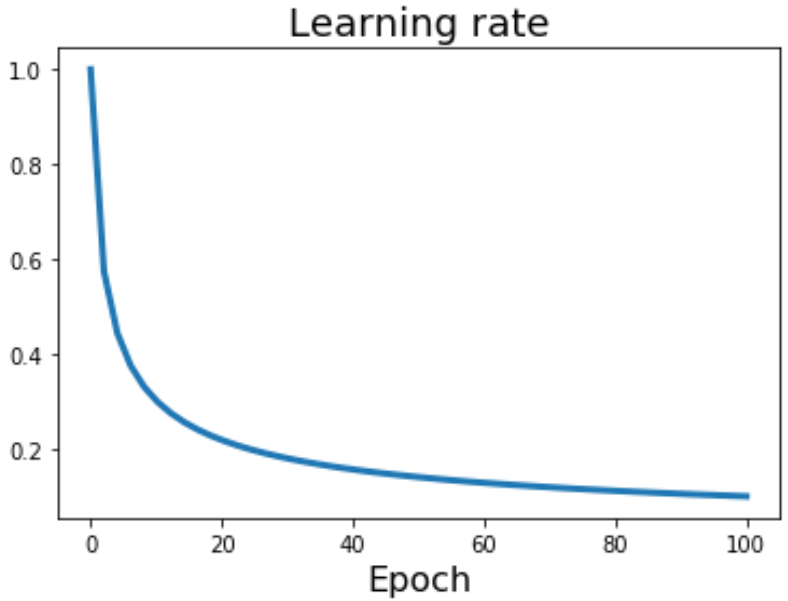
Cosine: $\alpha_t = \frac{1}{2}\alpha_0 \left(1 + \cos(t\pi/T)\right)$

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

α_0 : Initial learning rate
α_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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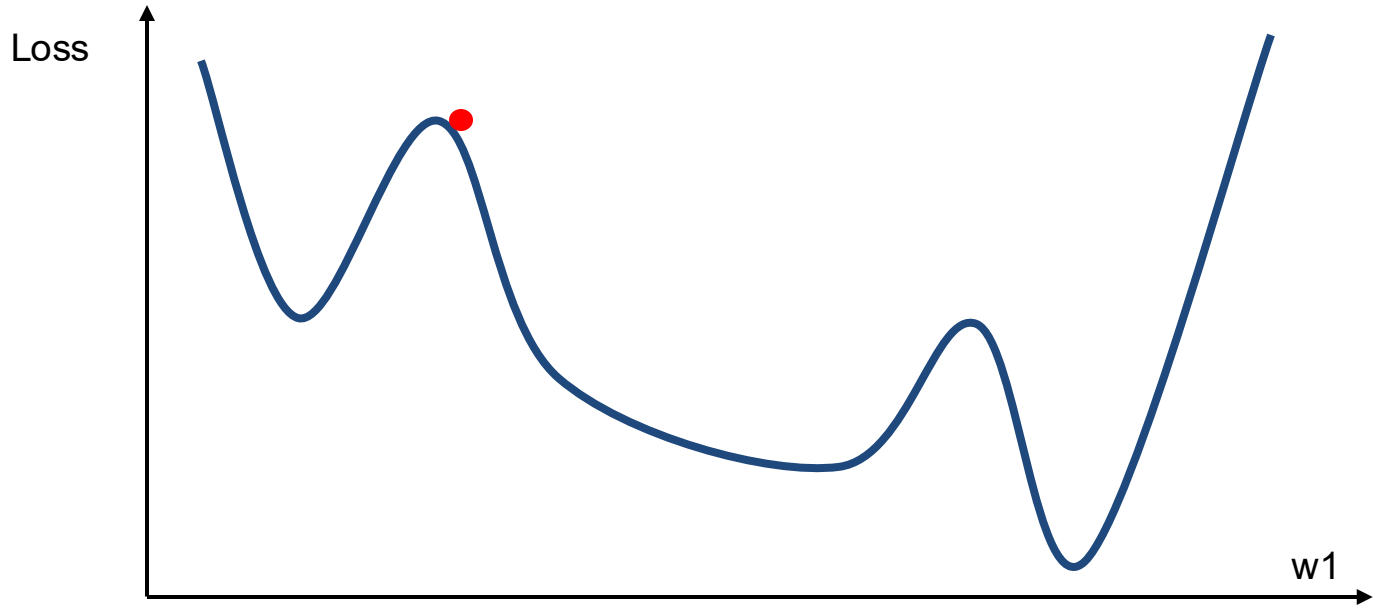
Linear: $\alpha_t = \alpha_0(1 - t/T)$

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

α_0 : Initial learning rate
α_t : Learning rate at epoch t
T : Total number of epochs

