

# Lecture 3: Regularization and Optimization

# Administrative: Assignment 1

Released last week, due **Fri 4/21 at 11:59pm**

Office hours: help with high-level questions only, no code debugging. [[No Code Show Policy](#)]

# Administrative: Project proposal

Due **Mon 4/24**

TA expertise are posted on the webpage.

([http://cs231n.stanford.edu/office\\_hours.html](http://cs231n.stanford.edu/office_hours.html))

# Administrative: Ed

Please make sure to check and read all pinned Ed posts.

- AWS credit: create an account, submit the number ID using google form by 4/13.
- Project group: fill in your information in the google form and/or look through existing responses and reach out
- SCPD: if you would like to take the midterm on-campus, make a private Ed post to let us know by 4/12.

# Image Classification: A core task in Computer Vision



This image by [Nikita](#) is  
licensed under [CC-BY 2.0](#)

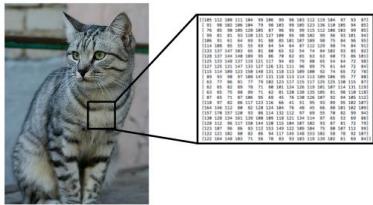
(assume given a set of labels)  
{dog, cat, truck, plane, ...}



cat  
dog  
bird  
deer  
truck

# Recall from last time: Challenges of recognition

Viewpoint

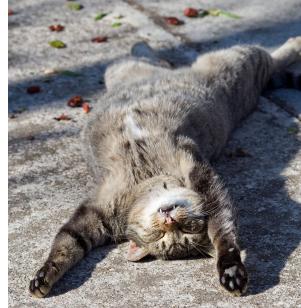


Illumination



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Deformation



[This image](#) by Umberto Salvagnin  
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Occlusion



[This image](#) by ionsson is licensed  
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Clutter



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Intraclass Variation



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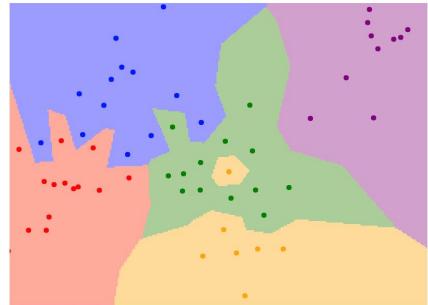
## Recall from last time: data-driven approach, kNN

The image displays a 10x10 grid of 100 small square images, each representing a different object category from the ImageNet dataset. The categories are listed vertically on the left side of the grid:

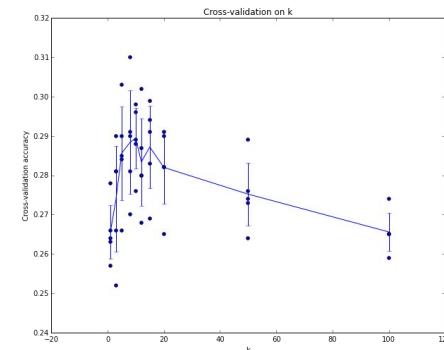
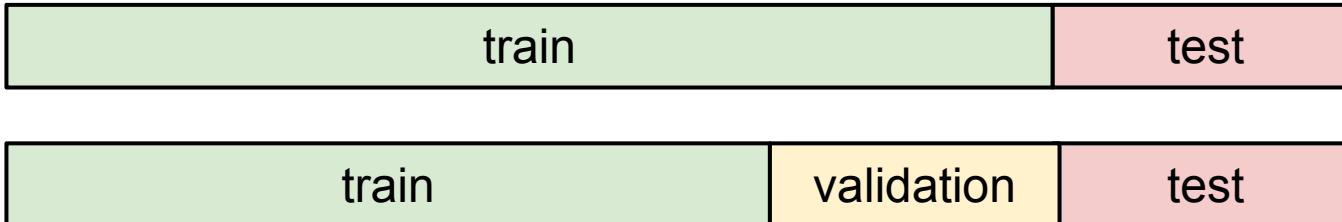
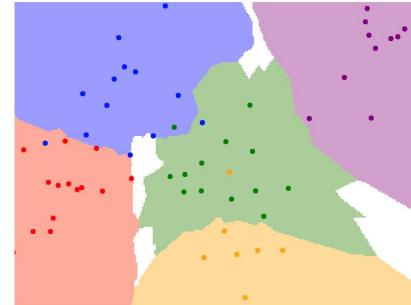
- airplane
- automobile
- bird
- cat
- deer
- dog
- frog
- horse
- ship
- truck

Each image in the grid shows a different example of the corresponding object, such as various types of aircraft, cars, birds, felines, cervids, canines, anurans, equines, vessels, and vehicles.

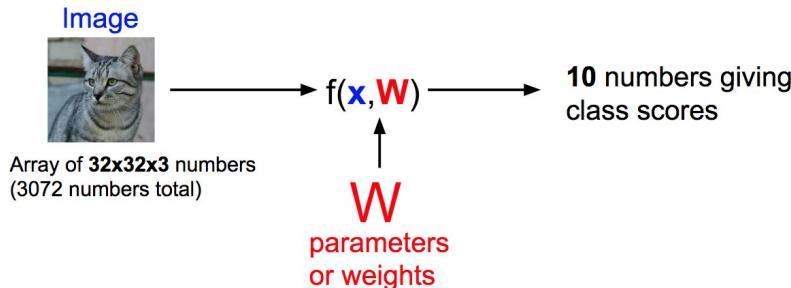
## 1-NN classifier



## 5-NN classifier



# Recall from last time: Linear Classifier



$$f(\mathbf{x}, \mathbf{W}) = \mathbf{W}\mathbf{x} + \mathbf{b}$$

## Algebraic Viewpoint

$$f(\mathbf{x}, \mathbf{W}) = \mathbf{W}\mathbf{x}$$

Stretch pixels into column:

Input image

$\begin{matrix} 56 & 231 \\ 24 & 2 \end{matrix}$

$\begin{matrix} 0.2 & -0.5 & 0.1 & 2.0 \\ 1.5 & 1.3 & 2.1 & 0.0 \\ 0 & 0.25 & 0.2 & -0.3 \end{matrix}$

$\begin{matrix} 56 \\ 231 \\ 24 \\ 2 \end{matrix}$

$\begin{matrix} 1.1 \\ 3.2 \\ -1.2 \end{matrix}$

$\begin{matrix} -96.8 \\ 437.9 \\ 61.95 \end{matrix}$

Cat score  
Dog score  
Ship score

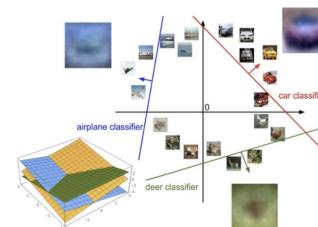
## Visual Viewpoint

One template per class



## Geometric Viewpoint

Hyperplanes cutting up space

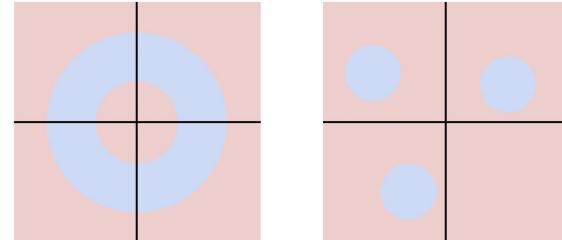


**Class 1:**  
 $1 \leq L_2 \text{ norm} \leq 2$

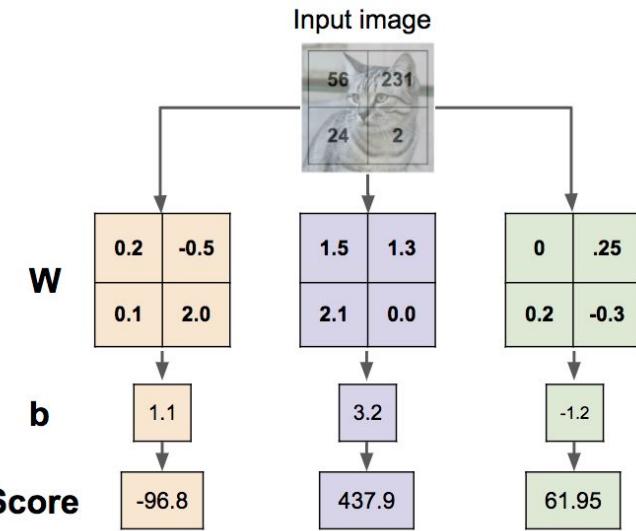
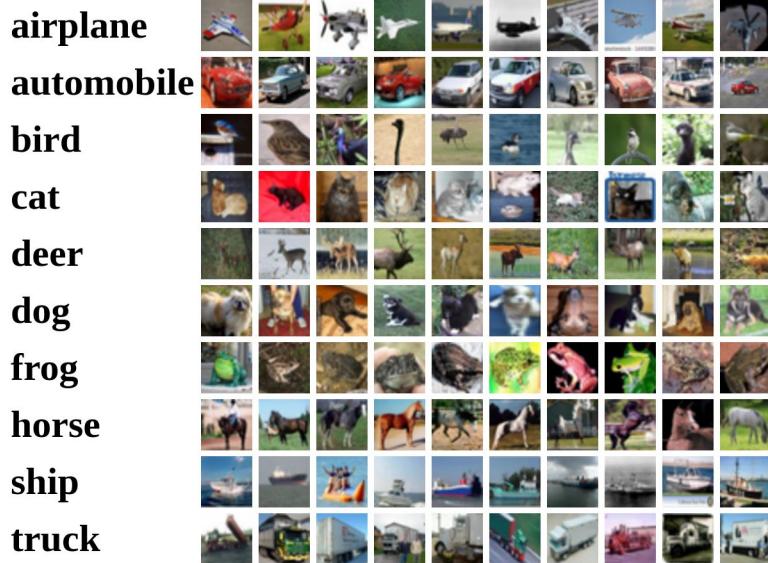
**Class 2:**  
Everything else

