

COMP541

DEEP LEARNING

Lecture #04 – Training Deep Neural Networks

MODE CONNECTIVITY

OPTIMA OF A LOSS FUNCTION CONNECTED BY SIMPLE CURVES OVER WHICH TRAINING AND ACCURACY ARE NEARLY CONSTANT

BASED ON THE WORK OF MURAT GARIPOV, PAVEL MELNIKOV, DMITRII VASILYENOK, YUAN ZHANG, JON WILSON

VISUALIZATION & ANALYSIS IS A COLLABORATION BETWEEN MURAT GARIPOV, PAVEL MELNIKOV, D. JAVIER IDEAMI javier@losslandscape.com

NeurIPS 2018, ARXIV:1802.10026 | LOSSLANDSCAPE.COM



KOÇ
UNIVERSITY

Aykut Erdem // Koç University // Fall 2023

0.16

2.8

3.0

3.2

MINIMA

MINIMA

0.15

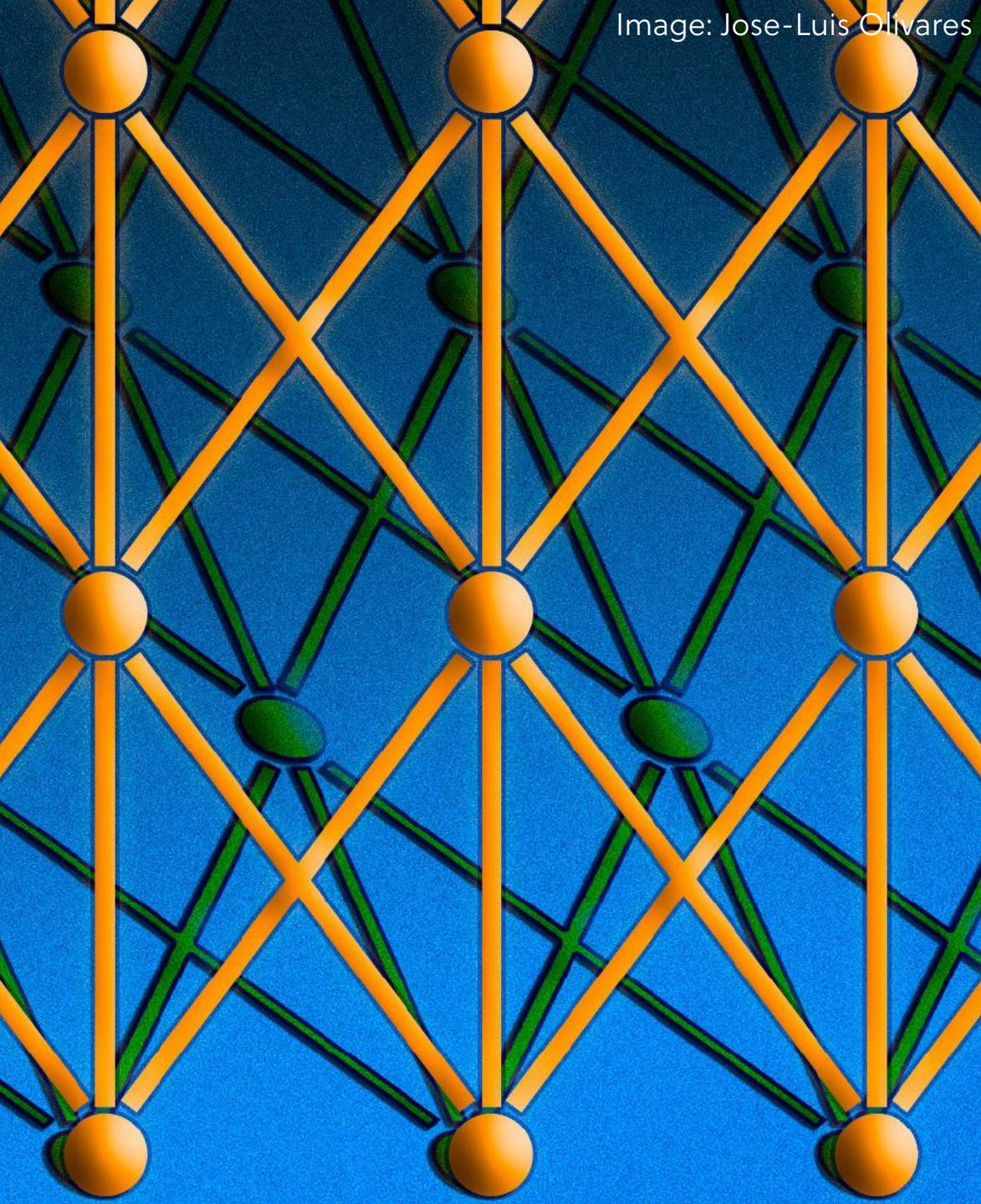
3.75

LOSS (TRAIN MODE)

REAL DATA, RESNET-20 NO-SKIP,
CIFAR10, SGD-MOM, BS=128
WD=3e-4, MOM=0.9
BN, TRAIN MOD, 90K PTS
LOG SCALED (ORIG LOSS NUMS)

Previously on COMP541

- multi-layer perceptrons
- activation functions
- chain rule
- backpropagation algorithm
- computational graph
- distributed word representations



Lecture overview

- data preprocessing and normalization
- weight initializations
- ways to improve generalization
- optimization
- babysitting the learning process
- hyperparameter selection

Disclaimer: Much of the material and slides for this lecture were borrowed from

- Fei-Fei Li, Andrej Karpathy and Justin Johnson's CS231n class
- Roger Grosse's CSC321 class
- Shubhendu Trivedi and Risi Kondor's CMSC 35246 class
- Efstratios Gavves and Max Welling's UvA deep learning class
- Hinton's Neural Networks for Machine Learning class
- Justin Johnson's EECS 498/598 class

Paper presentations start next week

- Paper presentations will start next week!
- Paper critiques
 - More info on Wednesday

Beyond BatchNorm: Towards a Unified Understanding of Normalization in Deep Learning. Ekdeep Singh Lubana, Robert P. Dick, Hidenori Tanaka. NeurIPS 2021.

Beyond BatchNorm: Towards a Unified Understanding of Normalization in Deep Learning

Ekdeep Singh Lubana^{1,*}, Robert P. Dick², Hidenori Tanaka^{2,3}

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²Department of Applied Physics, Stanford University

³Physics & Informatics Laboratories, NTT Research, Inc.

Abstract

Inspired by BatchNorm, there has been an explosion of normalization layers in deep learning. Recent works have identified a multitude of beneficial properties in BatchNorm to explain its success. However, given the paucity of alternative normalization layers, these properties need to be extended so that any given layer's success/failure can be accurately predicted. In this work, we take a first step towards this goal by extending known properties of BatchNorm to randomly initialized deep neural networks (DNNs) to several recently proposed normalization layers. Our primary findings follow: (i) similar to BatchNorm, activation-based normalization layers can prevent exponential growth of activations in ResNets, but normmetric techniques require explicit remedies; (ii) use of GroupNorm can ensure an informative forward propagation with different samples being assigned dissimilar activations, but increasing group size results in increasingly indistinguishable activations for different samples, explaining how convergence speed in ReLU with LayerNorm and (iii) small group sizes result in large gradient norm in ReLU layers, hence explaining training instability issues in Instance Normalization and confirming a speed-stability tradeoff in GroupNorm. Overall, our analysis reveals a unified set of mechanisms that underpin the success of normalization methods in deep learning, providing us with a compass to systematically explore the vast design space of DNN normalization layers.

1 Introduction

Normalizing techniques are often necessary to effectively train deep neural networks (DNNs) [1, 2]. Arguably, the most popular of these is BatchNorm [1], whose success can be attributed to several beneficial properties that allow it to stabilize a DNN's training dynamics: for example, ability to propagate informative activation patterns in deeper layers [4, 5]; reduced dependence on initialization [6, 7, 8]; faster convergence via removal of outliers eigenvalues [9, 10]; and training of learning rates [11], equivalent to modern adaptive optimizers [12]; and smoothing of loss landscape [13, 14]. However, depending on the application scenario, BatchNorm's use can be of limited benefit or even a curse: for example, BatchNorm struggles when training with small batch-sizes [3, 15]; in settings with train-test distribution shifts, BatchNorm can undermine a model's accuracy [16, 17]; in meta-learning, it can lead to transductive inference [18]; and in adversarial training, it can hamper accuracy on both clean and adversarial examples by estimating incorrect statistics [19, 20].

To either address specific shortcomings or to replace BatchNorm in general, several recent works propose alternative normalization layers (interchangeably called normalizers in this paper). For example, Brock et al. [23] propose to match BatchNorm's forward propagation behavior in Residual

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[†]Work partially performed during an internship at Physics & Informatics Laboratories, NTT Research.

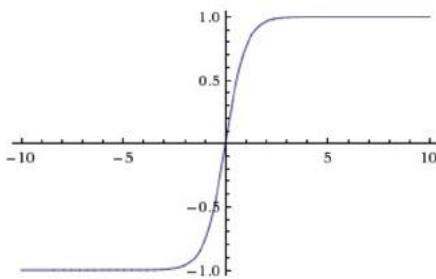
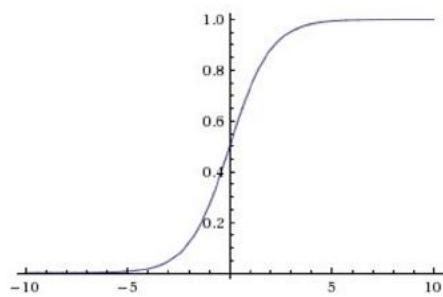
35th Conference on Neural Information Processing Systems (NeurIPS 2021).

Activation Functions

Activation Functions

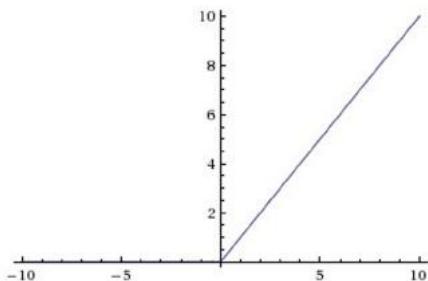
Sigmoid

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

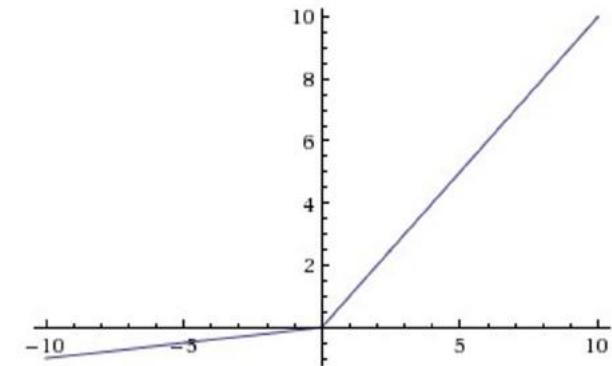


tanh $\tanh(x)$

ReLU $\max(0, x)$



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

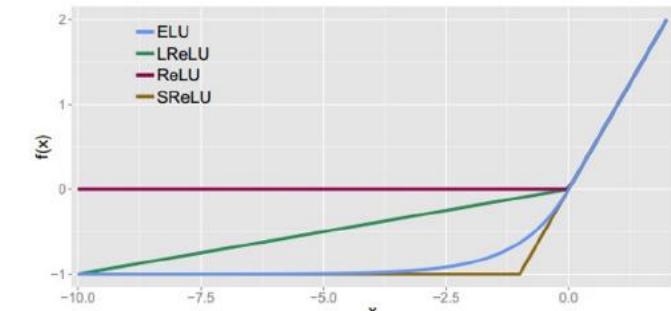


Maxout

ELU

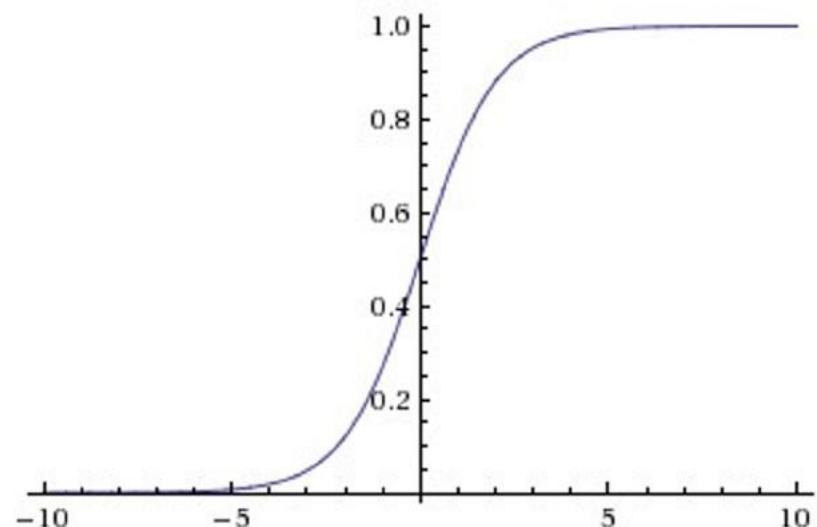
$$\max(w_1^T x + b_1, w_2^T x + b_2)$$

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha (\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$



Activation Functions

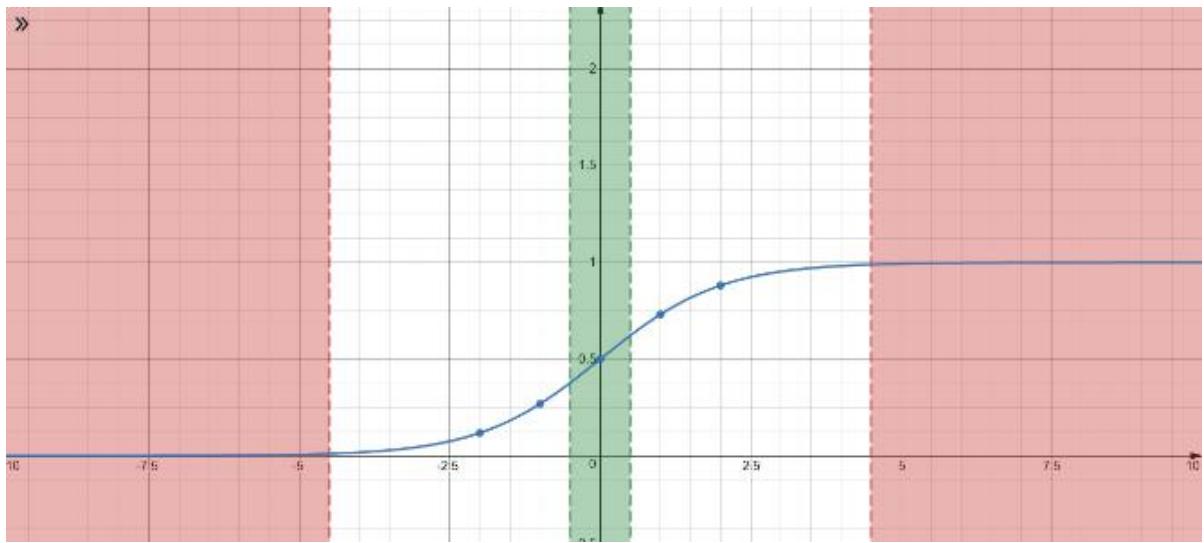
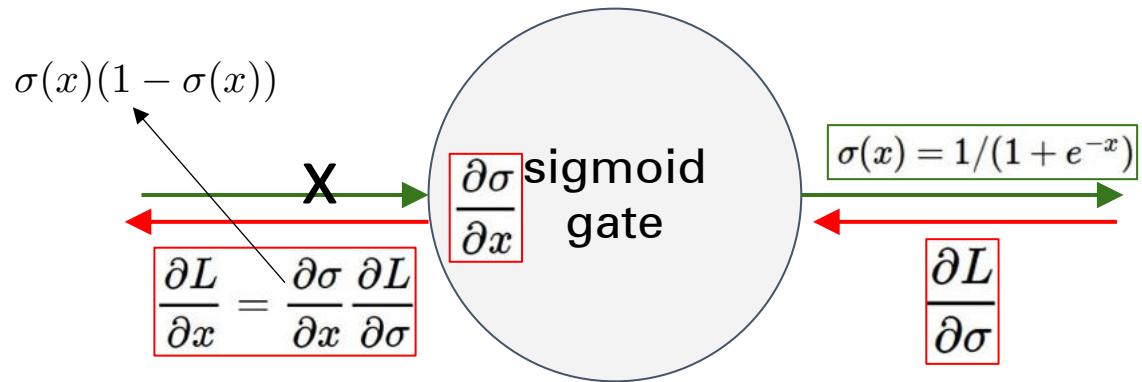
$$\sigma(x) = 1/(1 + e^{-x})$$



Sigmoid

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

Activation Functions



Sigmoid

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

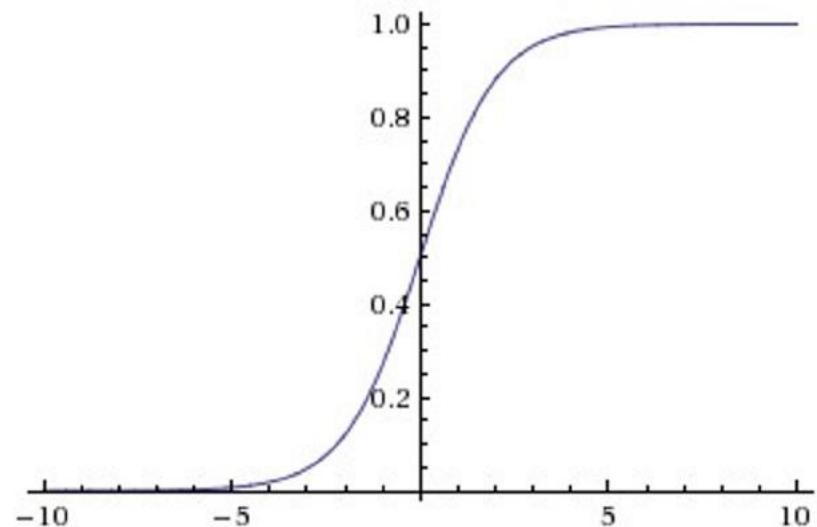
- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating “firing rate” of a neuron

3 problems:

1. Saturated neurons “kill” the gradients

Activation Functions

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



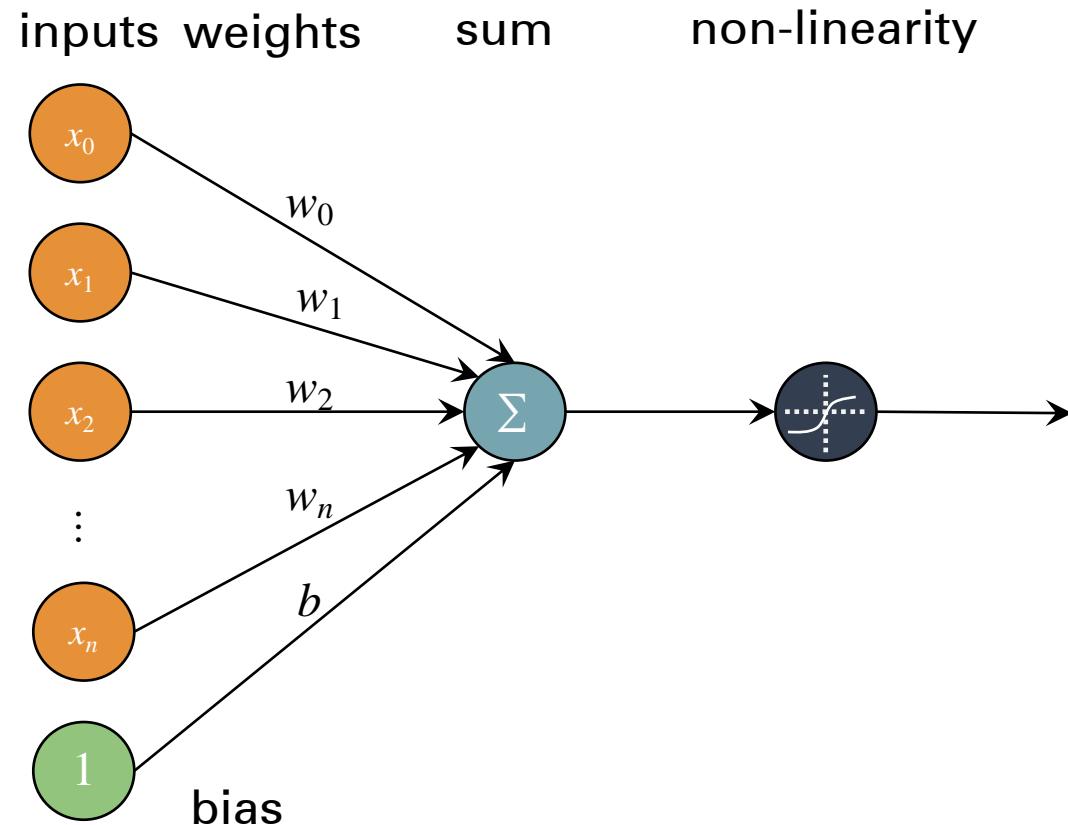
Sigmoid

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

3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered

Consider what happens when the input to a neuron (x) is always positive:

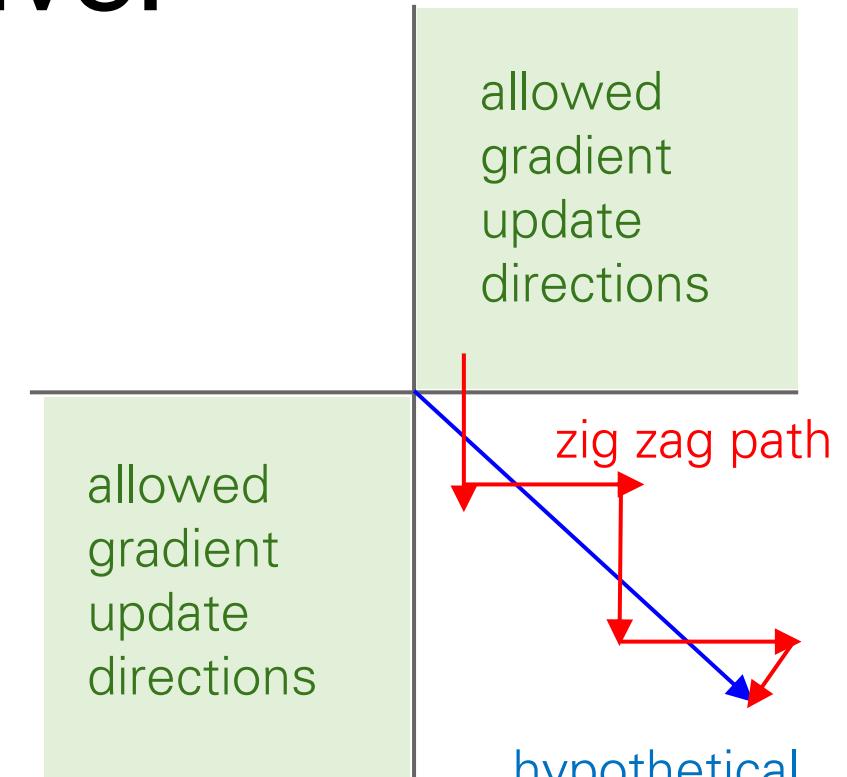


$$f \left(\sum_i w_i x_i + b \right)$$

What can we say about the gradients on w ?

Consider what happens when the input to a neuron (x) is always positive:

$$f \left(\sum_i w_i x_i + b \right)$$

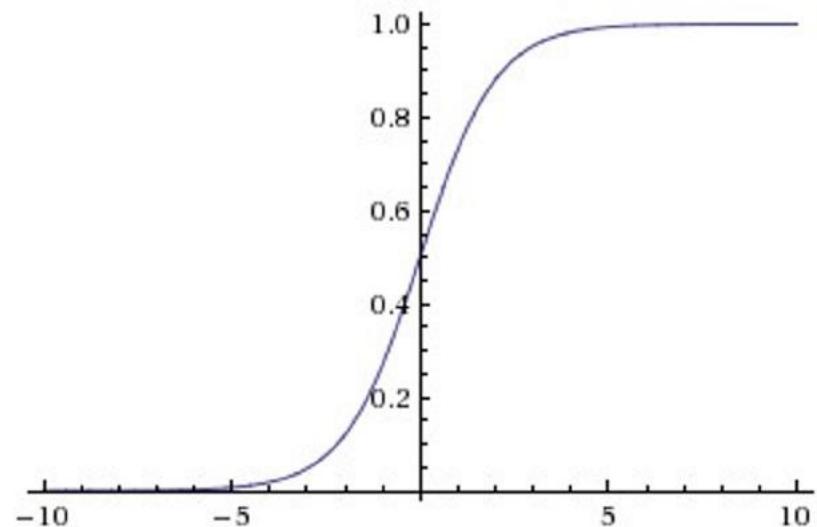


What can we say about the gradients on w ?

Always all positive or all negative :(
(this is also why you want zero-mean data!)

Activation Functions

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



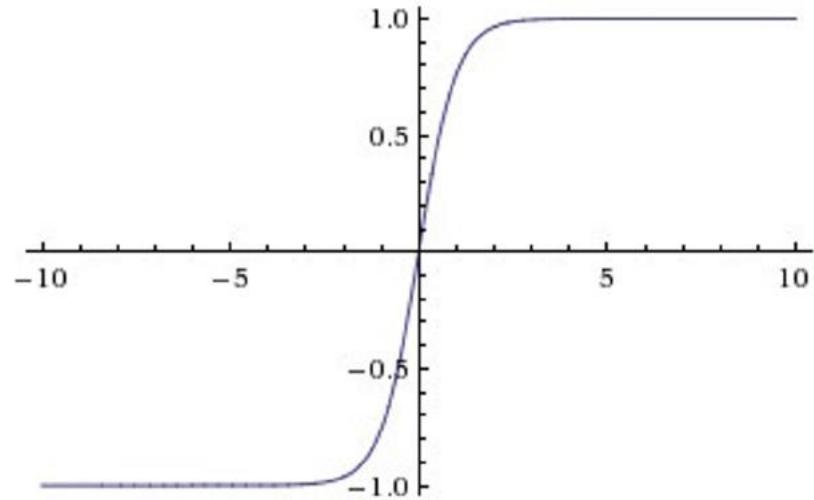
Sigmoid

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

3 problems:

1. Saturated neurons “kill” the gradients
2. Sigmoid outputs are not zero-centered
3. $\exp()$ is a bit compute expensive

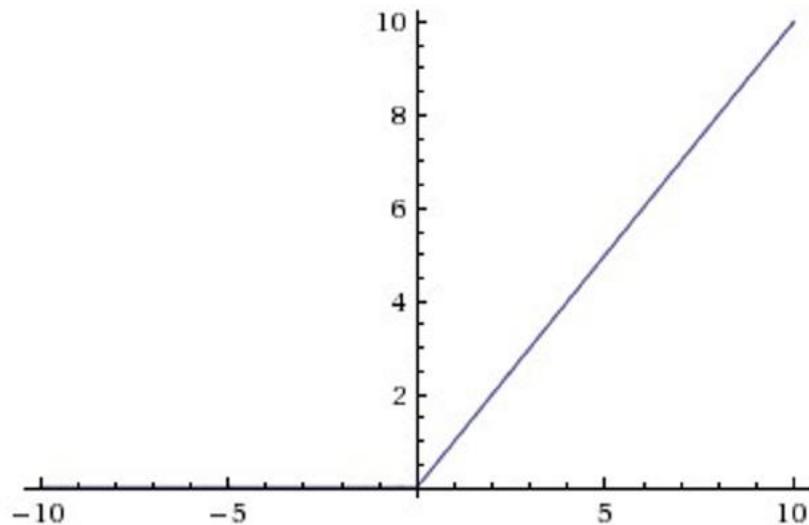
Activation Functions



$\tanh(x)$

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

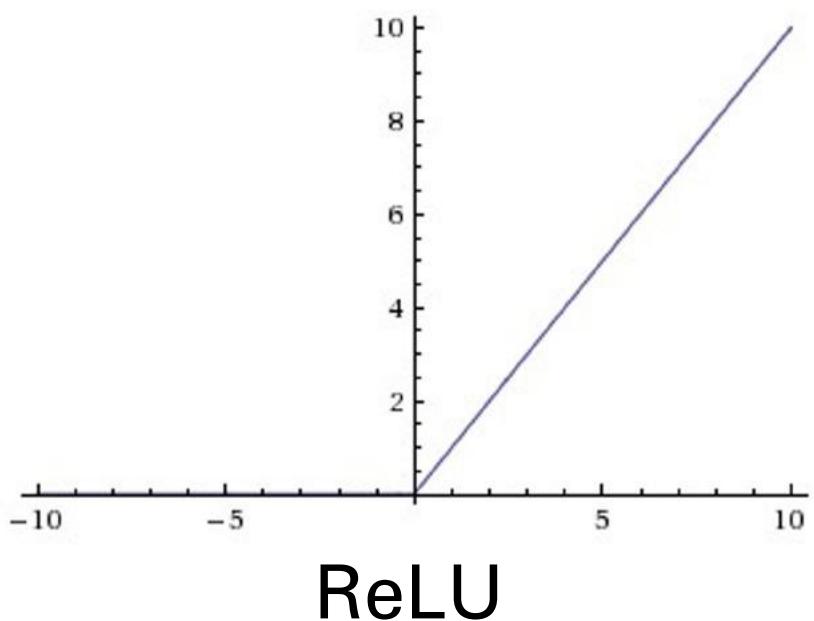
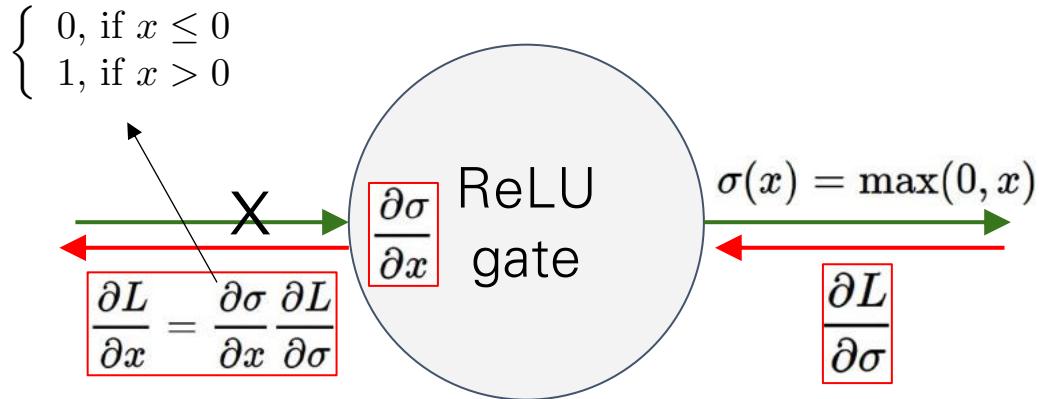
Activation Functions



- Computes $f(x) = \max(0, x)$
- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

ReLU
(Rectified Linear Unit)

Activation Functions



- Computes $f(x) = \max(0, x)$
 - Does not saturate (in +region)
 - Very computationally efficient
 - Converges much faster than sigmoid/tanh in practice (e.g. 6x)
 - Not zero-centered output
 - An annoyance:
- Hint:** what is the gradient when $x < 0$?

DATA CLOUD

active ReLU

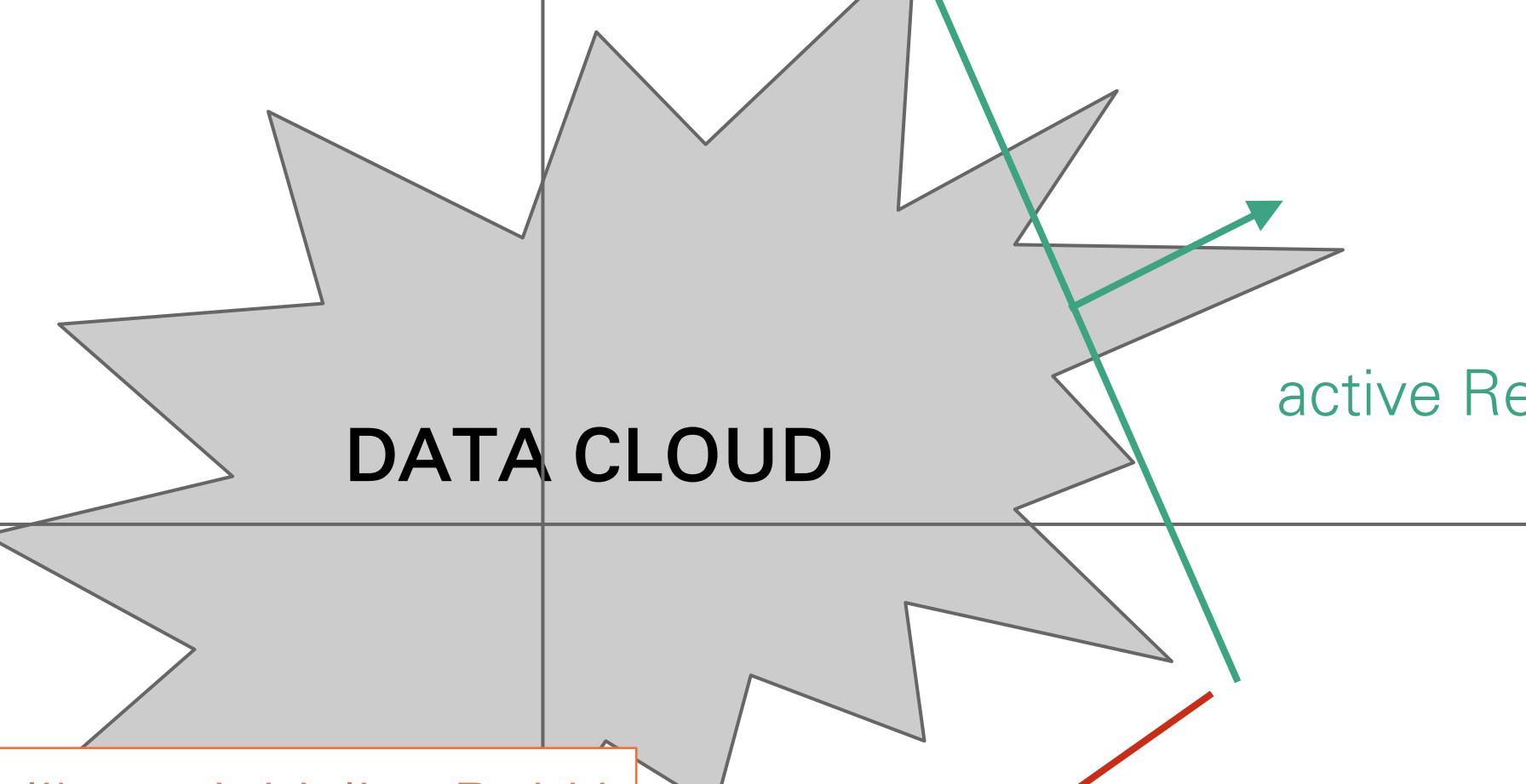
dead ReLU
will never activate
→ never update

DATA CLOUD

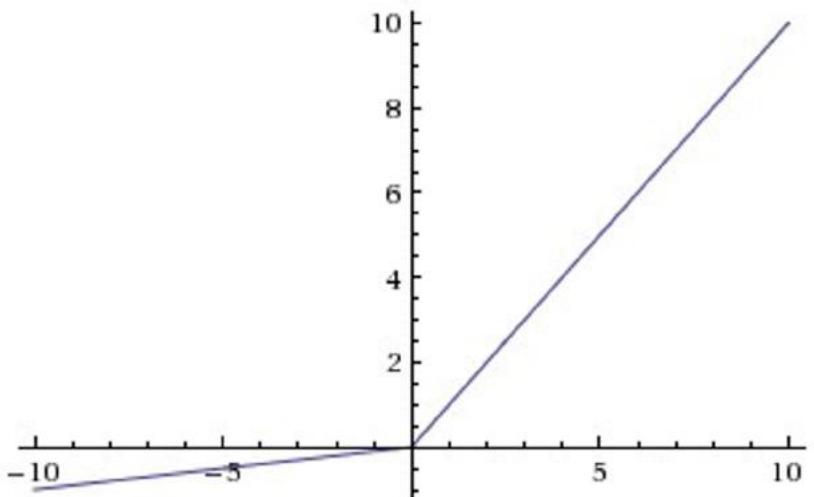
→ people like to initialize ReLU neurons with slightly positive biases (e.g. 0.01)

dead ReLU
will never activate
→ never update

active ReLU



Activation Functions



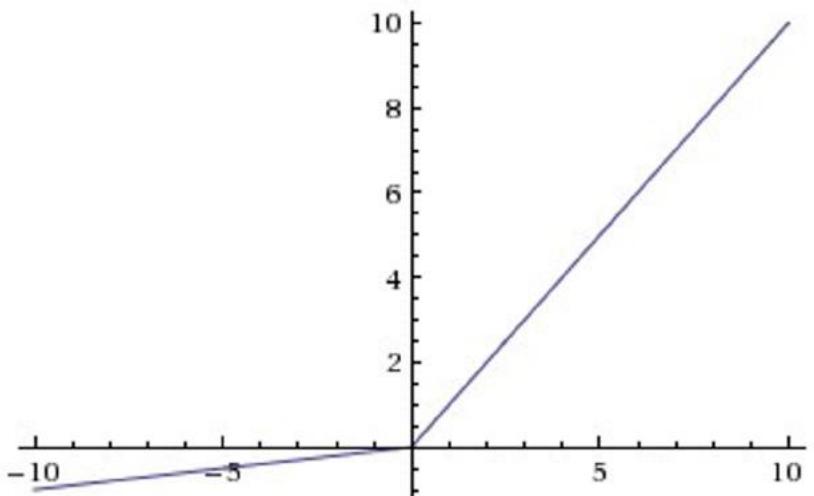
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- will not “die”.

Leaky ReLU

$$f(x) = \max(0.01x, x)$$

[Mass et al., 2013]
[He et al., 2015]

Activation Functions



Leaky ReLU

$$f(x) = \max(0.01x, x)$$

- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- will not “die”.

Parametric Rectifier (PReLU)

$$f(x) = \max(\alpha x, x)$$

backprop into α
(parameter)

[Mass et al., 2013]
[He et al., 2015]

Maxout “Neuron”

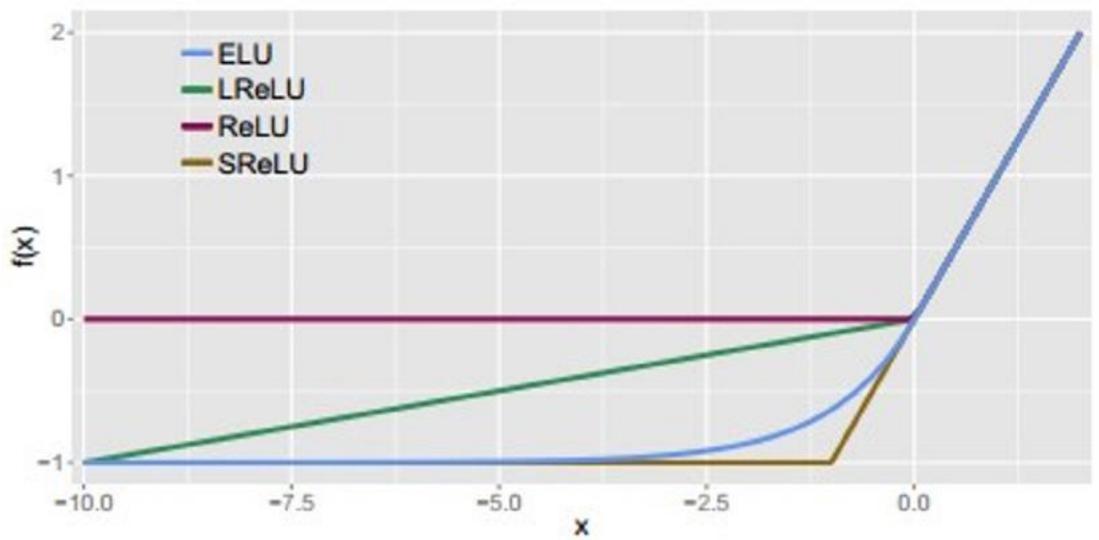
- Does not have the basic form of dot product -> nonlinearity
- Generalizes ReLU and Leaky ReLU
- Linear Regime! Does not saturate! Does not die!

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

Problem: doubles the number of parameters/neuron :(

Activation Functions

Exponential Linear Units (ELU)

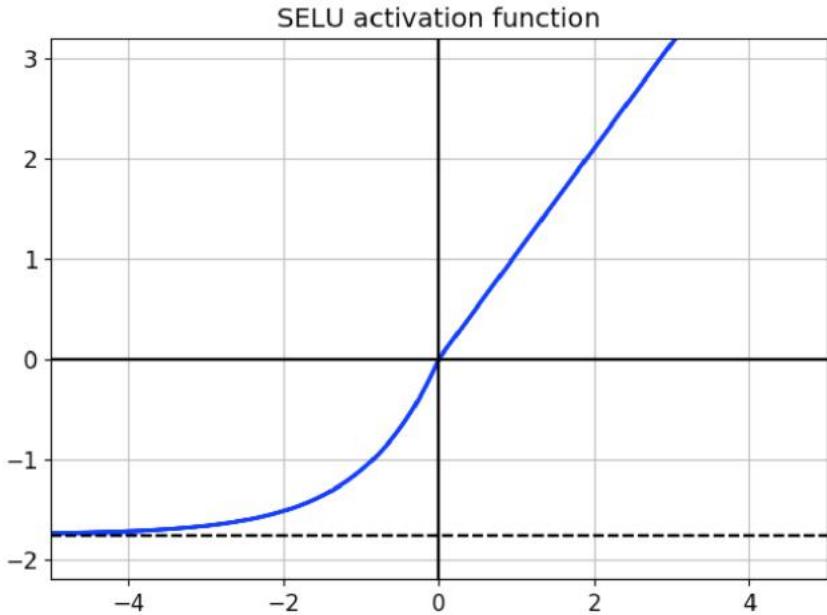


- All benefits of ReLU
- Does not die
- Closer to zero mean outputs
- Computation requires $\exp()$

$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

Activation Functions

Scaled Exponential Linear Units (SELU)



$$f(x) = \lambda \begin{cases} x & \text{if } x > 0 \\ \alpha(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

$$\alpha = 1.6732632423543772848170429916717$$

$$\lambda = 1.0507009873554804934193349852946$$

- Scaled version of ELU
- Stable and attracting fixed points for the mean and variance
- No need for batch normalization
- ~100 pages long of pure math

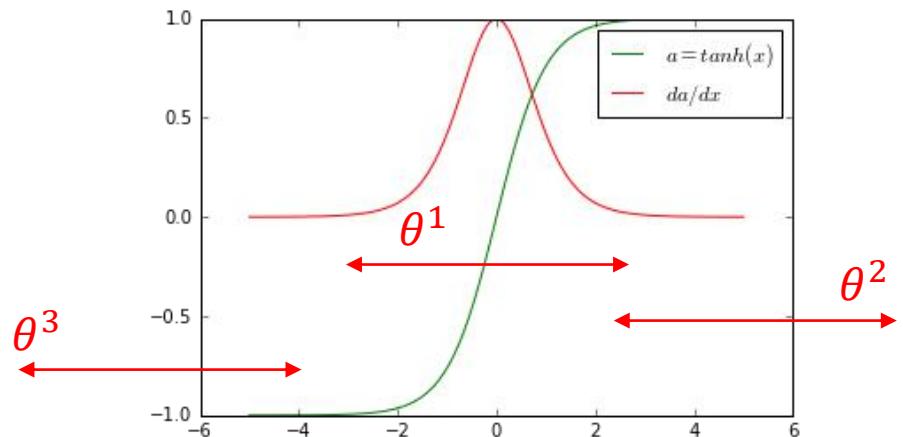
"Using the Banach fixed-point theorem, we prove that activations close to zero mean and unit variance that are propagated through many network layers will converge towards zero mean and unit variance — even under the presence of noise and perturbations."