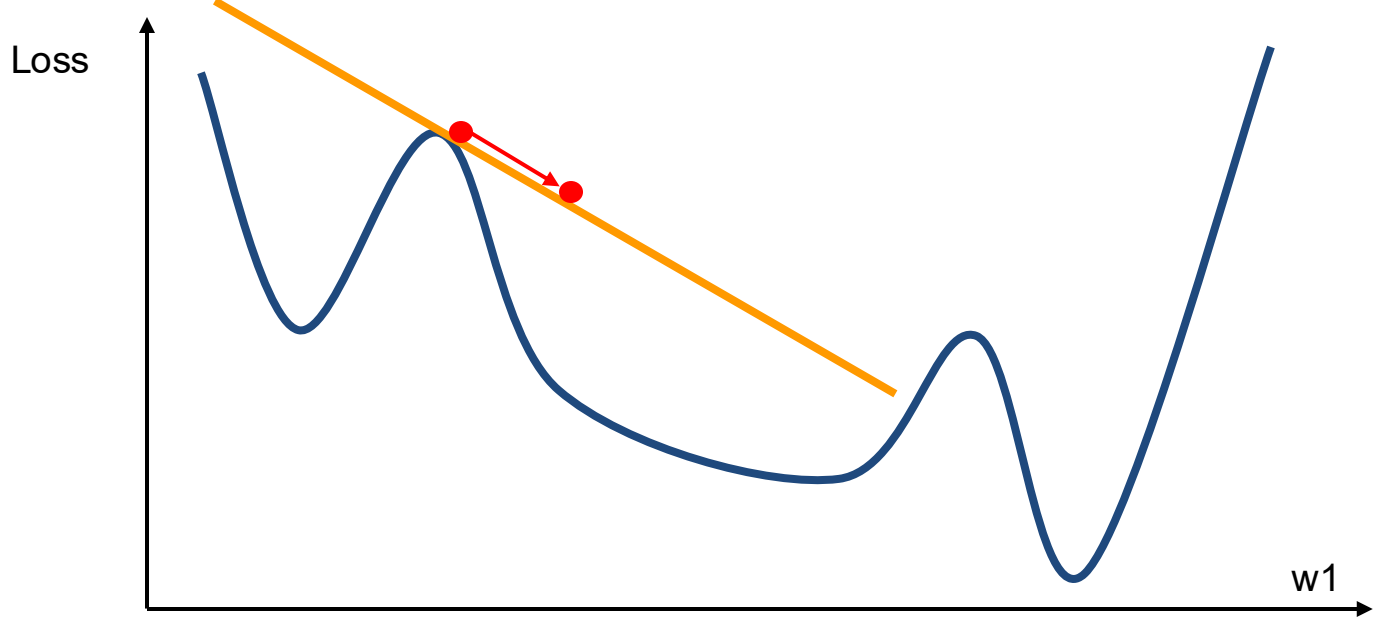
Vaswani et al, “Attention is all you need”, NIPS 2017

First-Order Optimization



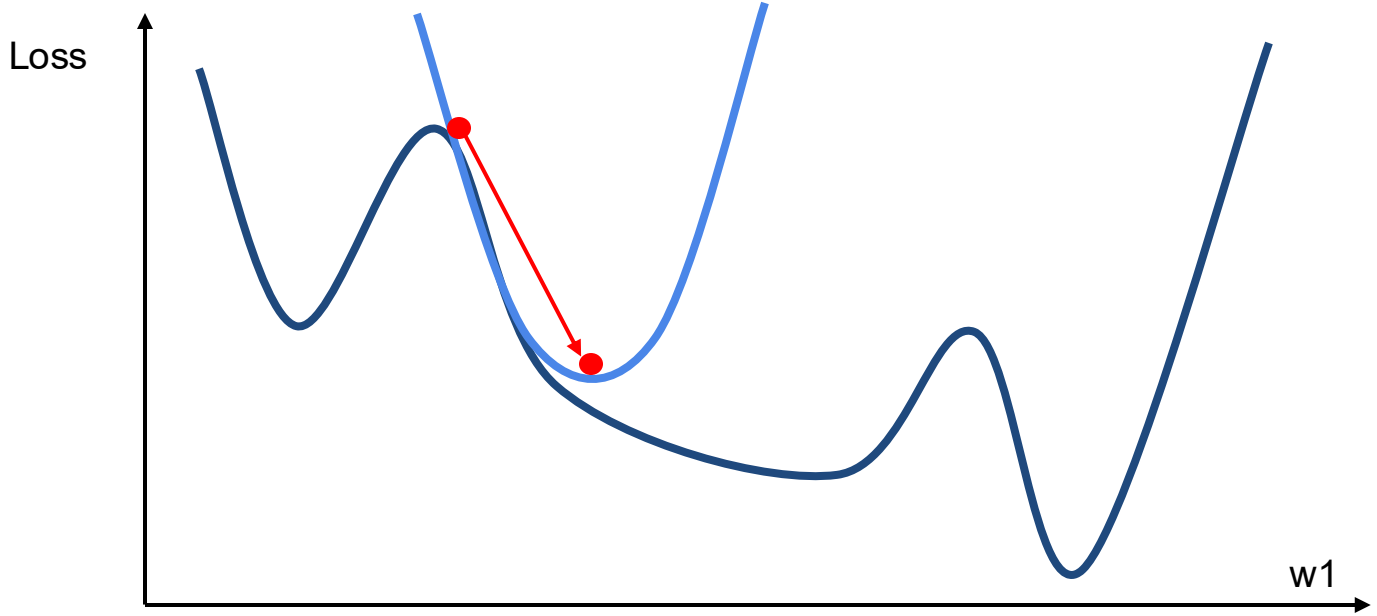
First-Order Optimization

(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

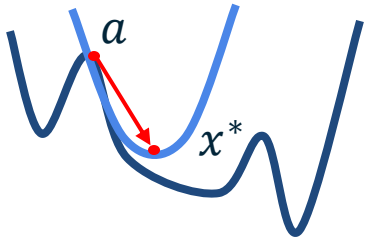
second-order Taylor Expansion of $f(x)$ at a:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2$$