**Class 1:**  
Three modes

**Class 2:**  
Everything else



# Interpreting a Linear Classifier: Visual Viewpoint



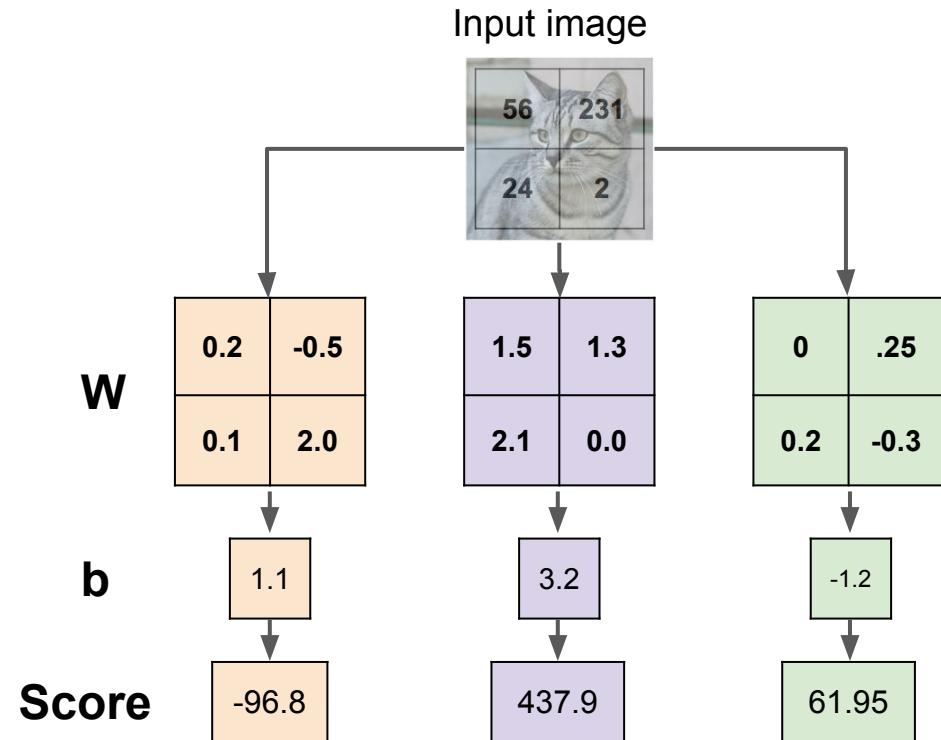
# Example with an image with 4 pixels, and 3 classes (cat/dog/ship)

## Algebraic Viewpoint

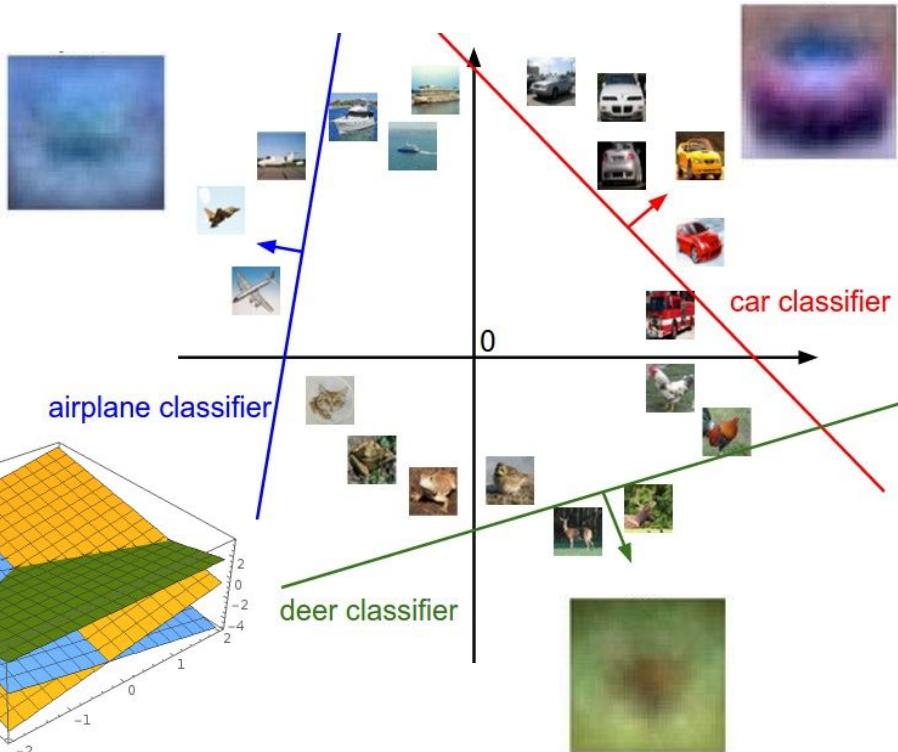
$$f(x, W) = Wx$$

Stretch pixels into column

$$\begin{matrix} \text{Input image} \\ \begin{bmatrix} 56 & 231 \\ 24 & 2 \end{bmatrix} \end{matrix} \xrightarrow{\text{Stretch pixels into column}} \begin{matrix} \text{Input image} \\ \begin{bmatrix} 56 \\ 231 \\ 24 \\ 2 \end{bmatrix} \end{matrix}$$
$$\begin{matrix} \text{W} \\ \begin{bmatrix} 0.2 & -0.5 & 0.1 & 2.0 \\ 1.5 & 1.3 & 2.1 & 0.0 \\ 0 & 0.25 & 0.2 & -0.3 \end{bmatrix} \end{matrix} + \begin{matrix} \text{b} \\ \begin{bmatrix} 1.1 \\ 3.2 \\ -1.2 \end{bmatrix} \end{matrix} = \begin{matrix} \text{Cat score} \\ -96.8 \end{matrix} \quad \begin{matrix} \text{Dog score} \\ 437.9 \end{matrix} \quad \begin{matrix} \text{Ship score} \\ 61.95 \end{matrix}$$



# Interpreting a Linear Classifier: Geometric Viewpoint



$$f(x, W) = Wx + b$$



Array of **32x32x3** numbers  
(3072 numbers total)

Plot created using [Wolfram Cloud](#)

[Cat image](#) by [Nikita](#) is licensed under [CC-BY 2.0](#)

Suppose: 3 training examples, 3 classes.  
With some  $W$  the scores  $f(x, W) = Wx$  are:



cat	<b>3.2</b>	1.3	2.2
car	5.1	<b>4.9</b>	2.5
frog	-1.7	2.0	<b>-3.1</b>

A **loss function** tells how good our current classifier is

Given a dataset of examples

$$\{(x_i, y_i)\}_{i=1}^N$$

Where  $x_i$  is image and  
 $y_i$  is (integer) label

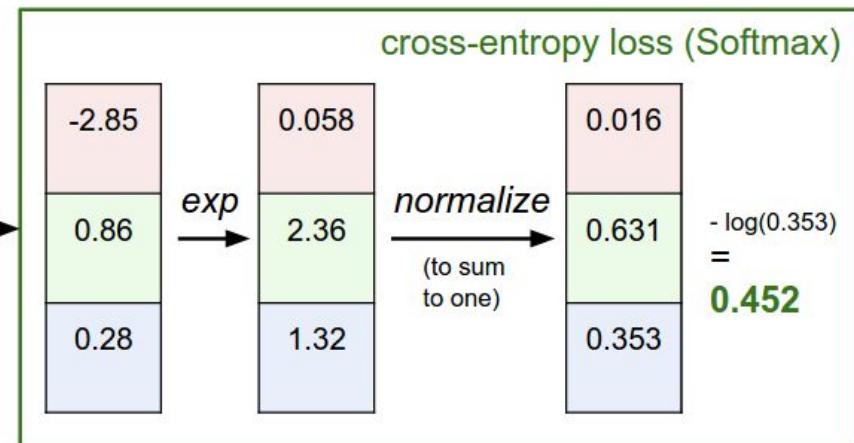
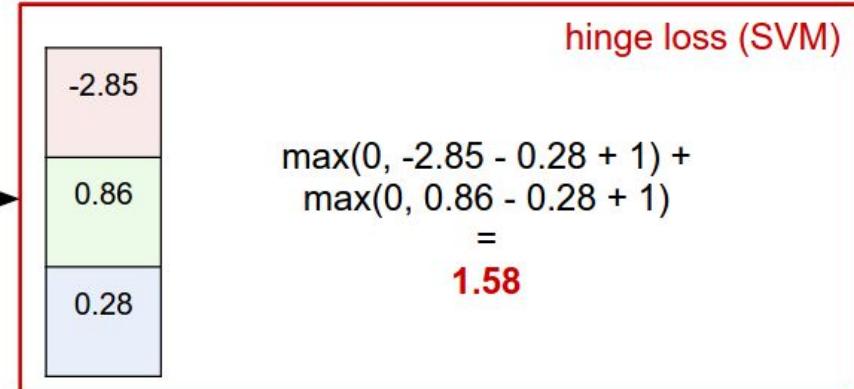
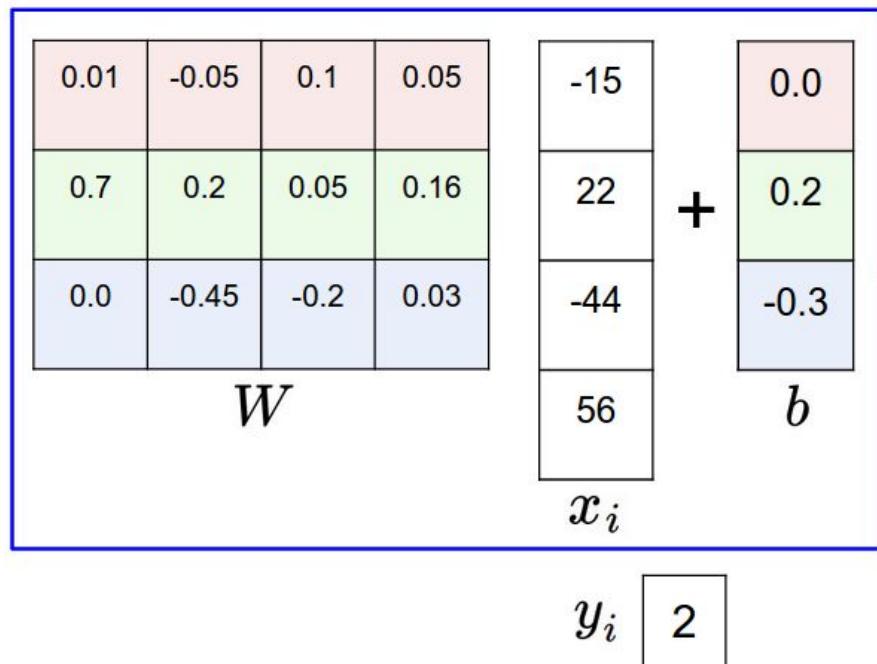
Loss over the dataset is a average of loss over examples:

$$L = \frac{1}{N} \sum_i L_i(f(x_i, W), y_i)$$

# Softmax vs. SVM

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right) \quad L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

matrix multiply + bias offset



$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

Q: Suppose that we found a  $W$  such that  $L = 0$ .  
Is this  $W$  unique?

$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

Q: Suppose that we found a  $W$  such that  $L = 0$ .  
Is this  $W$  unique?

**No!  $2W$  is also has  $L = 0$ !**

Suppose: 3 training examples, 3 classes.  
With some  $W$  the scores  $f(x, W) = Wx$  are:



cat	<b>3.2</b>	1.3	2.2
car	5.1	<b>4.9</b>	2.5
frog	-1.7	2.0	<b>-3.1</b>
Losses:	2.9	<b>0</b>	

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

**Before:**

$$\begin{aligned}
 &= \max(0, 1.3 - 4.9 + 1) \\
 &\quad + \max(0, 2.0 - 4.9 + 1) \\
 &= \max(0, -2.6) + \max(0, -1.9) \\
 &= 0 + 0 \\
 &= 0
 \end{aligned}$$

**With  $W$  twice as large:**

$$\begin{aligned}
 &= \max(0, 2.6 - 9.8 + 1) \\
 &\quad + \max(0, 4.0 - 9.8 + 1) \\
 &= \max(0, -6.2) + \max(0, -4.8) \\
 &= 0 + 0 \\
 &= 0
 \end{aligned}$$

$$f(x, W) = Wx$$

$$L = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1)$$

E.g. Suppose that we found a  $W$  such that  $L = 0$ .  
Is this  $W$  unique?

**No!  $2W$  is also has  $L = 0$ !**

**How do we choose between  $W$  and  $2W$ ?**

# Regularization -

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

**Data loss:** Model predictions  
should match training data

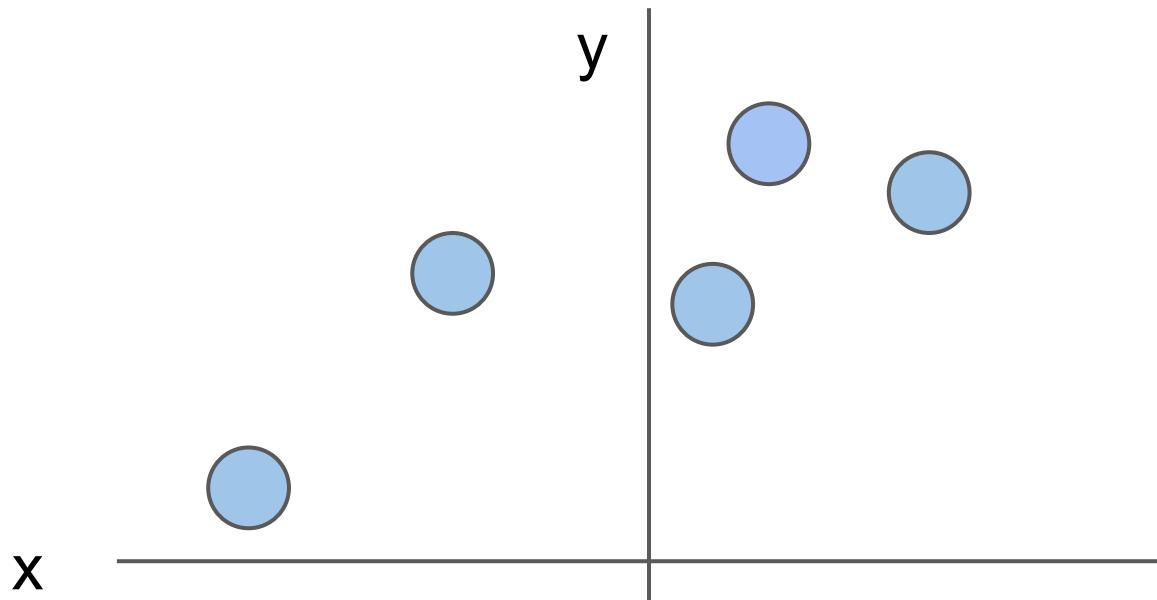
# Regularization

$$L(W) = \underbrace{\frac{1}{N} \sum_{i=1}^N L_i(f(x_i, W), y_i)}_{\text{Data loss: Model predictions should match training data}} + \lambda R(W)$$