Data Preprocessing and Normalization

Data preprocessing

- Scale input variables to have similar diagonal covariances $c_i = \sum_j (x_i^{(j)})^2$
 - Similar covariances \rightarrow more balanced rate of learning for different weights
 - Rescaling to 1 is a good choice, unless some dimensions are less important

$$x = [x^1, x^2, x^3]^T, \theta = [\theta^1, \theta^2, \theta^3]^T, a = \tanh(\theta^T x)$$



$x^1, x^2, x^3 \rightarrow$ much different covariances

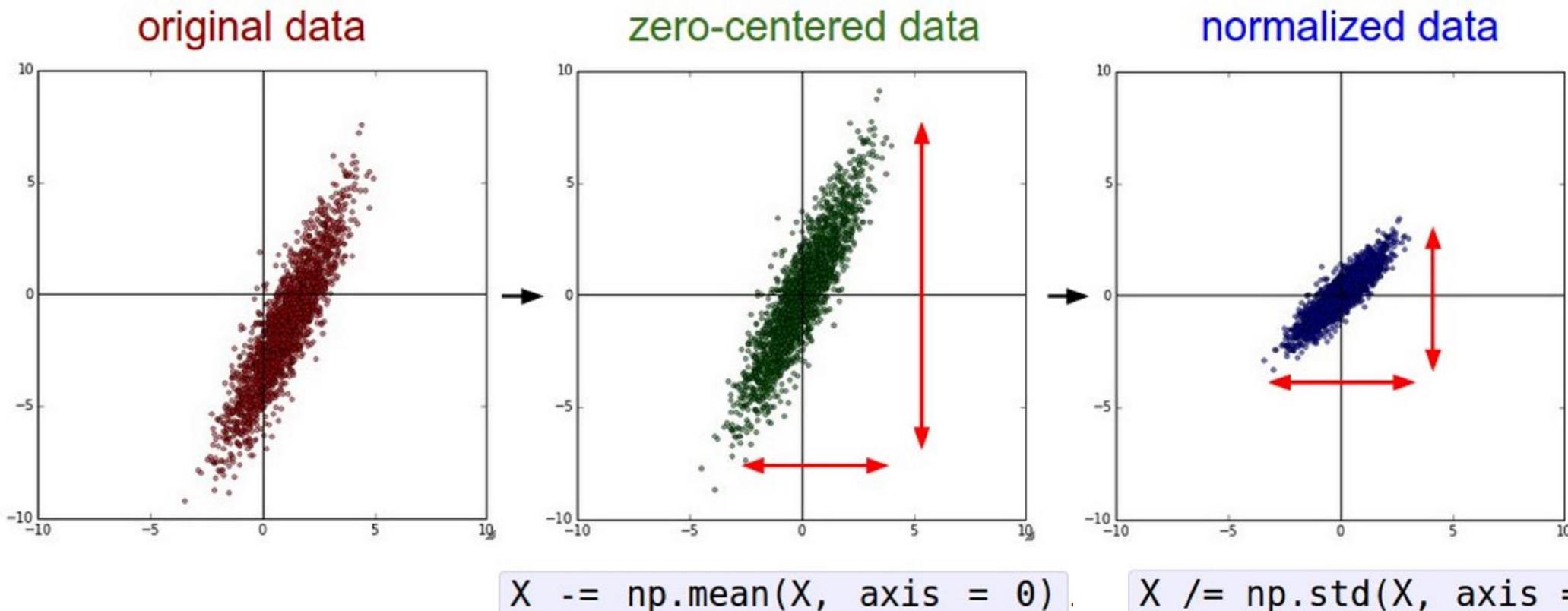
Generated gradients $\left. \frac{\partial \mathcal{L}}{\partial \theta} \right|_{x^1, x^2, x^3}$: much different

Gradient update harder: $\theta^{t+1} = \theta^t - \eta_t \begin{bmatrix} \partial \mathcal{L} / \partial \theta^1 \\ \partial \mathcal{L} / \partial \theta^2 \\ \partial \mathcal{L} / \partial \theta^3 \end{bmatrix}$

Data preprocessing

- Input variables should be as decorrelated as possible
 - Input variables are “more independent”
 - Network is forced to find non-trivial correlations between inputs
 - Decorrelated inputs → Better optimization
 - Obviously not the case when inputs are by definition correlated (sequences)

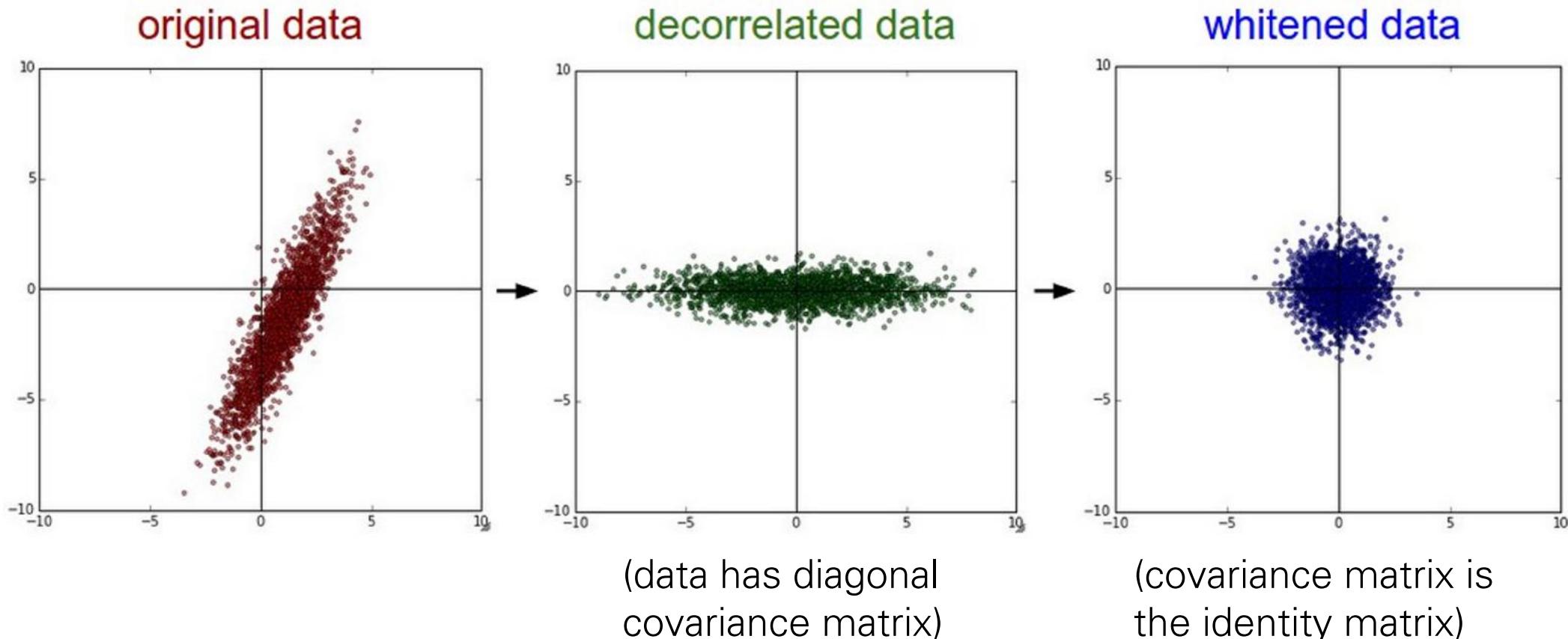
Data preprocessing



(Assume $X [NxD]$ is data matrix, each example in a row)

Data preprocessing

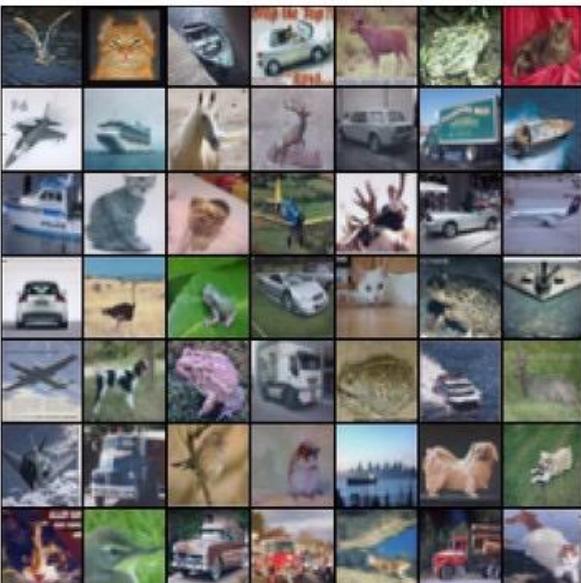
In practice, you may also see **PCA** and **Whitening** of the data



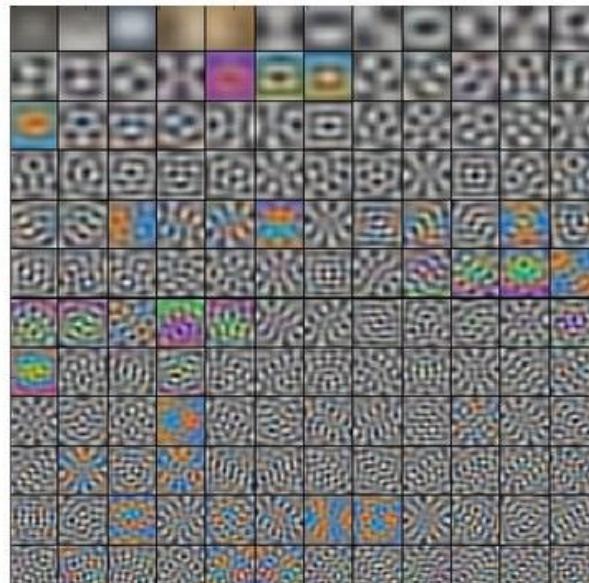
Data preprocessing

In practice, you may also see **PCA** and **Whitening** of the data

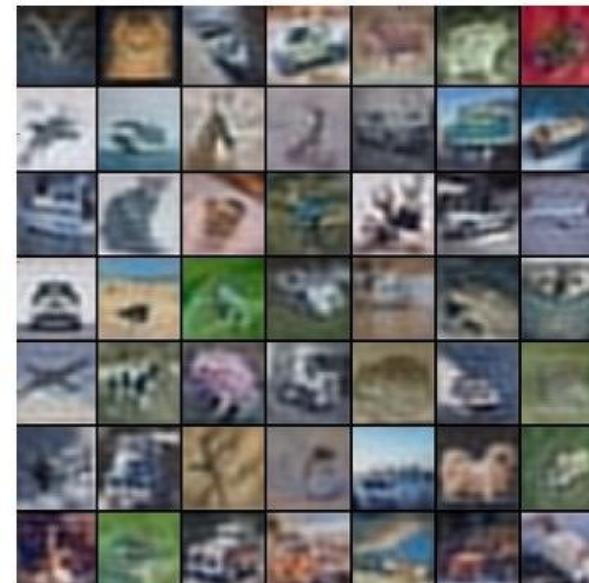
original images



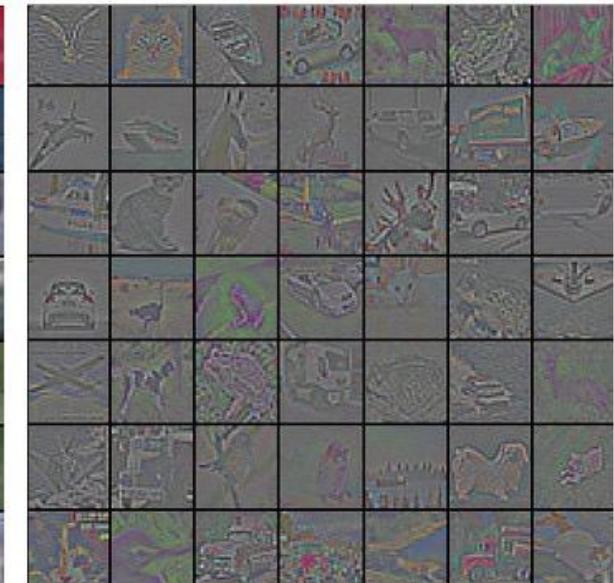
top 144 eigenvectors



reduced images



whitened images



TLDR: In practice for Images: center only

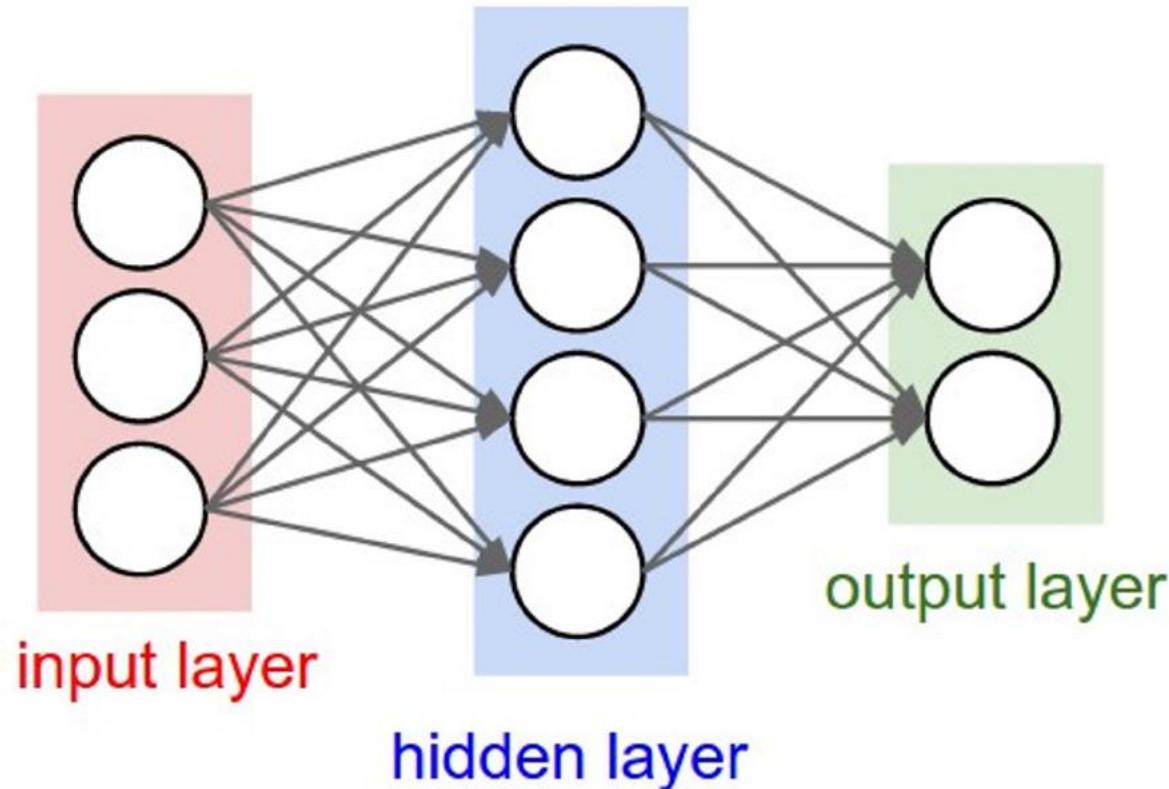
e.g. consider CIFAR-10 example with [32,32,3] images

- Subtract the mean image (e.g. AlexNet)
(mean image = [32,32,3] array)
- Subtract per-channel mean (e.g. VGGNet)
(mean along each channel = 3 numbers)

Not common to normalize variance, to do PCA or whitening

Weight Initialization

Q: what happens when $W=0$ init is used?



First idea: Small random numbers

(Gaussian with zero mean and 1e-2 standard deviation)

```
W = 0.01* np.random.randn(D,H)
```

First idea: Small random numbers

(Gaussian with zero mean and 1e-2 standard deviation)

```
W = 0.01* np.random.randn(D,H)
```

Works ~okay for small networks, but can lead to non-homogeneous distributions of activations across the layers of a network.

Lets look at some activation statistics

E.g. 10-layer net with 500 neurons on each layer, using tanh non-linearities, and initializing as described in last slide.

```
# assume some unit gaussian 10-D input data
D = np.random.randn(1000, 500)
hidden_layer_sizes = [500]*10
nonlinearities = ['tanh']*len(hidden_layer_sizes)

act = {'relu':lambda x:np.maximum(0,x), 'tanh':lambda x:np.tanh(x)}
Hs = {}
for i in xrange(len(hidden_layer_sizes)):
    X = D if i == 0 else Hs[i-1] # input at this layer
    fan_in = X.shape[1]
    fan_out = hidden_layer_sizes[i]
    W = np.random.randn(fan_in, fan_out) * 0.01 # layer initialization

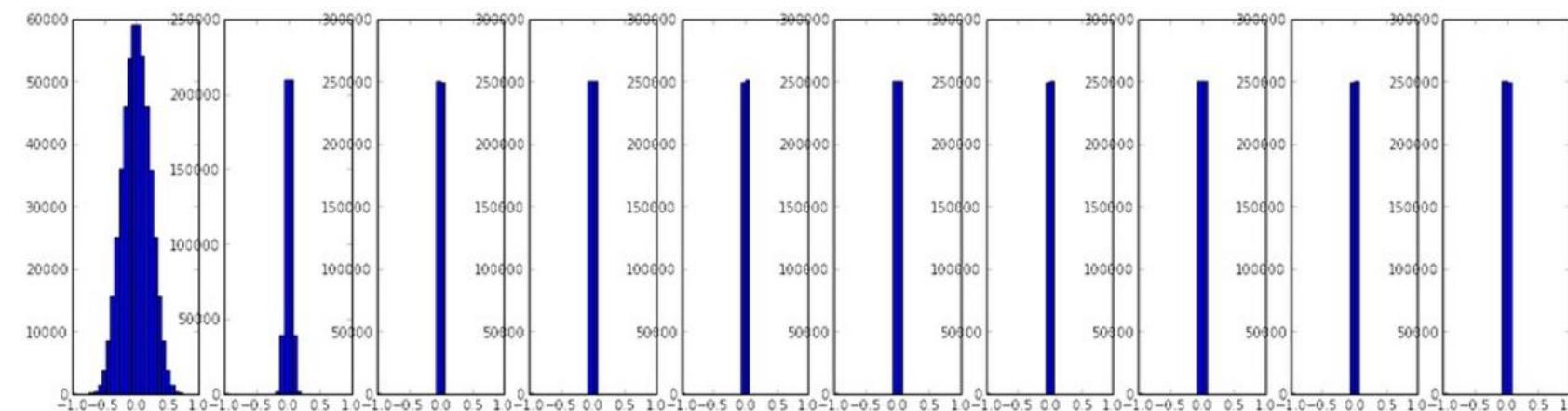
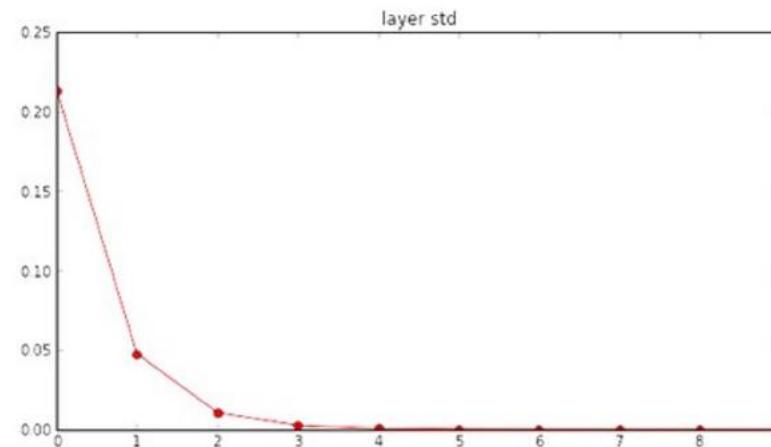
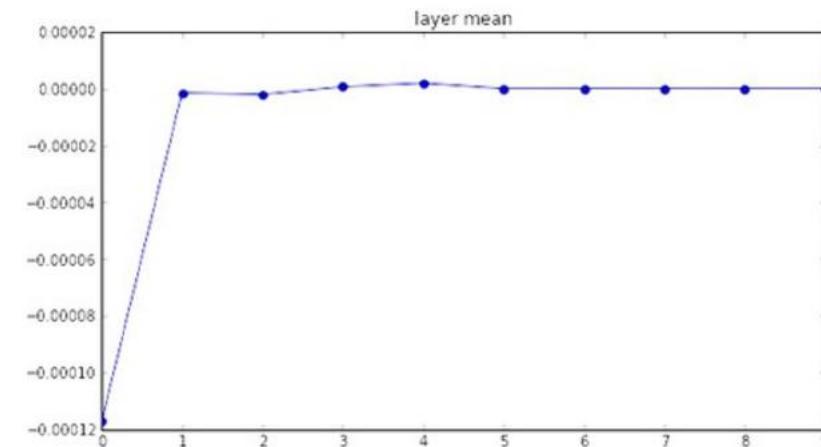
    H = np.dot(X, W) # matrix multiply
    H = act[nonlinearities[i]](H) # nonlinearity
    Hs[i] = H # cache result on this layer

# look at distributions at each layer
print 'input layer had mean %f and std %f' % (np.mean(D), np.std(D))
layer_means = [np.mean(H) for i,H in Hs.iteritems()]
layer_stds = [np.std(H) for i,H in Hs.iteritems()]
for i,H in Hs.iteritems():
    print 'hidden layer %d had mean %f and std %f' % (i+1, layer_means[i], layer_stds[i])

# plot the means and standard deviations
plt.figure()
plt.subplot(121)
plt.plot(Hs.keys(), layer_means, 'ob-')
plt.title('layer mean')
plt.subplot(122)
plt.plot(Hs.keys(), layer_stds, 'or-')
plt.title('layer std')

# plot the raw distributions
plt.figure()
for i,H in Hs.iteritems():
    plt.subplot(1,len(Hs),i+1)
    plt.hist(H.ravel(), 30, range=(-1,1))
```

```
input layer had mean 0.000927 and std 0.998388  
hidden layer 1 had mean -0.000117 and std 0.213081  
hidden layer 2 had mean -0.000001 and std 0.047551  
hidden layer 3 had mean -0.000002 and std 0.010630  
hidden layer 4 had mean 0.000001 and std 0.002378  
hidden layer 5 had mean 0.000002 and std 0.000532  
hidden layer 6 had mean -0.000000 and std 0.000119  
hidden layer 7 had mean 0.000000 and std 0.000026  
hidden layer 8 had mean -0.000000 and std 0.000006  
hidden layer 9 had mean 0.000000 and std 0.000001  
hidden layer 10 had mean -0.000000 and std 0.000000
```



All activations become zero!

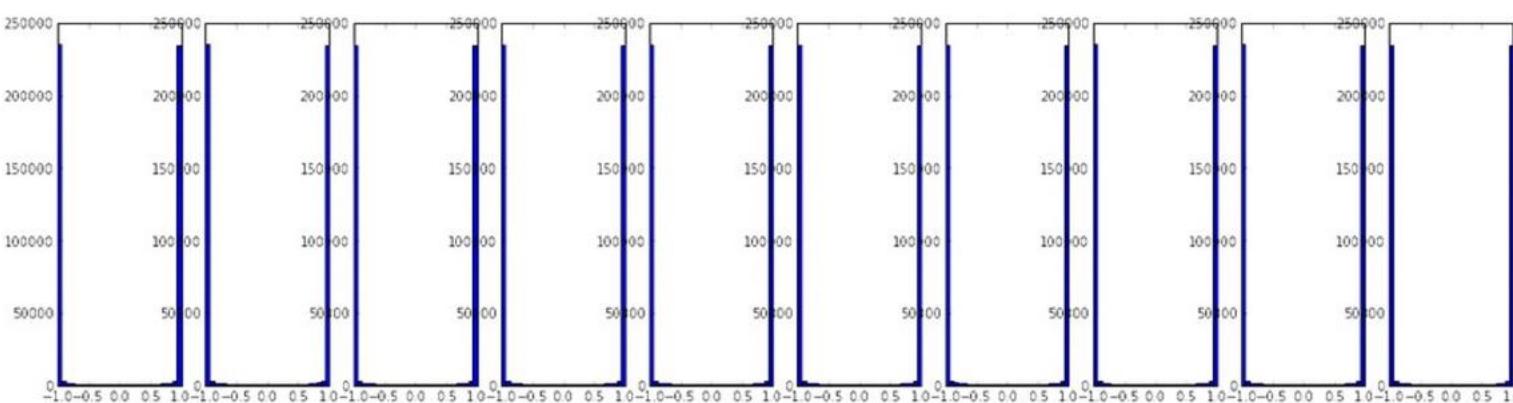
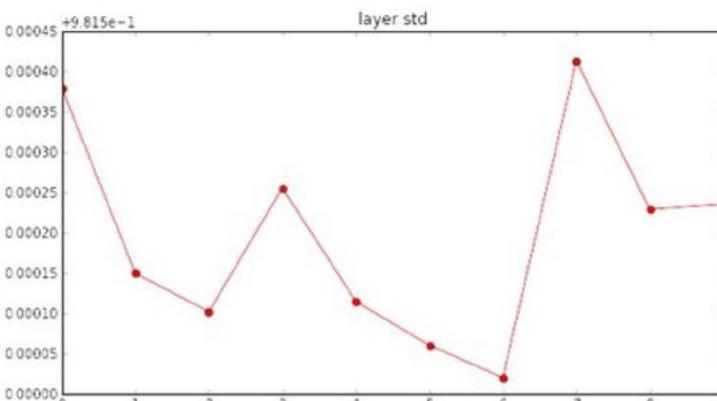
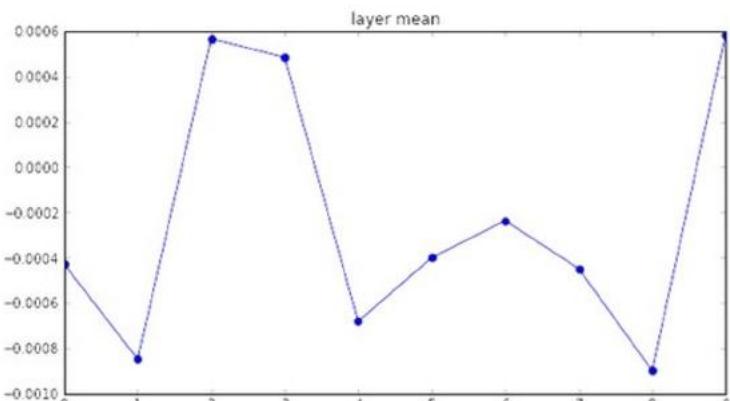
Q: think about the backward pass. What do the gradients look like?

Hint: think about backward pass for a W^*X gate.

```
W = np.random.randn(fan_in, fan_out) * 1.0 # layer initialization
```

```
input layer had mean 0.001800 and std 1.001311  
hidden layer 1 had mean -0.000430 and std 0.981879  
hidden layer 2 had mean -0.000849 and std 0.981649  
hidden layer 3 had mean 0.000566 and std 0.981601  
hidden layer 4 had mean 0.000483 and std 0.981755  
hidden layer 5 had mean -0.000682 and std 0.981614  
hidden layer 6 had mean -0.000401 and std 0.981560  
hidden layer 7 had mean -0.000237 and std 0.981520  
hidden layer 8 had mean -0.000448 and std 0.981913  
hidden layer 9 had mean -0.000899 and std 0.981728  
hidden layer 10 had mean 0.000584 and std 0.981736
```

*1.0 instead of *0.01



Almost all neurons completely saturated, either -1 and 1. Gradients will be all zero.

```

input layer had mean 0.001800 and std 1.001311
hidden layer 1 had mean 0.001198 and std 0.627953
hidden layer 2 had mean -0.000175 and std 0.486051
hidden layer 3 had mean 0.000055 and std 0.407723
hidden layer 4 had mean -0.000306 and std 0.357108
hidden layer 5 had mean 0.000142 and std 0.320917
hidden layer 6 had mean -0.000389 and std 0.292116
hidden layer 7 had mean -0.000228 and std 0.273387
hidden layer 8 had mean -0.000291 and std 0.254935
hidden layer 9 had mean 0.000361 and std 0.239266
hidden layer 10 had mean 0.000139 and std 0.228008

```

```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

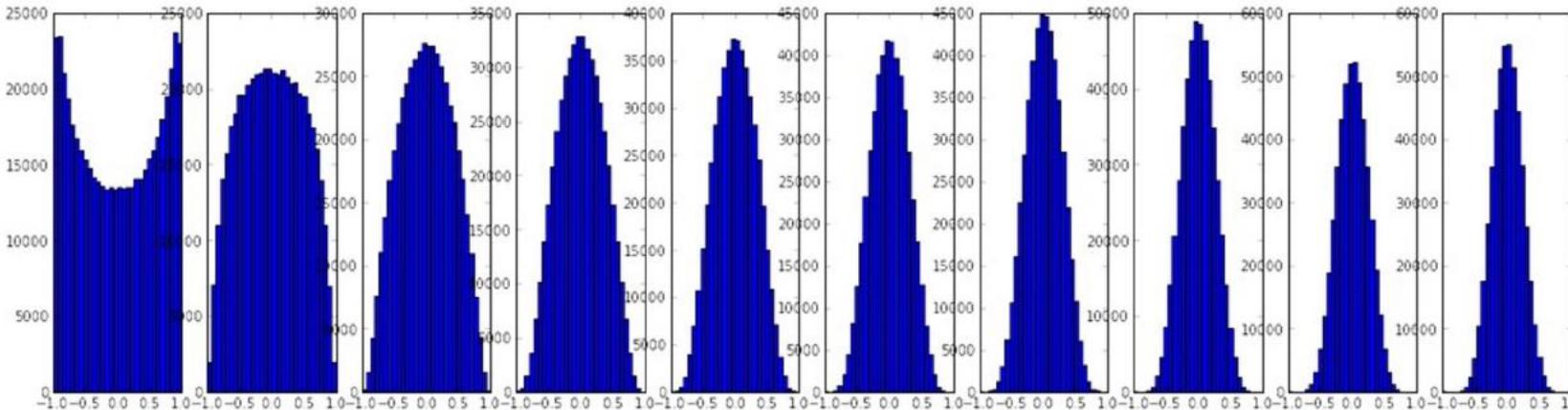
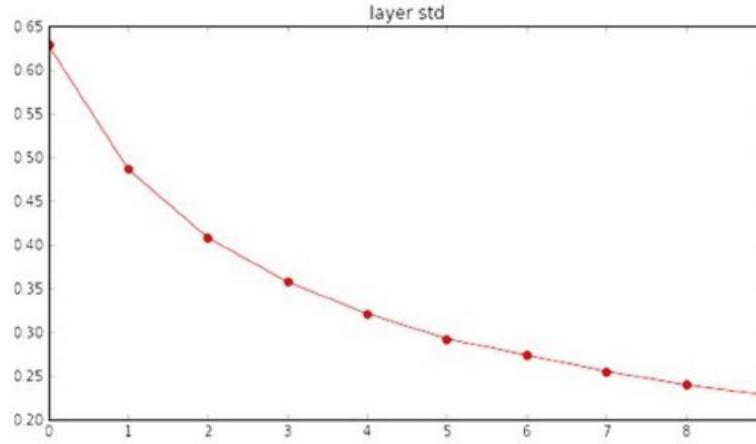
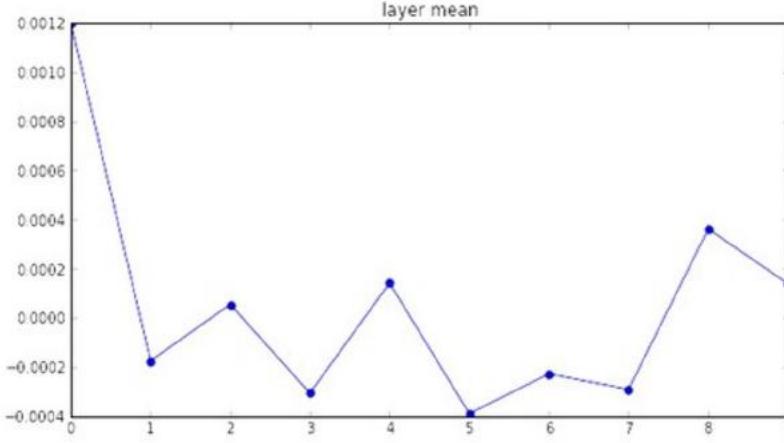
Keep the variance the same
across every layer!

"Xavier initialization"
[Glorot et al., 2010]

Reasonable initialization.
(Mathematical derivation
assumes linear activations)

- If a hidden unit has a big fan-in, small changes on many of its incoming weights can cause the learning to overshoot.
 - We generally want smaller incoming weights when the fan-in is big, so initialize the weights to be proportional to $\text{sqrt}(\text{fan-in})$.
- We can also scale the learning rate the same way. More on this later!

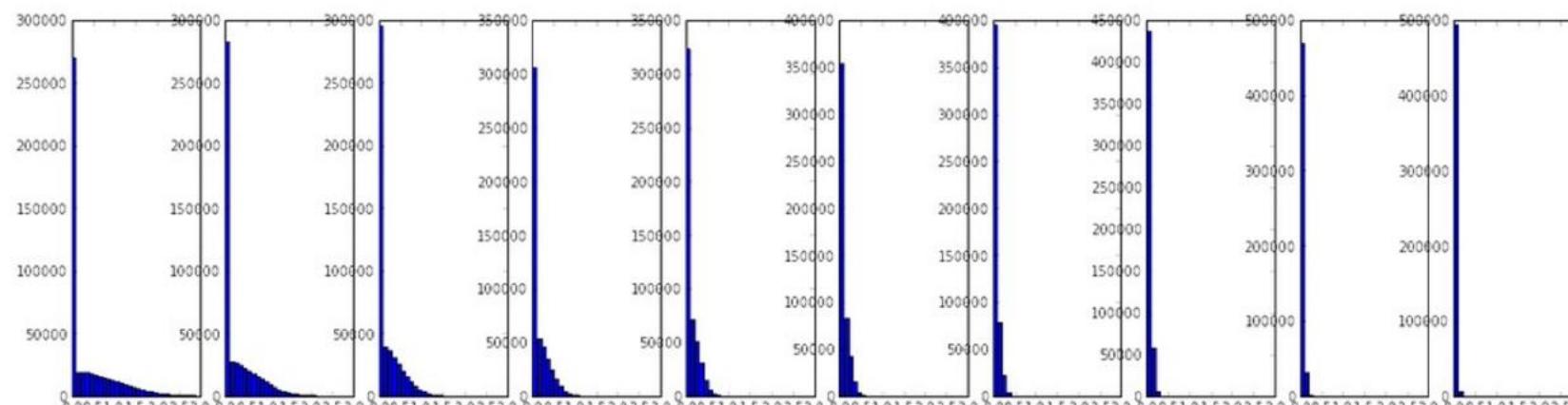
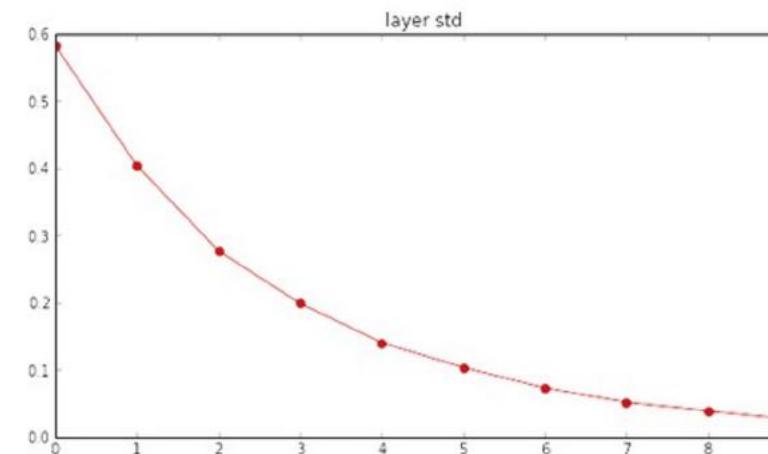
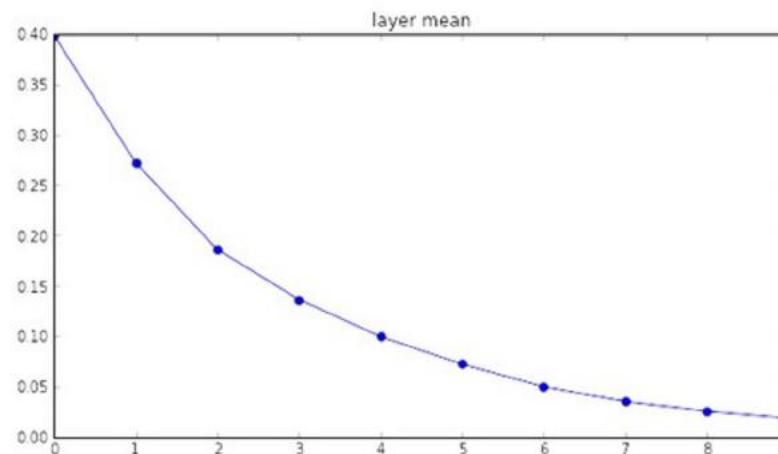
(from Hinton's notes)



```
input layer had mean 0.000501 and std 0.999444  
hidden layer 1 had mean 0.398623 and std 0.582273  
hidden layer 2 had mean 0.272352 and std 0.403795  
hidden layer 3 had mean 0.186076 and std 0.276912  
hidden layer 4 had mean 0.136442 and std 0.198685  
hidden layer 5 had mean 0.099568 and std 0.140299  
hidden layer 6 had mean 0.072234 and std 0.103280  
hidden layer 7 had mean 0.049775 and std 0.072748  
hidden layer 8 had mean 0.035138 and std 0.051572  
hidden layer 9 had mean 0.025404 and std 0.038583  
hidden layer 10 had mean 0.018408 and std 0.026076
```

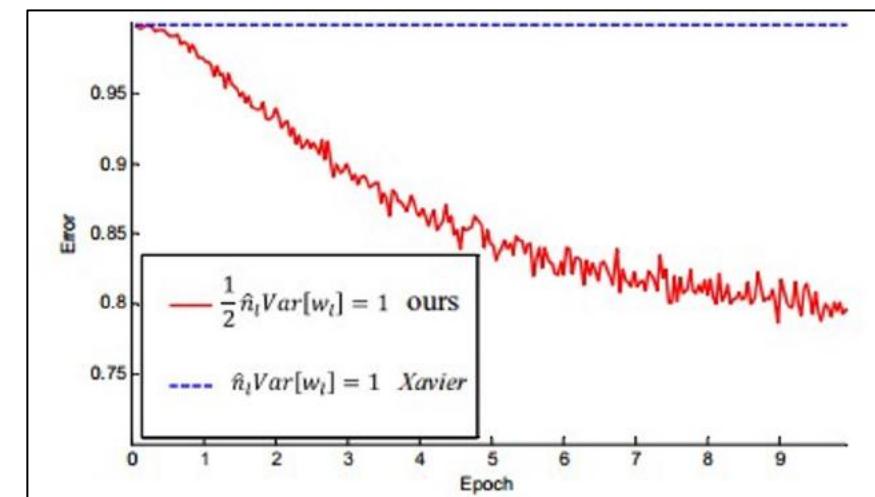
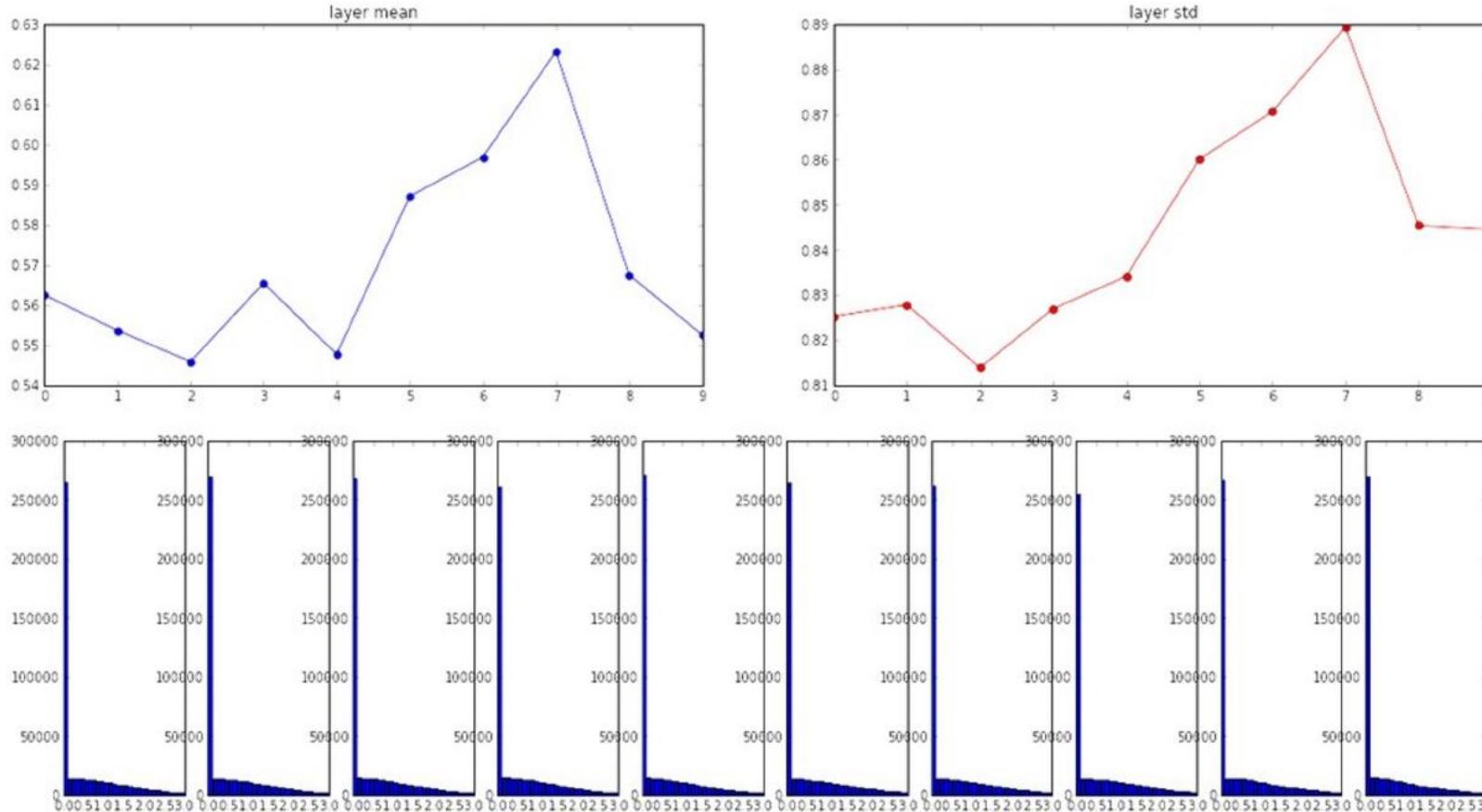
```
W = np.random.randn(fan_in, fan_out) / np.sqrt(fan_in) # layer initialization
```

but when using the ReLU nonlinearity
it breaks.