Newton's method for optimization: solving for the critical point $f'(x) = 0$, we obtain the Newton update rule

$$f'(x) = f'(a) + f''(a)(x-a) = 0$$

$$x^* = a - \frac{1}{f''(a)} f'(a)$$



Think of a as the current params, x^* as the updated params

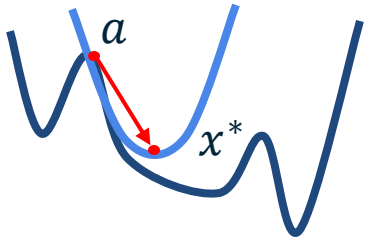
Second-Order Optimization (multivariate)

second-order Taylor Expansion of $f(\boldsymbol{x})$ at $\boldsymbol{a}$:

$$f(w) = f(\boldsymbol{a}) + (\boldsymbol{x} - \boldsymbol{a})^T \nabla f \; + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{a})^T H(\boldsymbol{x} - \boldsymbol{a})$$

Newton's method for optimization: solving for the critical point we obtain the Newton update rule:

$$\boldsymbol{x}^* = \boldsymbol{a} - H^{-1} \nabla f$$



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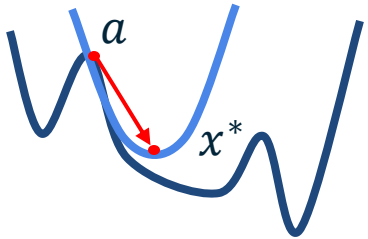


Q: Why is this unsuitable for deep learning?

Hessian Matrix

$$\mathbf{H}_f = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \dfrac{\partial^2 f}{\partial x_2\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \dfrac{\partial^2 f}{\partial x_n\,\partial x_1} & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

N

N

Second-Order Optimization

second-order Taylor expansion:

$$f(\boldsymbol{x}) = f(\boldsymbol{a}) + (x-a)^T \nabla f \; + \frac{1}{2}(x-a)^T H (x-a)$$

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

$$x^* = a - H^{-1} \nabla f$$

Q: Why is this unsuitable for deep learning?

Hessian has O(N^2) elements for N->1 functions
Inverting takes O(N^3), N = Millions

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

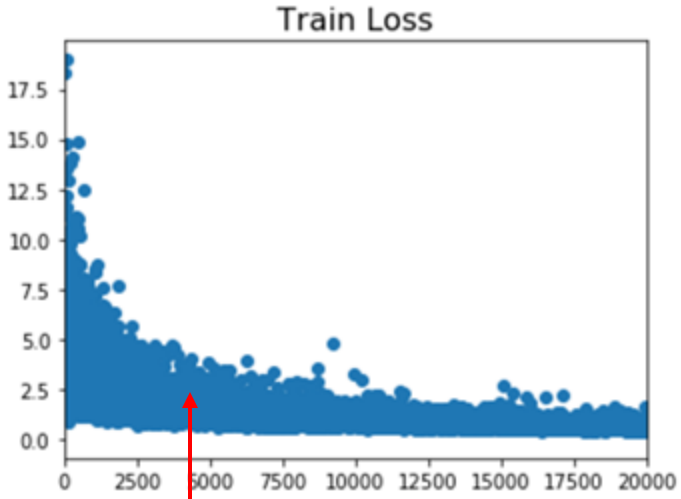
In practice:

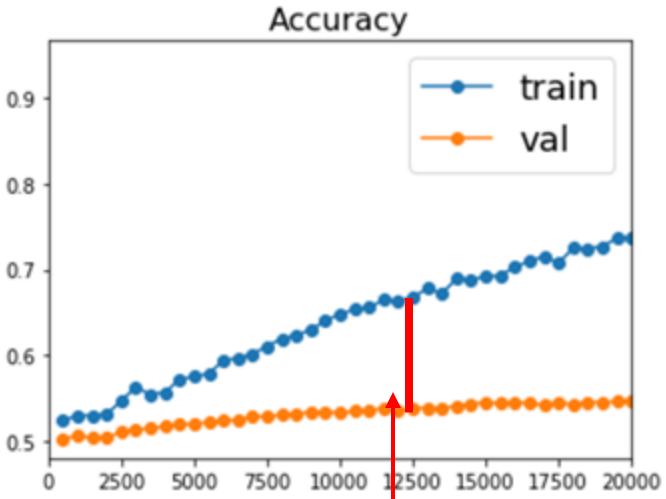
- **Adam** and its minor variants are good default choices in many cases; it often works ok even with constant learning rate
- **SGD+Momentum** can outperform Adam but may require more tuning of LR and schedule
  - Try cosine schedule, very few hyperparameters!