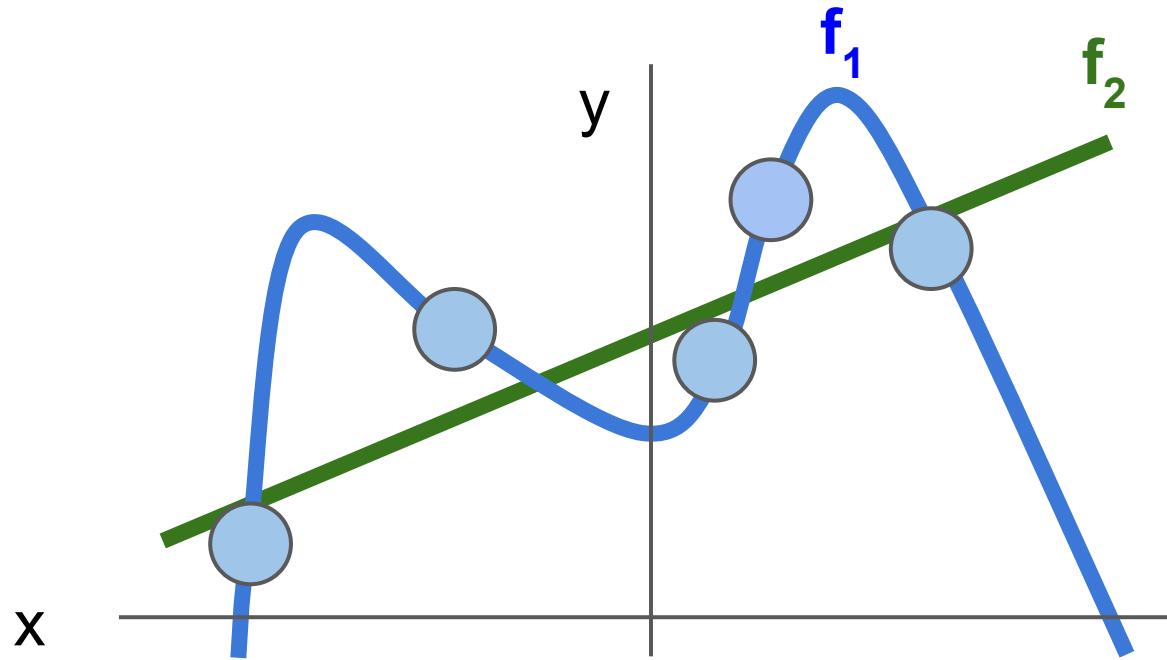

**Data loss:** Model predictions should match training data

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

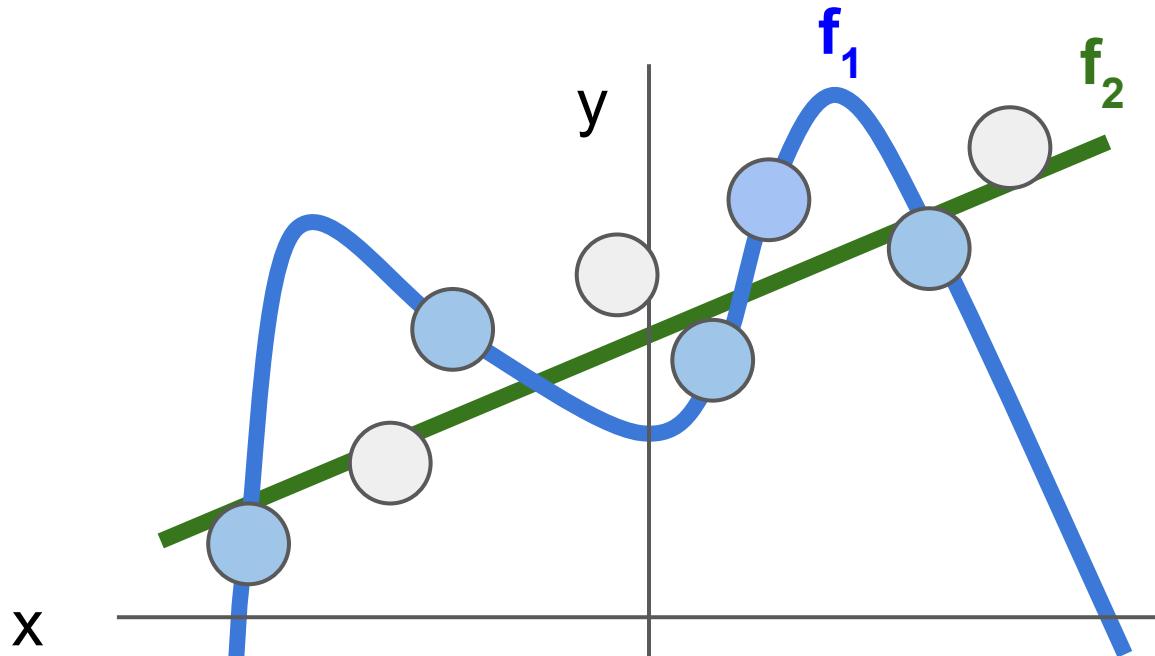
# Regularization intuition: toy example training data



# Regularization intuition: Prefer Simpler Models



# Regularization: Prefer Simpler Models



Regularization pushes against fitting the data  
too well so we don't fit noise in the data

# Regularization

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

**Data loss:** Model predictions should match training data



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

**Occam's Razor:** Among multiple competing hypotheses, the simplest is the best, William of Ockham 1285-1347

# Regularization

$\lambda$  = regularization strength  
(hyperparameter)

$$L(W) = \underbrace{\frac{1}{N} \sum_{i=1}^N L_i(f(x_i, W), y_i)}_{\text{Data loss: Model predictions should match training data}} + \lambda R(W)$$



**Data loss:** Model predictions should match training data

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

# Regularization

$\lambda$  = regularization strength  
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$$L(W) = \underbrace{\frac{1}{N} \sum_{i=1}^N L_i(f(x_i, W), y_i)}_{\text{Data loss: Model predictions should match training data}} + \lambda R(W)$$



**Data loss:** Model predictions should match training data

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

## Simple examples

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

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

Elastic net (L1 + L2):  $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

# Regularization

$\lambda$  = regularization strength  
(hyperparameter)

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

**Data loss:** Model predictions should match training data



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

## Simple examples

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

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

Elastic net (L1 + L2):  $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$

## More complex:

Dropout

Batch normalization

Stochastic depth, fractional pooling, etc

# Regularization

$\lambda$  = regularization strength  
(hyperparameter)

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

**Data loss:** Model predictions should match training data

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

Why regularize?

- Express preferences over weights
- Make the model *simple* so it works on test data
- Improve optimization by adding curvature

# Regularization: Expressing Preferences

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

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

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

L2 Regularization

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

Which of w1 or w2 will  
the L2 regularizer prefer?

$$w_1^T x = w_2^T x = 1$$

# Regularization: Expressing Preferences

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

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

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

L2 Regularization

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

Which of w1 or w2 will  
the L2 regularizer prefer?

L2 regularization likes to  
“spread out” the weights

$$w_1^T x = w_2^T x = 1$$

# Regularization: Expressing Preferences

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

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

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

L2 Regularization

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

Which of w1 or w2 will  
the L2 regularizer prefer?

L2 regularization likes to  
“spread out” the weights

$$w_1^T x = w_2^T x = 1$$

Which one would L1  
regularization prefer?

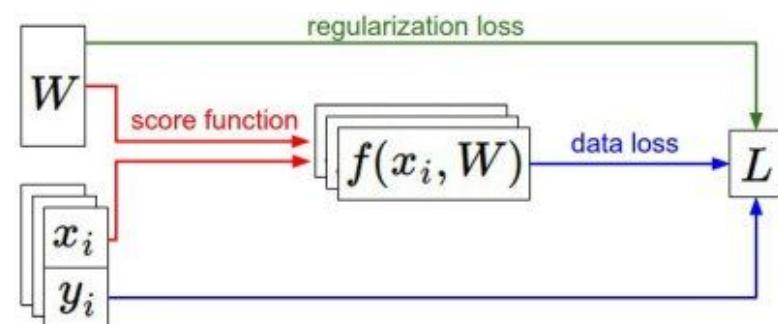
# Recap

- We have some dataset of  $(x, y)$
- We have a **score function**:  $s = f(x; W) = Wx$  e.g.
- We have a **loss function**:

$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{sj}}\right) \quad \text{Softmax}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \quad \text{SVM}$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + R(W) \quad \text{Full loss}$$



# Recap

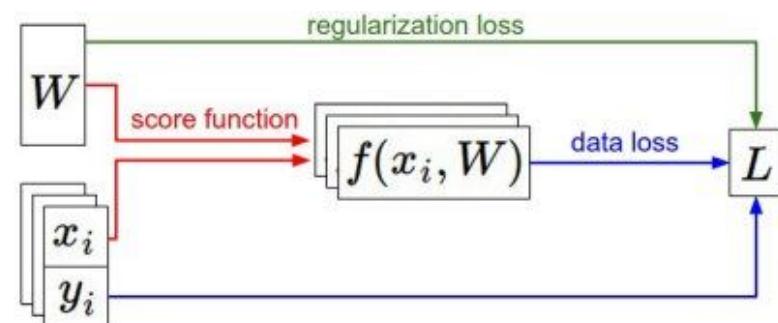
How do we find the best  $W$ ?

- We have some dataset of  $(x, y)$
- We have a **score function**:  $s = f(x; W) = Wx$  e.g.
- We have a **loss function**:

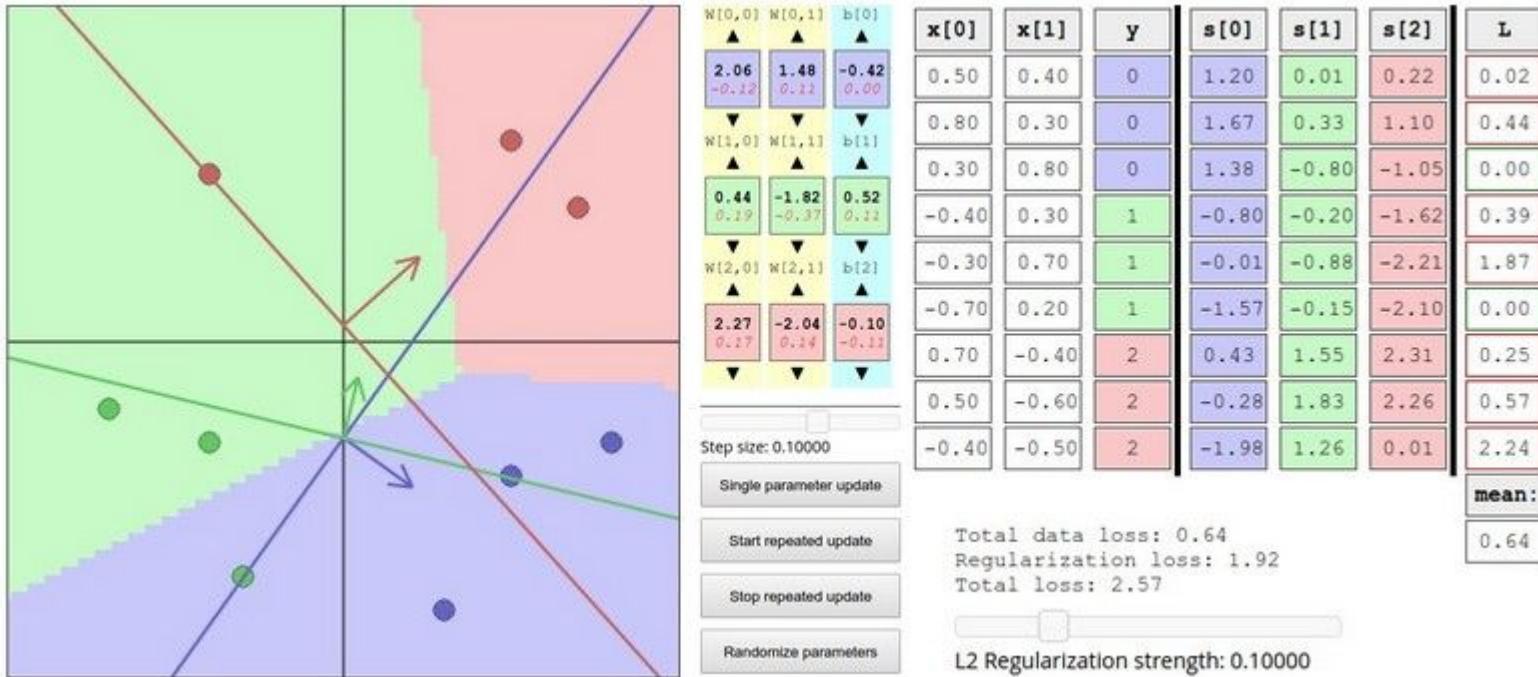
$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{sj}}\right) \quad \text{Softmax}$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1) \quad \text{SVM}$$

$$L = \frac{1}{N} \sum_{i=1}^N L_i + R(W) \quad \text{Full loss}$$



# Interactive Web Demo



<http://vision.stanford.edu/teaching/cs231n-demos/linear-classify/>

# Optimization



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[Walking man image](#) is CC0 1.0 public domain