```
input layer had mean 0.000501 and std 0.999444
hidden layer 1 had mean 0.562488 and std 0.825232
hidden layer 2 had mean 0.553614 and std 0.827835
hidden layer 3 had mean 0.545867 and std 0.813855
hidden layer 4 had mean 0.565396 and std 0.826902
hidden layer 5 had mean 0.547678 and std 0.834092
hidden layer 6 had mean 0.587103 and std 0.860035
hidden layer 7 had mean 0.596867 and std 0.870610
hidden layer 8 had mean 0.623214 and std 0.889348
hidden layer 9 had mean 0.567498 and std 0.845357
hidden layer 10 had mean 0.552531 and std 0.844523
```

He et al., 2015
(note additional /2)



Proper initialization is an active area of research...

- Understanding the difficulty of training deep feedforward neural networks. Glorot and Bengio, 2010
- Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. Saxe et al, 2013
- Random walk initialization for training very deep feedforward networks. Sussillo and Abbott, 2014
- Delving deep into rectifiers: Surpassing human-level performance on ImageNet classification. He et al., 2015
- Data-dependent Initializations of Convolutional Neural Networks. Krähenbühl et al., 2015
- All you need is a good init. Mishkin and Matas, 2015
- How to start training: The effect of initialization and architecture. Hanin and Rolnick, 2018
- How to Initialize your Network? Robust Initialization for WeightNorm & ResNets. Arpit et al., 2019

...

Batch Normalization

“you want unit Gaussian activations? just make them so.”

consider a batch of activations at some layer.
To make each dimension unit gaussian, apply:

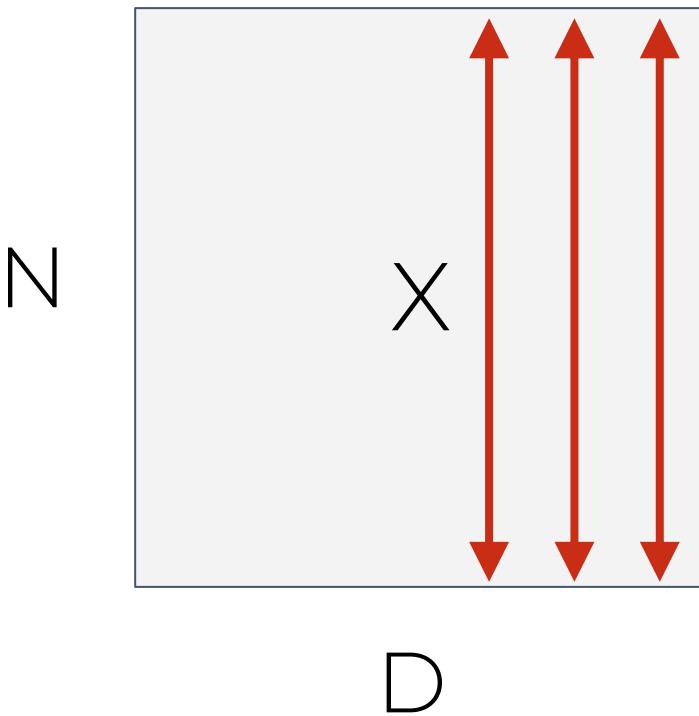
$$\hat{x}^{(k)} = \frac{x^{(k)} - \text{E}[x^{(k)}]}{\sqrt{\text{Var}[x^{(k)}]}}$$

this is a vanilla differentiable
function...

[Ioffe and Szegedy, 2015]

Batch Normalization

“you want unit gaussian activations? just make them so.”



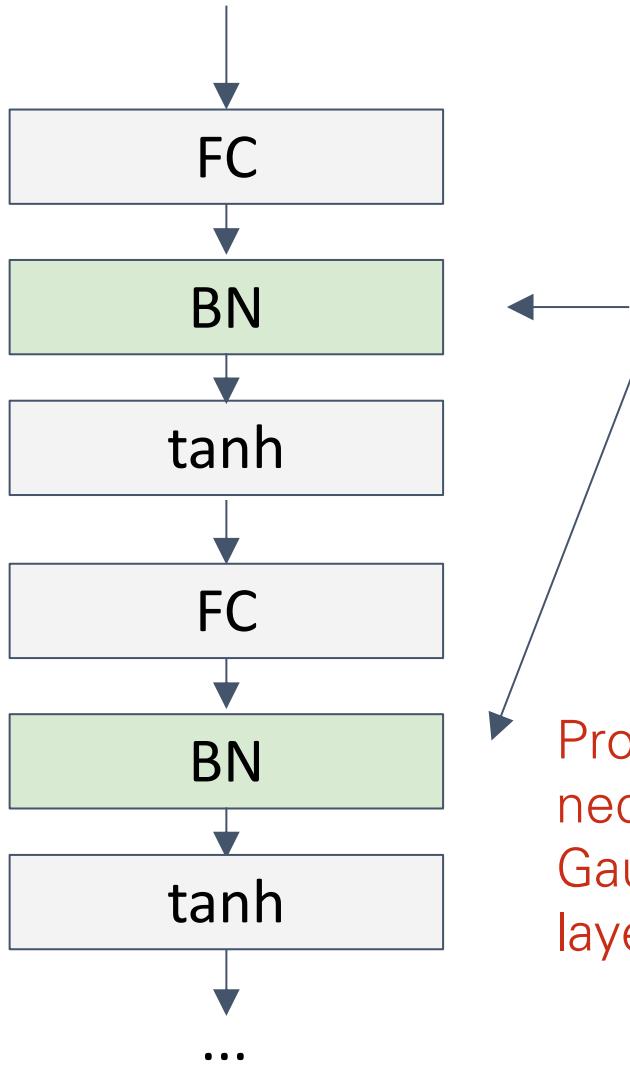
1. compute the empirical mean and variance independently for each dimension.

2. Normalize

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

[Ioffe and Szegedy, 2015]

Batch Normalization



Usually inserted after Fully Connected / (or Convolutional, as we'll see soon) layers, and before nonlinearity.

Problem: do we necessarily want a unit Gaussian input to a tanh layer?

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

[Ioffe and Szegedy, 2015]

Batch Normalization

Normalize:

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

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

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

Note, the network can learn:

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

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

to recover the identity mapping.

Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_1 \dots m\}$;

Parameters to be learned: γ, β

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

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

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

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

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

- Improves gradient flow through the network
- Allows higher learning rates
- Reduces the strong dependence on initialization
- Acts as a form of regularization in a funny way, and slightly reduces the need for dropout, maybe

[Ioffe and Szegedy, 2015]

Batch Normalization

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_1 \dots m\}$;

Parameters to be learned: γ, β

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

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

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

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

Note: at test time BatchNorm layer functions differently:

The mean/std are not computed based on the batch. Instead, a single fixed empirical mean of activations during training is used.

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

Other normalization schemes

- **Layer Normalization**

Ba et al., Layer Normalization, arXiv preprint, 2016

- **Weight Normalization**

Salimans, Weight Normalization: A Simple Reparameterization to Accelerate Training of Deep Neural Networks, NIPS, 2016

- **Instance Normalization**

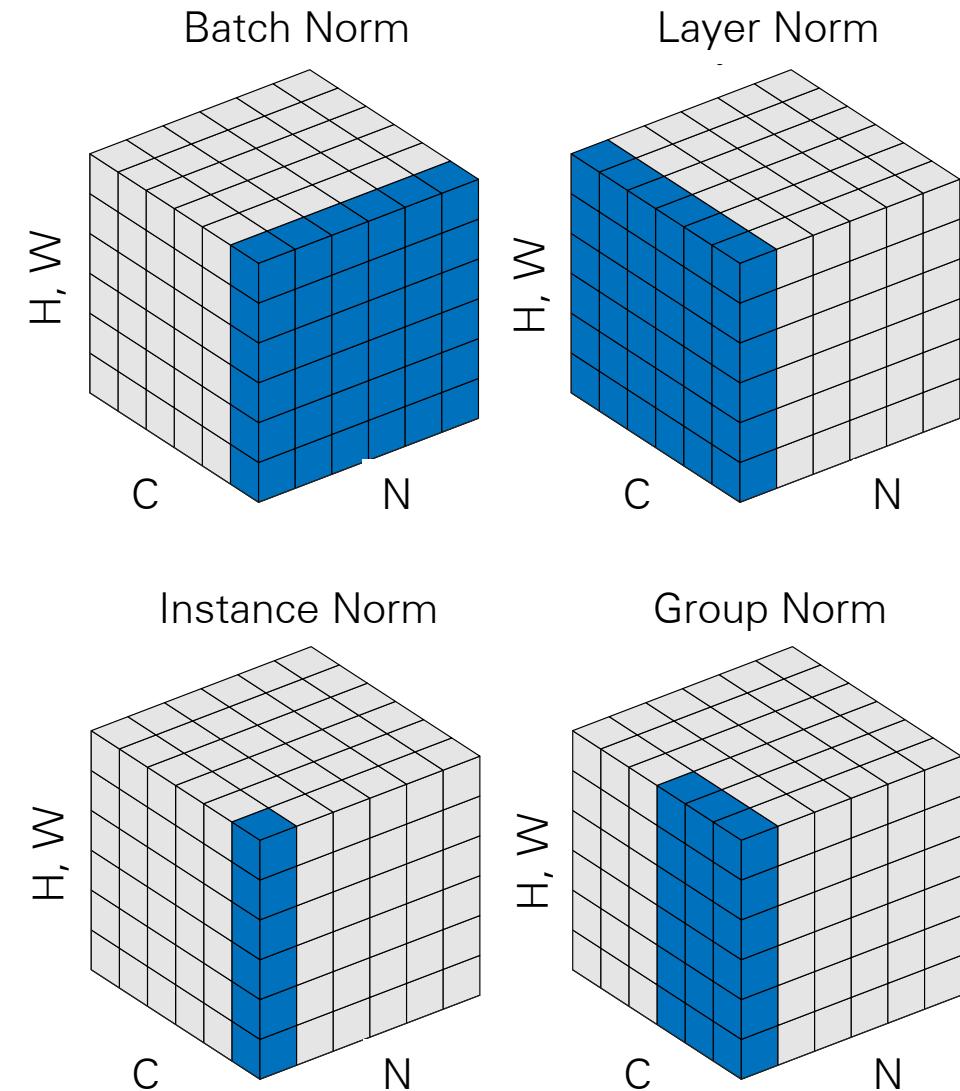
Ulyanov et al., Instance normalization: The missing ingredient for fast stylization. arXiv preprint, 2016

- **Batch Renormalization**

Ioffe, Batch Renormalization: Towards Reducing Minibatch Dependence in Batch-Normalized Models, NIPS 2017

- **Group Renormalization**

Wu and He, Group Normalization, ECCV 2018



Improving Generalization

Preventing Overfitting

- **Approach 1:** Get more data!
 - Almost always the best bet if you have enough compute power to train on more data.
- **Approach 2:** Use a model that has the right capacity:
 - enough to fit the true regularities.
 - not enough to also fit spurious regularities (if they are weaker).
- **Approach 3:** Average many different models.
 - Use models with different forms.
 - Or train the model on different subsets of the training data (this is called “bagging”).
- **Approach 4: (Bayesian)** Use a single neural network architecture, but average the predictions made by many different weight vectors.

Some ways to limit the capacity of a neural net

- The capacity can be controlled in many ways:
 - **Architecture:** Limit the number of hidden layers and the number of units per layer.
 - **Early stopping:** Start with small weights and stop the learning before it overfits.
 - **Weight-decay:** Penalize large weights using penalties or constraints on their squared values (L2 penalty) or absolute values (L1 penalty).
 - **Noise:** Add noise to the weights or the activities.
- Typically, a combination of several of these methods is used.

Regularization

- Neural networks typically have thousands, if not millions of parameters
 - Usually, the dataset size smaller than the number of parameters
- Overfitting is a grave danger
- Proper weight regularization is crucial to avoid overfitting

$$\theta^* \leftarrow \arg \min_{\theta} \sum_{(x,y) \subseteq (X,Y)} \ell(y, a_L(x; \theta_1, \dots, L)) + \lambda \Omega(\theta)$$

- Possible regularization methods
 - l_2 -regularization
 - l_1 -regularization
 - Dropout

l_2 -regularization

- Most important (or most popular) regularization

$$\theta^* \leftarrow \arg \min_{\theta} \sum_{(x,y) \subseteq (X,Y)} \ell(y, a_L(x; \theta_{1,\dots,L})) + \frac{\lambda}{2} \sum_l \|\theta_l\|^2$$

- The l_2 -regularization can pass inside the gradient descend update rule

$$\theta^{(t+1)} = \theta^{(t)} - \eta_t (\nabla_{\theta} \mathcal{L} + \lambda \theta_l) \Rightarrow$$

$$\theta^{(t+1)} = (1 - \lambda \eta_t) \theta^{(t)} - \eta_t \nabla_{\theta} \mathcal{L}$$

“Weight decay”, because
weights get smaller

- λ is usually about $10^{-1}, 10^{-2}$

l_1 -regularization

- l_1 -regularization is one of the most important techniques

$$\theta^* \leftarrow \arg \min_{\theta} \sum_{(x,y) \subseteq (X,Y)} \ell(y, a_L(x; \theta_{1,\dots,L})) + \frac{\lambda}{2} \sum_l \|\theta_l\|$$

- Also l_1 -regularization passes inside the gradient descend update rule

$$\theta^{(t+1)} = \theta^{(t)} - \lambda \eta_t \frac{\theta^{(t)}}{|\theta^{(t)}|} - \eta_t \nabla_{\theta} \mathcal{L}$$

Sign function

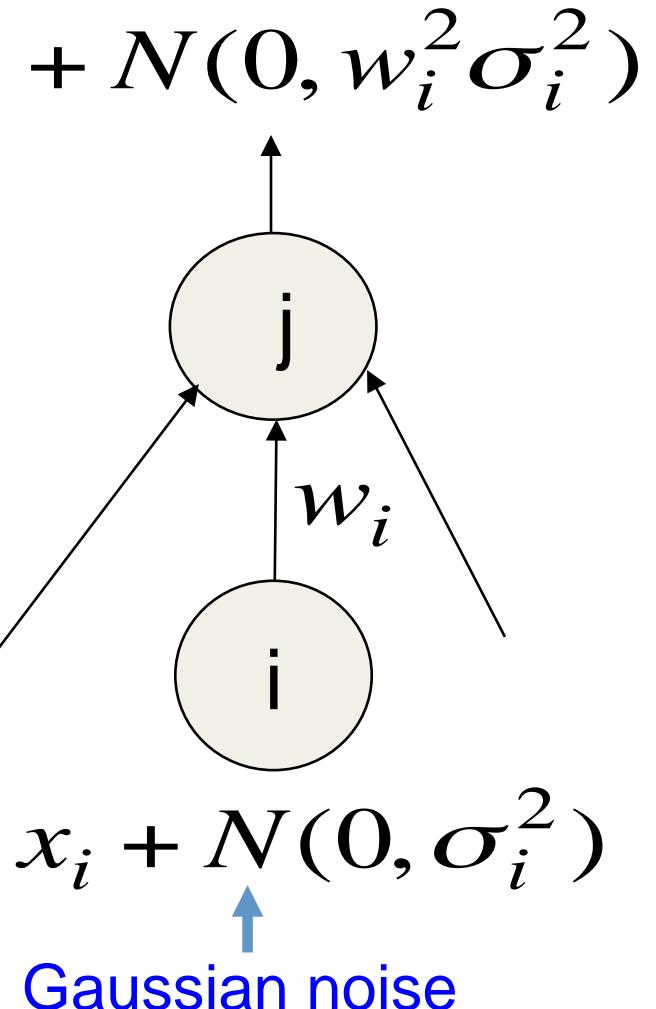
- l_1 -regularization → sparse weights
- $\lambda \uparrow \rightarrow$ more weights become 0

Data augmentation [Krizhevsky2012]



Noise as a regularizer

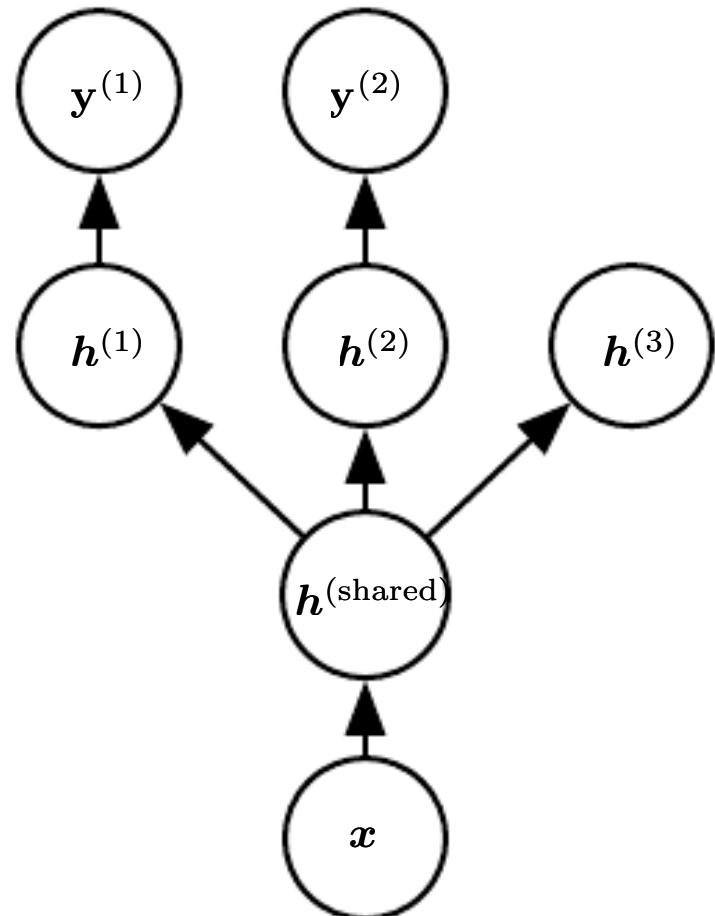
- Suppose we add Gaussian noise to the inputs.
 - The variance of the noise is amplified by the squared weight before going into the next layer.
- In a simple net with a linear output unit directly connected to the inputs, the amplified noise gets added to the output.
- This makes an additive contribution to the squared error.
 - So minimizing the squared error tends to minimize the squared weights when the inputs are noisy.



Not exactly equivalent to using an L2 weight penalty.

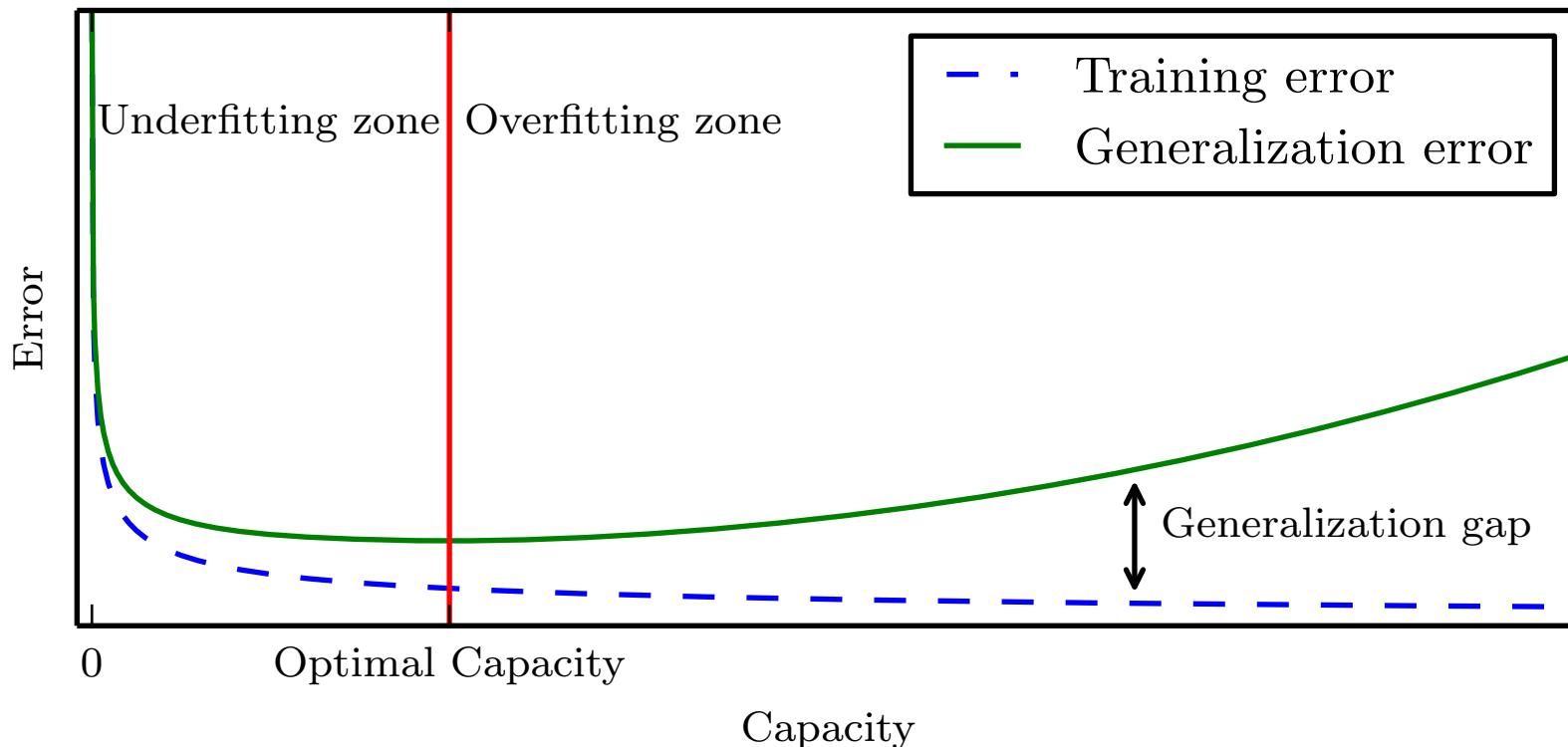
Multi-task Learning

- Improving generalization by pooling the examples arising out of several tasks.
- Different supervised tasks share the same input x , as well as some intermediate-level representation h (shared)
 - Task-specific parameters
 - Generic parameters (shared across all the tasks)



Early stopping

- Start with small weights and stop the learning before it overfits.
- Think early stopping as a very efficient hyperparameter selection.
 - The number of training steps is just another hyperparameter.

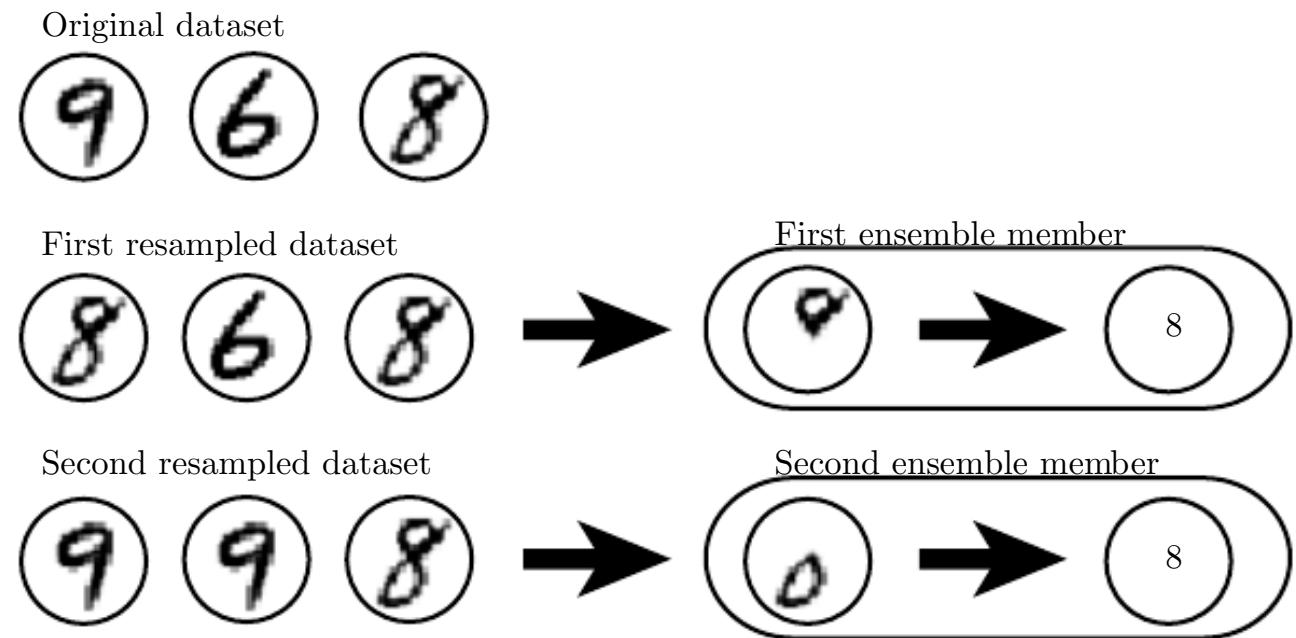


Model Ensembles: The bias-variance trade-off

- When the amount of training data is limited, we get overfitting.
 - Averaging the predictions of many different models is a good way to reduce overfitting.
 - It helps most when the models make very different predictions.
- For regression, the squared error can be decomposed into a “bias” term and a “variance” term.
 - The bias term is big if the model has too little capacity to fit the data.
 - The variance term is big if the model has so much capacity that it is good at fitting the sampling error in each particular training set.
- By averaging away the variance we can use individual models with high capacity. These models have high variance but low bias.

Model Ensembles

- Train several different models separately, then have all of the models vote on the output for test examples.
- Different models will usually not make all the same errors on the test set.
- Usually ~2% gain!



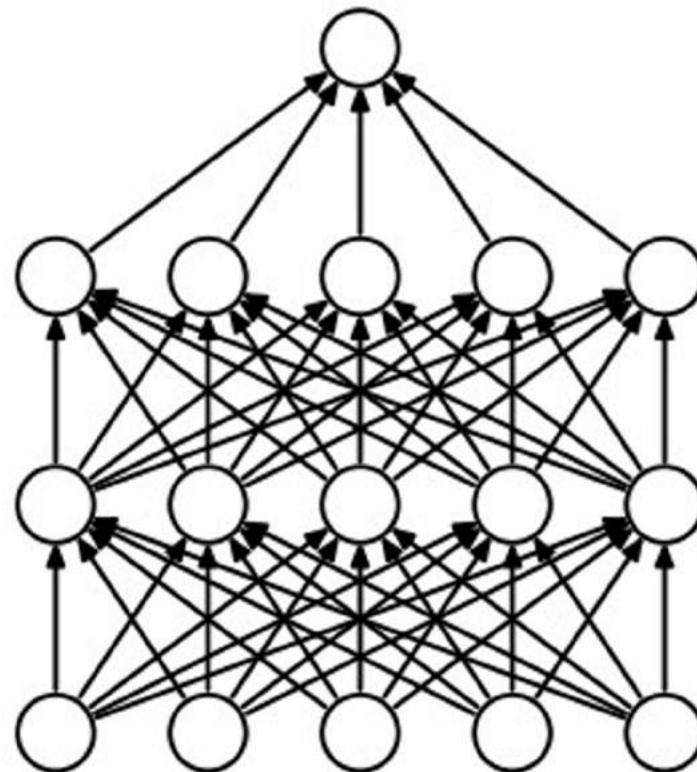
Model Ensembles

- We can also get a small boost from averaging multiple model checkpoints of a single model.
- keep track of (and use at test time) a running average parameter vector:

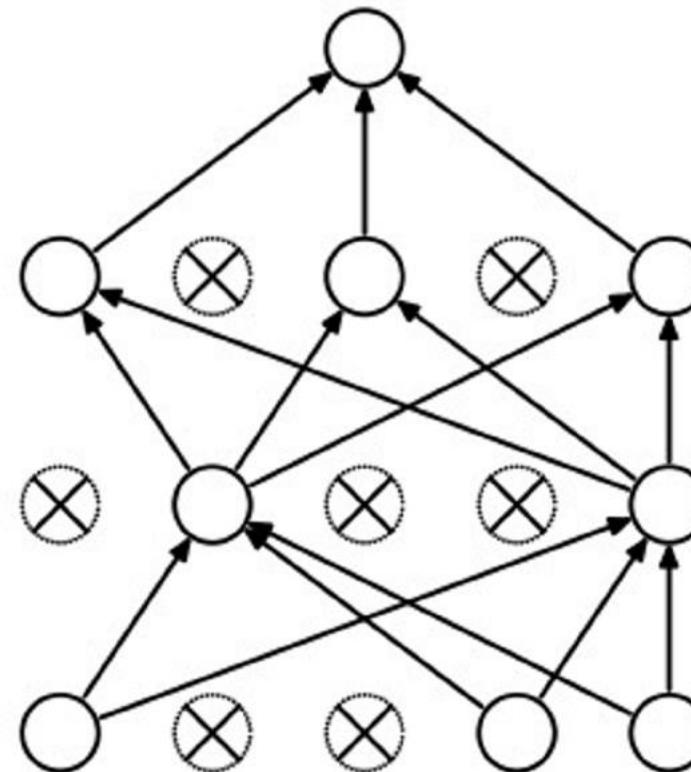
```
while True:  
    data_batch = dataset.sample_data_batch()  
    loss = network.forward(data_batch)  
    dx = network.backward()  
    x += - learning_rate * dx  
    x_test = 0.995*x_test + 0.005*x # use for test set
```

Dropout

- “randomly set some neurons to zero in the forward pass”



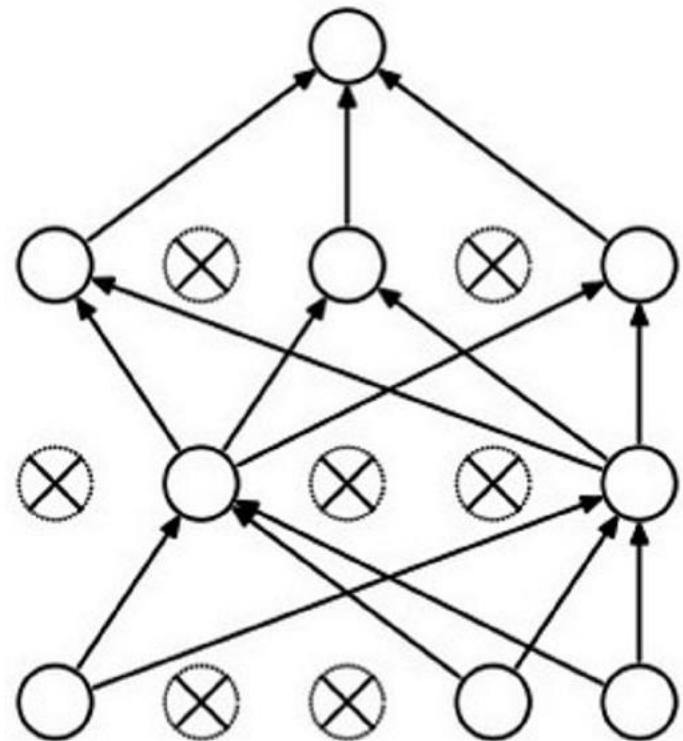
(a) Standard Neural Net



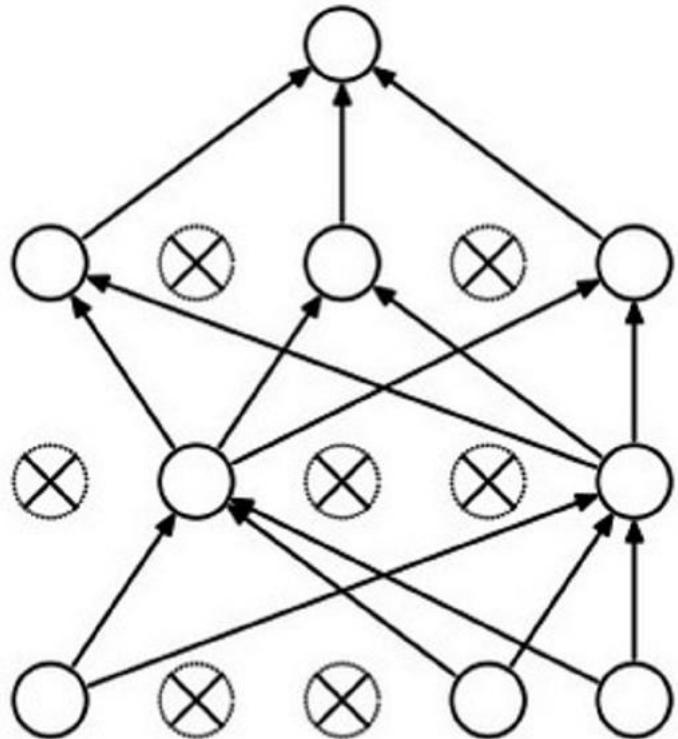
(b) After applying dropout.

[Srivastava et al., 2014]

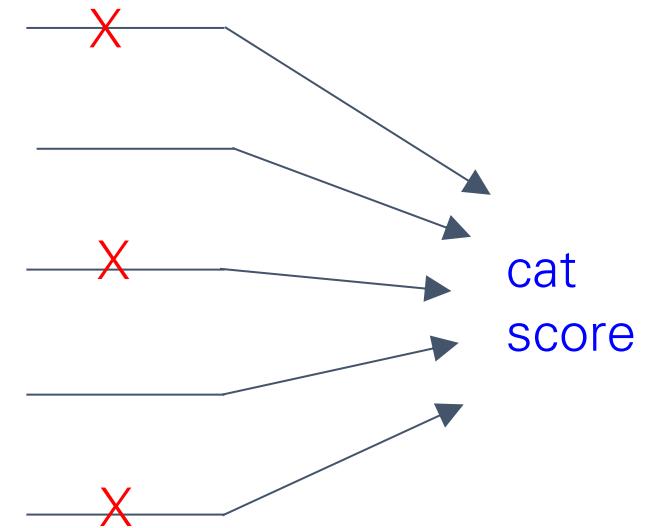
Waaaaait a second...
How could this possibly be a good idea?



Waaaait a second... How could this possibly be a good idea?



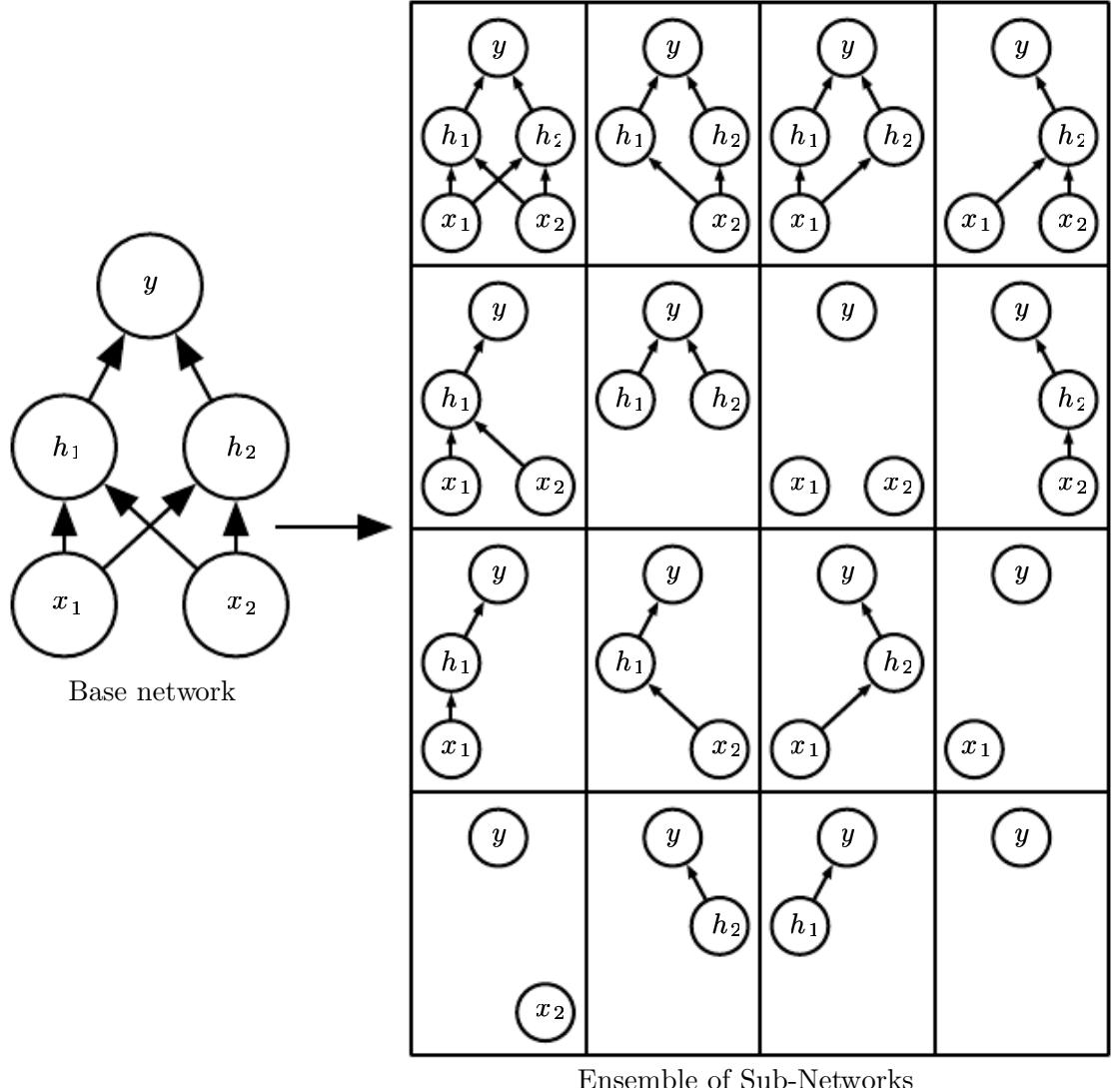
Forces the network to have a redundant representation.



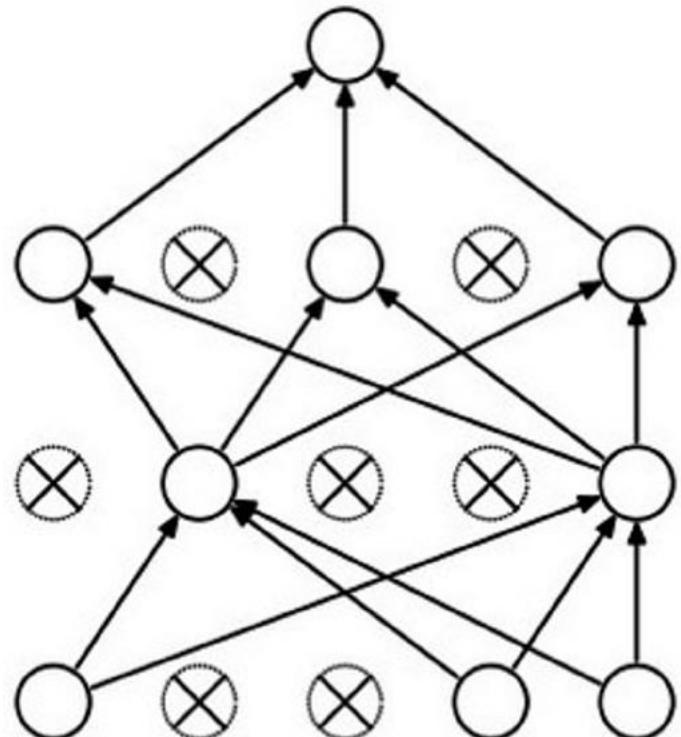
Waaaaait a second... How could this possibly be a good idea?

Another interpretation:

- Dropout is training a large ensemble of models (that share parameters).
- Each binary mask is one model, gets trained on only ~one datapoint.



At test time....



Ideally:

want to integrate out all the noise

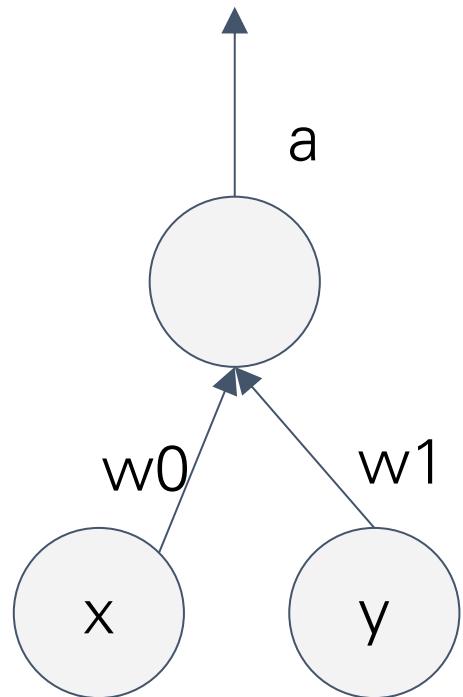
Monte Carlo approximation:

do many forward passes with different dropout masks, average all predictions

At test time....

Can in fact do this with a single forward pass! (approximately)

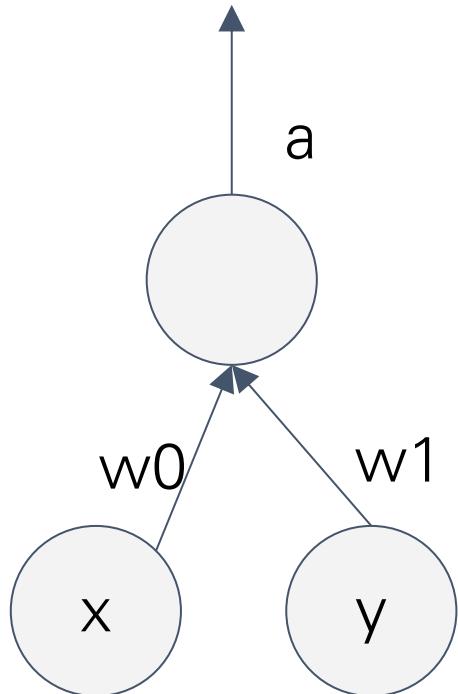
Leave all input neurons turned on (no dropout).



At test time....

Can in fact do this with a single forward pass! (approximately)

Leave all input neurons turned on (no dropout).

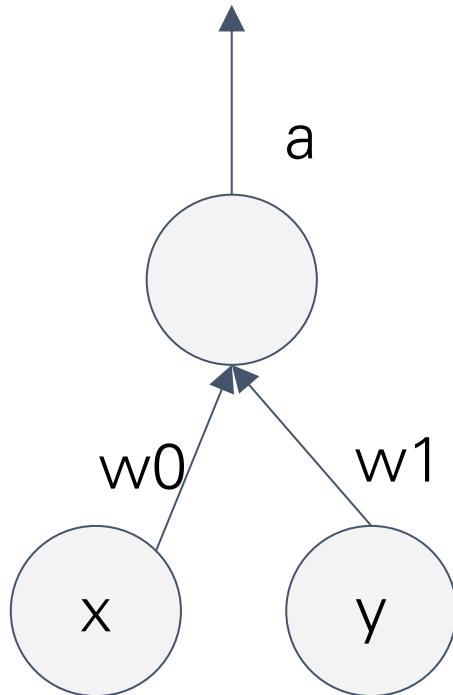


(this can be shown to be an
approximation to evaluating the
whole ensemble)

At test time....

Can in fact do this with a single forward pass! (approximately)

Leave all input neurons turned on (no dropout).



during test: $\mathbf{a = w0*x + w1*y}$

during train:

$$\begin{aligned} E[a] &= \frac{1}{4} * (w0*0 + w1*0 \\ &\quad w0*0 + w1*y \\ &\quad w0*x + w1*0 \\ &\quad w0*x + w1*y) \\ &= \frac{1}{4} * (2 w0*x + 2 w1*y) \\ &= \frac{1}{2} * (\mathbf{w0*x + w1*y}) \end{aligned}$$

With $p=0.5$, using all inputs in the forward pass would inflate the activations by 2x from what the network was "used to" during training!

=> Have to compensate by scaling the activations back down by $\frac{1}{2}$

We can do something approximate analytically