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

Regularization

Beyond Training Error

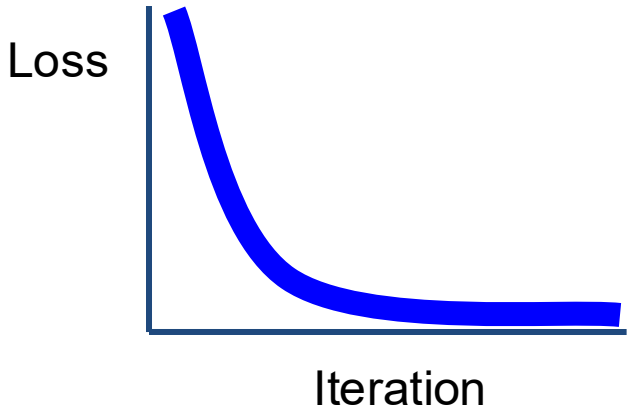


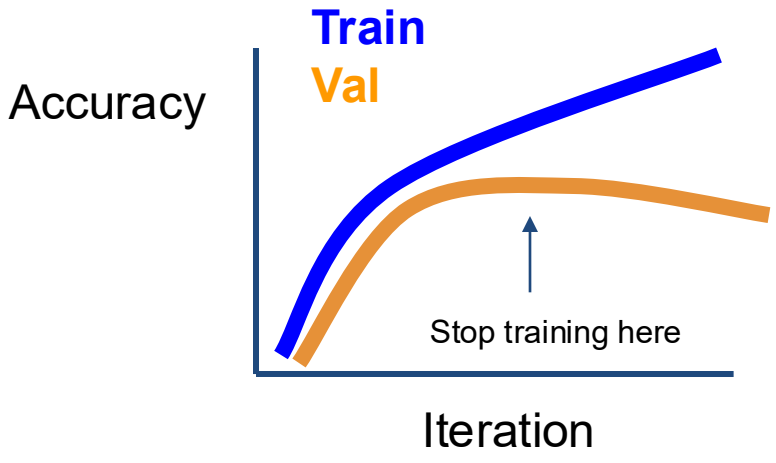


Better optimization algorithms help reduce training loss

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

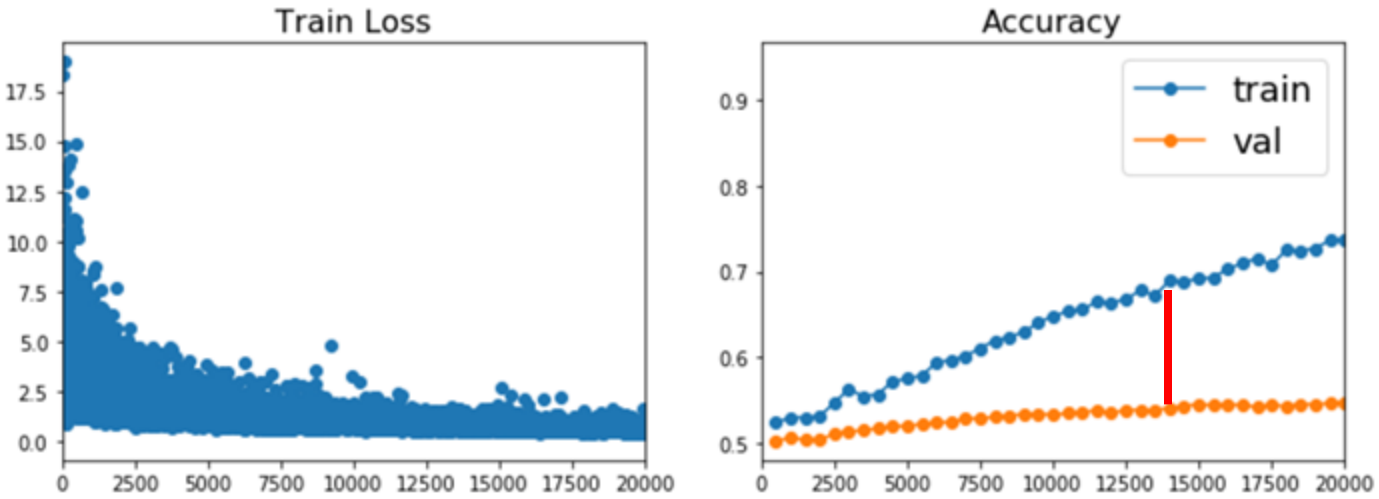
Early Stopping: Always do this





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

How to improve generalization?



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)

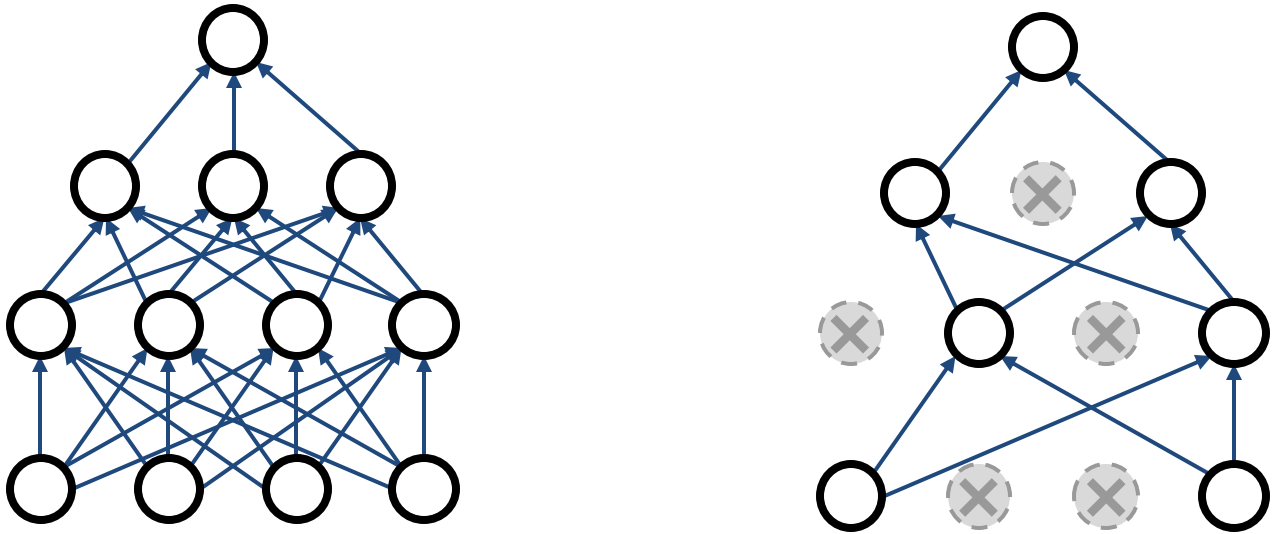
L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$