# Strategy #1: A first very bad idea solution: Random search

```
# assume X_train is the data where each column is an example (e.g. 3073 x 50,000)
# assume Y_train are the labels (e.g. 1D array of 50,000)
# assume the function L evaluates the loss function

bestloss = float("inf") # Python assigns the highest possible float value
for num in xrange(1000):
    W = np.random.randn(10, 3073) * 0.0001 # generate random parameters
    loss = L(X_train, Y_train, W) # get the loss over the entire training set
    if loss < bestloss: # keep track of the best solution
        bestloss = loss
        bestW = W
    print 'in attempt %d the loss was %f, best %f' % (num, loss, bestloss)

# prints:
# in attempt 0 the loss was 9.401632, best 9.401632
# in attempt 1 the loss was 8.959668, best 8.959668
# in attempt 2 the loss was 9.044034, best 8.959668
# in attempt 3 the loss was 9.278948, best 8.959668
# in attempt 4 the loss was 8.857370, best 8.857370
# in attempt 5 the loss was 8.943151, best 8.857370
# in attempt 6 the loss was 8.605604, best 8.605604
# ... (truncated: continues for 1000 lines)
```

# Lets see how well this works on the test set...

```
# Assume X_test is [3073 x 10000], Y_test [10000 x 1]
scores = Wbest.dot(Xte_cols) # 10 x 10000, the class scores for all test examples
# find the index with max score in each column (the predicted class)
Yte_predict = np.argmax(scores, axis = 0)
# and calculate accuracy (fraction of predictions that are correct)
np.mean(Yte_predict == Yte)
# returns 0.1555
```

15.5% accuracy! not bad!  
(SOTA is ~99.7%)

## Strategy #2: Follow the slope



## Strategy #2: Follow the slope

In 1-dimension, the derivative of a function:

$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h}$$

In multiple dimensions, the **gradient** is the vector of (partial derivatives) along each dimension

The slope in any direction is the **dot product** of the direction with the gradient  
The direction of steepest descent is the **negative gradient**

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,  
?,...]

current W:	W + h (first dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...] <b>loss 1.25347</b>	[0.34 + 0.0001, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...] <b>loss 1.25322</b>	[?, , , , , , , , ,...]

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (first dim):**

[0.34 + 0.0001,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25322**

**gradient dW:**

**[-2.5,**  
?,  
?,

$$\frac{(1.25322 - 1.25347)}{0.0001} = -2.5$$

$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h}$$

?,  
?,...]

current W:	W + h (second dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...]	[0.34, -1.11 + <b>0.0001</b> , 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...]	[-2.5, ?, ?, ?, ?, ?, ?, ?, ?, ?,...]
<b>loss 1.25347</b>	<b>loss 1.25353</b>	

current W:

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

loss 1.25347

W + h (second dim):

[0.34,  
-1.11 + 0.0001,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

loss 1.25353

gradient dW:

[-2.5,  
0.6,  
?,  
?]

$$\frac{(1.25353 - 1.25347)}{0.0001} = 0.6$$

$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h}$$

?,...]

current W:	W + h (third dim):	gradient dW:
[0.34, -1.11, 0.78, 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...]	[0.34, -1.11, 0.78 + <b>0.0001</b> , 0.12, 0.55, 2.81, -3.1, -1.5, 0.33,...]	[-2.5, 0.6, ?, ?, ?, ?, ?, ?, ?, ?,...]
<b>loss 1.25347</b>	<b>loss 1.25347</b>	

current W:

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

loss 1.25347

W + h (third dim):

[0.34,  
-1.11,  
0.78 + 0.0001,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

loss 1.25347

gradient dW:

[-2.5,  
0.6,  
0,  
?,  
?]

$$\frac{(1.25347 - 1.25347)}{0.0001} = 0$$

$$\frac{df(x)}{dx} = \lim_{h \rightarrow 0} \frac{f(x + h) - f(x)}{h}$$

?, ...]

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**W + h (third dim):**

[0.34,  
-1.11,  
0.78 + **0.0001**,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[-2.5,  
0.6,  
**0**,  
?,  
?]

### Numeric Gradient

- Slow! Need to loop over all dimensions
- Approximate

[,...]

This is silly. The loss is just a function of  $W$ :

$$L = \frac{1}{N} \sum_{i=1}^N L_i + \sum_k W_k^2$$

$$L_i = \sum_{j \neq y_i} \max(0, s_j - s_{y_i} + 1)$$

$$s = f(x; W) = Wx$$

want  $\nabla_W L$

This is silly. The loss is just a function of W:

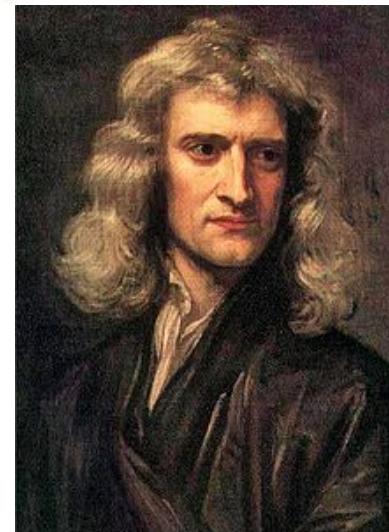
$$L = \frac{1}{N} \sum_{i=1}^N L_i + \sum_k W_k^2$$

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$$s = f(x; W) = Wx$$

want  $\nabla_W L$

Use calculus to compute an analytic gradient



[This image](#) is in the public domain



[This image](#) is in the public domain

**current W:**

[0.34,  
-1.11,  
0.78,  
0.12,  
0.55,  
2.81,  
-3.1,  
-1.5,  
0.33,...]

**loss 1.25347**

**gradient dW:**

[-2.5,  
0.6,  
0,  
0.2,  
0.7,  
-0.5,  
1.1,  
1.3,  
-2.1,...]

dW = ...  
(some function  
data and W)



# In summary:

- Numerical gradient: approximate, slow, easy to write
- Analytic gradient: exact, fast, error-prone

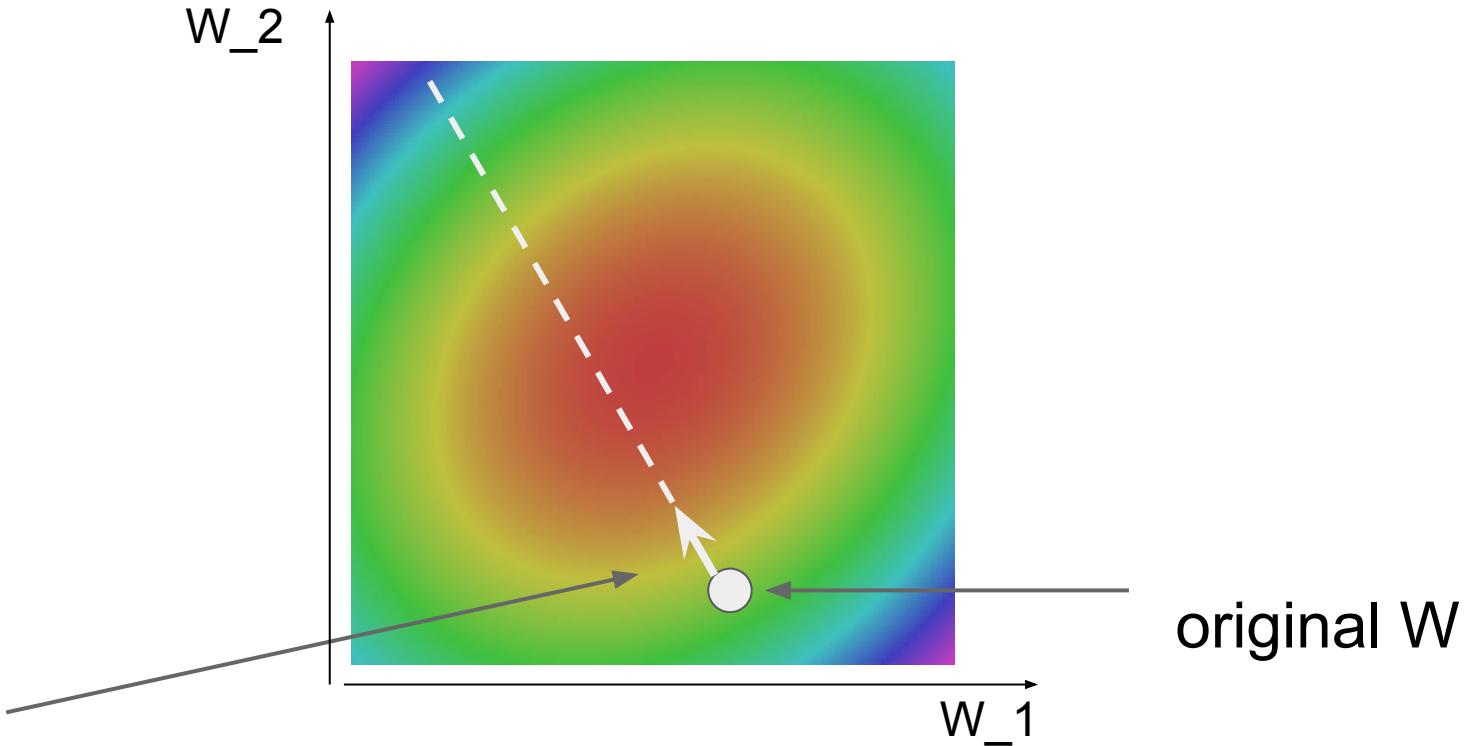
=>

In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check**.