```
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 forward pass

scale at test time

More common: “Inverted dropout”

```
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!



Optimization

Training a neural network, main loop:

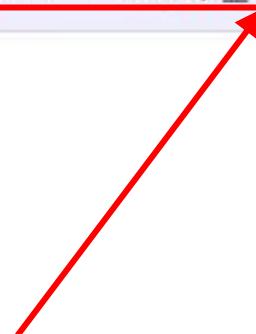
```
# Vanilla Gradient Descent

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

Training a neural network, main loop:

```
# Vanilla Gradient Descent

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



simple gradient descent update
now: complicate.

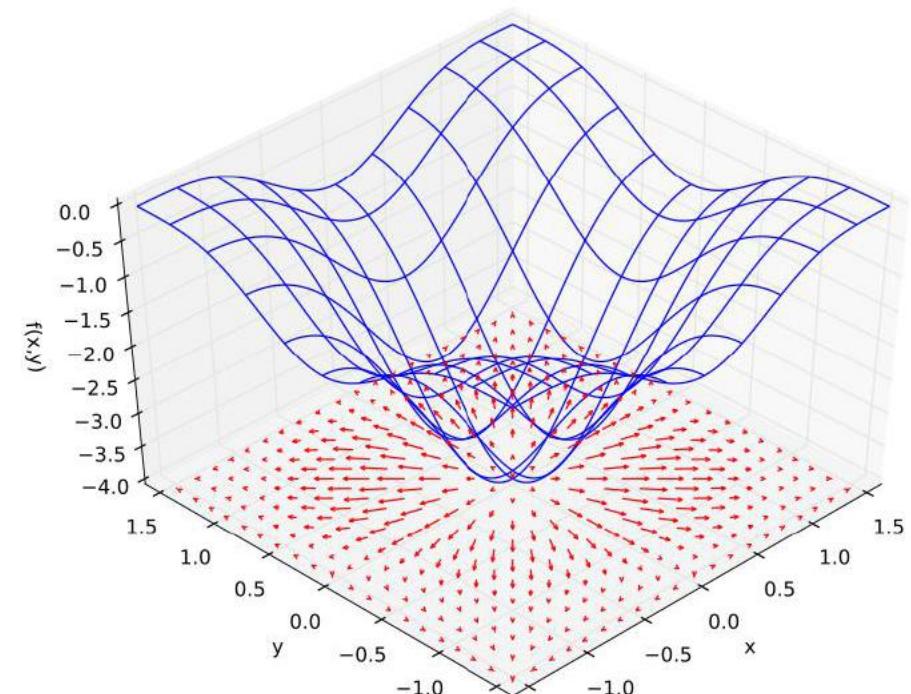
Gradients

- When we write $\nabla_W L(W)$, we mean the vector of partial derivatives wrt all coordinates of W :

$$\nabla_W L(W) = \left[\frac{\partial L}{\partial W_1}, \frac{\partial L}{\partial W_2}, \dots, \frac{\partial L}{\partial W_m} \right]^T$$

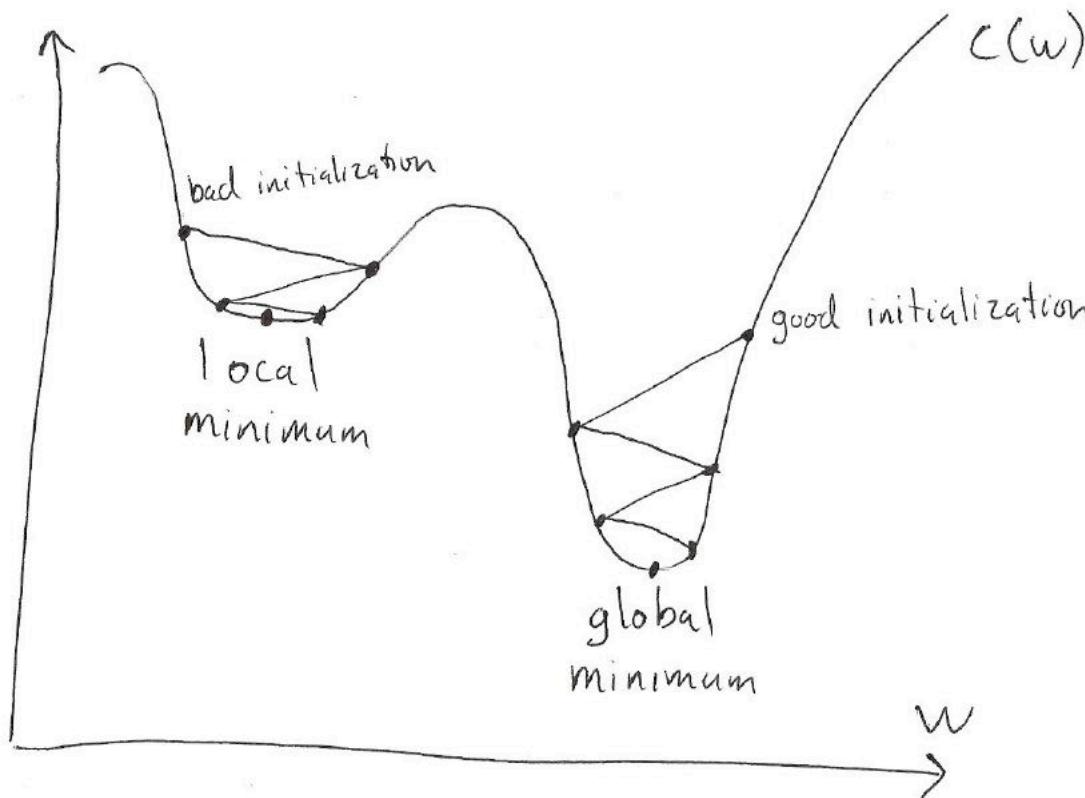
where $\frac{\partial L}{\partial W_i}$ measures how fast the loss changes vs. change in W_i

- In figure:** loss surface is blue, gradient vectors are red:
- When $\nabla_W L(W) = 0$, it means all the partials are zero, i.e. the loss is not changing in any direction.
- Note: arrows point out from a minimum, in toward a maximum



Optimization

- Visualizing gradient descent in one dimension:



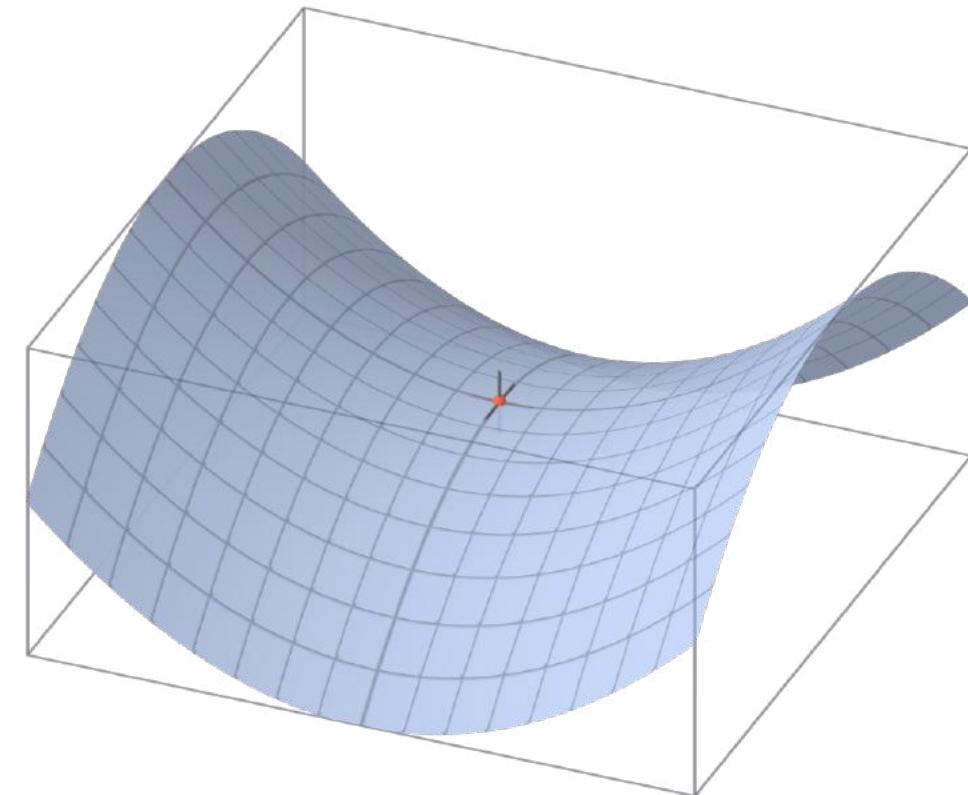
- The regions where gradient descent converges to a particular local minimum are called **basins of attraction**.

Local Minima

- Since the optimization problem is non-convex, it probably has local minima.
- This kept people from using neural nets for a long time, because they wanted guarantees they were getting the optimal solution.
- But are local minima really a problem?
 - Common view among practitioners: yes, there are local minima, but they're probably still pretty good.
 - Maybe your network wastes some hidden units, but then you can just make it larger.
 - It's very hard to demonstrate the existence of local minima in practice.
 - In any case, other optimization-related issues are much more important.

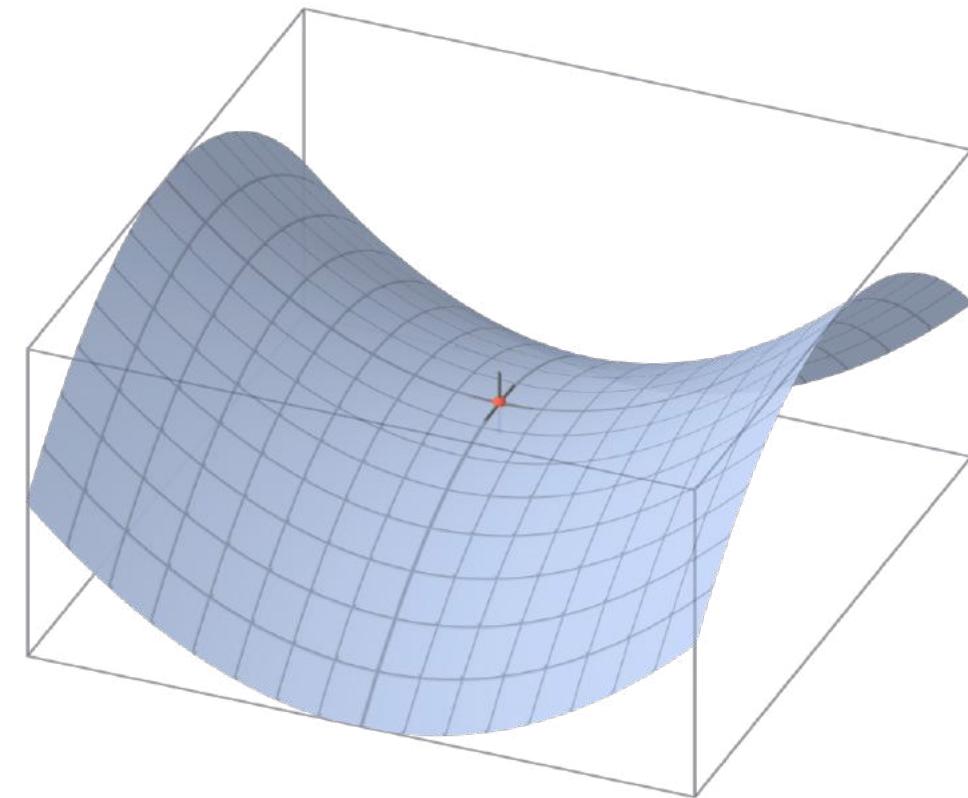
Saddle Points

- At a **saddle point**, $\frac{\partial L}{\partial W} = 0$ even though we are not at a minimum. Some directions curve upwards, and others curve downwards.
- When would saddle points be a problem?
 - If we're exactly on the saddle point, then we're stuck.
 - If we're slightly to the side, then we can get unstuck.



Saddle Points

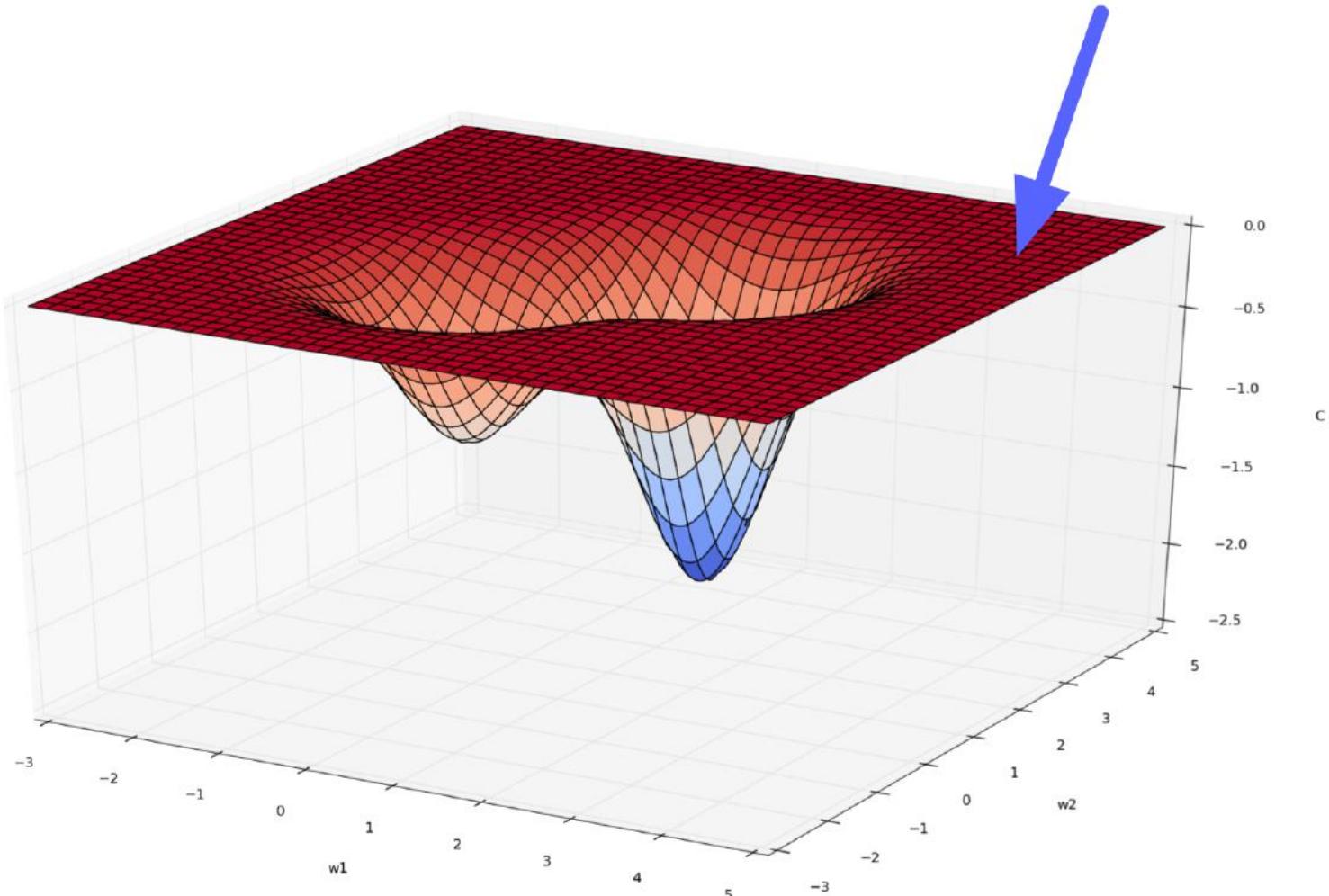
- At a **saddle point**, $\frac{\partial L}{\partial W} = 0$ even though we are not at a minimum. Some directions curve upwards, and others curve downwards.
- When would saddle points be a problem?
 - If we're exactly on the saddle point, then we're stuck.
 - If we're slightly to the side, then we can get unstuck.



Saddle points much more common in high dimensions!

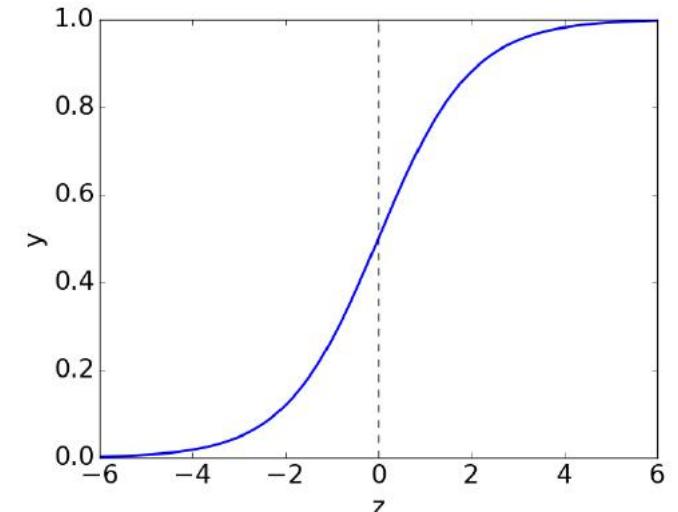
Plateaux

- A flat region is called a **plateau**. (Plural: plateaux)

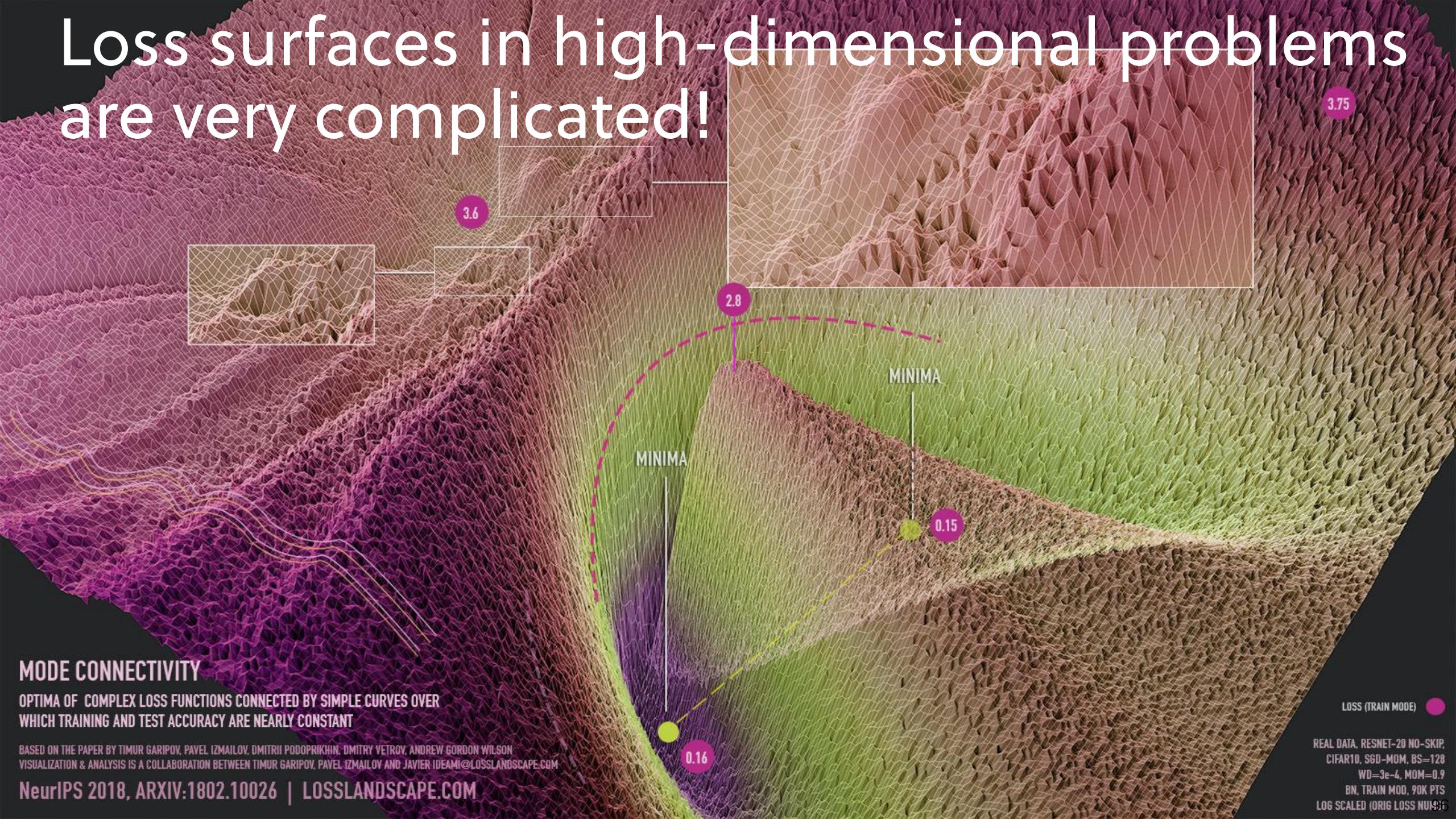


Plateaux

- An important example of a plateau is a **saturated unit**. This is when it is in the flat region of its activation function.
- If $\phi'(z_i)$ is always close to zero, then the weights will get stuck.
- If there is a ReLU unit whose input z_i is always negative, the weight derivatives will be exactly 0. We call this a **dead unit**.



Loss surfaces in high-dimensional problems are very complicated!



Batch Gradient Descent

Algorithm 1 Batch Gradient Descent at Iteration k

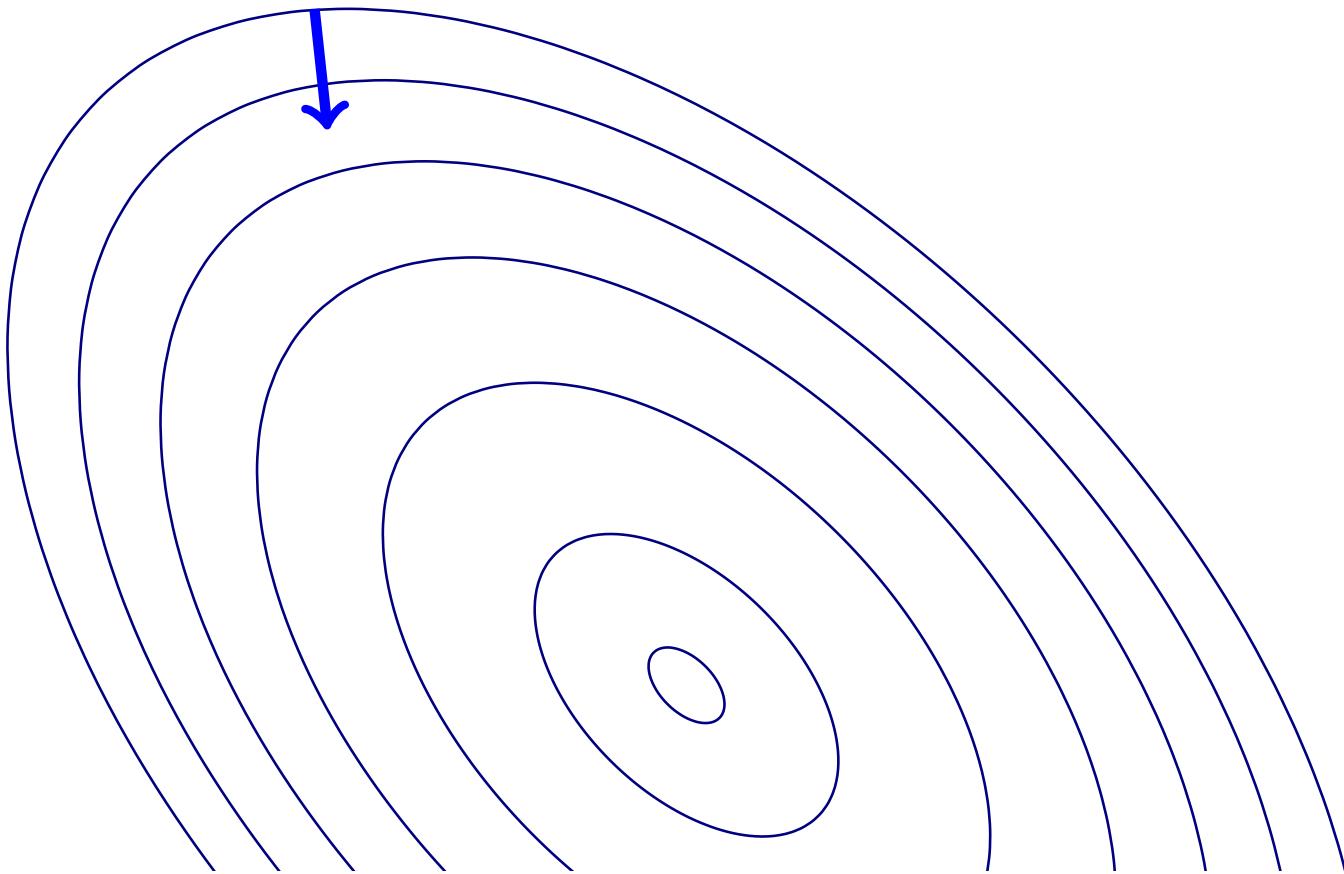
Require: Learning rate ϵ_k

Require: Initial Parameter θ

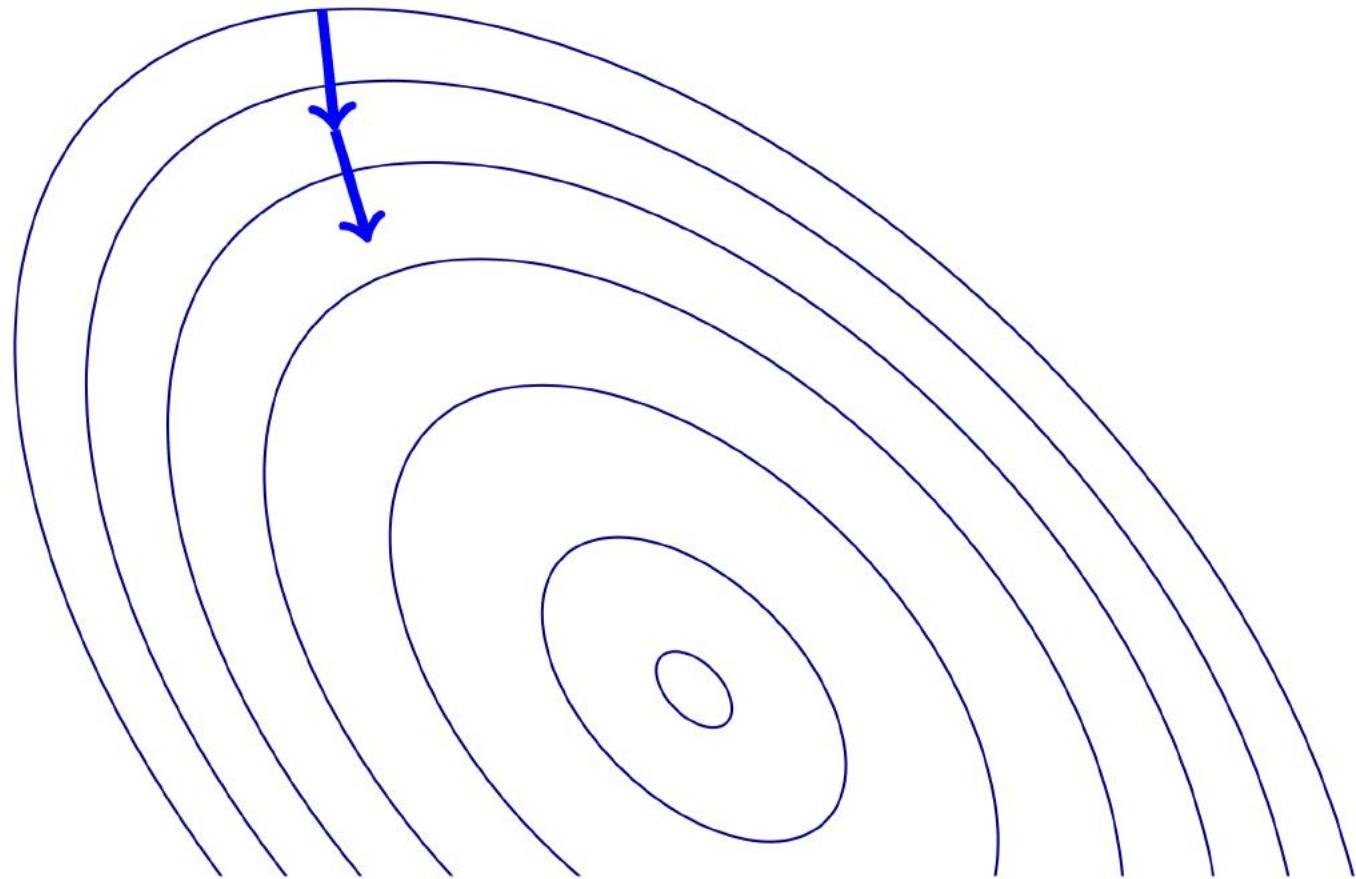
- 1: **while** stopping criteria not met **do**
 - 2: Compute gradient estimate over N examples:
 - 3: $\hat{\mathbf{g}} \leftarrow +\frac{1}{N} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$
 - 4: Apply Update: $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$
 - 5: **end while**
-

- Positive: Gradient estimates are stable
- Negative: Need to compute gradients over the entire training for one update

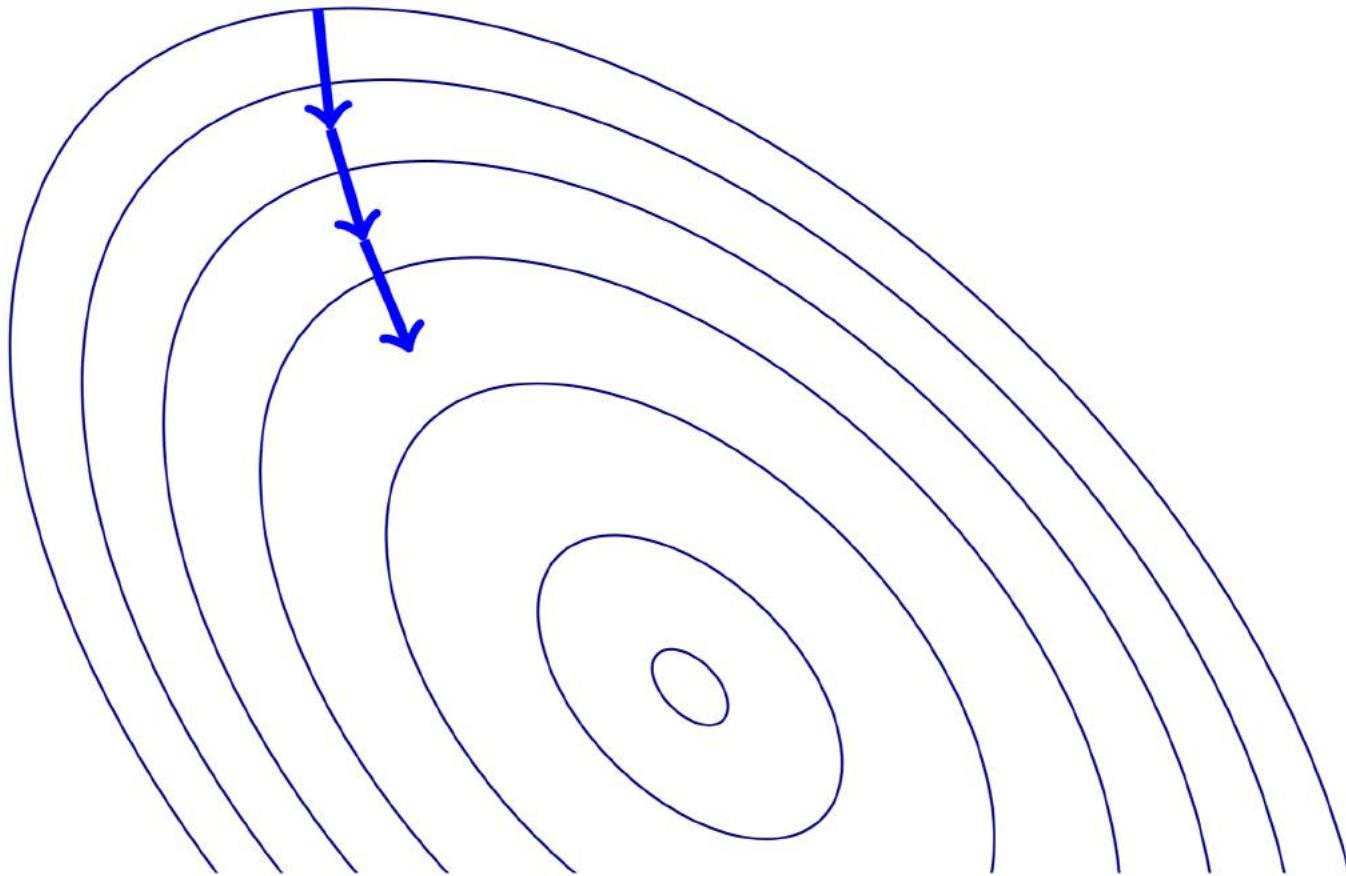
Gradient Descent



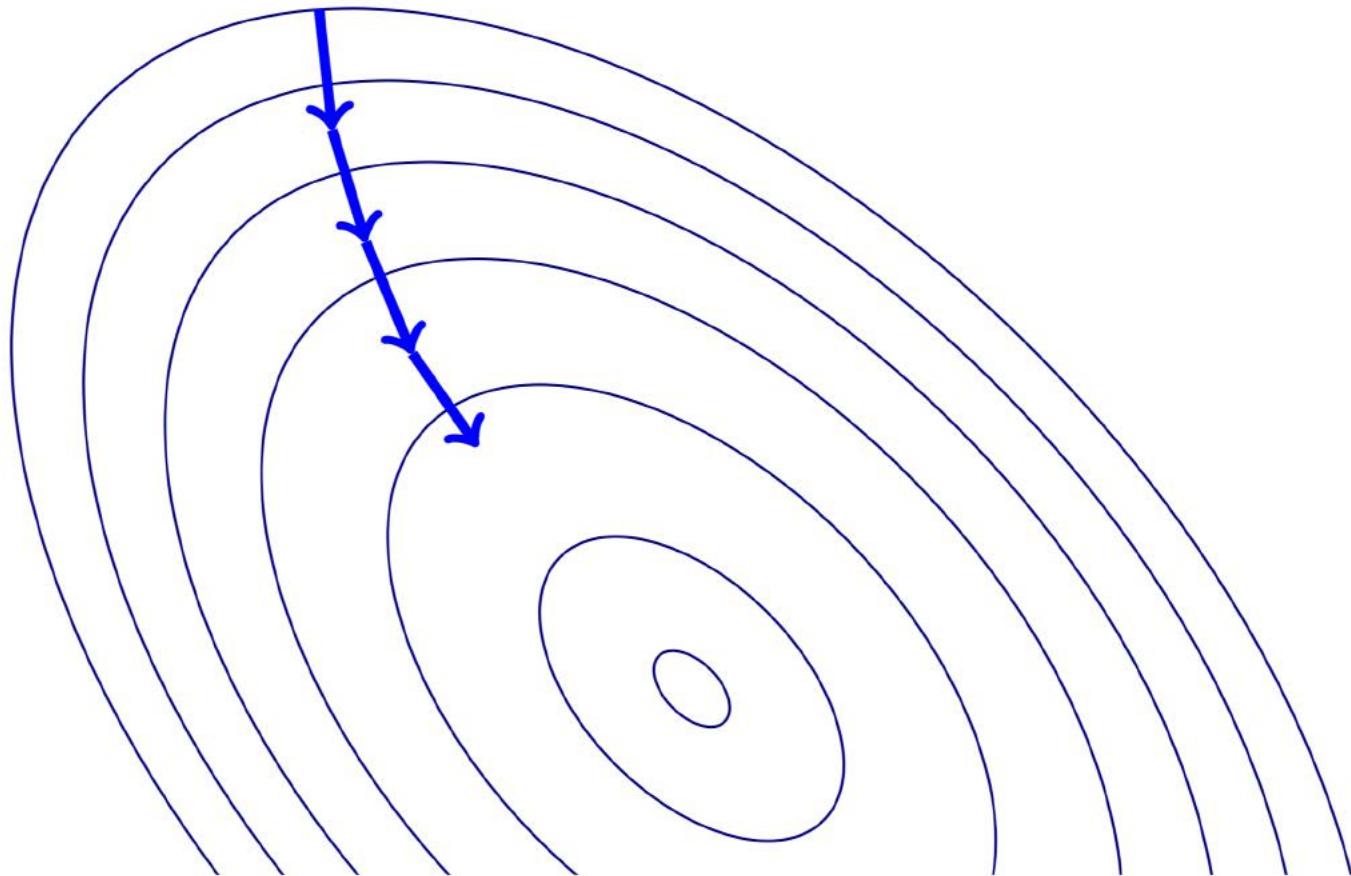
Gradient Descent



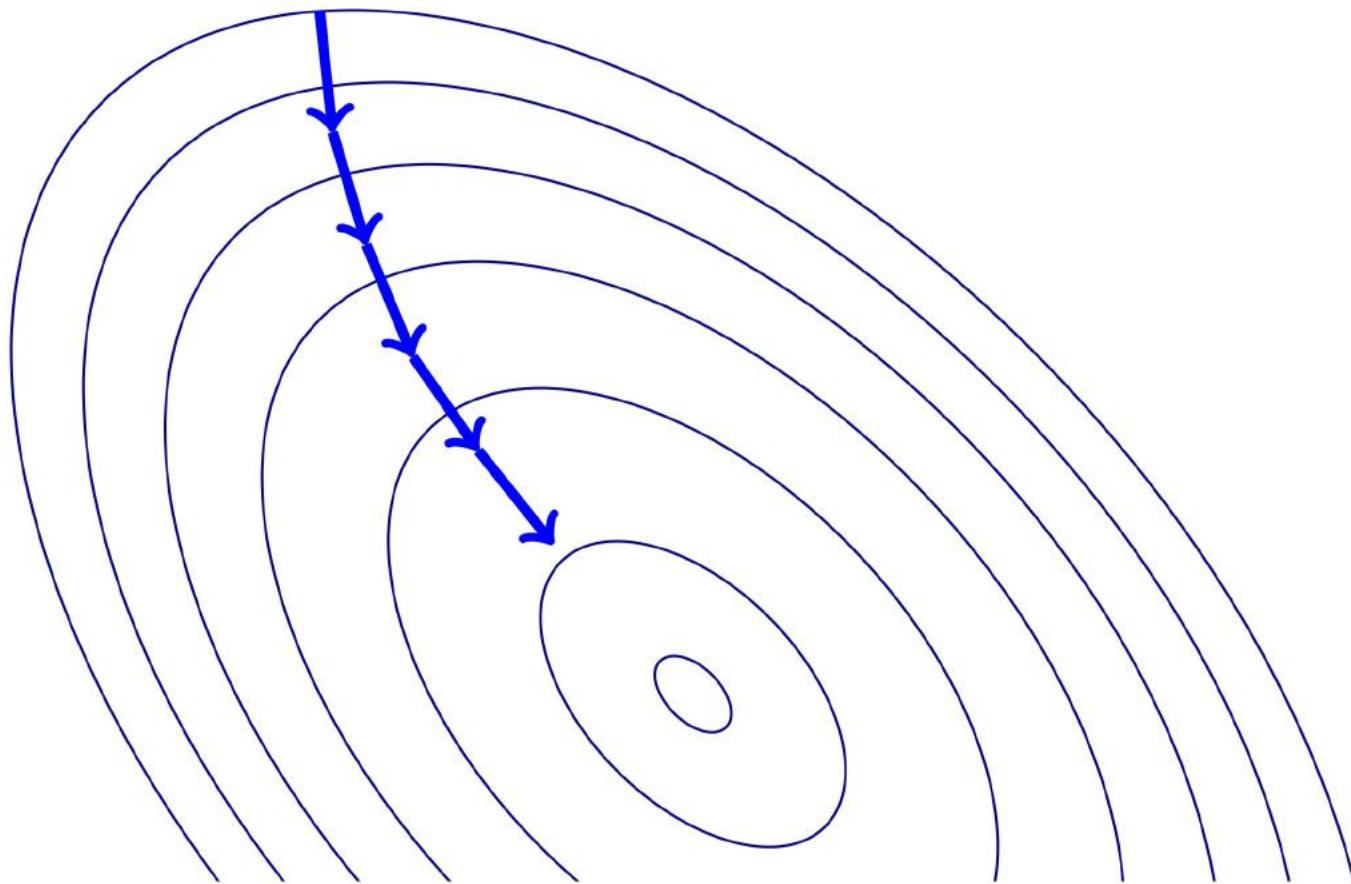
Gradient Descent



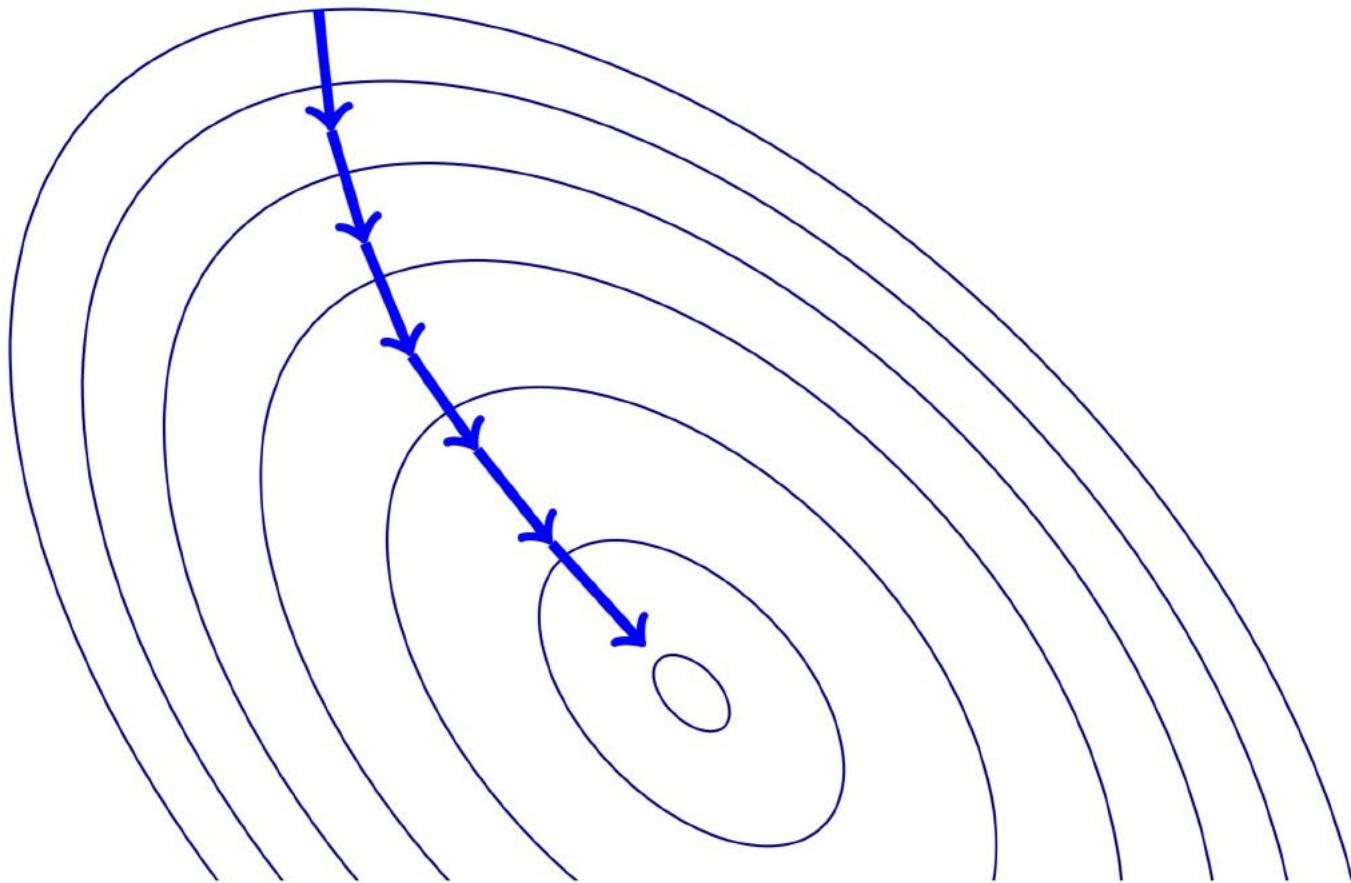
Gradient Descent



Gradient Descent