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

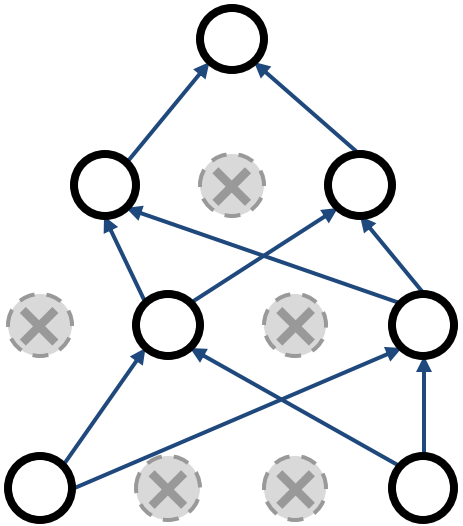
```
p = 0.5 # probability of keeping a unit active. higher = less dropout

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

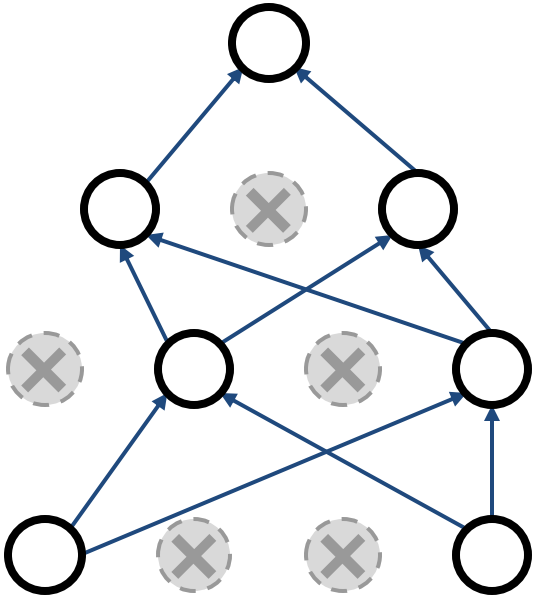
  # backward pass: compute gradients... (not shown)
  # perform parameter update... (not shown)
```

Example forward pass with a 3-layer network using dropout



Regularization: Dropout

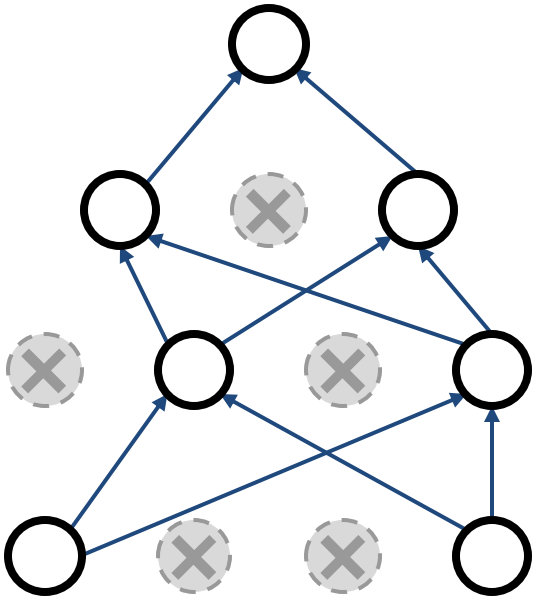
How can this possibly be a good idea?



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

Output (label)

Input (image)

Dropout makes our output random!

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

Random mask

Test-time behavior should be deterministic

Want to “average out” the randomness at test-time

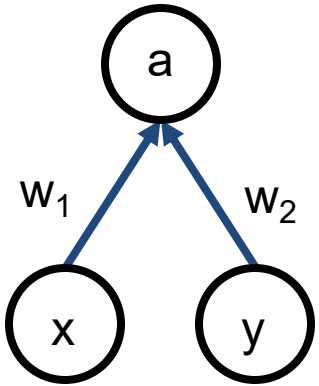
$$y = f(x) = E_z\left[f(x, z)\right] = \int p(z) f(x, z) dz$$

Dropout: Test time

Compute the expectation

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

Consider a single neuron.