# Gradient Descent

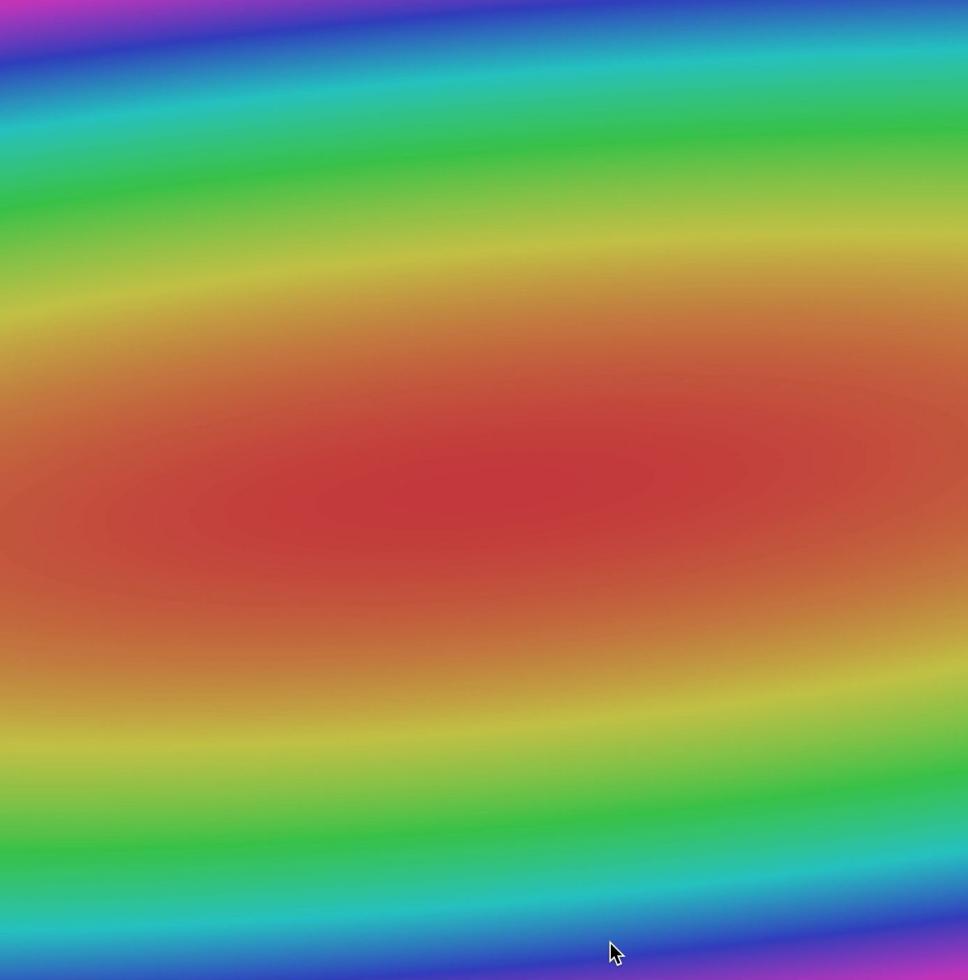
```
# Vanilla Gradient Descent

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



negative gradient direction

original  $W$



# Stochastic Gradient Descent (SGD)

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

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

Full sum expensive  
when N is large!

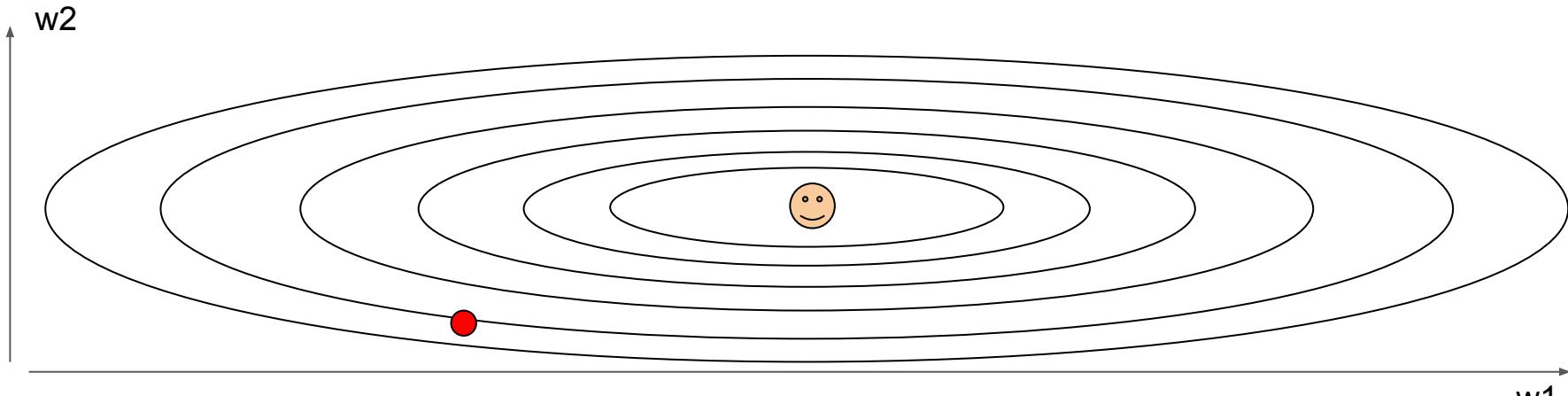
Approximate sum  
using a **minibatch** of  
examples  
32 / 64 / 128 common