Gradient Descent



Stochastic Batch Gradient Descent

Algorithm 2 Stochastic Gradient Descent at Iteration k

Require: Learning rate ϵ_k

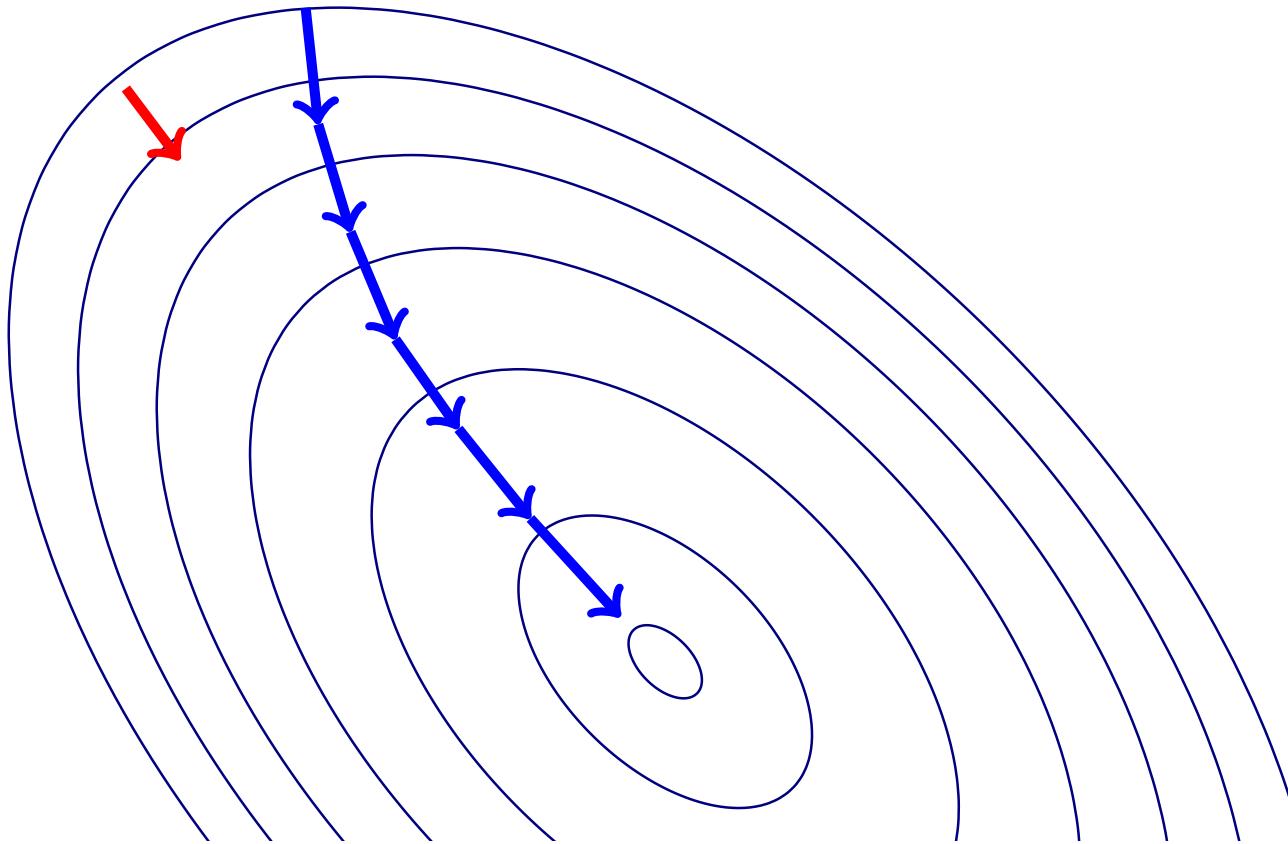
Require: Initial Parameter θ

- 1: **while** stopping criteria not met **do**
 - 2: Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set
 - 3: Compute gradient estimate:
 - 4: $\hat{\mathbf{g}} \leftarrow +\nabla_{\theta} L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$
 - 5: Apply Update: $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$
 - 6: **end while**
-

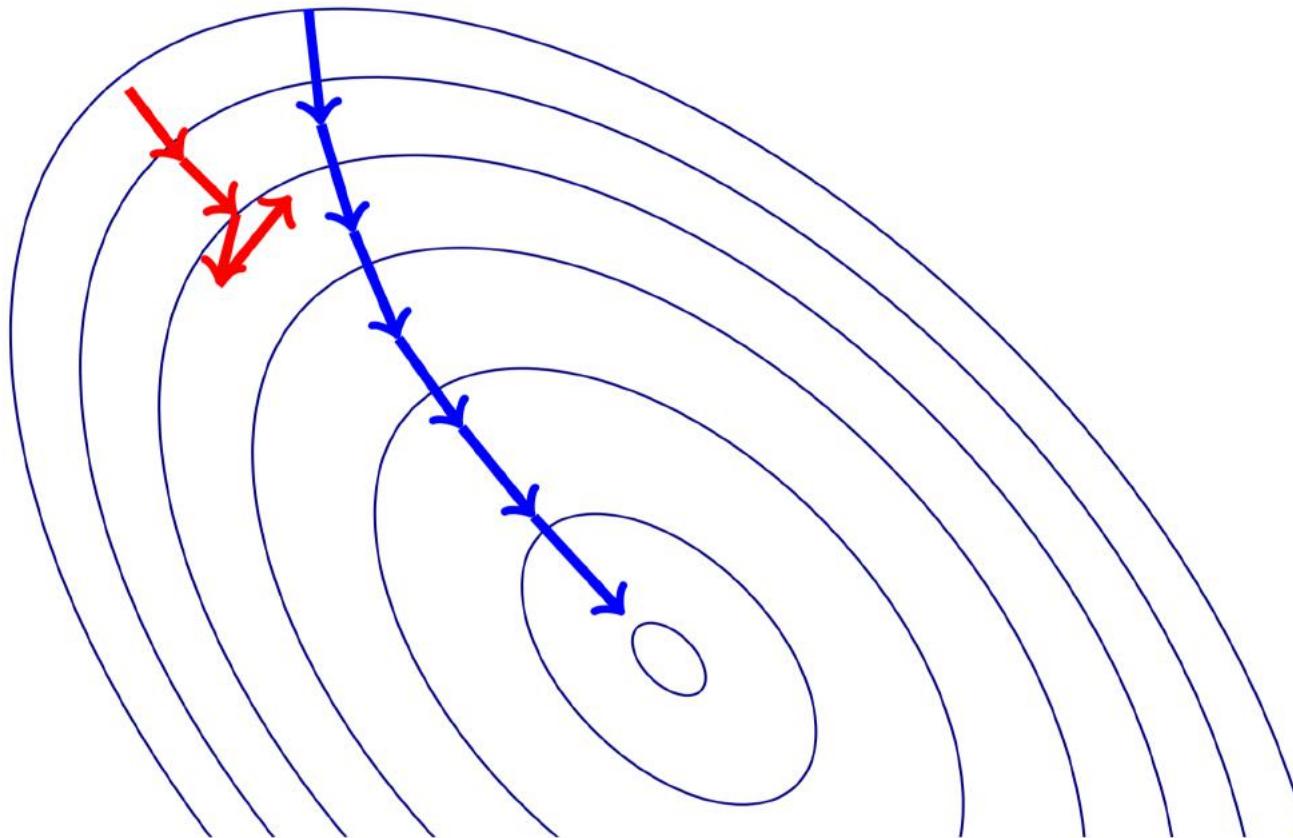
Minibatching

- Potential Problem: Gradient estimates can be very noisy
- Obvious Solution: Use larger mini-batches
- Advantage: Computation time per update does not depend on number of training examples N
- This allows convergence on extremely large datasets
- See: Large Scale Learning with Stochastic Gradient Descent by Leon Bottou

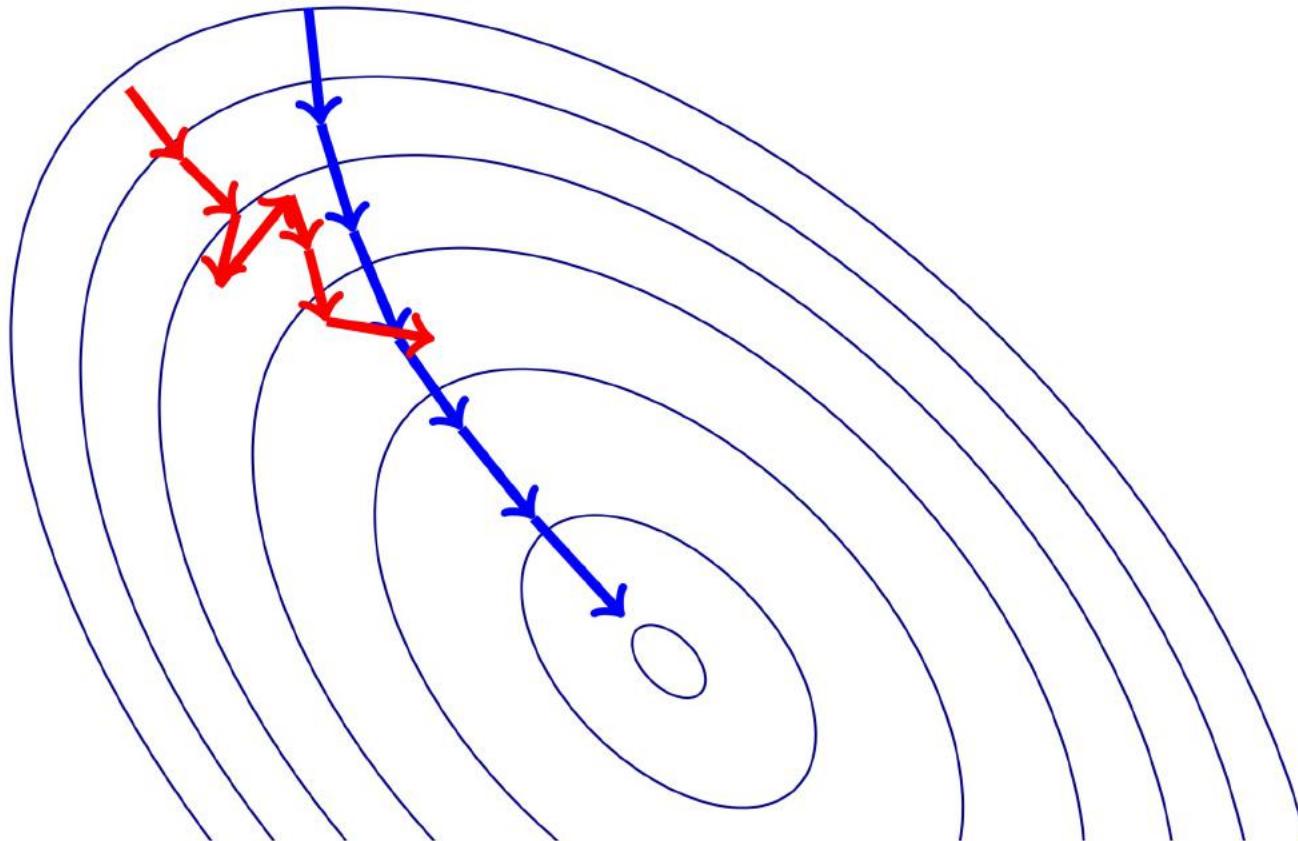
Stochastic Gradient Descent



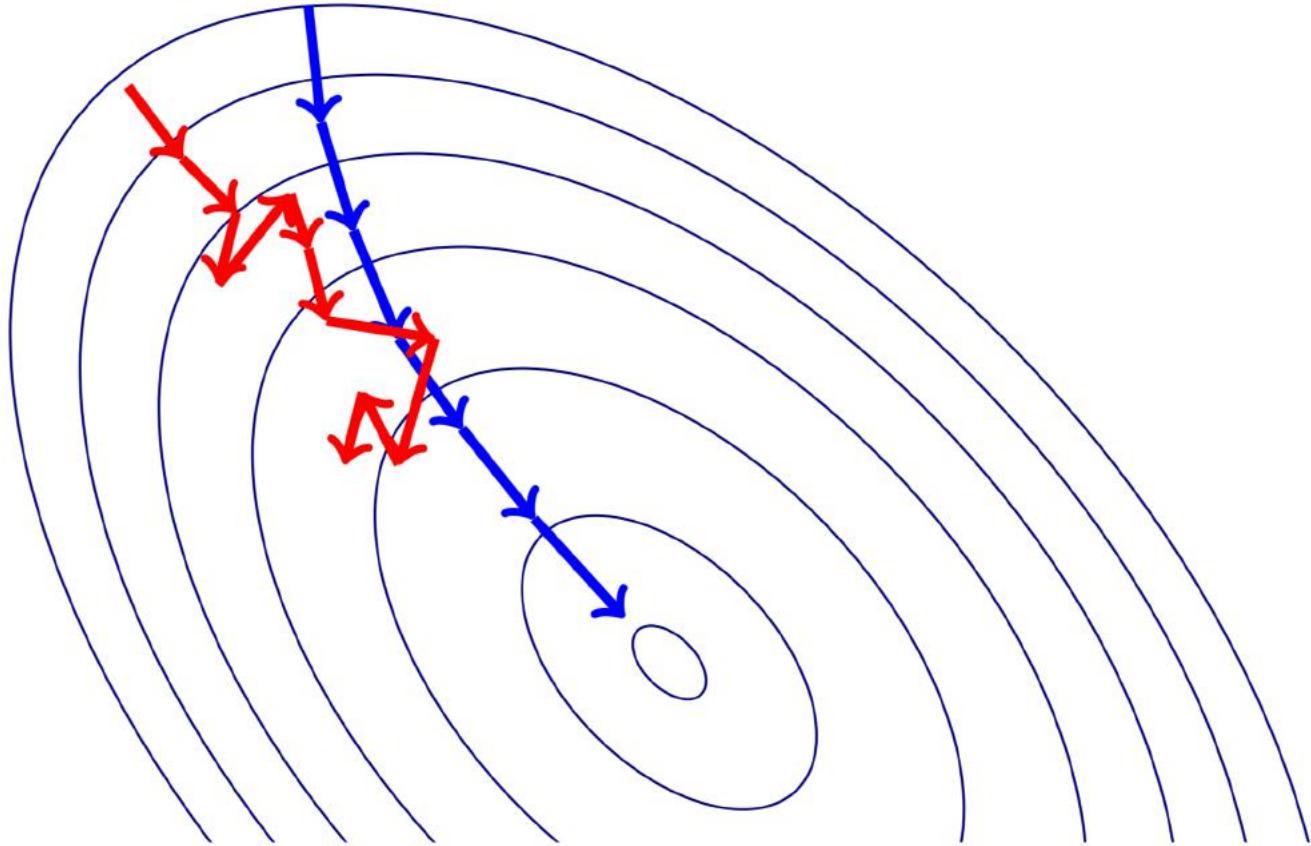
Stochastic Gradient Descent



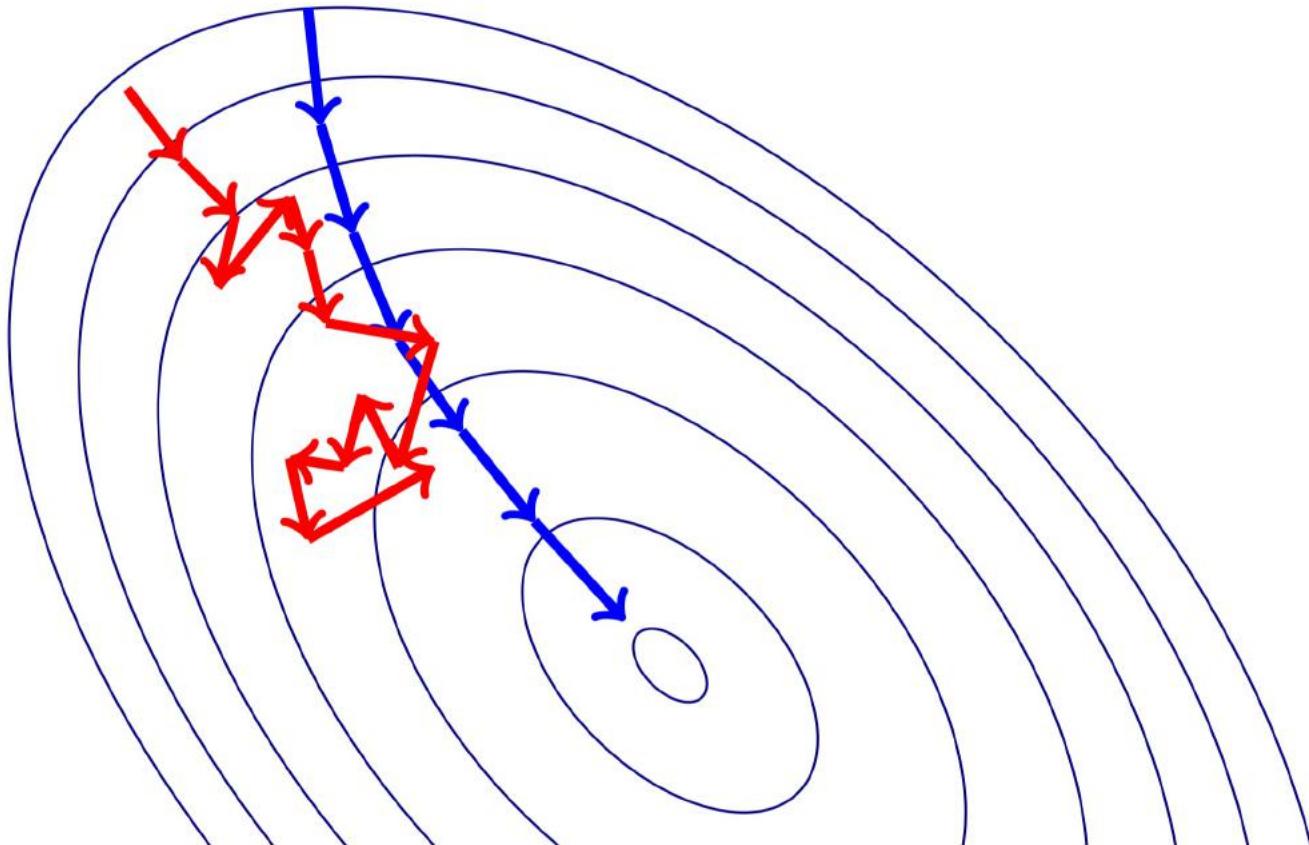
Stochastic Gradient Descent



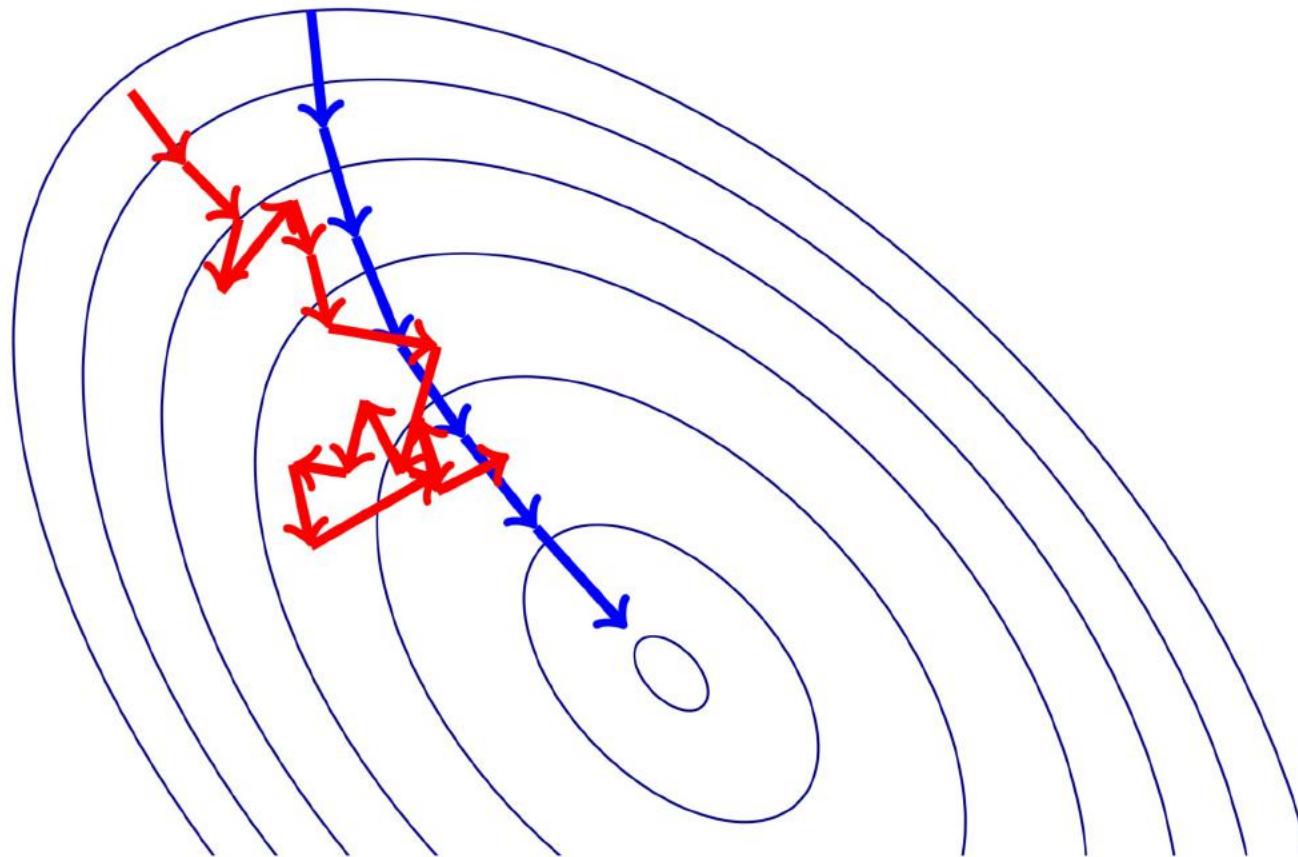
Stochastic Gradient Descent



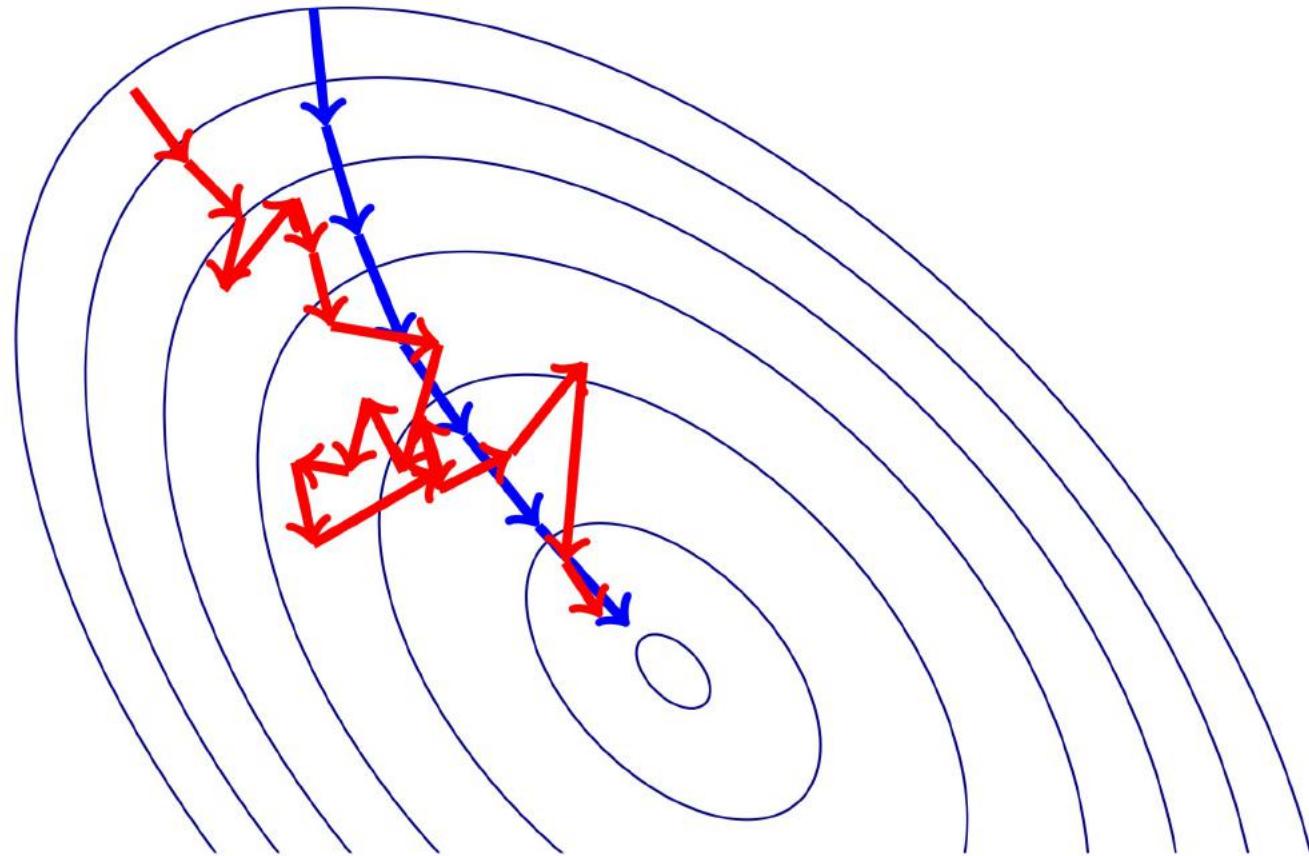
Stochastic Gradient Descent



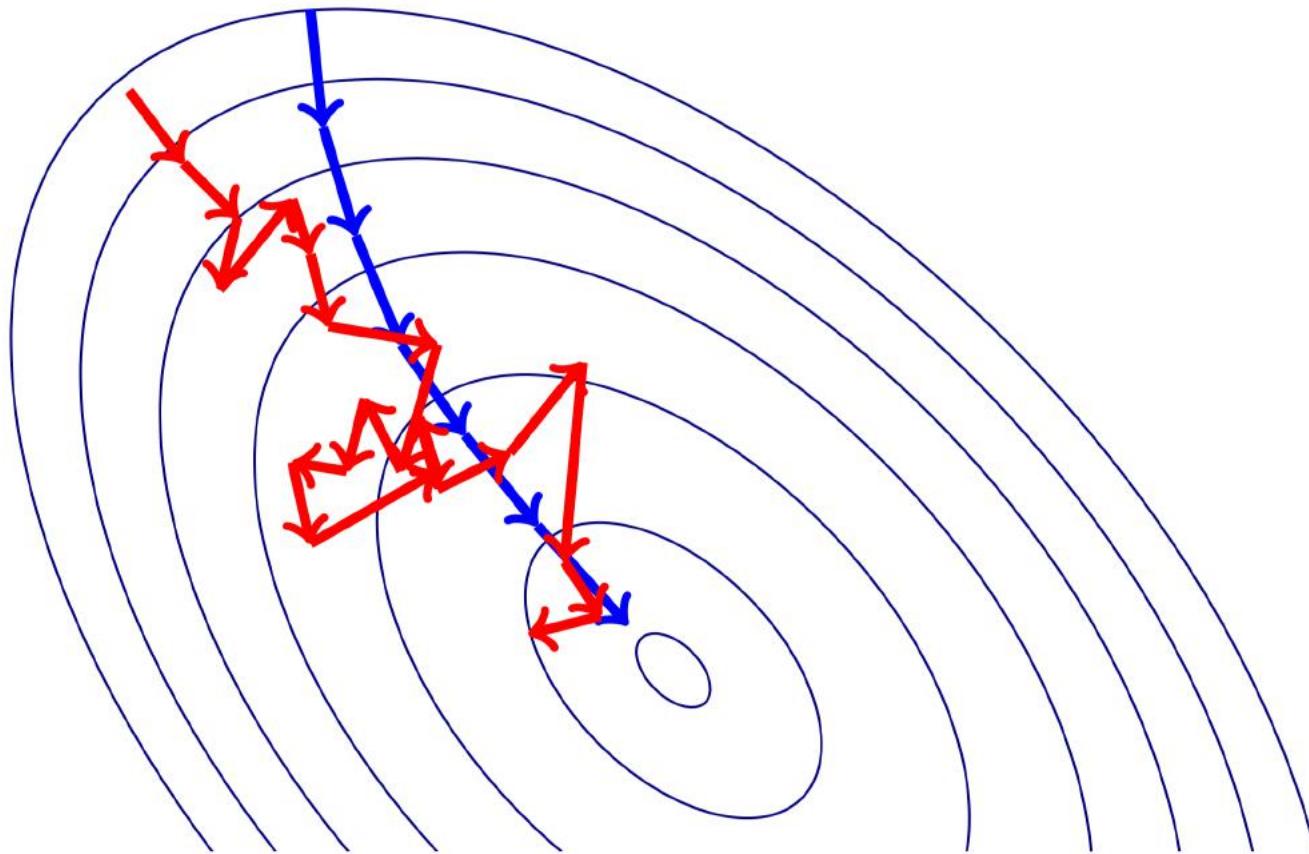
Stochastic Gradient Descent



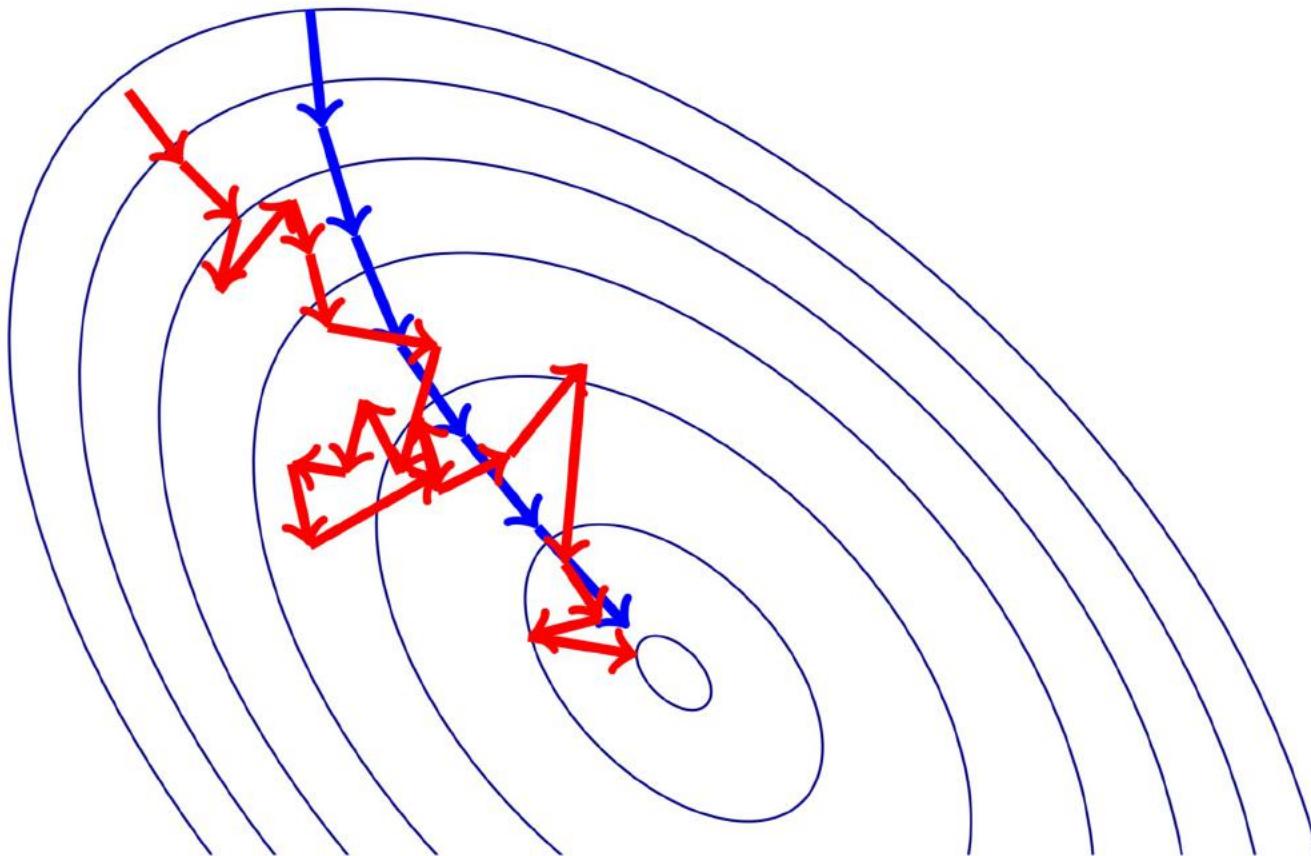
Stochastic Gradient Descent



Stochastic Gradient Descent



Stochastic Gradient Descent



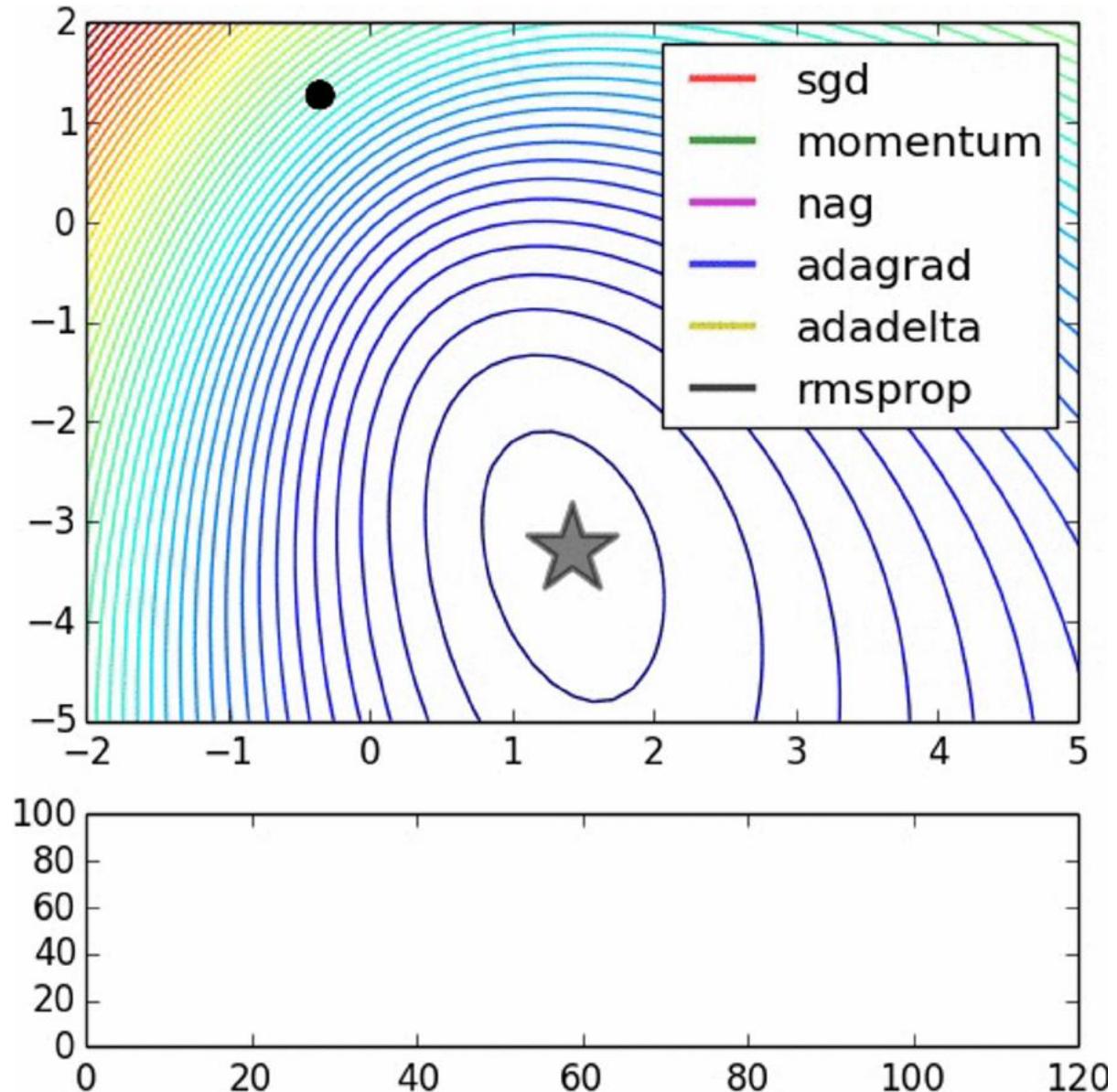
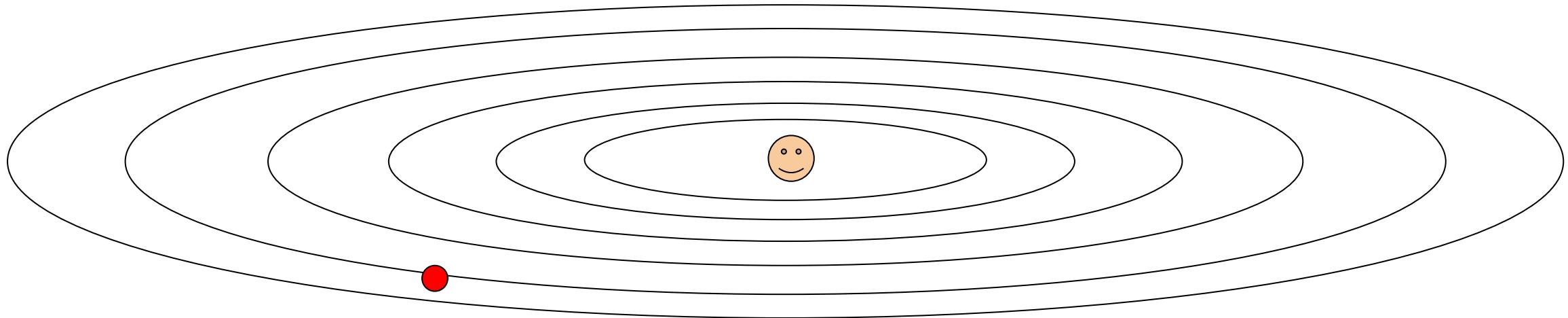


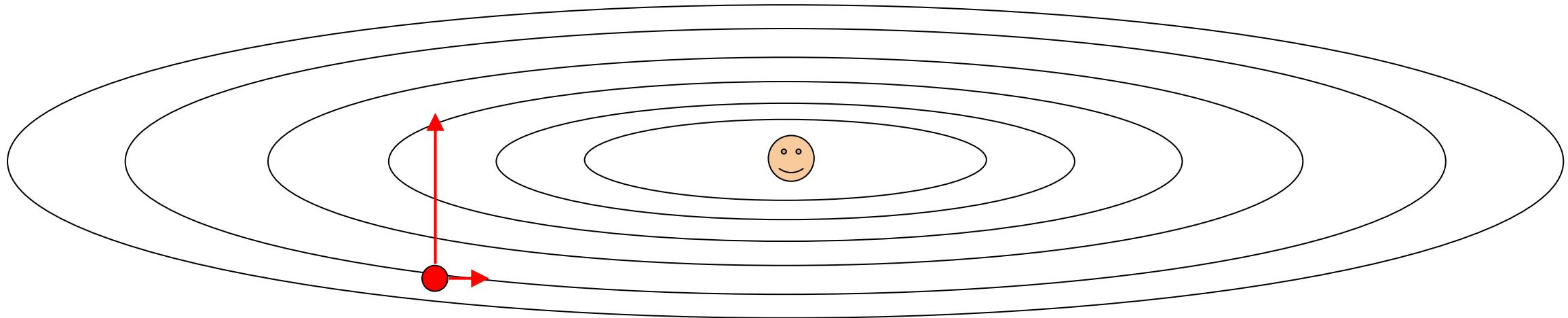
Image credits: Alec Radford

Suppose loss function is steep vertically but shallow horizontally:



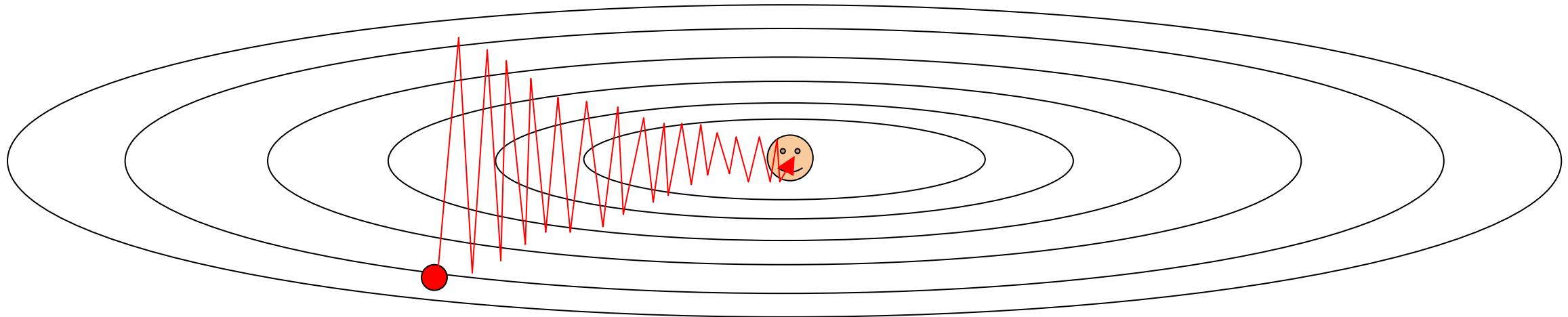
Q: What is the trajectory along which we converge towards the minimum with SGD?

Suppose loss function is steep vertically but shallow horizontally:



Q: What is the trajectory along which we converge towards the minimum with SGD?

Suppose loss function is steep vertically but shallow horizontally:



Q: What is the trajectory along which we converge towards the minimum with SGD?
very slow progress along flat direction, jitter along steep one

Momentum update

SGD

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

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

SGD+Momentum

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

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

Momentum update

SGD

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

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

SGD+Momentum

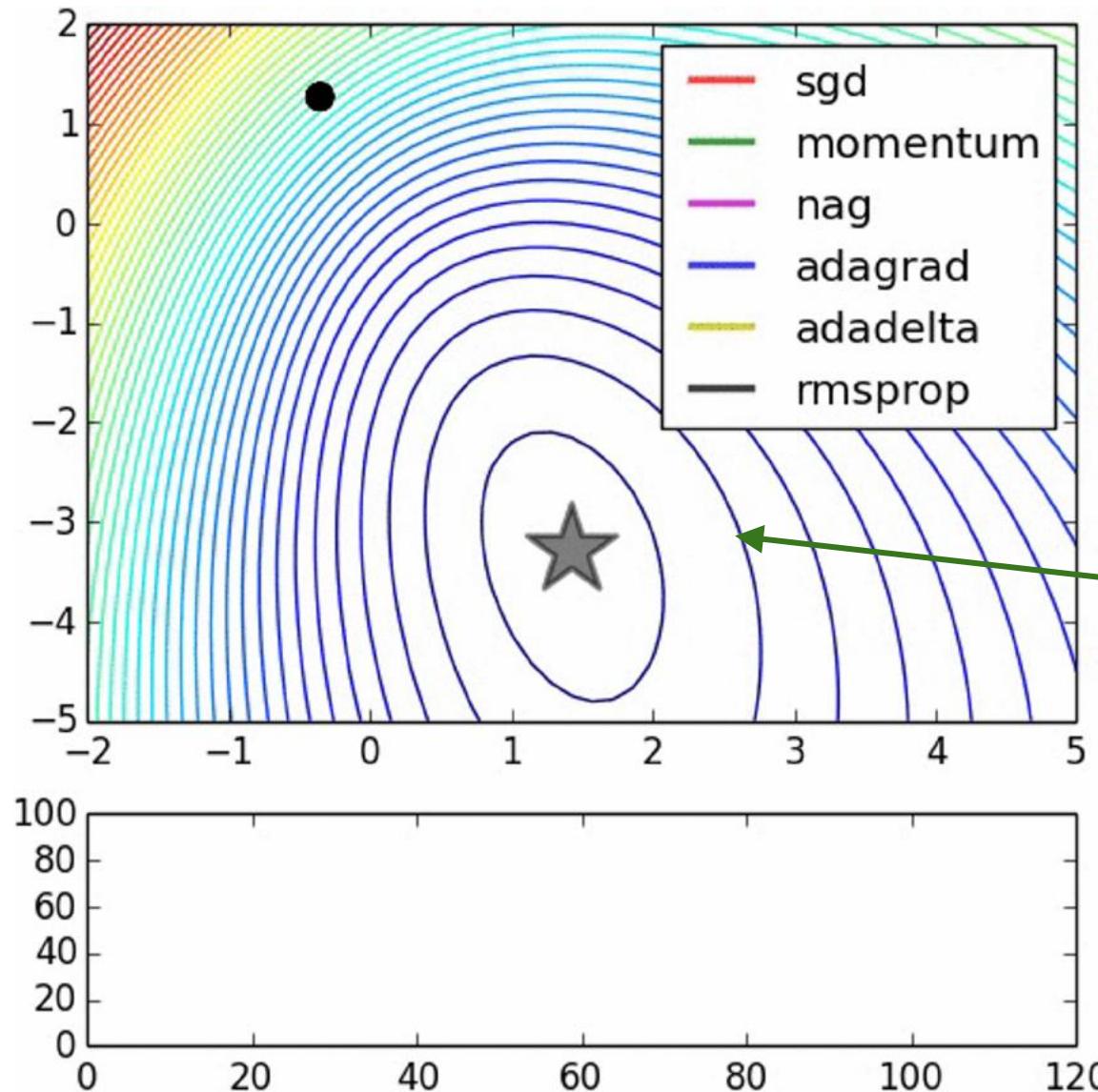
$$\begin{aligned}v_{t+1} &= \rho v_t + \nabla f(x_t) \\x_{t+1} &= x_t - \alpha v_{t+1}\end{aligned}$$

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



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

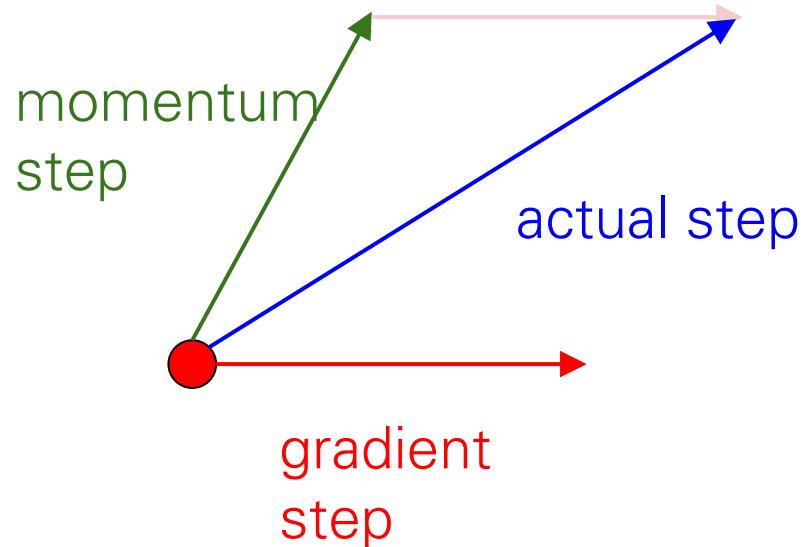
SGD vs Momentum



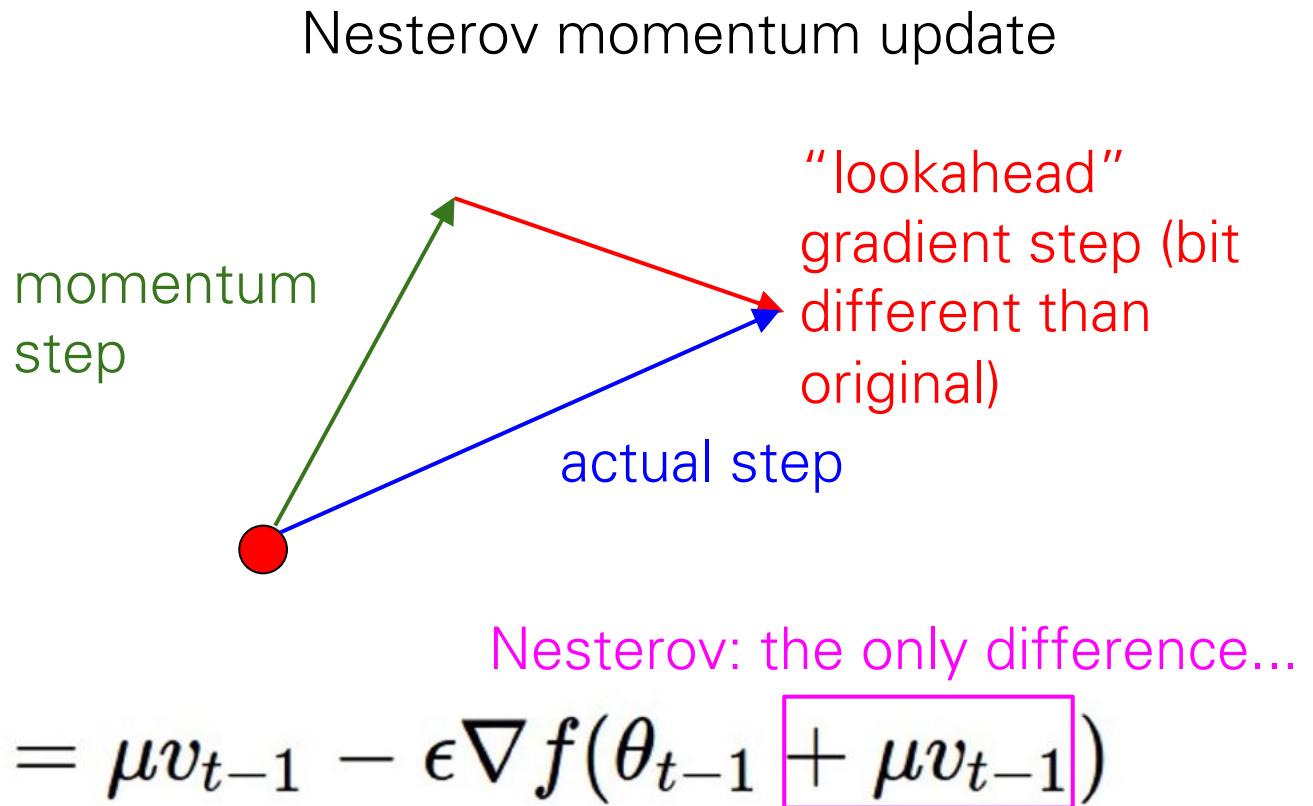
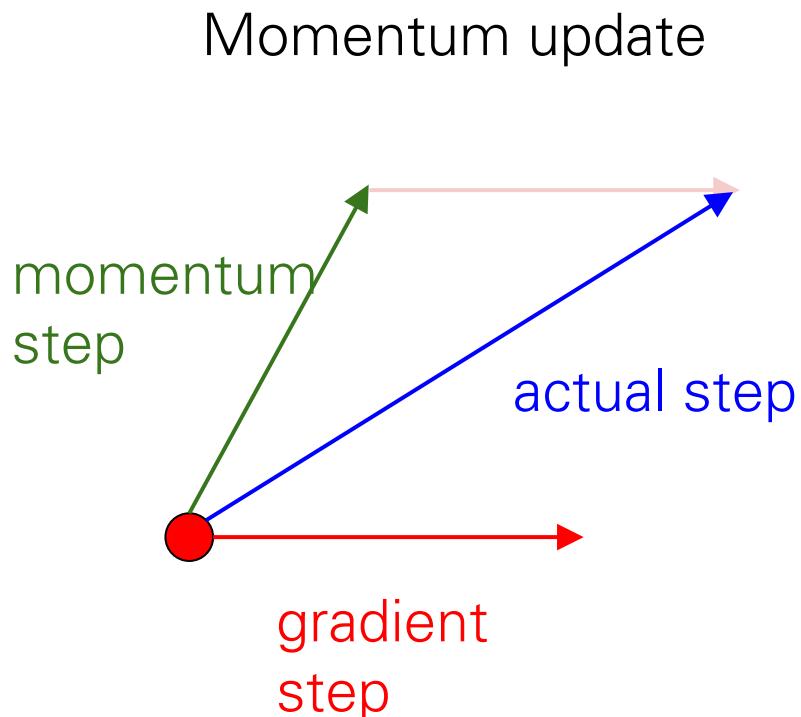
notice momentum
overshooting the target,
but overall getting to the
minimum much faster.

SGD + Momentum

Momentum update



Nesterov Momentum



$$\theta_t = \theta_{t-1} + v_t$$

Nesterov Momentum

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

$$x_{t+1} = x_t + v_{t+1}$$

Nesterov Momentum

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

$$x_{t+1} = x_t + v_{t+1}$$

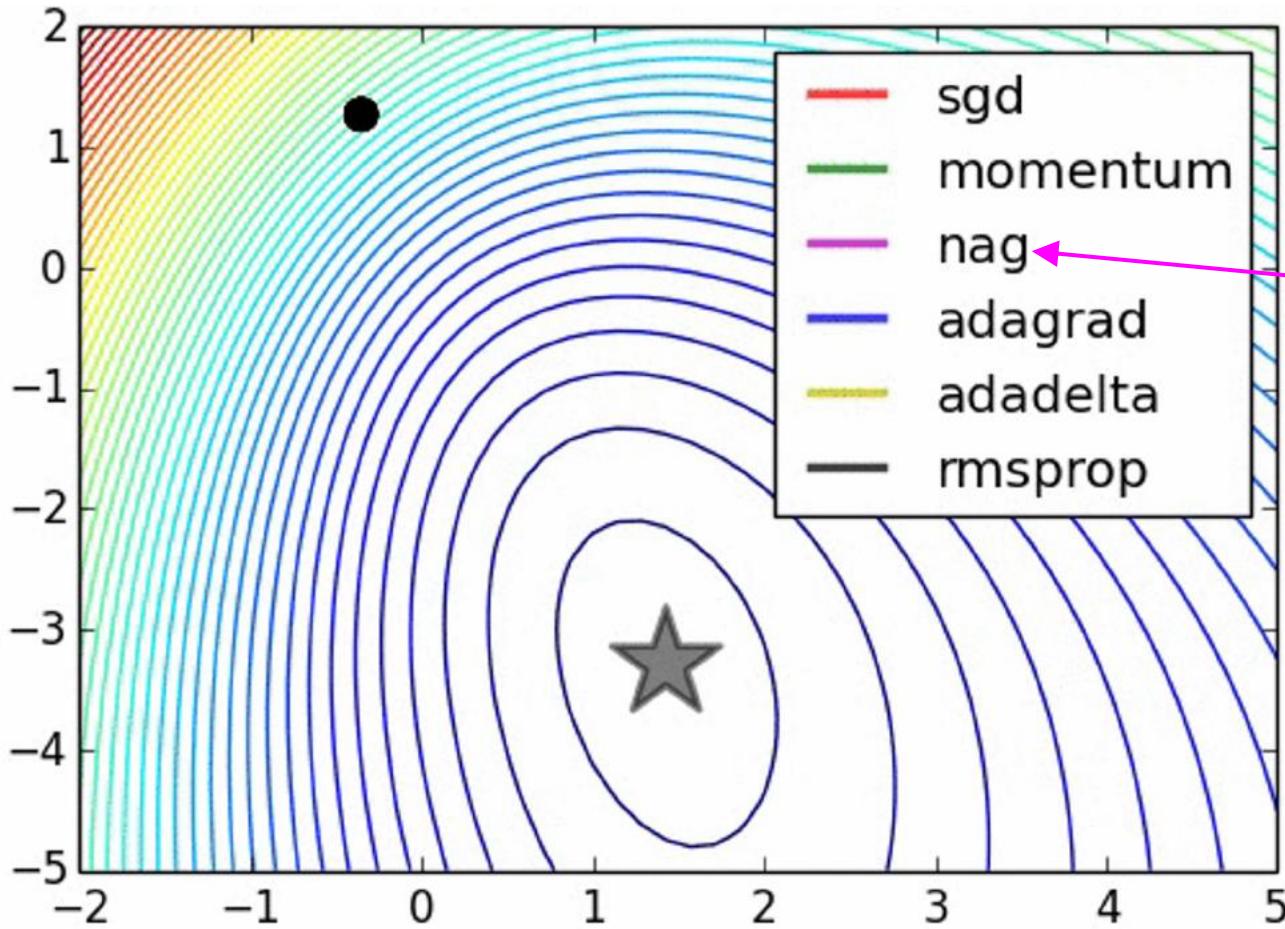
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$

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

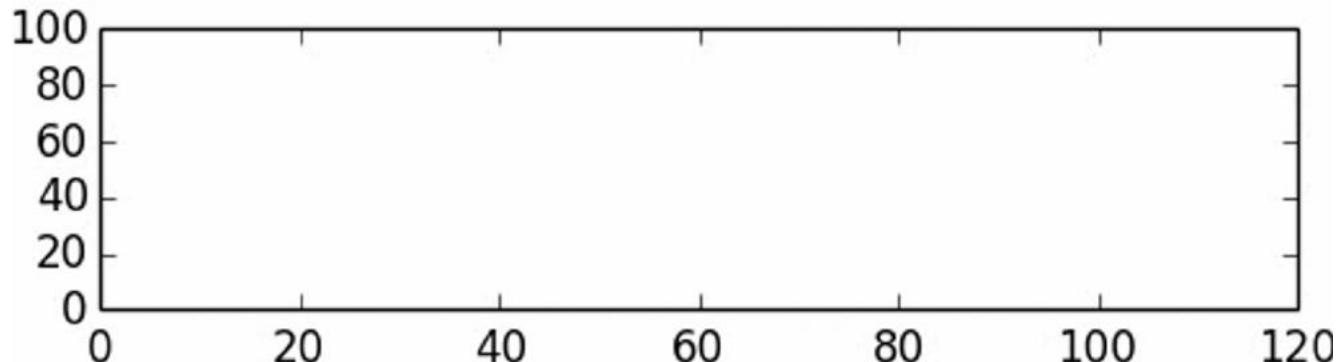
$$v_{t+1} = \rho v_t - \alpha \nabla f(\tilde{x}_t)$$

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

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



nag =
Nesterov
Accelerated
Gradient



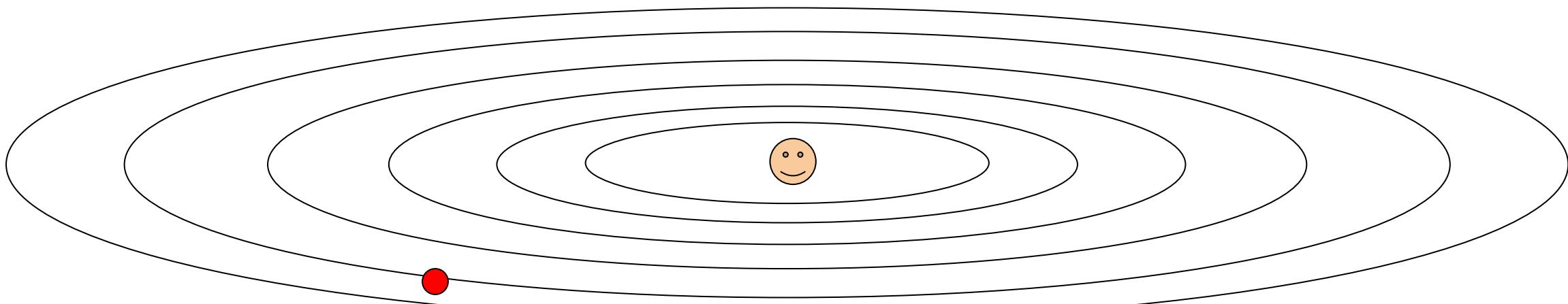
AdaGrad update

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

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

AdaGrad update

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

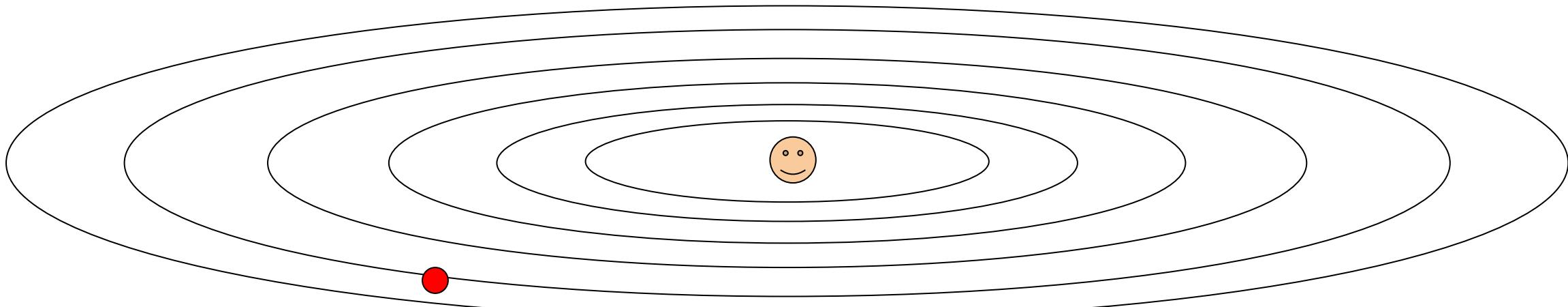


Q: What happens with AdaGrad?

Weights that receive high gradients will have their effective learning rate reduced, while weights that receive small updates will have their effective learning rate increased!

AdaGrad update