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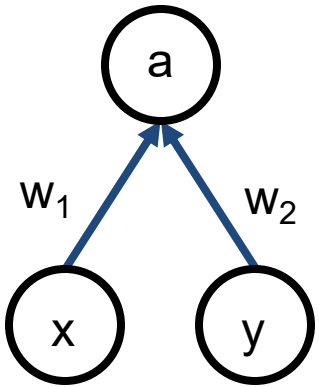


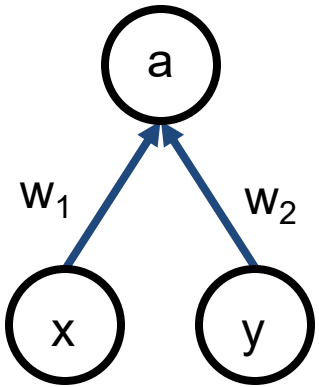
Consider a single neuron.

Without dropout: $E\big[a\big] = w_1 x + w_2 y$

Dropout: Test time

Compute the expectation

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



Consider a single neuron.

Without dropout: $E[a] = w_1 x + w_2 y$

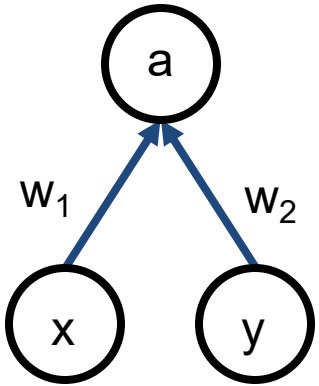
With dropout we have:

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

Dropout: Test time

Compute the expectation

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



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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:
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!

Similar to BatchNorm, different behavior train vs test!