```
# Vanilla Minibatch Gradient Descent
```

```
while True:  
    data_batch = sample_training_data(data, 256) # sample 256 examples  
    weights_grad = evaluate_gradient(loss_fun, data_batch, weights)  
    weights += - step_size * weights_grad # perform parameter update
```

# Optimization: Problem #1 with SGD

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



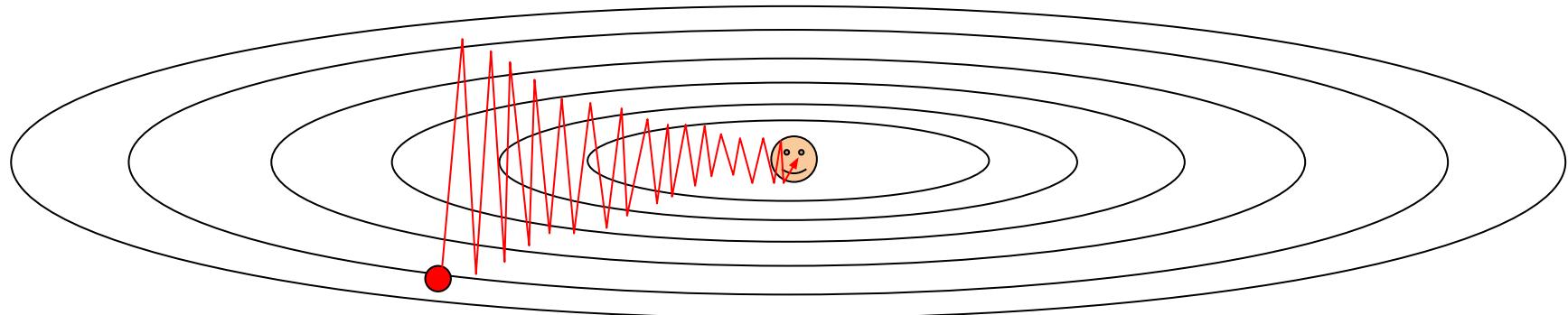
Aside: Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

# Optimization: Problem #1 with SGD

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

What does gradient descent do?

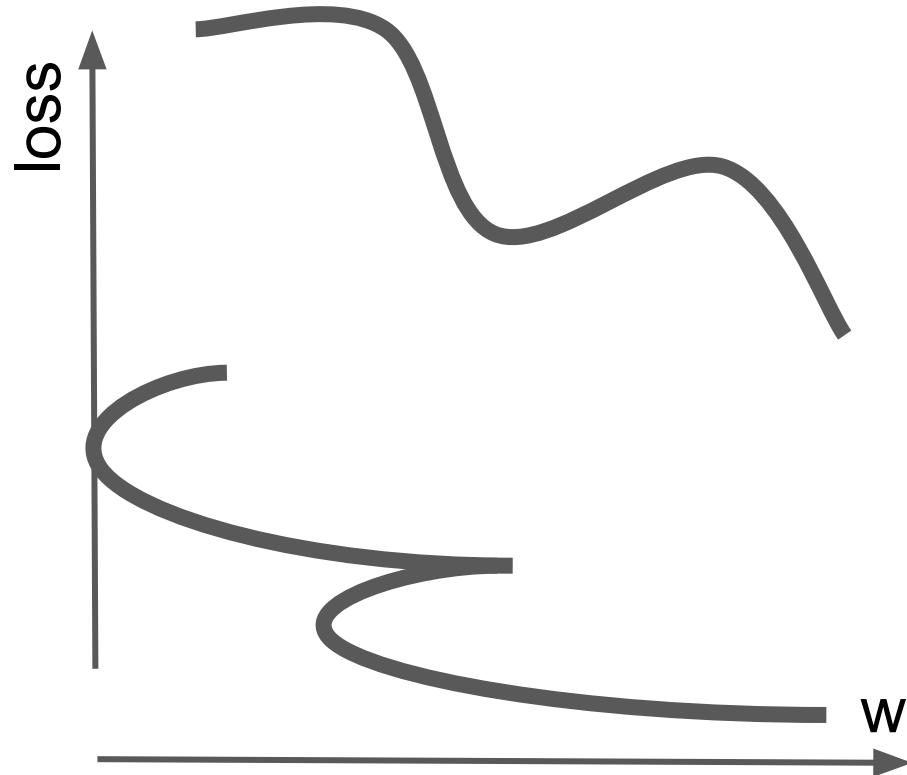
Very slow progress along shallow dimension, jitter along steep direction



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

# Optimization: Problem #2 with SGD

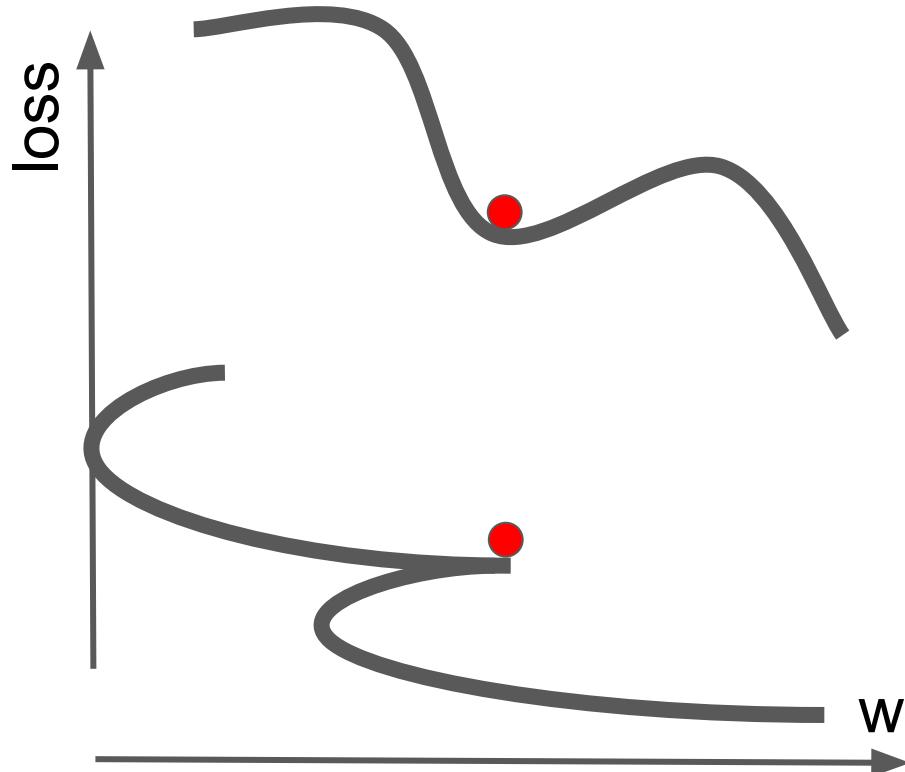
What if the loss  
function has a  
**local minima** or  
**saddle point**?



# Optimization: Problem #2 with SGD

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

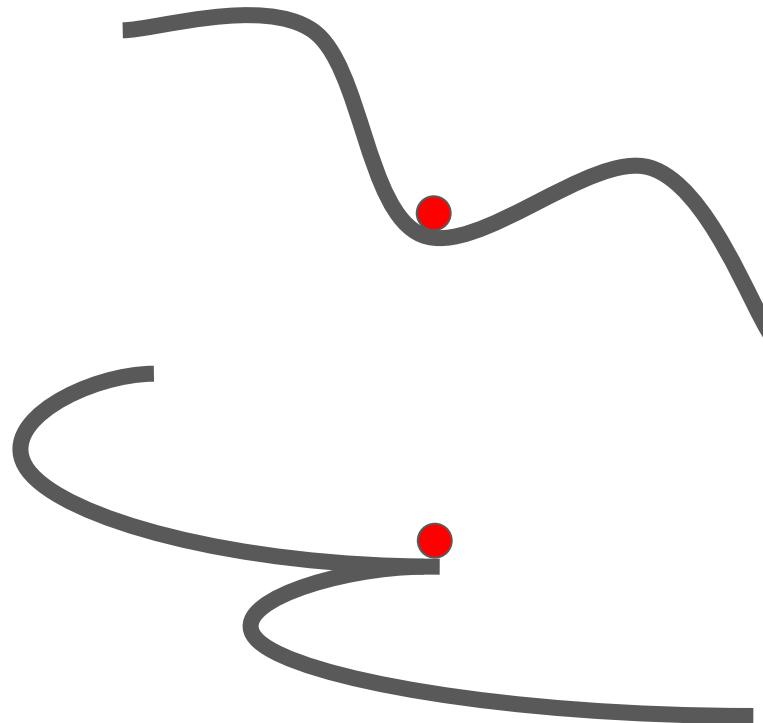
Zero gradient,  
gradient descent  
gets stuck



# Optimization: Problem #2 with SGD

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

Saddle points much  
more common in  
high dimension



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

# Optimization: Problem #2 with SGD

**saddle point** in two dimension

$$f(x, y) = x^2 - y^2$$

$$\frac{\partial}{\partial \textcolor{teal}{x}} (\textcolor{teal}{x}^2 - y^2) = 2x \rightarrow 2(\textcolor{teal}{0}) = 0$$

$$\frac{\partial}{\partial \textcolor{red}{y}} (x^2 - \textcolor{red}{y}^2) = -2y \rightarrow -2(\textcolor{red}{0}) = 0$$

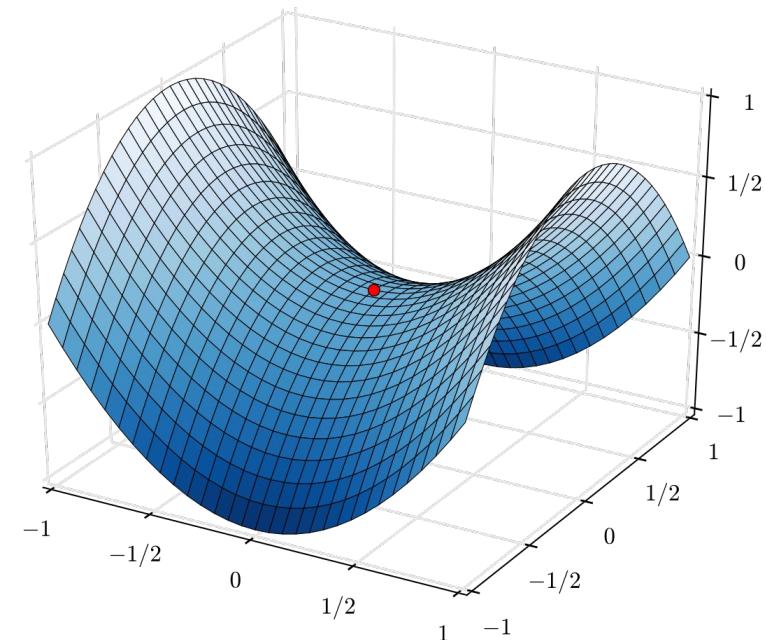


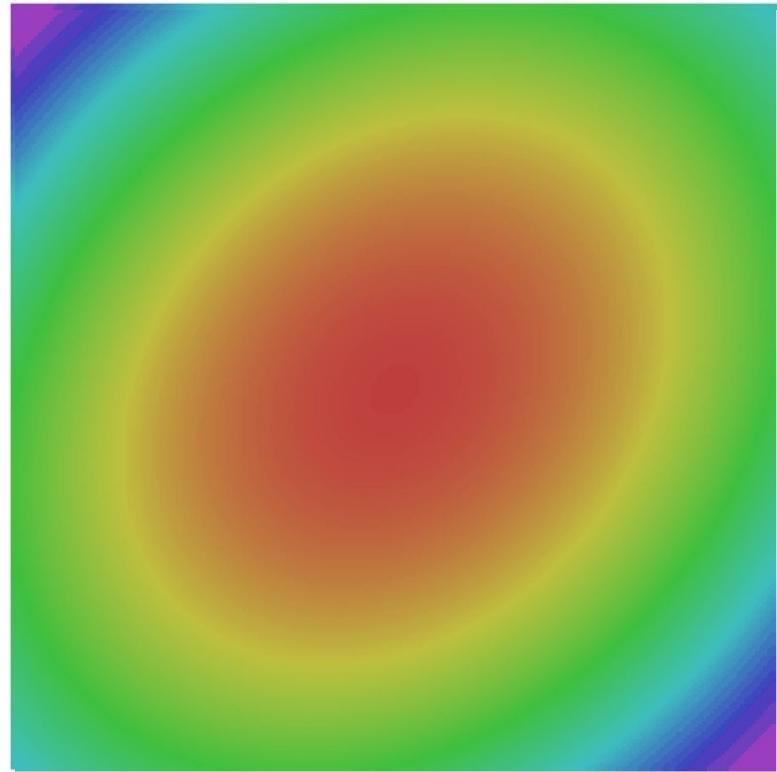
Image source: [https://en.wikipedia.org/wiki/Saddle\\_point](https://en.wikipedia.org/wiki/Saddle_point)

# Optimization: Problem #3 with SGD

Our gradients come from  
minibatches so they can be noisy!

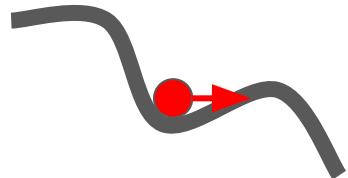
$$L(W) = \frac{1}{N} \sum_{i=1}^N L_i(x_i, y_i, W)$$

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

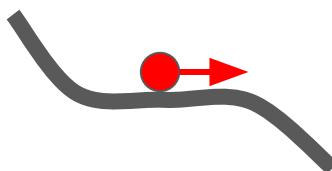


# SGD + Momentum

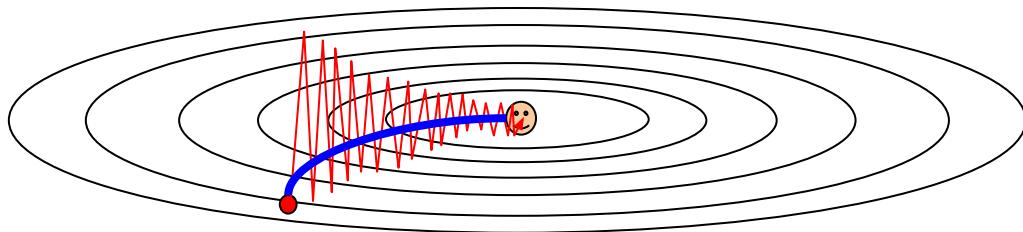
Local Minima



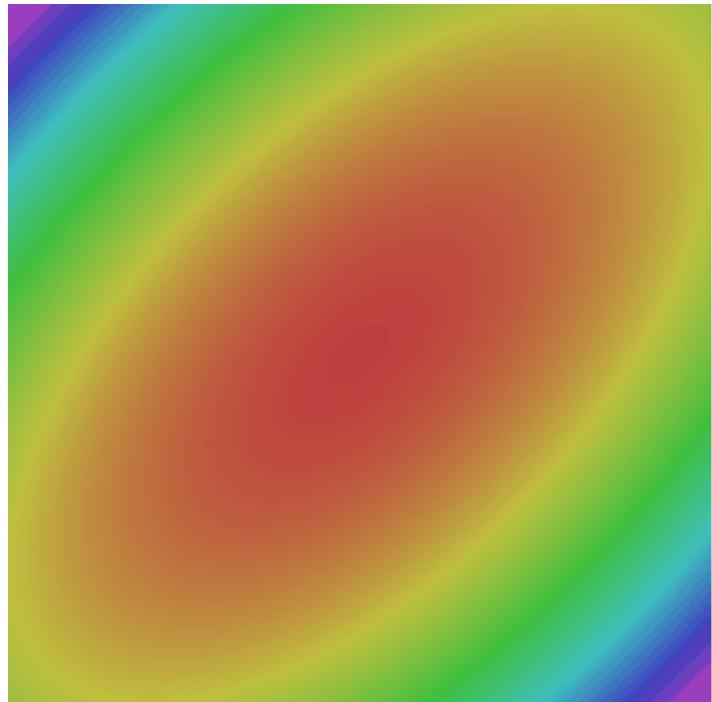
Saddle points



Poor Conditioning



## Gradient Noise



SGD

SGD+Momentum

# SGD: the simple two line update code

## SGD

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

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

# SGD + Momentum:

continue moving in the general direction as the previous iterations

SGD

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

SGD+Momentum

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

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

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

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