```
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?

The adaptive learning scheme is monotonic, which is usually too aggressive and stops the learning process too early.

RMSProp

AdaGrad

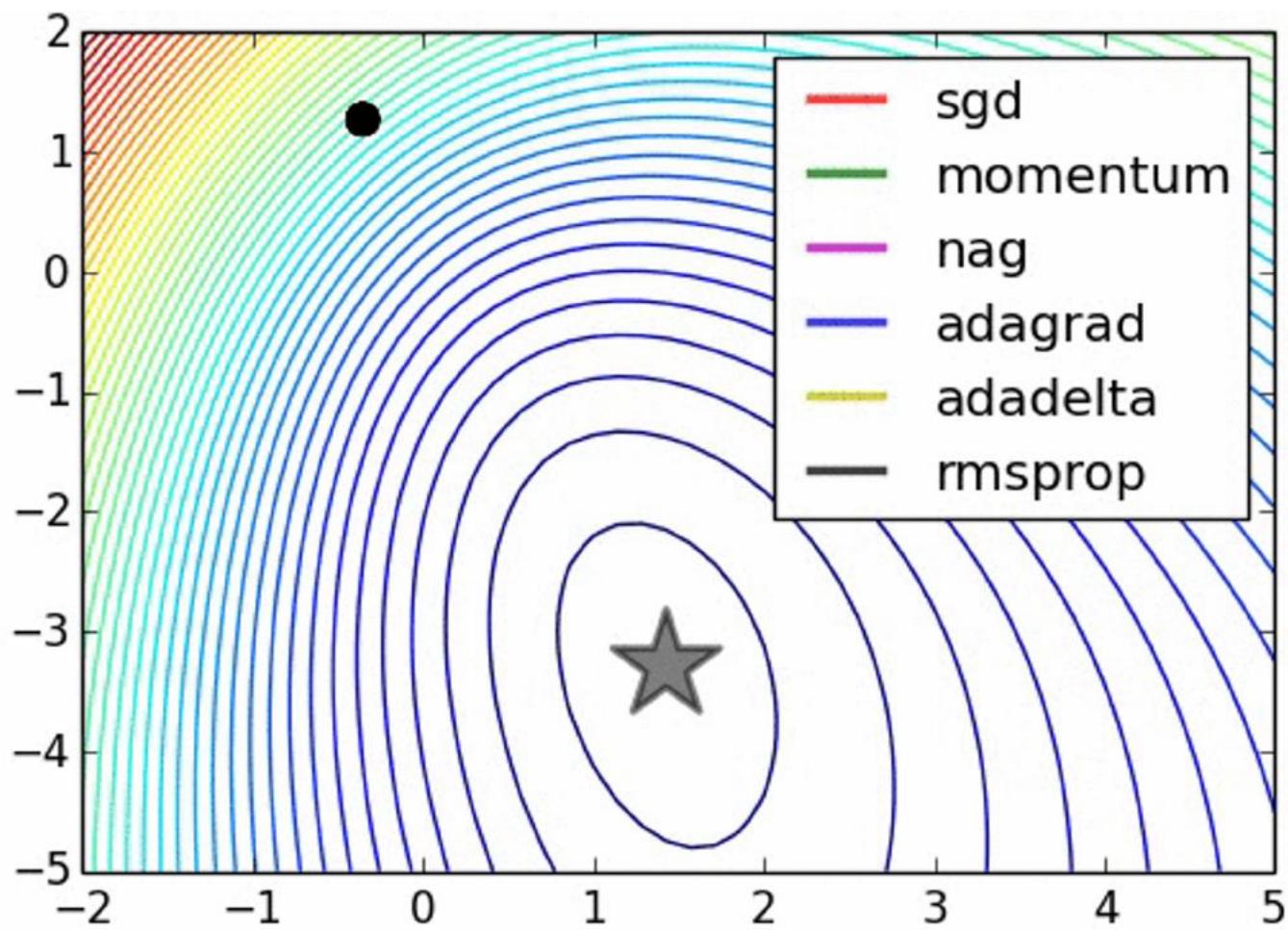
```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



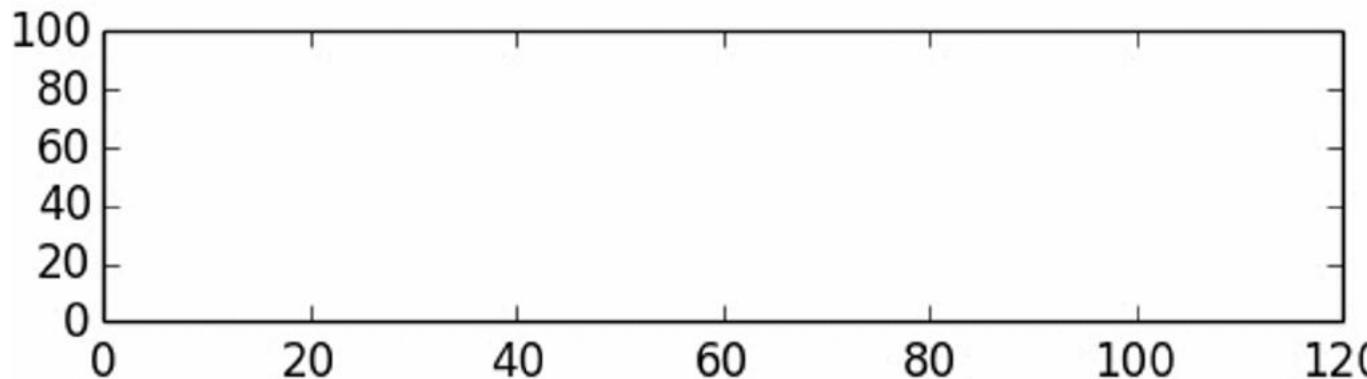
RMSProp

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

[Tieleman and Hinton, 2012]



adagrad
rmsprop



Adaptive Moment Estimation (Adam)

(incomplete, but close)

```
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

Looks a bit like RMSProp with momentum

Adam (full form)

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

momentum

Bias correction

AdaGrad / RMSProp

The bias correction compensates for the fact that m, v are initialized at zero and need some time to “warm up”.

Adam (full form)

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

momentum

Bias correction

AdaGrad / RMSProp

The bias correction compensates for the fact that m, v are initialized at zero and need some time to “warm up”.

Adam with $\beta_1 = 0.9$,
 $\beta_2 = 0.999$, and
 $\text{learning_rate} = 1e-3$ or $5e-4$
is a great starting point for many models!

[Kingma and Ba, 2014]

Optimization Algorithm Comparison

Algorithm	Tracks first moments (Momentum)	Tracks second moments (Adaptive learning rates)	Leaky second moments	Bias correction for moment estimates
SGD	✗	✗	✗	✗
SGD+Momentum	✓	✗	✗	✗
Nesterov	✓	✗	✗	✗
AdaGrad	✗	✓	✗	✗
RMSProp	✗	✓	✓	✗
Adam	✓	✓	✓	✓

L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$

$$g_t = \nabla L(w_t)$$

$$s_t = \text{optimizer}(g_t)$$

$$w_{t+1} = w_t - \alpha s_t$$

L2 Regularization vs Weight Decay

Optimization Algorithm

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$$g_t = \nabla L(w_t)$$

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L2 Regularization

$$L(w) = L_{data}(w) + \lambda |w|^2$$

$$g_t = \nabla L(w_t) = \nabla L_{data}(w_t) + 2\lambda w_t$$

$$s_t = \text{optimizer}(g_t)$$

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L2 Regularization vs Weight Decay

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Weight Decay

$$L(w) = L_{data}(w)$$

$$g_t = \nabla L_{data}(w_t)$$

$$s_t = \text{optimizer}(g_t) + 2\lambda w_t$$

$$w_{t+1} = w_t - \alpha s_t$$

L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$

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L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

L2 Regularization

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L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$

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L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

But they are not the same for adaptive methods (AdaGrad, RMSProp, Adam, etc)

L2 Regularization

$$L(w) = L_{data}(w) + \lambda |w|^2$$

$$g_t = \nabla L(w_t) = \nabla L_{data}(w_t) + 2\lambda w_t$$

$$s_t = \text{optimizer}(g_t)$$

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Weight Decay

$$L(w) = L_{data}(w)$$

$$g_t = \nabla L_{data}(w_t)$$

$$s_t = \text{optimizer}(g_t) + 2\lambda w_t$$

$$w_{t+1} = w_t - \alpha s_t$$

AdamW: Decoupled Weight Decay

Algorithm 2 Adam with L₂ regularization and Adam with decoupled weight decay (AdamW)

- 1: **given** $\alpha = 0.001, \beta_1 = 0.9, \beta_2 = 0.999, \epsilon = 10^{-8}, \lambda \in \mathbb{R}$
- 2: **initialize** time step $t \leftarrow 0$, parameter vector $\boldsymbol{\theta}_{t=0} \in \mathbb{R}^n$, first moment vector $\mathbf{m}_{t=0} \leftarrow \boldsymbol{\theta}_0$, second moment vector $\mathbf{v}_{t=0} \leftarrow \boldsymbol{\theta}_0$, schedule multiplier $\eta_{t=0} \in \mathbb{R}$
- 3: **repeat**
- 4: $t \leftarrow t + 1$
- 5: $\nabla f_t(\boldsymbol{\theta}_{t-1}) \leftarrow \text{SelectBatch}(\boldsymbol{\theta}_{t-1})$ ▷ select batch and return the corresponding gradient
- 6: $\mathbf{g}_t \leftarrow \nabla f_t(\boldsymbol{\theta}_{t-1}) + \lambda \boldsymbol{\theta}_{t-1}$
- 7: $\mathbf{m}_t \leftarrow \beta_1 \mathbf{m}_{t-1} + (1 - \beta_1) \mathbf{g}_t$ ▷ here and below all operations are element-wise
- 8: $\mathbf{v}_t \leftarrow \beta_2 \mathbf{v}_{t-1} + (1 - \beta_2) \mathbf{g}_t^2$
- 9: $\hat{\mathbf{m}}_t \leftarrow \mathbf{m}_t / (1 - \beta_1^t)$ ▷ β_1 is taken to the power of t
- 10: $\hat{\mathbf{v}}_t \leftarrow \mathbf{v}_t / (1 - \beta_2^t)$ ▷ β_2 is taken to the power of t
- 11: $\eta_t \leftarrow \text{SetScheduleMultiplier}(t)$ ▷ can be fixed, decay, or also be used for warm restarts
- 12: $\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta_t \left(\alpha \hat{\mathbf{m}}_t / (\sqrt{\hat{\mathbf{v}}_t} + \epsilon) + \lambda \boldsymbol{\theta}_{t-1} \right)$
- 13: **until** stopping criterion is met
- 14: **return** optimized parameters $\boldsymbol{\theta}_t$

AdamW: Decoupled Weight Decay

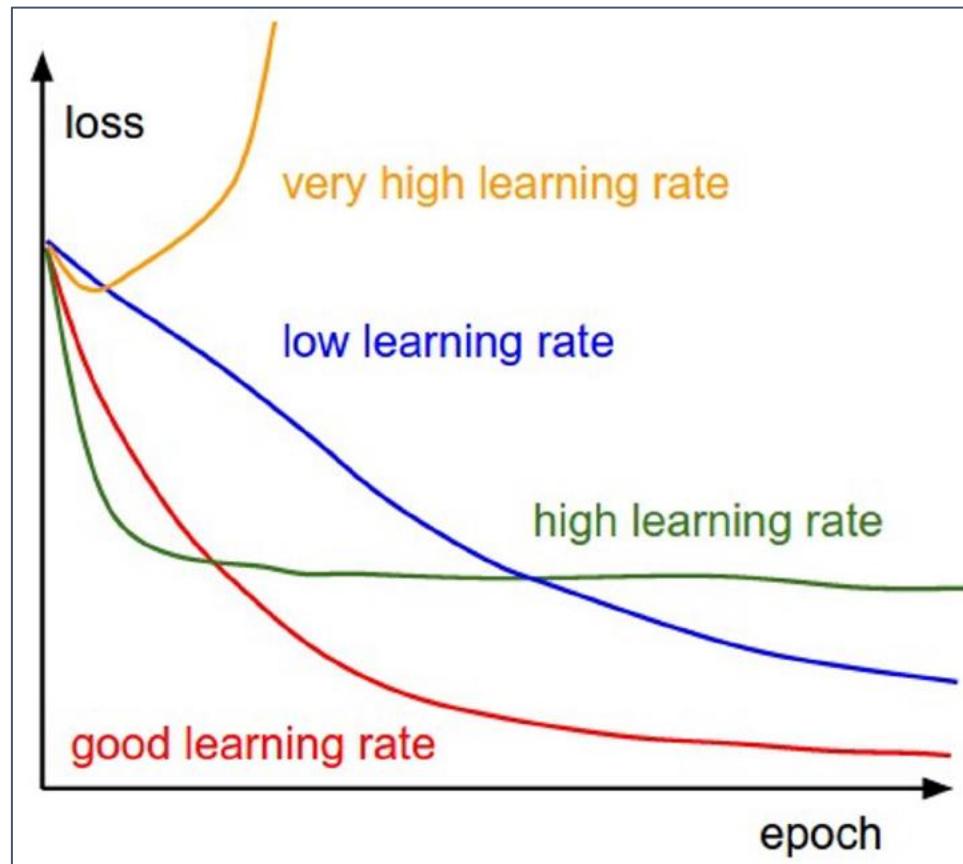
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- 2: ~~initialize time step $t \leftarrow 0$, parameter vector $\theta_{t=0} \in \mathbb{R}^n$, first moment vector $m_{t=0} \leftarrow \theta$, second moment vector $v_{t=0} \leftarrow \theta$, schedule multiplier $\eta_{t=0} \in \mathbb{R}$~~

AdamW should probably be your
“default” optimizer for new problems

- 8: $v_t \leftarrow \beta_2 v_{t-1} + (1 - \beta_2) g_t^2$
- 9: $\hat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ $\triangleright \beta_1$ is taken to the power of t
- 10: $\hat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ $\triangleright \beta_2$ is taken to the power of t
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- 13: **until** stopping criterion is met
- 14: **return** optimized parameters θ_t

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



=> Learning rate decay over time!

step decay:

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

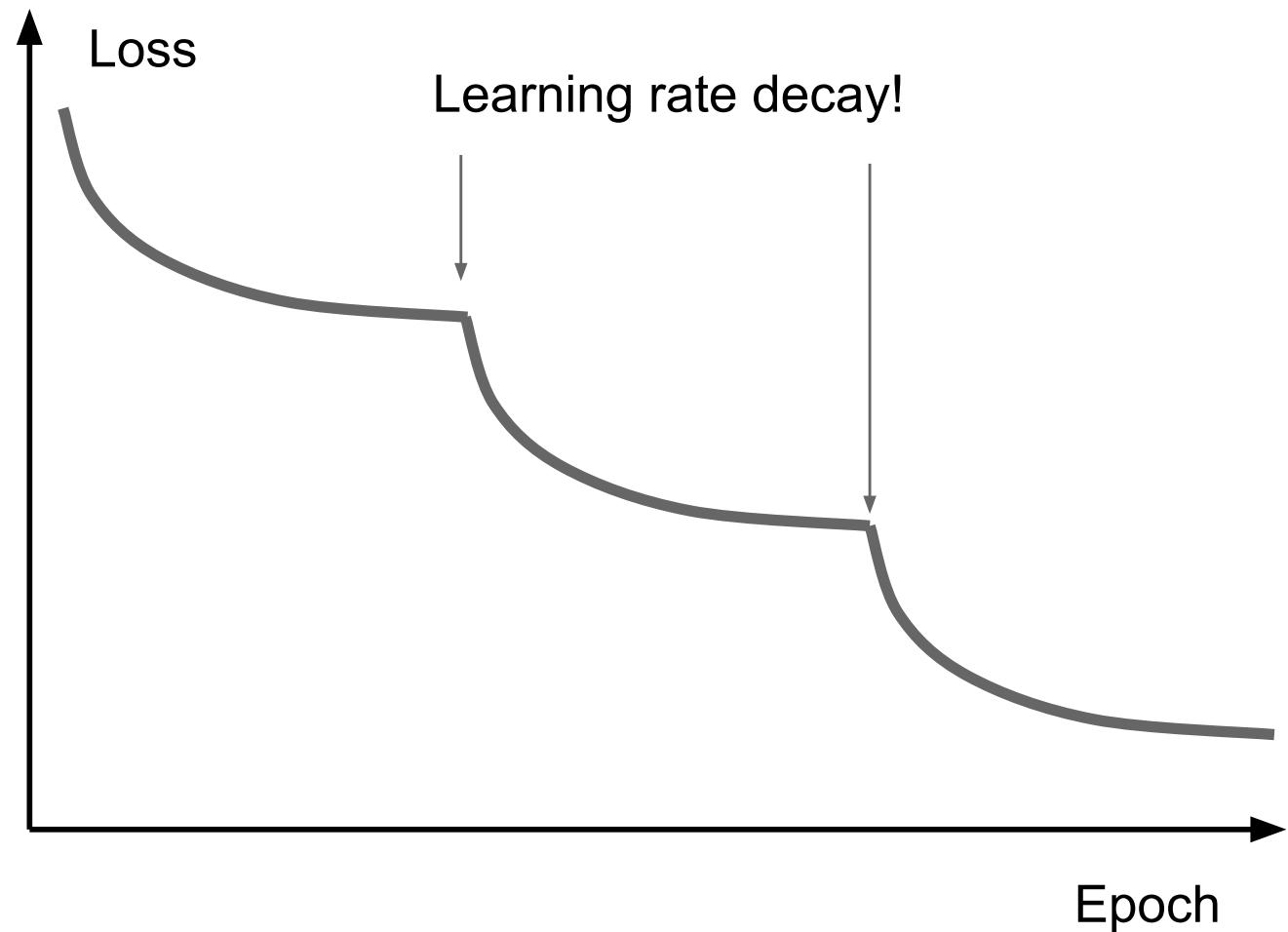
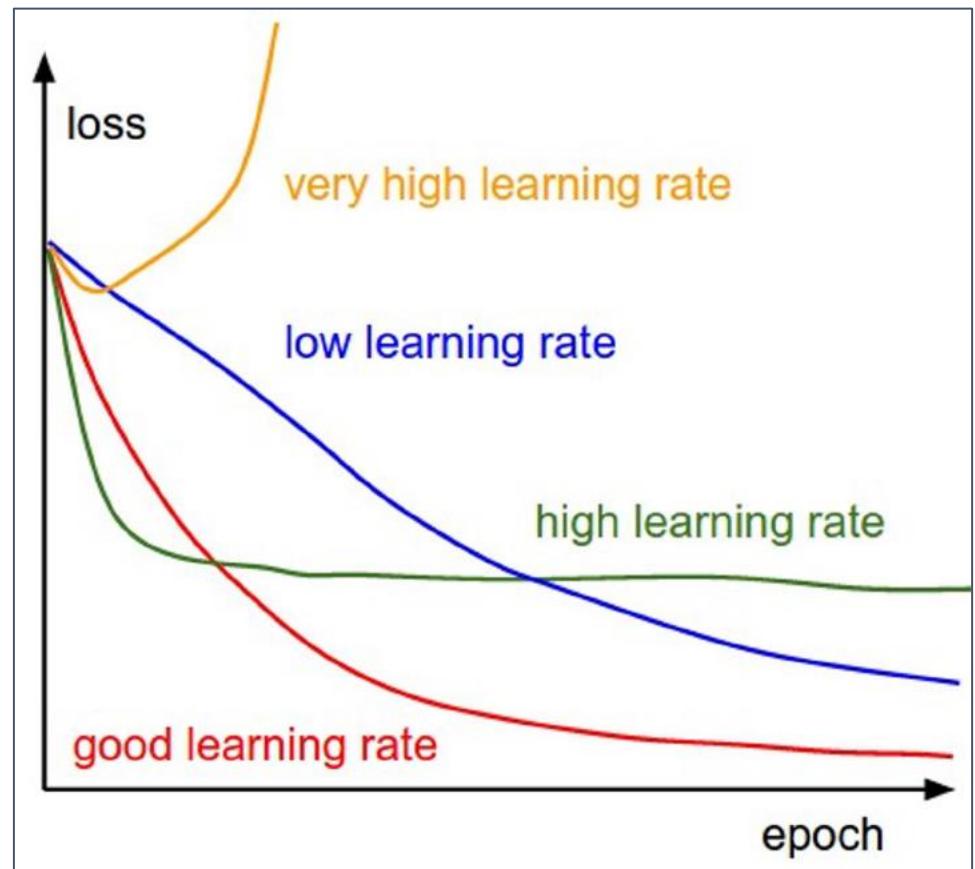
exponential decay:

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

1/t decay:

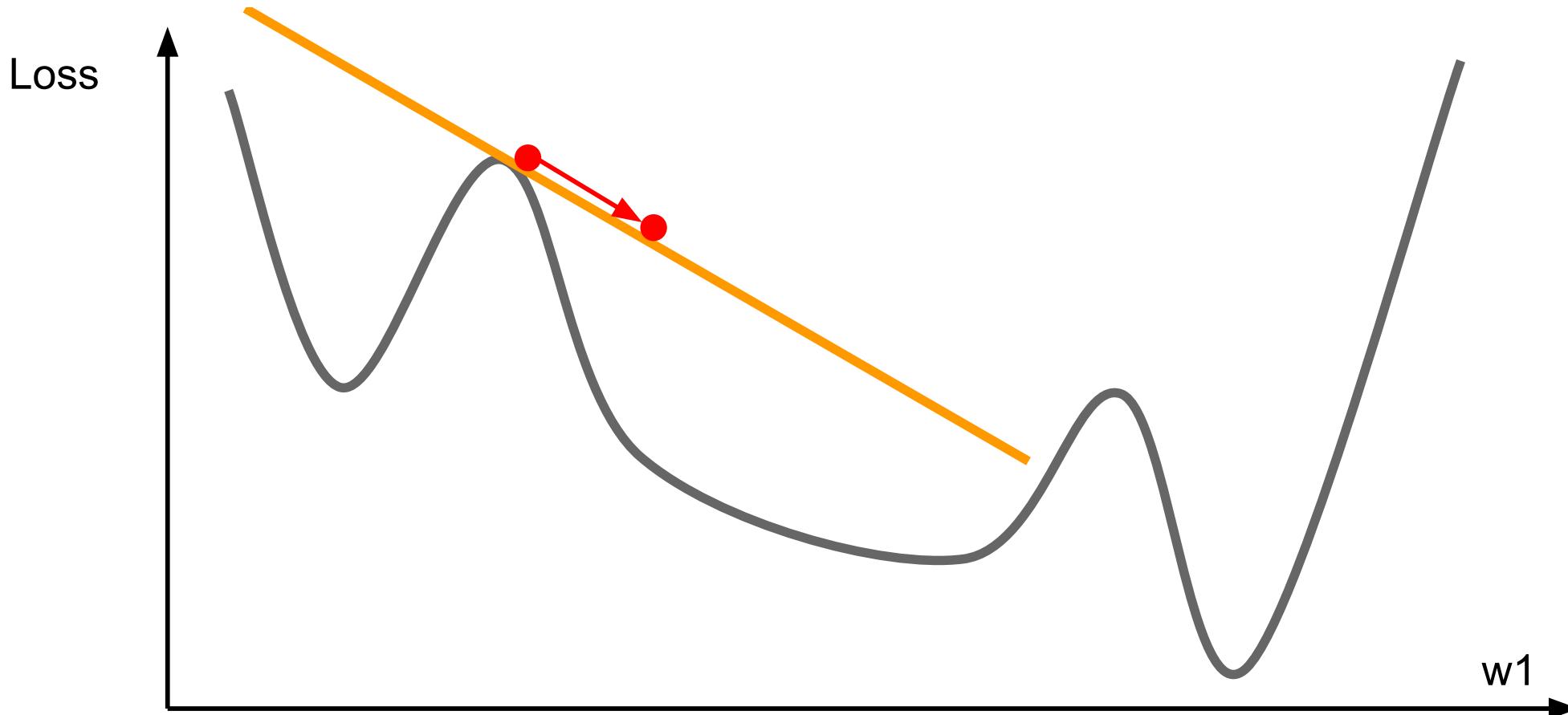
$$\alpha = \alpha_0 / (1 + kt)$$

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



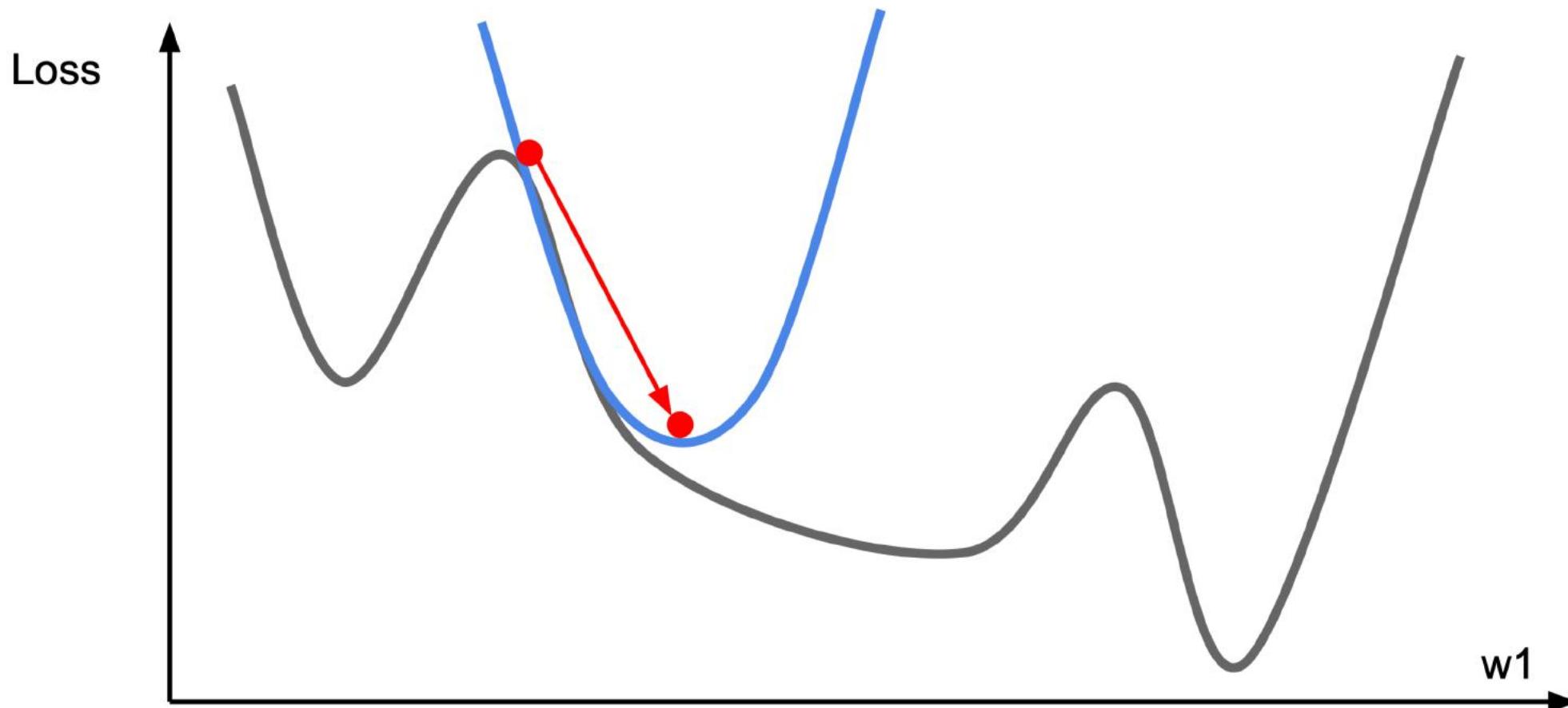
First-Order Optimization

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



Second-Order Optimization

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



Second order optimization methods

second-order Taylor expansion:

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

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

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

notice:
no hyperparameters! (e.g. learning rate)

Q: what is nice about this update?

Second order optimization methods

second-order Taylor expansion:

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

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

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

notice:
no hyperparameters! (e.g. learning rate)

Q2: why is this impractical for training Deep Neural Nets?

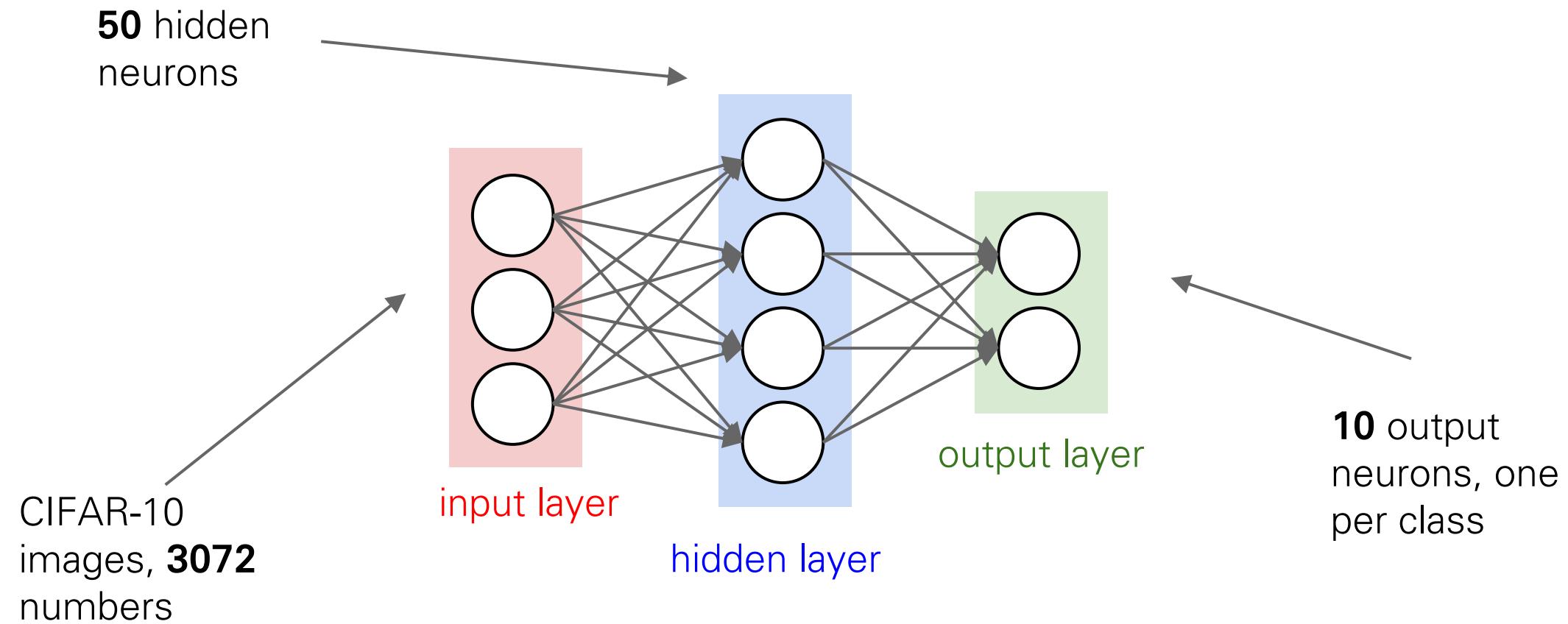
Second order optimization methods

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

- 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.

Babysitting the Learning Process

Say we start with one hidden layer of 50 neurons:



Double check that the loss is reasonable:

```
def init_two_layer_model(input_size, hidden_size, output_size):
    # initialize a model
    model = {}
    model['W1'] = 0.0001 * np.random.randn(input_size, hidden_size)
    model['b1'] = np.zeros(hidden_size)
    model['W2'] = 0.0001 * np.random.randn(hidden_size, output_size)
    model['b2'] = np.zeros(output_size)
    return model
```

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
loss, grad = two_layer_net(X_train, model, y_train, 0.0)      disable regularization
print loss
```

2.30261216167

loss ~2.3.
“correct” for
10 classes

returns the loss and the gradient for
all parameters

Double check that the loss is reasonable:

```
def init_two_layer_model(input_size, hidden_size, output_size):
    # initialize a model
    model = {}
    model['W1'] = 0.0001 * np.random.randn(input_size, hidden_size)
    model['b1'] = np.zeros(hidden_size)
    model['W2'] = 0.0001 * np.random.randn(hidden_size, output_size)
    model['b2'] = np.zeros(output_size)
    return model
```

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
loss, grad = two_layer_net(X_train, model, y_train, 1e3)      crank up regularization
print loss
```

3.06859716482

loss went up, good. (sanity check)

Lets try to train now...

Tip: Make sure that you can overfit very small portion of the training data

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
X_tiny = X_train[:20] # take 20 examples
y_tiny = y_train[:20]
best_model, stats = trainer.train(X_tiny, y_tiny, X_tiny, y_tiny,
                                  model, two_layer_net,
                                  num_epochs=200, reg=0.0,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = False,
                                  learning_rate=1e-3, verbose=True)
```

The above code:

- take the first 20 examples from CIFAR-10
- turn off regularization ($\text{reg} = 0.0$)
- use simple vanilla 'sgd'

Lets try to train now...

Tip: Make sure that you can overfit very small portion of the training data

Very small loss,
train accuracy 1.00,
nice!

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
X_tiny = X_train[:20] # take 20 examples
y_tiny = y_train[:20]
best_model, stats = trainer.train(X_tiny, y_tiny, X_tiny, y_tiny,
                                  model, two_layer_net,
                                  num_epochs=200, reg=0.0,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = False,
                                  learning_rate=1e-3, verbose=True)

Finished epoch 1 / 200: cost 2.302603, train: 0.400000, val 0.400000, lr 1.000000e-03
Finished epoch 2 / 200: cost 2.302258, train: 0.450000, val 0.450000, lr 1.000000e-03
Finished epoch 3 / 200: cost 2.301849, train: 0.600000, val 0.600000, lr 1.000000e-03
Finished epoch 4 / 200: cost 2.301196, train: 0.650000, val 0.650000, lr 1.000000e-03
Finished epoch 5 / 200: cost 2.300044, train: 0.650000, val 0.650000, lr 1.000000e-03
Finished epoch 6 / 200: cost 2.297864, train: 0.550000, val 0.550000, lr 1.000000e-03
Finished epoch 7 / 200: cost 2.293595, train: 0.600000, val 0.600000, lr 1.000000e-03
Finished epoch 8 / 200: cost 2.285096, train: 0.550000, val 0.550000, lr 1.000000e-03
Finished epoch 9 / 200: cost 2.268094, train: 0.550000, val 0.550000, lr 1.000000e-03
Finished epoch 10 / 200: cost 2.234787, train: 0.500000, val 0.500000, lr 1.000000e-03
Finished epoch 11 / 200: cost 2.173187, train: 0.500000, val 0.500000, lr 1.000000e-03
Finished epoch 12 / 200: cost 2.076862, train: 0.500000, val 0.500000, lr 1.000000e-03
Finished epoch 13 / 200: cost 1.974090, train: 0.400000, val 0.400000, lr 1.000000e-03
Finished epoch 14 / 200: cost 1.895885, train: 0.400000, val 0.400000, lr 1.000000e-03
Finished epoch 15 / 200: cost 1.820876, train: 0.450000, val 0.450000, lr 1.000000e-03
Finished epoch 16 / 200: cost 1.737430, train: 0.450000, val 0.450000, lr 1.000000e-03
Finished epoch 17 / 200: cost 1.642356, train: 0.500000, val 0.500000, lr 1.000000e-03
Finished epoch 18 / 200: cost 1.535239, train: 0.600000, val 0.600000, lr 1.000000e-03
Finished epoch 19 / 200: cost 1.421527, train: 0.600000, val 0.600000, lr 1.000000e-03
Finished epoch 20 / 200: cost 1.305760, train: 0.650000, val 0.650000, lr 1.000000e-03
-----
Finished epoch 195 / 200: cost 0.002694, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 196 / 200: cost 0.002674, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 197 / 200: cost 0.002655, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 198 / 200: cost 0.002635, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 199 / 200: cost 0.002617, train: 1.000000, val 1.000000, lr 1.000000e-03
Finished epoch 200 / 200: cost 0.002597, train: 1.000000, val 1.000000, lr 1.000000e-03
finished optimization. best validation accuracy: 1.000000
```

Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                   model, two_layer_net,
                                   num_epochs=10, reg=0.000001,
                                   update='sgd', learning_rate_decay=1,
                                   sample_batches = True,
                                   learning_rate=1e-6, verbose=True)
```

Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=1e-6, verbose=True)
```

```
Finished epoch 1 / 10: cost 2.302576, train: 0.080000, val 0.103000, lr 1.000000e-06
Finished epoch 2 / 10: cost 2.302582, train: 0.121000, val 0.124000, lr 1.000000e-06
Finished epoch 3 / 10: cost 2.302558, train: 0.119000, val 0.138000, lr 1.000000e-06
Finished epoch 4 / 10: cost 2.302519, train: 0.127000, val 0.151000, lr 1.000000e-06
Finished epoch 5 / 10: cost 2.302517, train: 0.158000, val 0.171000, lr 1.000000e-06
Finished epoch 6 / 10: cost 2.302518, train: 0.179000, val 0.172000, lr 1.000000e-06
Finished epoch 7 / 10: cost 2.302466, train: 0.180000, val 0.176000, lr 1.000000e-06
Finished epoch 8 / 10: cost 2.302452, train: 0.175000, val 0.185000, lr 1.000000e-06
Finished epoch 9 / 10: cost 2.302459, train: 0.206000, val 0.192000, lr 1.000000e-06
Finished epoch 10 / 10: cost 2.302420, train: 0.190000, val 0.192000, lr 1.000000e-06
finished optimization. best validation accuracy: 0.192000
```

Loss barely changing

Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

loss not going down:
learning rate too low

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=1e-6, verbose=True)
```

```
Finished epoch 1 / 10: cost 2.302576, train: 0.080000, val 0.103000, lr 1.000000e-06
Finished epoch 2 / 10: cost 2.302582, train: 0.121000, val 0.124000, lr 1.000000e-06
Finished epoch 3 / 10: cost 2.302558, train: 0.119000, val 0.138000, lr 1.000000e-06
Finished epoch 4 / 10: cost 2.302519, train: 0.127000, val 0.151000, lr 1.000000e-06
Finished epoch 5 / 10: cost 2.302517, train: 0.158000, val 0.171000, lr 1.000000e-06
Finished epoch 6 / 10: cost 2.302518, train: 0.179000, val 0.172000, lr 1.000000e-06
Finished epoch 7 / 10: cost 2.302466, train: 0.180000, val 0.176000, lr 1.000000e-06
Finished epoch 8 / 10: cost 2.302452, train: 0.175000, val 0.185000, lr 1.000000e-06
Finished epoch 9 / 10: cost 2.302459, train: 0.206000, val 0.192000, lr 1.000000e-06
Finished epoch 10 / 10: cost 2.302420, train: 0.190000, val 0.192000, lr 1.000000e-06
finished optimization. best validation accuracy: 0.192000
```

Loss barely changing: Learning rate is probably too low

Notice train/val accuracy goes to 20% though, what's up with that?
(remember this is softmax)

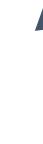
Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

loss not going down:
learning rate too low

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=1e6, verbose=True)
```

Okay now lets try learning rate 1e6. What could possibly go wrong?



Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=1e-6, verbose=True)

/home/karpathy/cs231n/code/cs231n/classifiers/neural_net.py:50: RuntimeWarning: divide by zero encountered in log
    data_loss = -np.sum(np.log(probs[range(N), y])) / N
/home/karpathy/cs231n/code/cs231n/classifiers/neural_net.py:48: RuntimeWarning: invalid value encountered in subtract
    probs = np.exp(scores - np.max(scores, axis=1, keepdims=True))
Finished epoch 1 / 10: cost nan, train: 0.091000, val 0.087000, lr 1.000000e+06
Finished epoch 2 / 10: cost nan, train: 0.095000, val 0.087000, lr 1.000000e+06
Finished epoch 3 / 10: cost nan, train: 0.100000, val 0.087000, lr 1.000000e+06
```

loss not going down:

learning rate too low

loss exploding:

learning rate too high

cost: NaN almost always means high learning rate...

Lets try to train now...

Start with small regularization and find learning rate that makes the loss go down.

loss not going down:

learning rate too low

loss exploding:

learning rate too high

```
model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
trainer = ClassifierTrainer()
best_model, stats = trainer.train(X_train, y_train, X_val, y_val,
                                  model, two_layer_net,
                                  num_epochs=10, reg=0.000001,
                                  update='sgd', learning_rate_decay=1,
                                  sample_batches = True,
                                  learning_rate=3e-3, verbose=True)
```

```
Finished epoch 1 / 10: cost 2.186654, train: 0.308000, val 0.306000, lr 3.000000e-03
Finished epoch 2 / 10: cost 2.176230, train: 0.330000, val 0.350000, lr 3.000000e-03
Finished epoch 3 / 10: cost 1.942257, train: 0.376000, val 0.352000, lr 3.000000e-03
Finished epoch 4 / 10: cost 1.827868, train: 0.329000, val 0.310000, lr 3.000000e-03
Finished epoch 5 / 10: cost inf, train: 0.128000, val 0.128000, lr 3.000000e-03
Finished epoch 6 / 10: cost inf, train: 0.144000, val 0.147000, lr 3.000000e-03
```

3e-3 is still too high. Cost explodes....

=> Rough range for learning rate we should be cross-validating is somewhere [1e-3 ... 1e-5]

Hyperparameter Selection

Everything is a hyperparameter

- Network size/depth
 - Small model variations
 - Minibatch creation strategy
 - Optimizer/learning rate
-
- Models are complicated and opaque, debugging can be difficult!

Cross-validation strategy

First do coarse -> fine cross-validation in stages

First stage: only a few epochs to get rough idea of what params work

Second stage: longer running time, finer search

... (repeat as necessary)

Tip for detecting explosions in the solver:

If the cost is ever $> 3 * \text{original cost}$, break out early

For example: run coarse search for 5 epochs

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-5, 5)
    lr = 10**uniform(-3, -6) ←

    trainer = ClassifierTrainer()
    model = init_two_layer_model(32*32*3, 50, 10) # input size, hidden size, number of classes
    trainer = ClassifierTrainer()
    best_model_local, stats = trainer.train(X_train, y_train, X_val, y_val,
                                              model, two_layer_net,
                                              num_epochs=5, reg=reg,
                                              update='momentum', learning_rate_decay=0.9,
                                              sample_batches = True, batch_size = 100,
                                              learning_rate=lr, verbose=False)
```

note it's best to optimize in log space!

```
val_acc: 0.412000, lr: 1.405206e-04, reg: 4.793564e-01, (1 / 100)
val_acc: 0.214000, lr: 7.231888e-06, reg: 2.321281e-04, (2 / 100)
val_acc: 0.208000, lr: 2.119571e-06, reg: 8.011857e+01, (3 / 100)
val_acc: 0.196000, lr: 1.551131e-05, reg: 4.374936e-05, (4 / 100)
val_acc: 0.079000, lr: 1.753300e-05, reg: 1.200424e+03, (5 / 100)
val_acc: 0.223000, lr: 4.215128e-05, reg: 4.196174e+01, (6 / 100)
val_acc: 0.441000, lr: 1.750259e-04, reg: 2.110807e-04, (7 / 100)
val_acc: 0.241000, lr: 6.749231e-05, reg: 4.226413e+01, (8 / 100)
val_acc: 0.482000, lr: 4.296863e-04, reg: 6.642555e-01, (9 / 100) ← nice
val_acc: 0.079000, lr: 5.401602e-06, reg: 1.599828e+04, (10 / 100)
val_acc: 0.154000, lr: 1.618508e-06, reg: 4.925252e-01, (11 / 100)
```

Now run finer search...

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-5, 5)
    lr = 10**uniform(-3, -6)
```

adjust range

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-4, 0)
    lr = 10**uniform(-3, -4)
```

```
val_acc: 0.527000, lr: 5.340517e-04, reg: 4.097824e-01, (0 / 100)
val_acc: 0.492000, lr: 2.279484e-04, reg: 9.991345e-04, (1 / 100)
val_acc: 0.512000, lr: 8.680827e-04, reg: 1.349727e-02, (2 / 100)
val_acc: 0.461000, lr: 1.028377e-04, reg: 1.220193e-02, (3 / 100)
val_acc: 0.460000, lr: 1.113730e-04, reg: 5.244309e-02, (4 / 100)
val_acc: 0.498000, lr: 9.477776e-04, reg: 2.001293e-03, (5 / 100)
val_acc: 0.469000, lr: 1.484369e-04, reg: 4.328313e-01, (6 / 100)
val_acc: 0.522000, lr: 5.586261e-04, reg: 2.312685e-04, (7 / 100)
val_acc: 0.530000, lr: 5.808183e-04, reg: 8.259964e-02, (8 / 100)
val_acc: 0.489000, lr: 1.979168e-04, reg: 1.010889e-04, (9 / 100)
val_acc: 0.490000, lr: 2.036031e-04, reg: 2.406271e-03, (10 / 100)
val_acc: 0.475000, lr: 2.021162e-04, reg: 2.287807e-01, (11 / 100)
val_acc: 0.460000, lr: 1.135527e-04, reg: 3.905040e-02, (12 / 100)
val_acc: 0.515000, lr: 6.947668e-04, reg: 1.562808e-02, (13 / 100)
val_acc: 0.531000, lr: 9.471549e-04, reg: 1.433895e-03, (14 / 100)
val_acc: 0.509000, lr: 3.140888e-04, reg: 2.857518e-01, (15 / 100)
val_acc: 0.514000, lr: 6.438349e-04, reg: 3.033781e-01, (16 / 100)
val_acc: 0.502000, lr: 3.921784e-04, reg: 2.707126e-04, (17 / 100)
val_acc: 0.509000, lr: 9.752279e-04, reg: 2.850865e-03, (18 / 100)
val_acc: 0.500000, lr: 2.412048e-04, reg: 4.997821e-04, (19 / 100)
val_acc: 0.466000, lr: 1.319314e-04, reg: 1.189915e-02, (20 / 100)
val_acc: 0.516000, lr: 8.039527e-04, reg: 1.528291e-02, (21 / 100)
```

53% - relatively good
for a 2-layer neural net
with 50 hidden
neurons.

Now run finer search...

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-5, 5)
    lr = 10**uniform(-3, -6)
```

adjust range

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-4, 0)
    lr = 10**uniform(-3, -4)
```

```
val_acc: 0.527000, lr: 5.340517e-04, reg: 4.097824e-01, (0 / 100)
val_acc: 0.492000, lr: 2.279484e-04, reg: 9.991345e-04, (1 / 100)
val_acc: 0.512000, lr: 8.680827e-04, reg: 1.349727e-02, (2 / 100)
val_acc: 0.461000, lr: 1.028377e-04, reg: 1.220193e-02, (3 / 100)
val_acc: 0.460000, lr: 1.113730e-04, reg: 5.244309e-02, (4 / 100)
val_acc: 0.498000, lr: 9.477776e-04, reg: 2.001293e-03, (5 / 100)
val_acc: 0.469000, lr: 1.484369e-04, reg: 4.328313e-01, (6 / 100)
val_acc: 0.522000, lr: 5.586261e-04, reg: 2.312685e-04, (7 / 100)
val_acc: 0.530000, lr: 5.808183e-04, reg: 8.259964e-02, (8 / 100)
val_acc: 0.489000, lr: 1.979168e-04, reg: 1.010889e-04, (9 / 100)
val_acc: 0.490000, lr: 2.036031e-04, reg: 2.406271e-03, (10 / 100)
val_acc: 0.475000, lr: 2.021162e-04, reg: 2.287807e-01, (11 / 100)
val_acc: 0.460000, lr: 1.135527e-04, reg: 3.905040e-02, (12 / 100)
val_acc: 0.515000, lr: 6.947668e-04, reg: 1.562808e-02, (13 / 100)
val_acc: 0.531000, lr: 9.471549e-04, reg: 1.433895e-03, (14 / 100)
val_acc: 0.509000, lr: 3.140888e-04, reg: 2.857518e-01, (15 / 100)
val_acc: 0.514000, lr: 6.438349e-04, reg: 3.033781e-01, (16 / 100)
val_acc: 0.502000, lr: 3.921784e-04, reg: 2.707126e-04, (17 / 100)
val_acc: 0.509000, lr: 9.752279e-04, reg: 2.850865e-03, (18 / 100)
val_acc: 0.500000, lr: 2.412048e-04, reg: 4.997821e-04, (19 / 100)
val_acc: 0.466000, lr: 1.319314e-04, reg: 1.189915e-02, (20 / 100)
val_acc: 0.516000, lr: 8.039527e-04, reg: 1.528291e-02, (21 / 100)
```

53% - relatively good
for a 2-layer neural net
with 50 hidden
neurons.

But this best cross-validation result is worrying. Why?

Now run finer search...

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-5, 5)
    lr = 10**uniform(-3, -6)
```

adjust range