Regularization: A common strategy

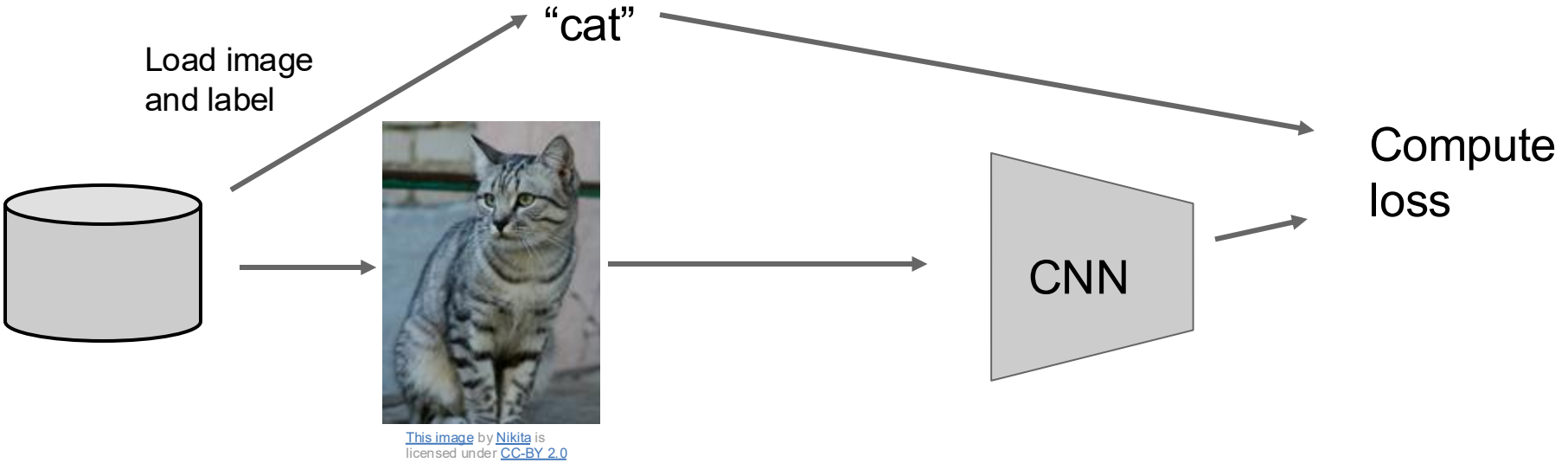
Training: Add some kind of randomness

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

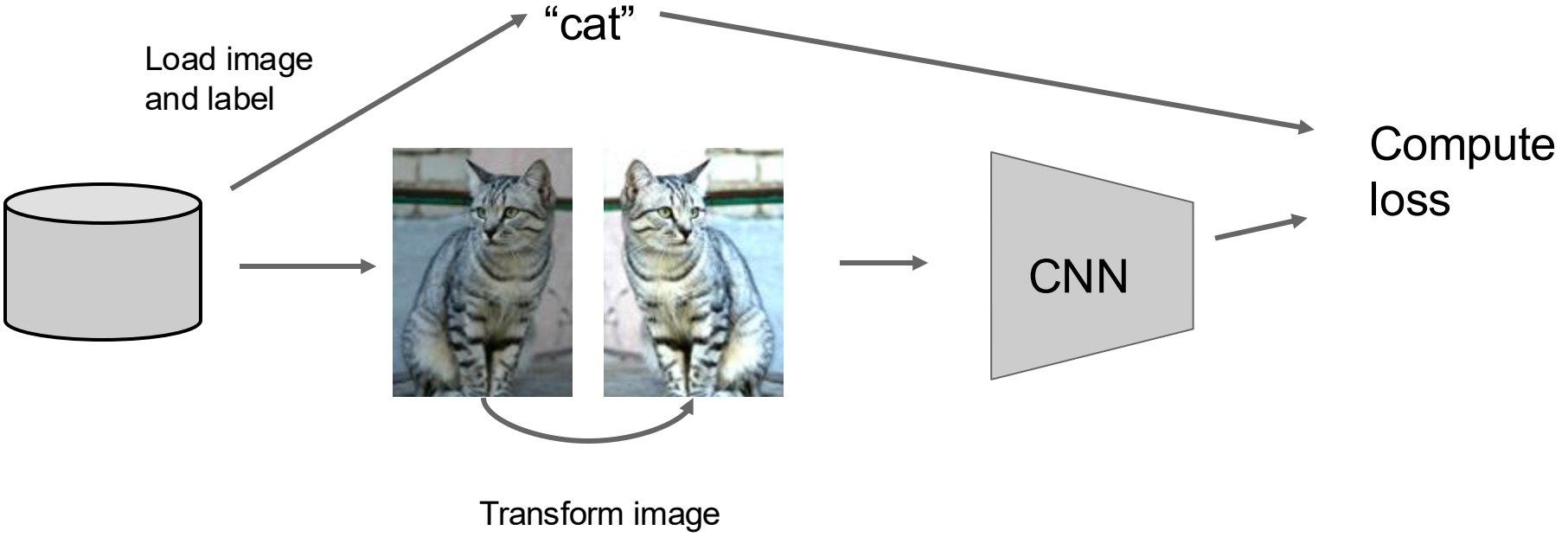
Testing: Average out randomness (sometimes approximate)

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

Regularization: Data Augmentation

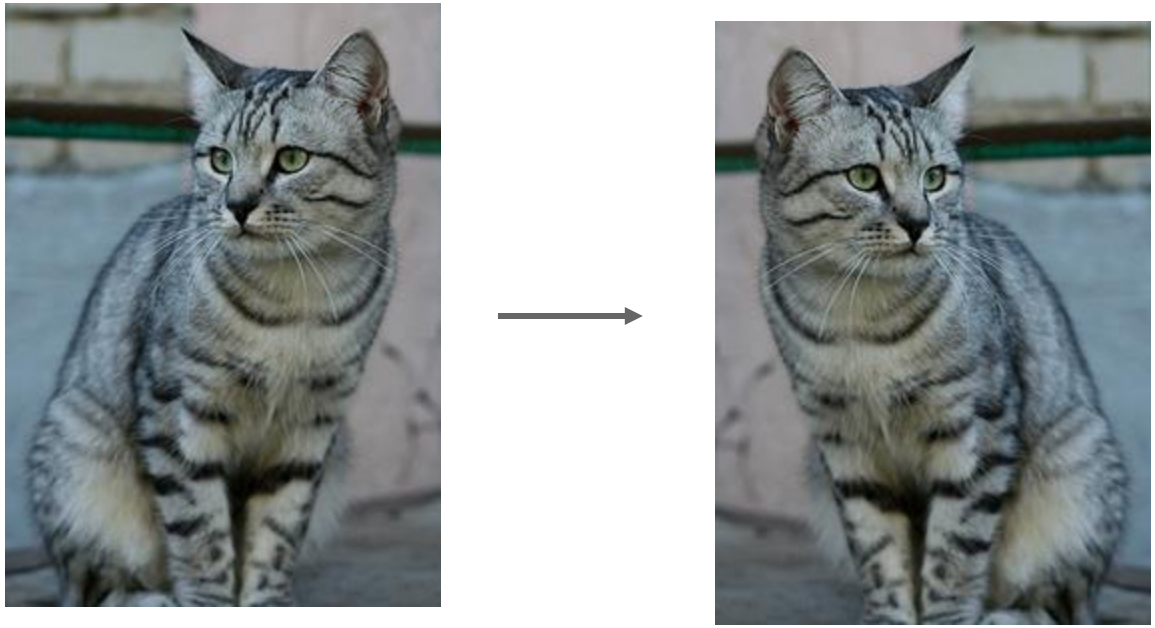


Regularization: Data Augmentation



Data Augmentation

Horizontal Flips



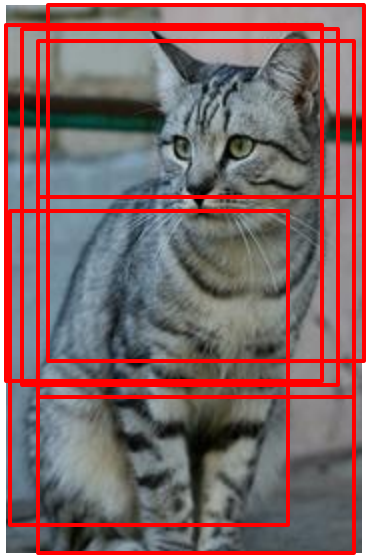
Data Augmentation

Random crops and scales

Training: sample random crops / scales

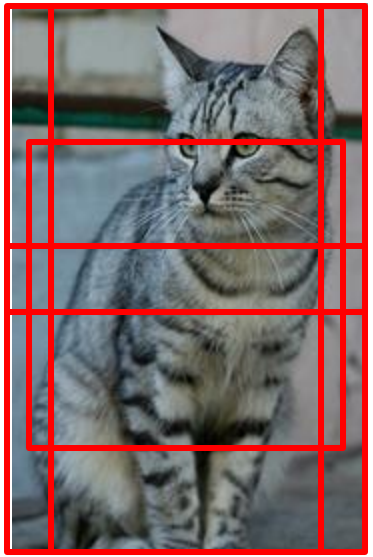
ResNet:

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 (test-time augmentation):

take votes / average from a fixed set of crops

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
3. Make prediction on all crops, use the majority vote as the final output.

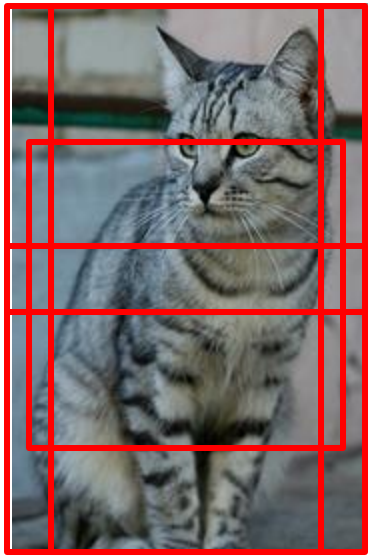
Data Augmentation

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 (deterministic):

- Take a center crop of 224 by 224.
- Or crop by longer dimension and resize.

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)

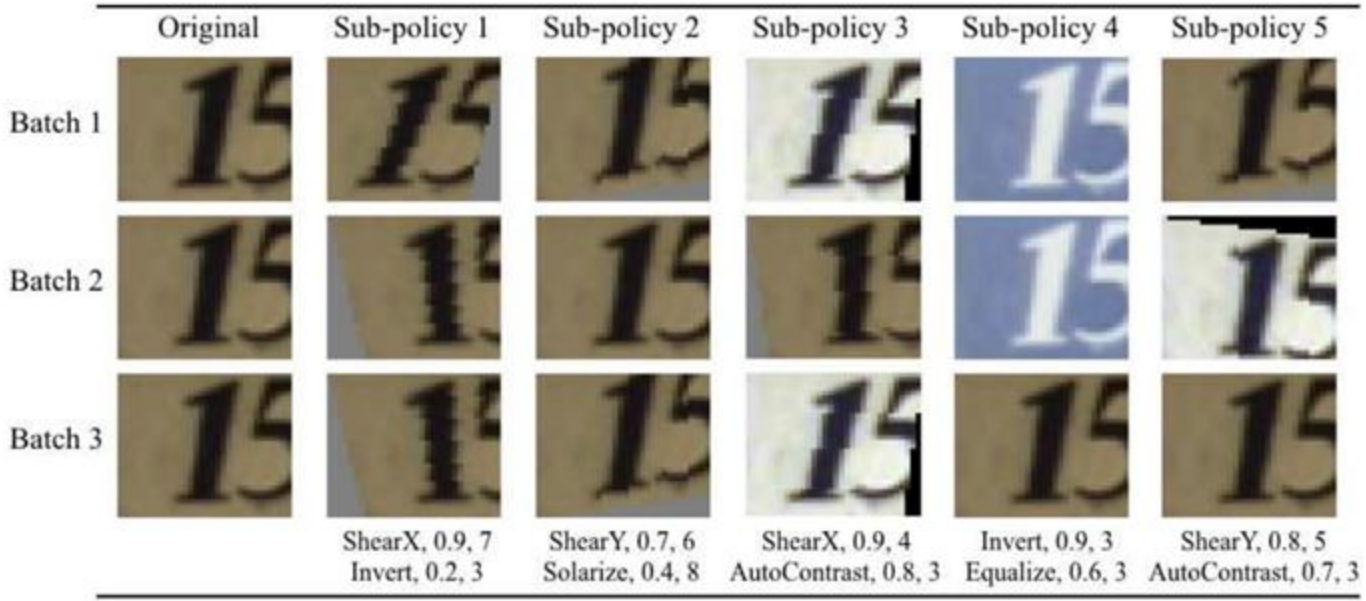
Data Augmentation

Get creative for your problem!

Examples of data augmentations:

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

Automatic Data Augmentation



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

Gradient clipping: prevent large gradient step

Large gradient step will likely destabilize training (gradients are noisy!)

Large gradient update can be caused by many issues, e.g., large weights, large input, bad loss function / activation function, …

Should always first try to fix the root cause (normalization, better loss / activation function, etc.)

But if all things fail … just clip the gradient

$$g_{new} = \min\left(1, \frac{\lambda}{||g||}\right) \times g$$

g: original gradient

λ: clipping threshold

If $||g|| \leq \lambda$, no effect

```
# Zero the gradients.
optimizer.zero_grad()

# Perform forward pass.
outputs = model(inputs)

# Compute the loss.
loss = loss_function(outputs, targets)

# Perform backward pass (compute gradients).
loss.backward()

# Clip the gradients.
torch.nn.utils.clip_grad_norm_(model.parameters(), max_norm=1.0)

# Update the model parameters.
optimizer.step()
```

Next Time:

Training Deep Neural Networks

- Details of the non-linear activation functions
- Data normalization
- Weight Initialization
- Batch Normalization
- Advanced Optimization
- Regularization
- Data Augmentation
- Transfer learning
- Hyperparameter Tuning
- Model Ensemble