```
max_count = 100
for count in xrange(max_count):
    reg = 10**uniform(-4, 0)
    lr = 10**uniform(-3, -4)
```

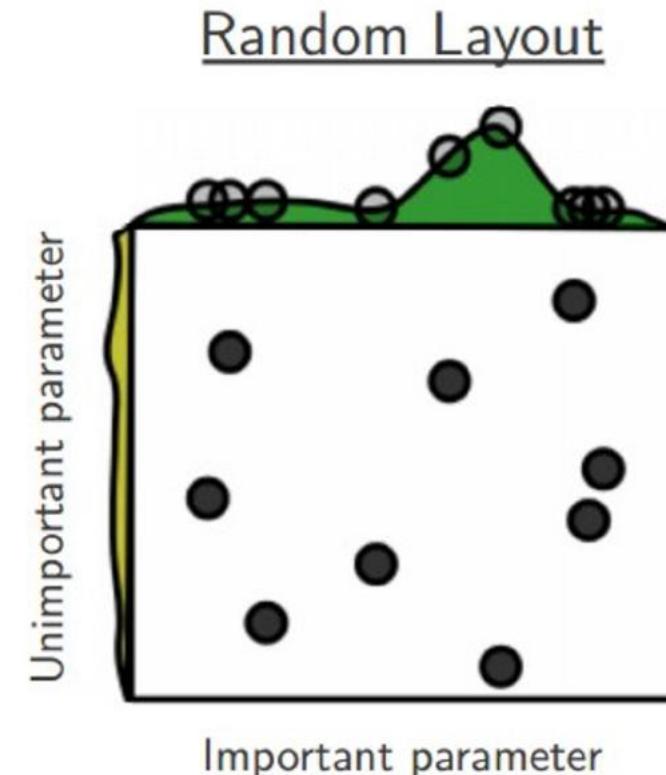
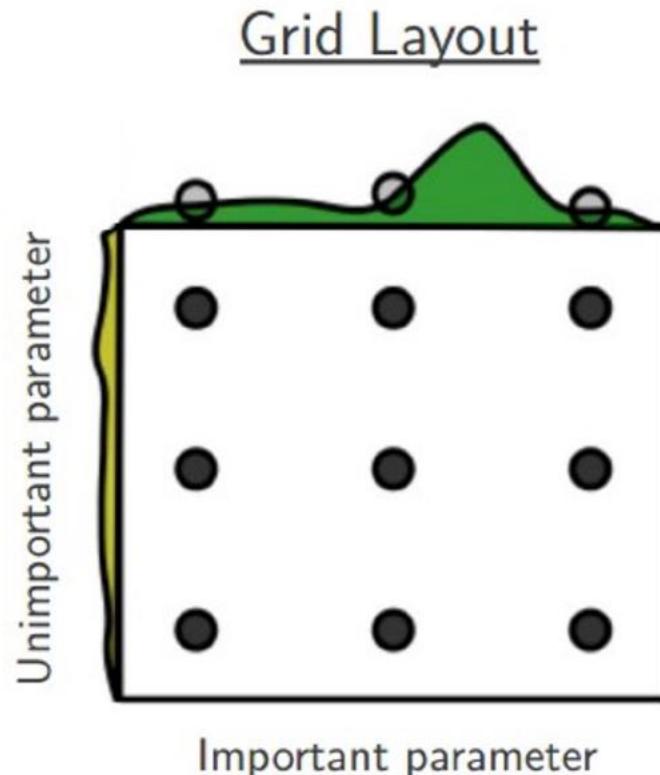
```
val_acc: 0.527000, lr: 5.340517e-04, reg: 4.097824e-01, (0 / 100)
val_acc: 0.492000, lr: 2.279484e-04, reg: 9.991345e-04, (1 / 100)
val_acc: 0.512000, lr: 8.680827e-04, reg: 1.349727e-02, (2 / 100)
val_acc: 0.461000, lr: 1.028377e-04, reg: 1.220193e-02, (3 / 100)
val_acc: 0.460000, lr: 1.113730e-04, reg: 5.244309e-02, (4 / 100)
val_acc: 0.498000, lr: 9.477776e-04, reg: 2.001293e-03, (5 / 100)
val_acc: 0.469000, lr: 1.484369e-04, reg: 4.328313e-01, (6 / 100)
val_acc: 0.522000, lr: 5.586261e-04, reg: 2.312685e-04, (7 / 100)
val_acc: 0.530000, lr: 5.808183e-04, reg: 8.259964e-02, (8 / 100)
val_acc: 0.489000, lr: 1.979168e-04, reg: 1.010889e-04, (9 / 100)
val_acc: 0.490000, lr: 2.036031e-04, reg: 2.406271e-03, (10 / 100)
val_acc: 0.475000, lr: 2.021162e-04, reg: 2.287807e-01, (11 / 100)
val_acc: 0.460000, lr: 1.135527e-04, reg: 3.905040e-02, (12 / 100)
val_acc: 0.515000, lr: 6.947668e-04, reg: 1.562808e-02, (13 / 100)
val_acc: 0.531000, lr: 9.471549e-04, reg: 1.433895e-03, (14 / 100)
val_acc: 0.509000, lr: 3.140888e-04, reg: 2.857518e-01, (15 / 100)
val_acc: 0.514000, lr: 6.438349e-04, reg: 3.033781e-01, (16 / 100)
val_acc: 0.502000, lr: 3.921784e-04, reg: 2.707126e-04, (17 / 100)
val_acc: 0.509000, lr: 9.752279e-04, reg: 2.850865e-03, (18 / 100)
val_acc: 0.500000, lr: 2.412048e-04, reg: 4.997821e-04, (19 / 100)
val_acc: 0.466000, lr: 1.319314e-04, reg: 1.189915e-02, (20 / 100)
val_acc: 0.516000, lr: 8.039527e-04, reg: 1.528291e-02, (21 / 100)
```

53% - relatively good
for a 2-layer neural net
with 50 hidden
neurons.

But this best cross-validation result is worrying.

Learning rate close
to the edge, need
more wider search!

Random Search vs. Grid Search

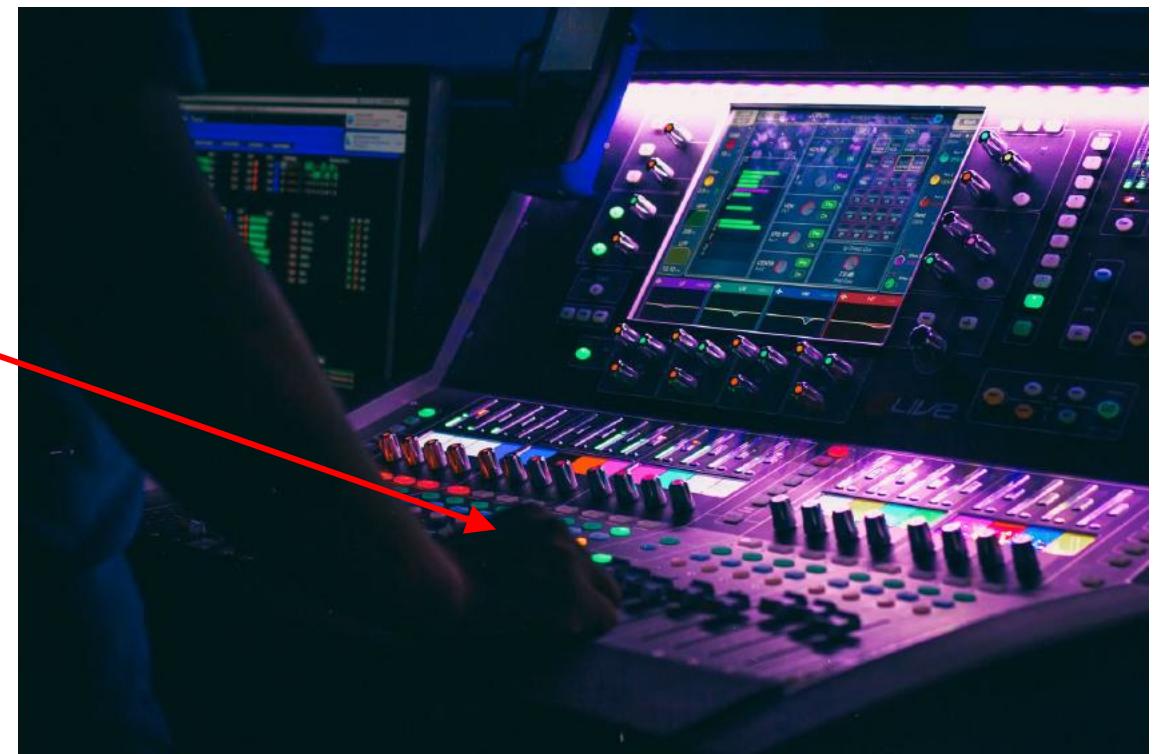


Random Search for Hyper-Parameter Optimization
Bergstra and Bengio, 2012

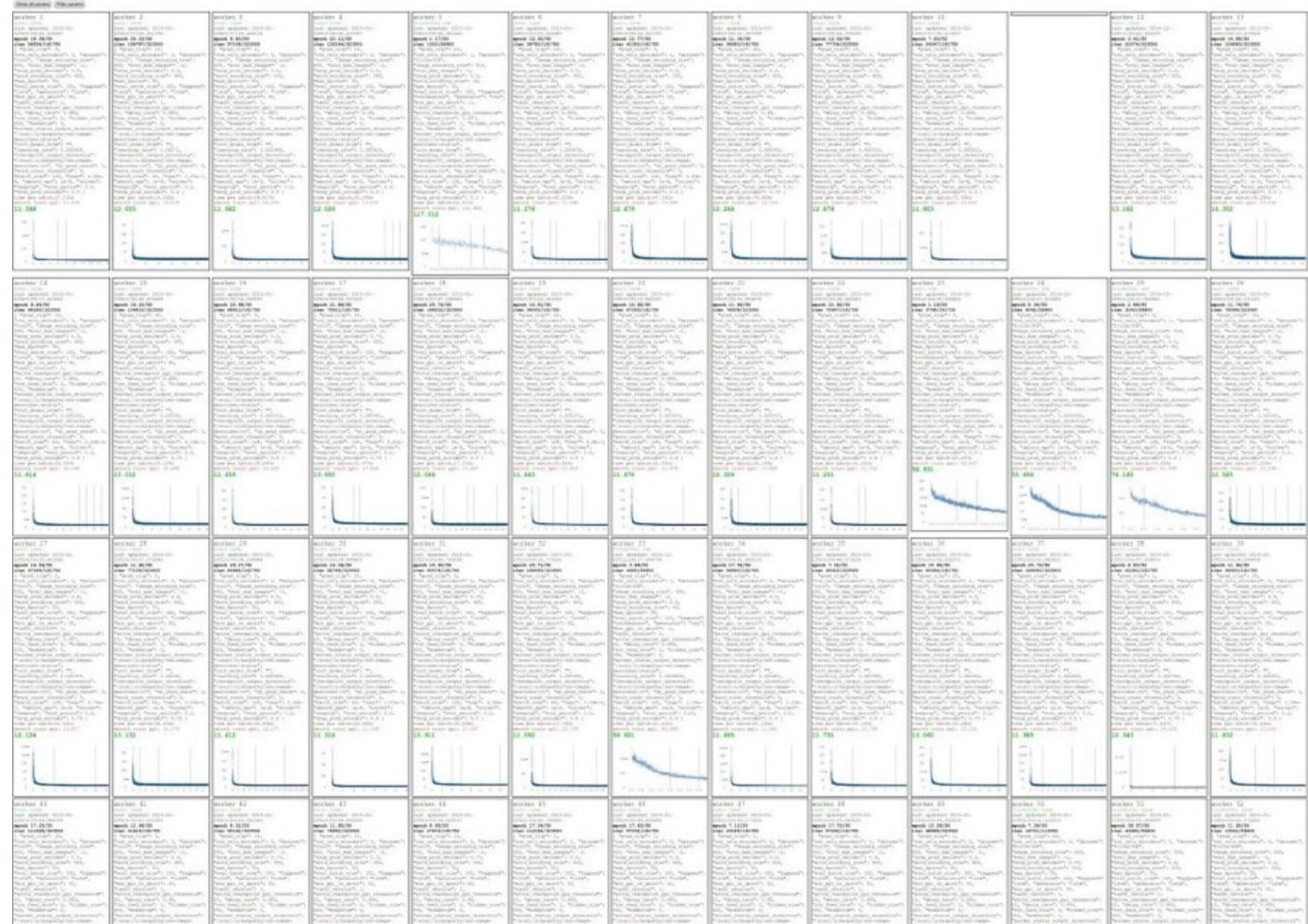
Hyperparameters to play with:

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

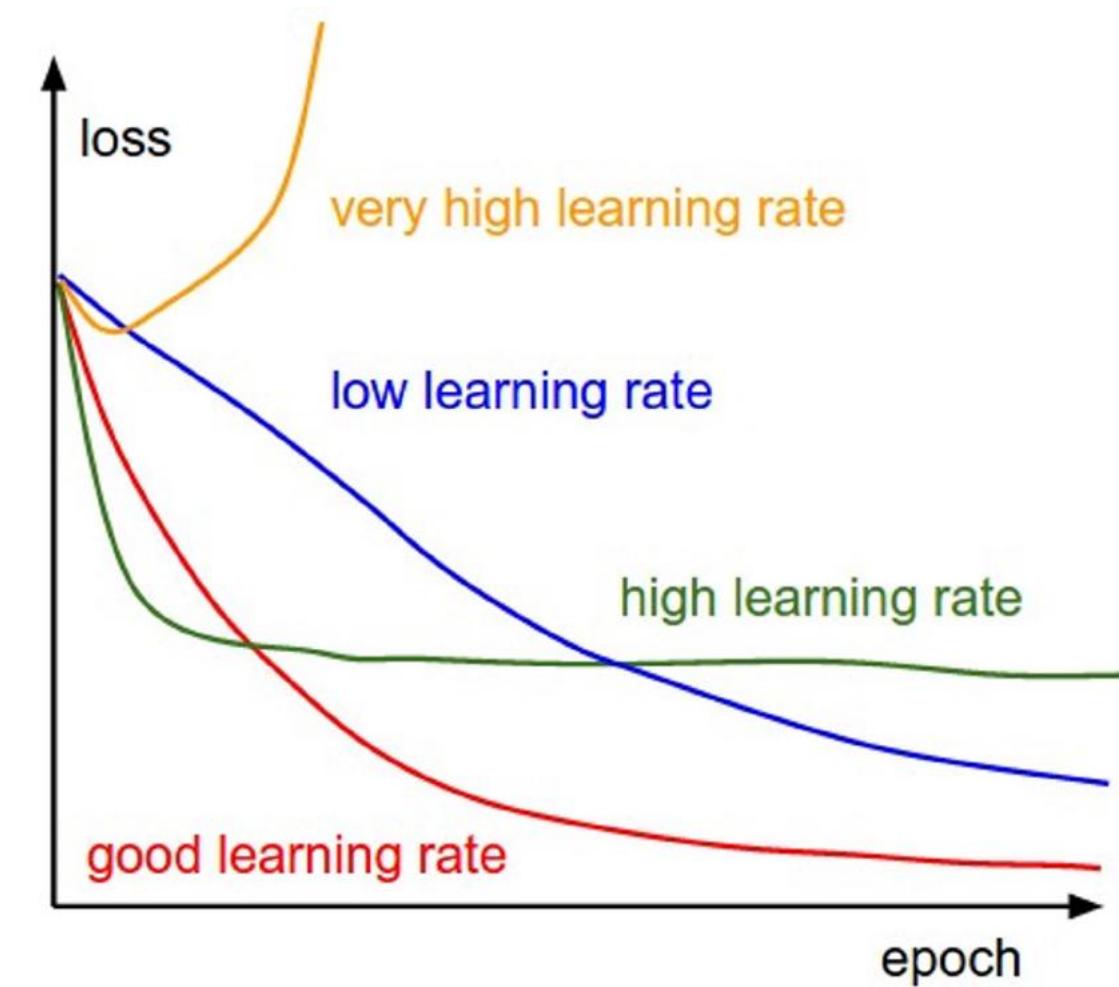
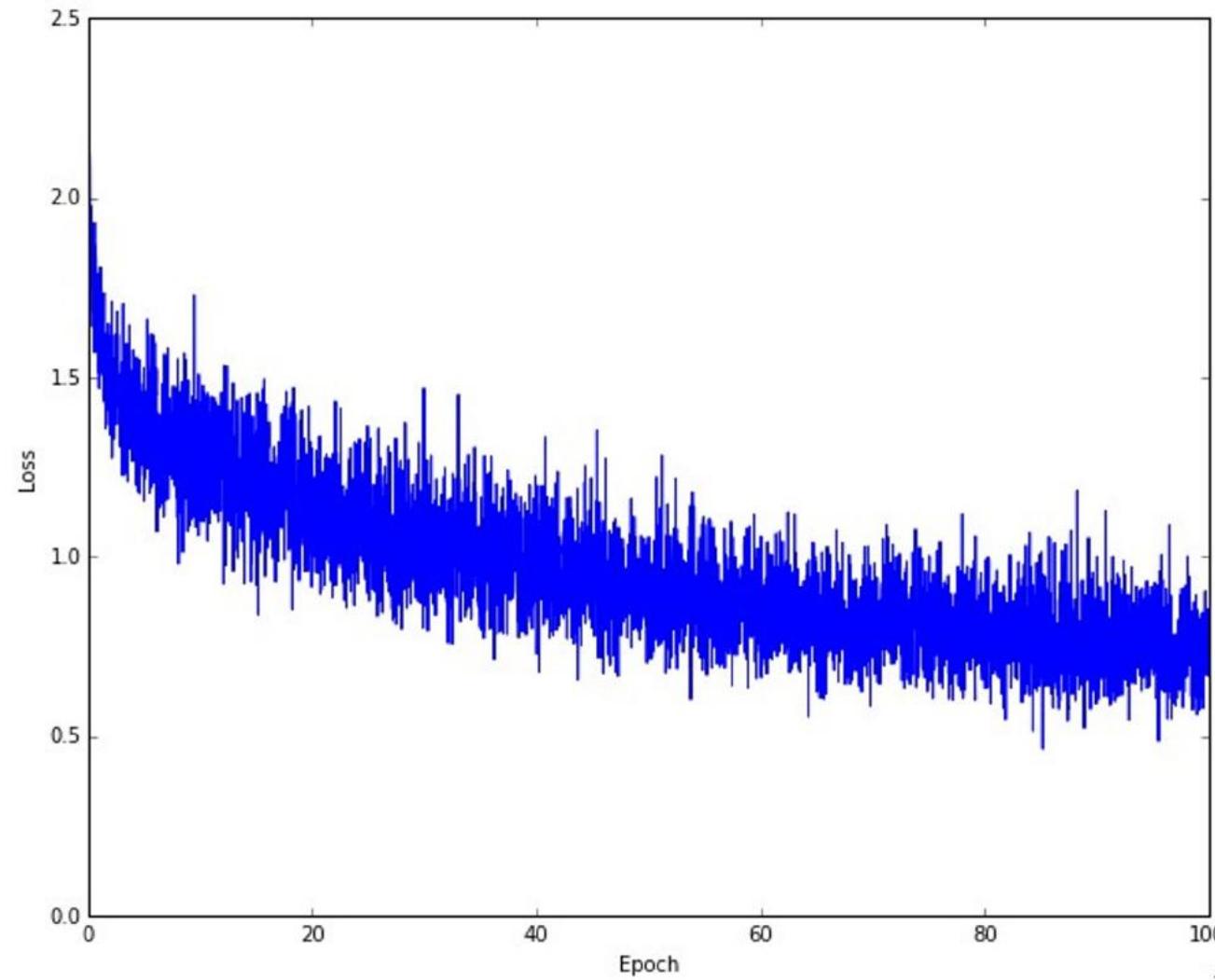
neural networks practitioner
music = loss function

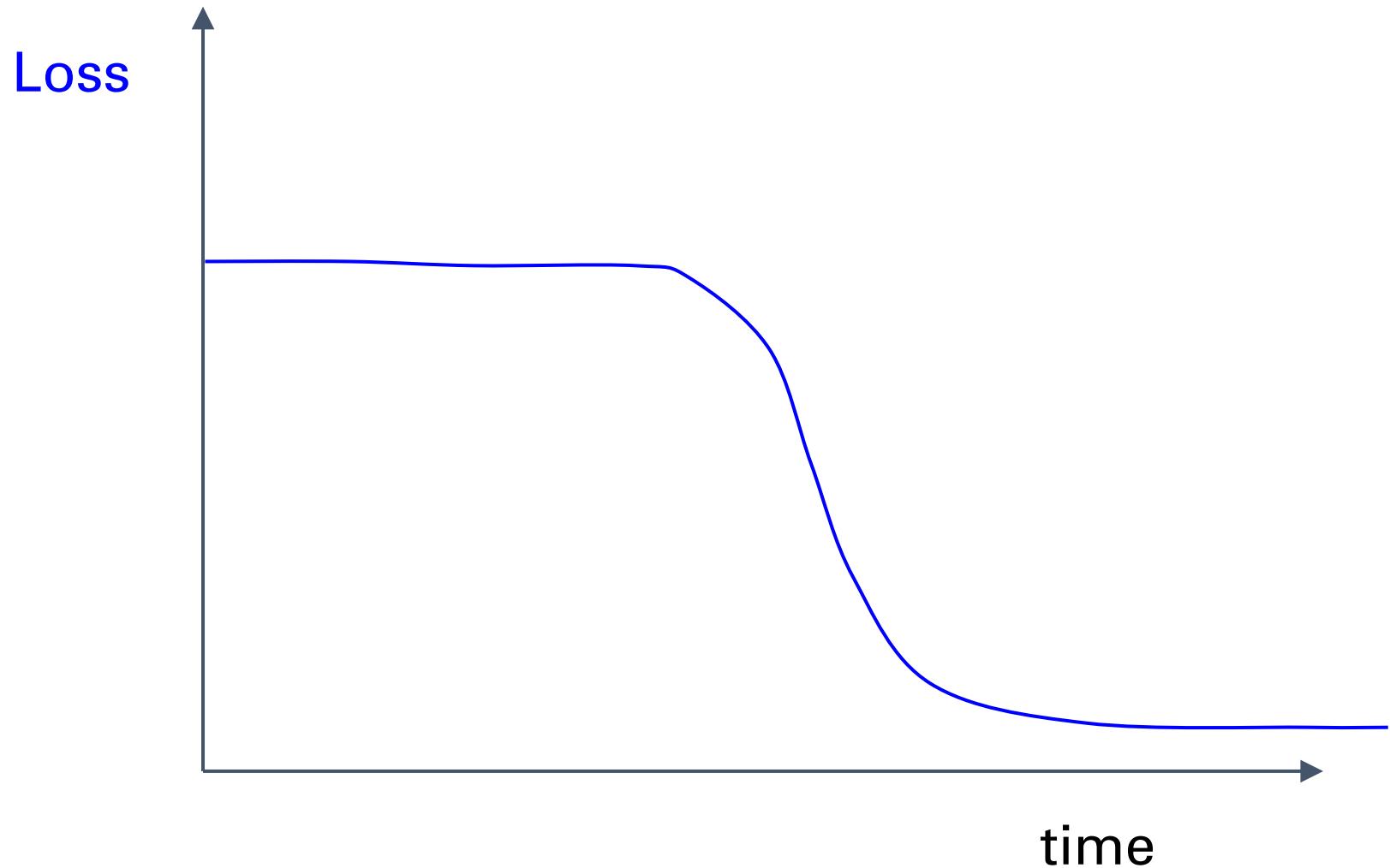


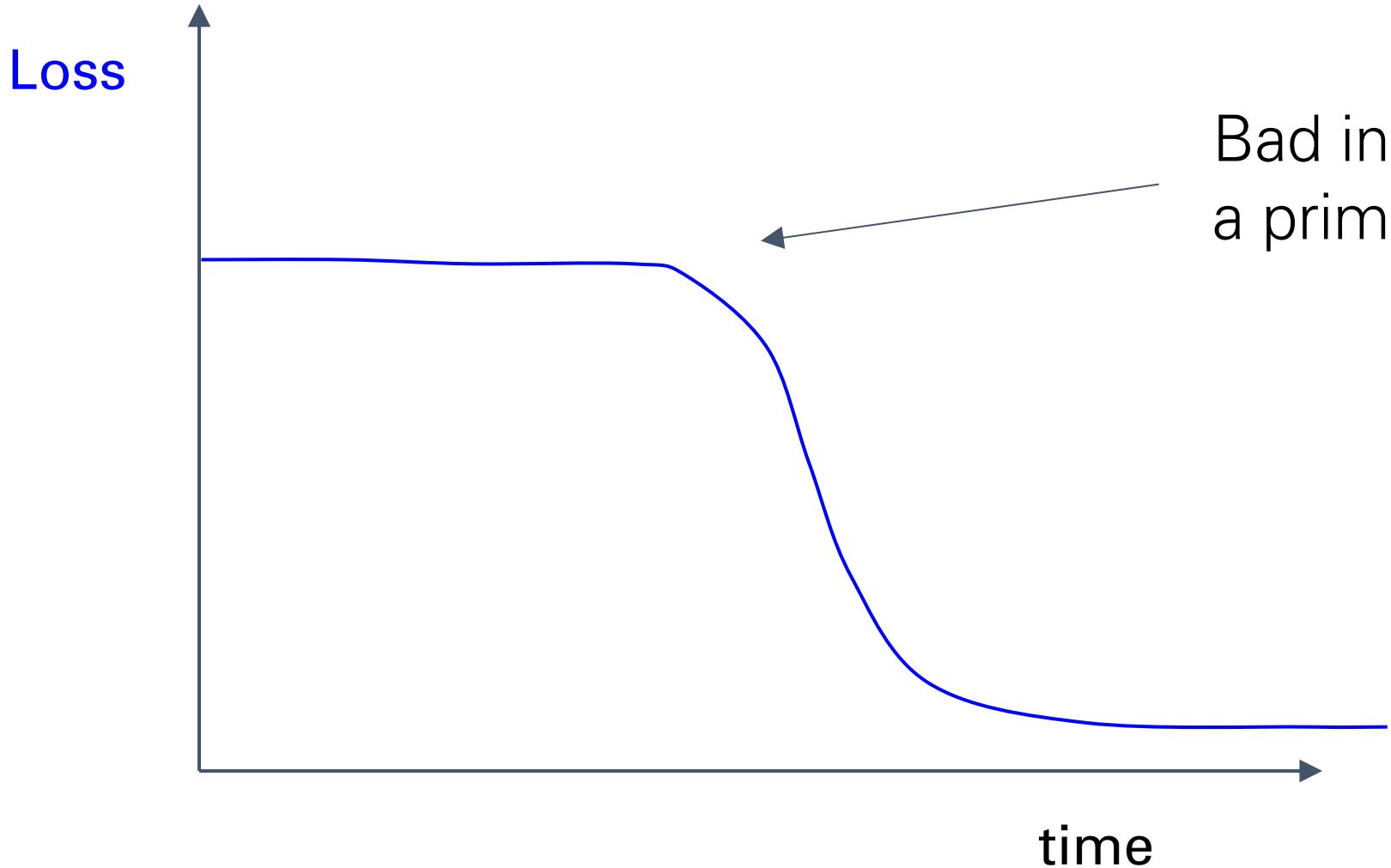
Cross-validation “command center”



Monitor and visualize the loss curve



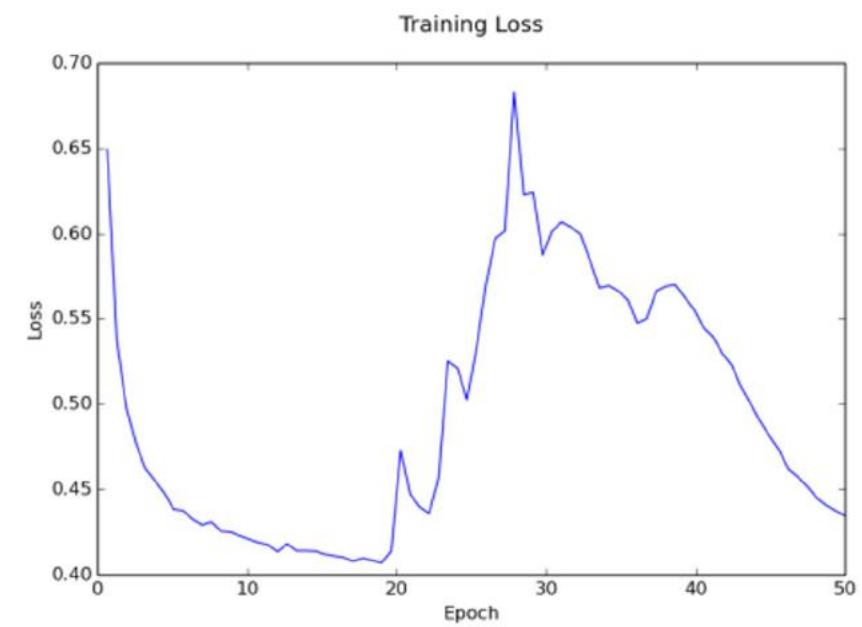
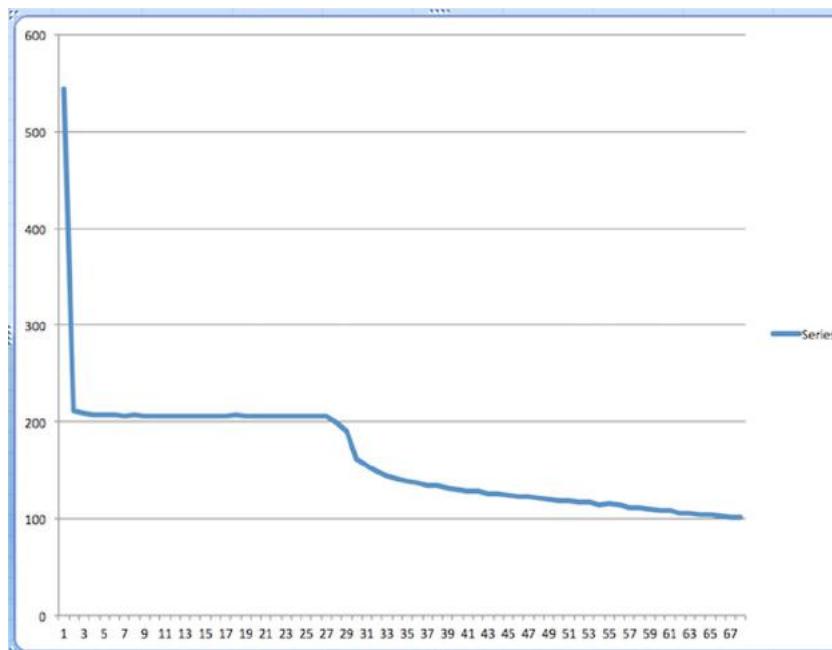
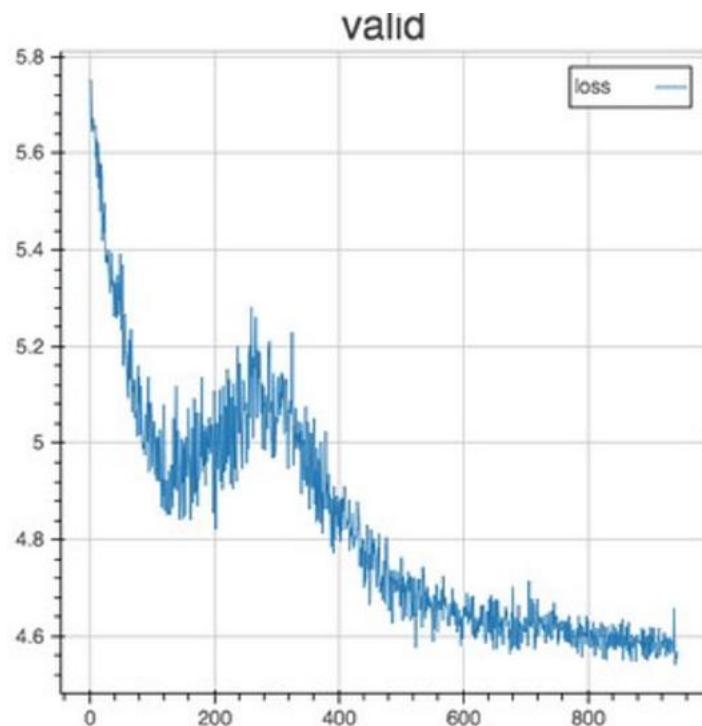




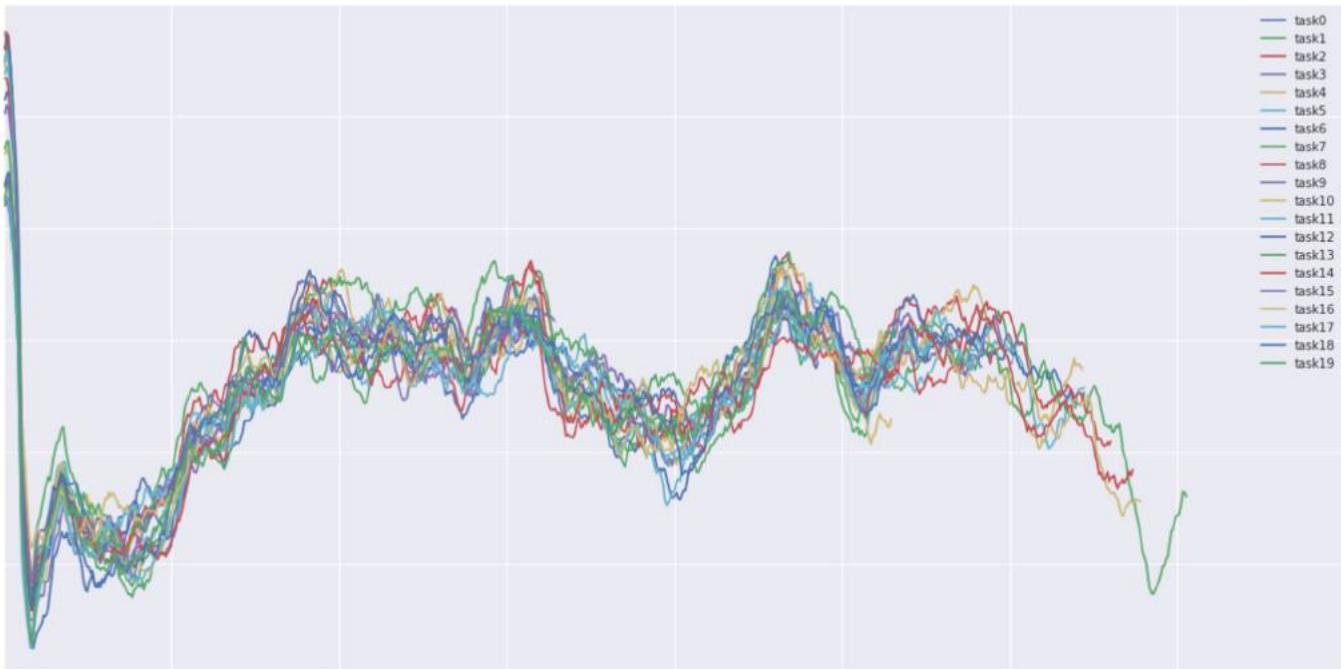
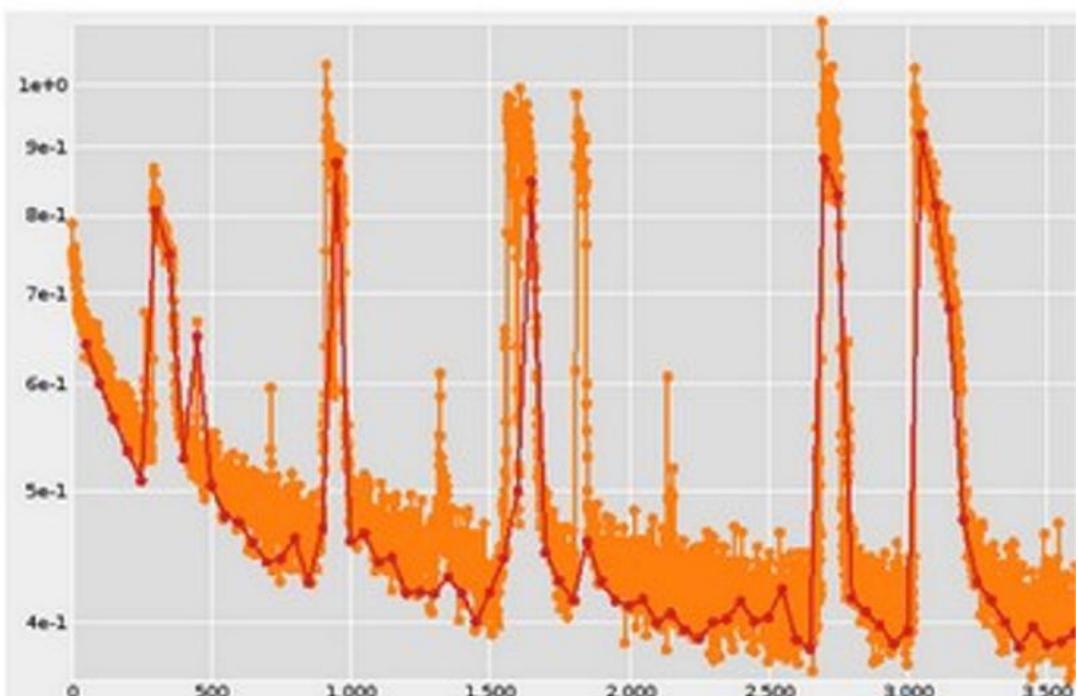
Bad initialization
a prime suspect

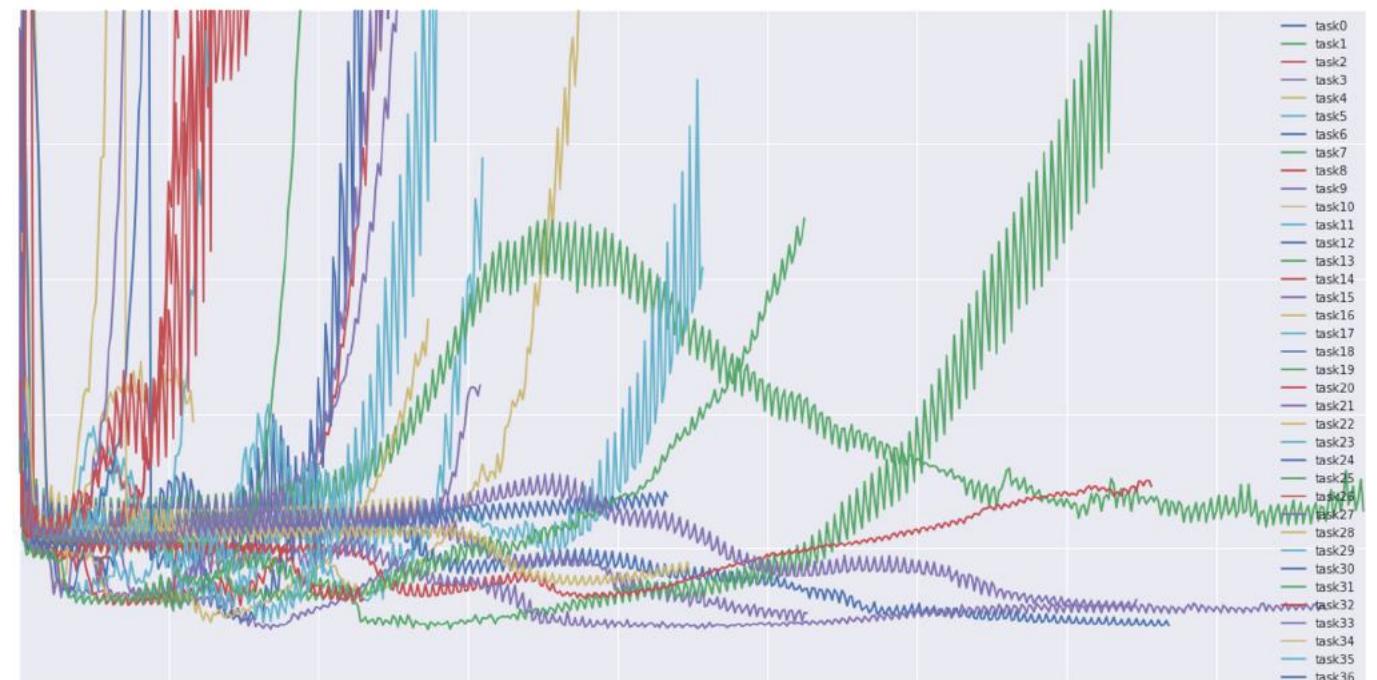
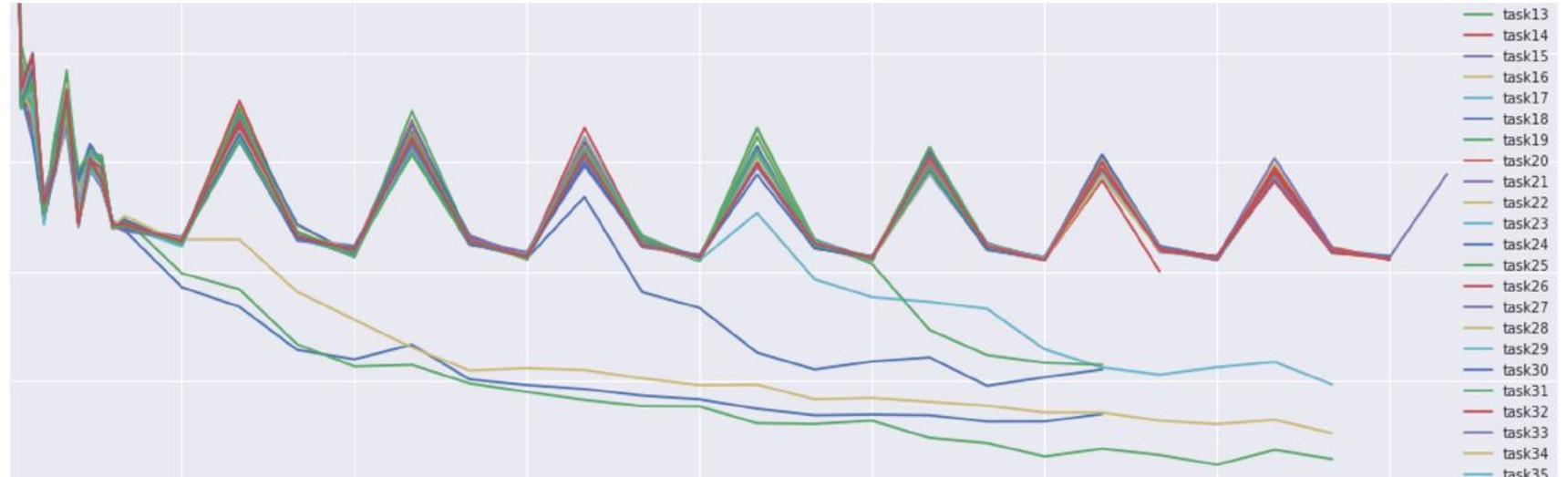
lossfunctions.tumblr.com

Loss function specimen



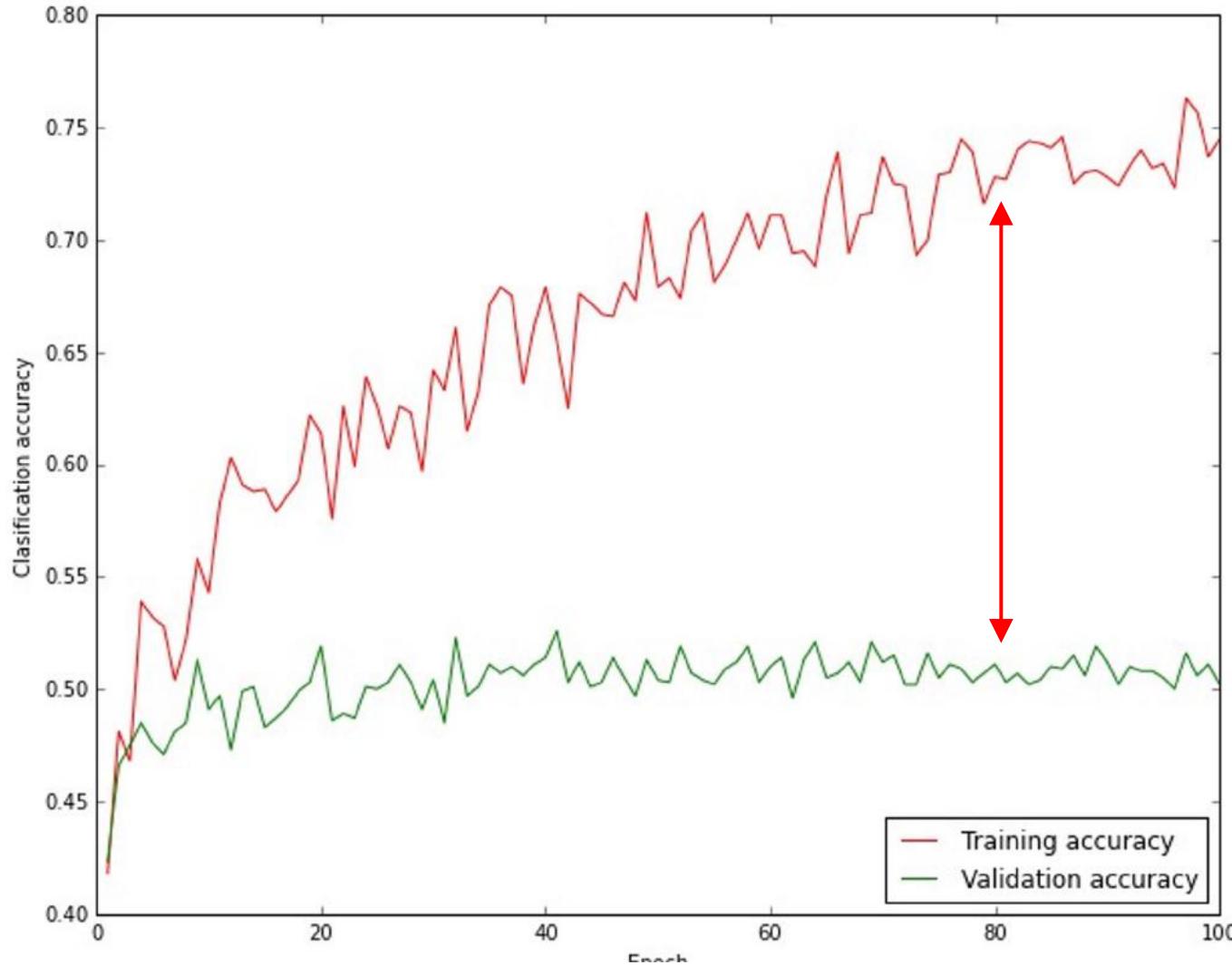
lossfunctions.tumblr.com





lossfunctions.tumblr.com

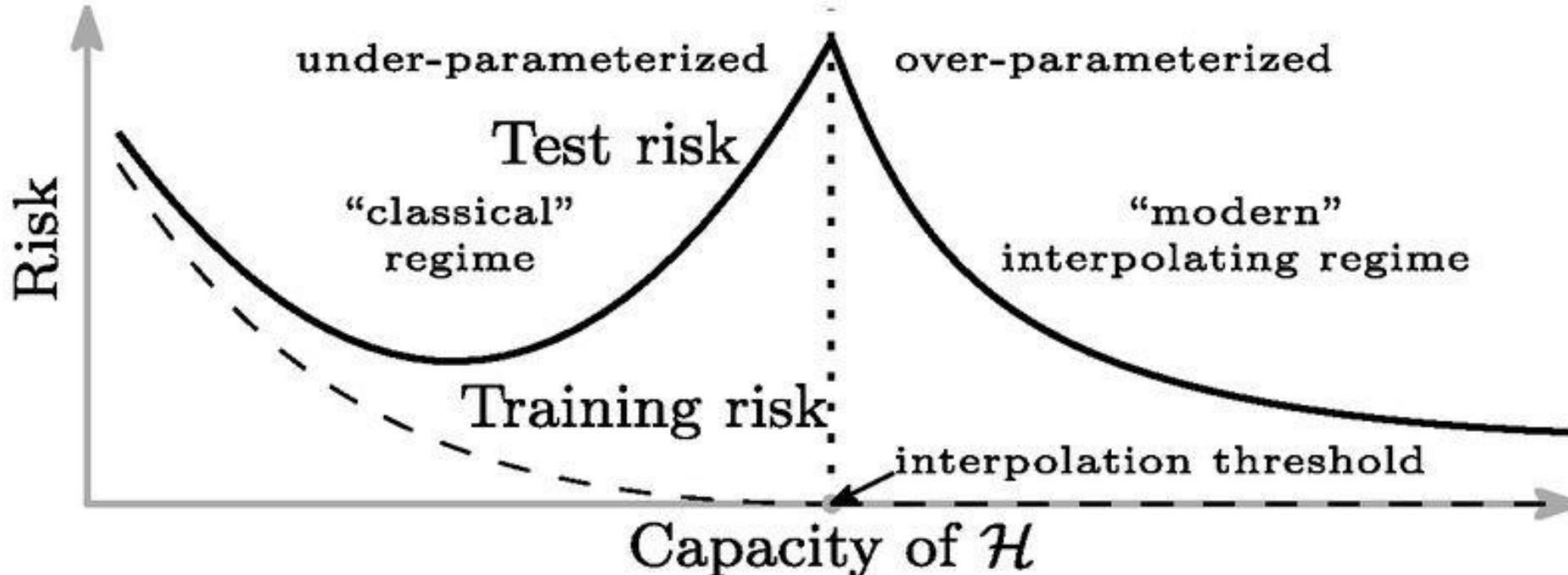
Monitor and visualize the accuracy:



big gap = overfitting
=> increase regularization strength

no gap
=> increase model capacity?

The Double Descent Phenomenon

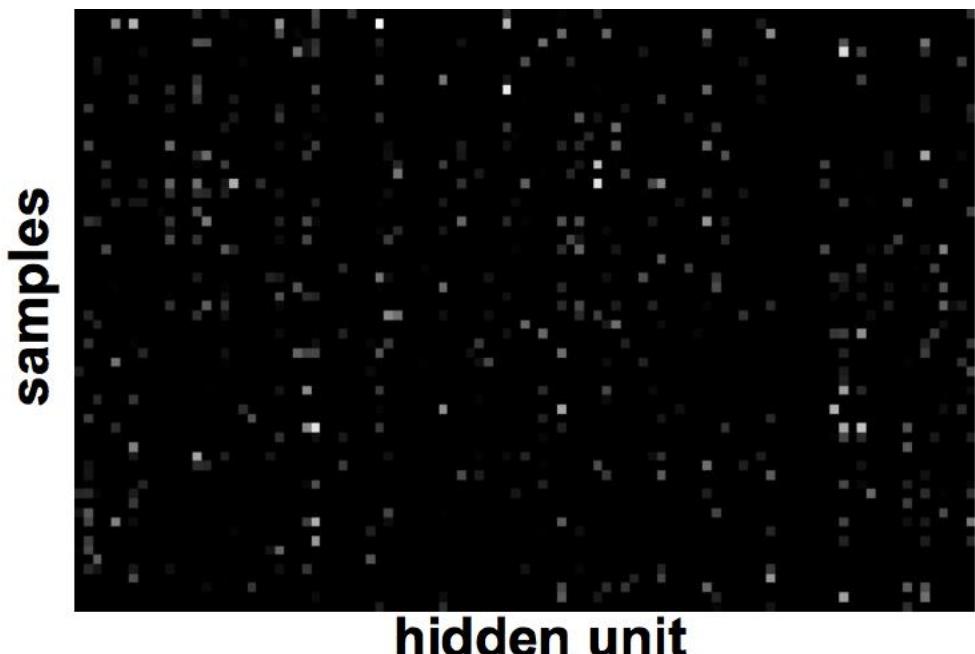


- Test error follows the traditional U-shaped curve in the under-parameterized case and monotonically decreases in the over-parameterized case.

(Neal et al., 2018).
(Spigler et al., 2018)
(Geiger et al., 2019)
(Belkin et al., 2019)

Visualization

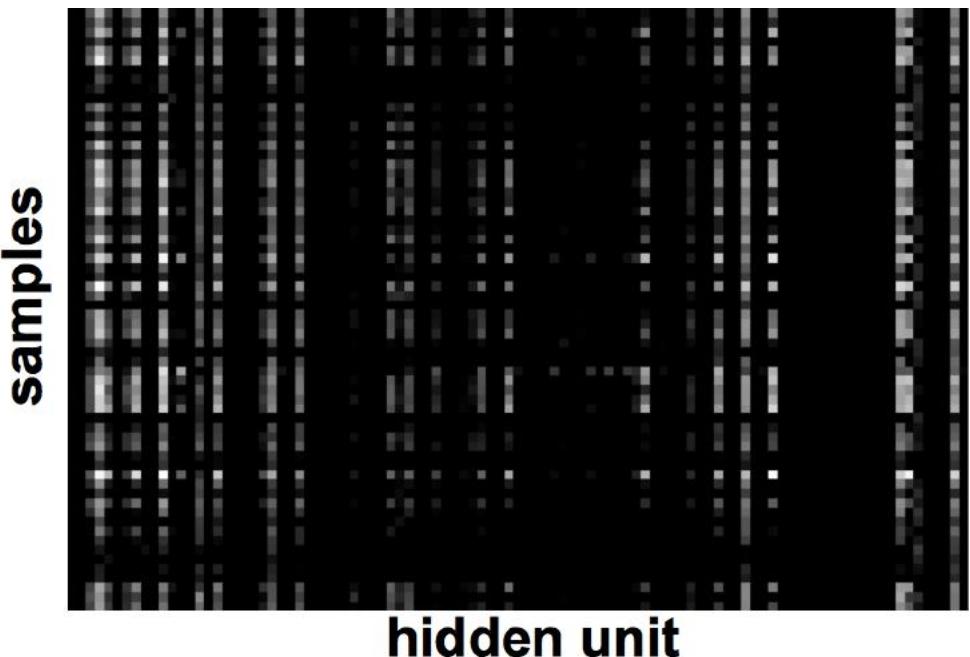
- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance



- Good training: hidden units are sparse across samples

Visualization

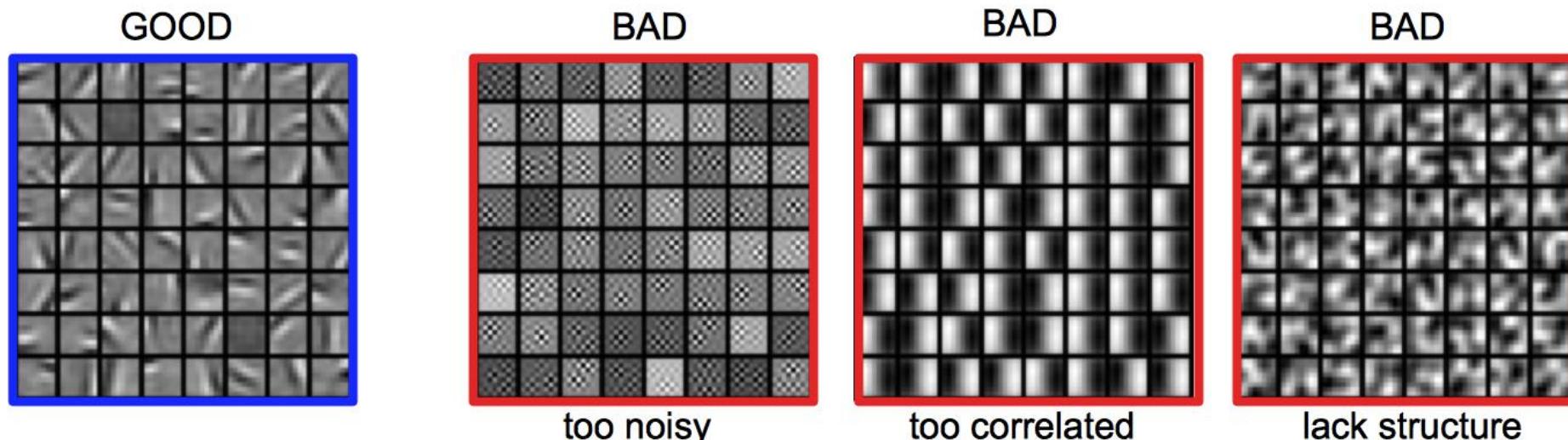
- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance



- Bad training: many hidden units ignore the input and/or exhibit strong correlations

Visualization

- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance
- Visualize parameters: learned features should exhibit structure and should be uncorrelated and are uncorrelated



Take Home Messages

Optimization Tricks

- SGD with momentum, batch-normalization, and dropout usually works very well
- Pick learning rate by running on a subset of the data
 - Start with large learning rate & divide by 2 until loss does not diverge
 - Decay learning rate by a factor of ~100 or more by the end of training
- Use ReLU nonlinearity
- Initialize parameters so that each feature across layers has similar variance. Avoid units in saturation.

Ways To Improve Generalization

- Weight sharing (greatly reduce the number of parameters)
- Dropout
- Weight decay (L2, L1)
- Sparsity in the hidden units

Babysitting

- Check gradients numerically by finite differences
- Visualize features (features need to be uncorrelated) and have high variance
- Visualize parameters: learned features should exhibit structure and should be uncorrelated and are uncorrelated
- Measure error on both training and validation set
- Test on a small subset of the data and check the error → 0.

Next lecture:
Convolutional
Neural Networks