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

# SGD + Momentum:

continue moving in the general direction as the previous iterations

## SGD

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

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

## SGD+Momentum

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

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

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

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

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

# SGD + Momentum:

## alternative equivalent formulation

### SGD+Momentum

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

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

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

### SGD+Momentum

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

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

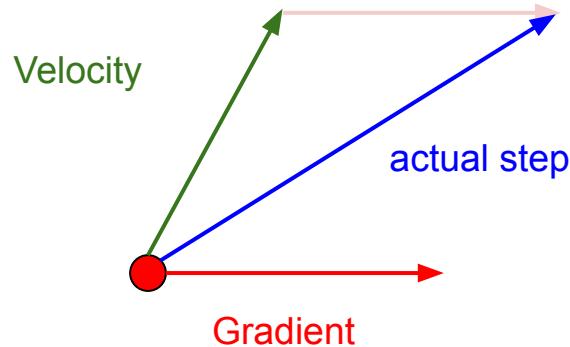
```
vx = 0
while True:
    dx = compute_gradient(x)
    vx = rho * vx + dx
    x -= learning_rate * vx
```

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

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

# SGD+Momentum

Momentum update:



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

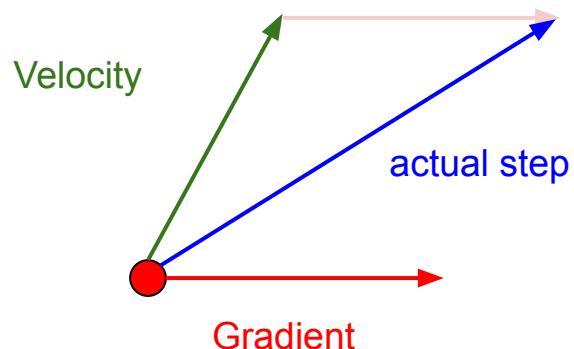
Nesterov, "A method of solving a convex programming problem with convergence rate  $O(1/k^2)$ ", 1983

Nesterov, "Introductory lectures on convex optimization: a basic course", 2004

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

# Nesterov Momentum

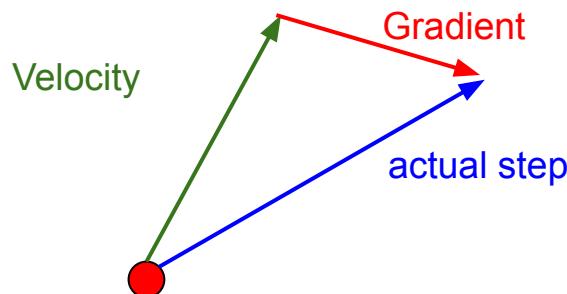
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Nesterov Momentum

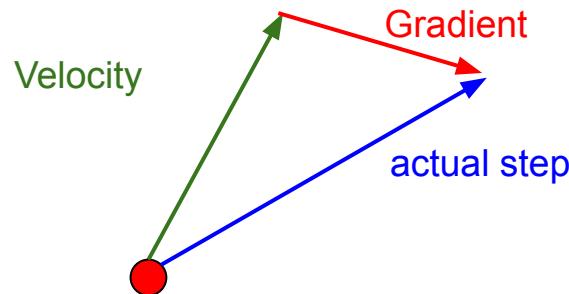


"Look ahead" to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

# Nesterov Momentum

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

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



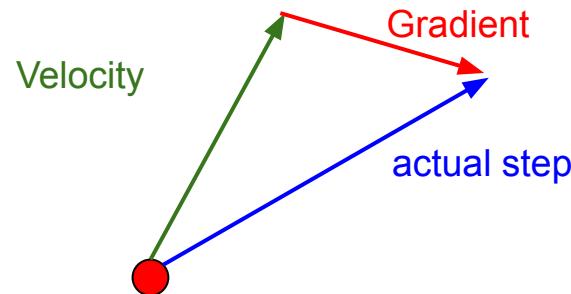
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$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$

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

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



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

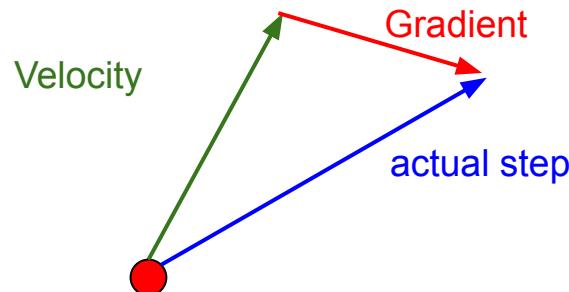
# Nesterov Momentum

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

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

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

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



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

# Nesterov Momentum

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

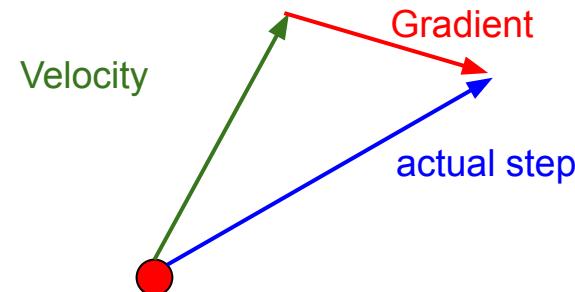
$$x_{t+1} = x_t + v_{t+1}$$

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

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

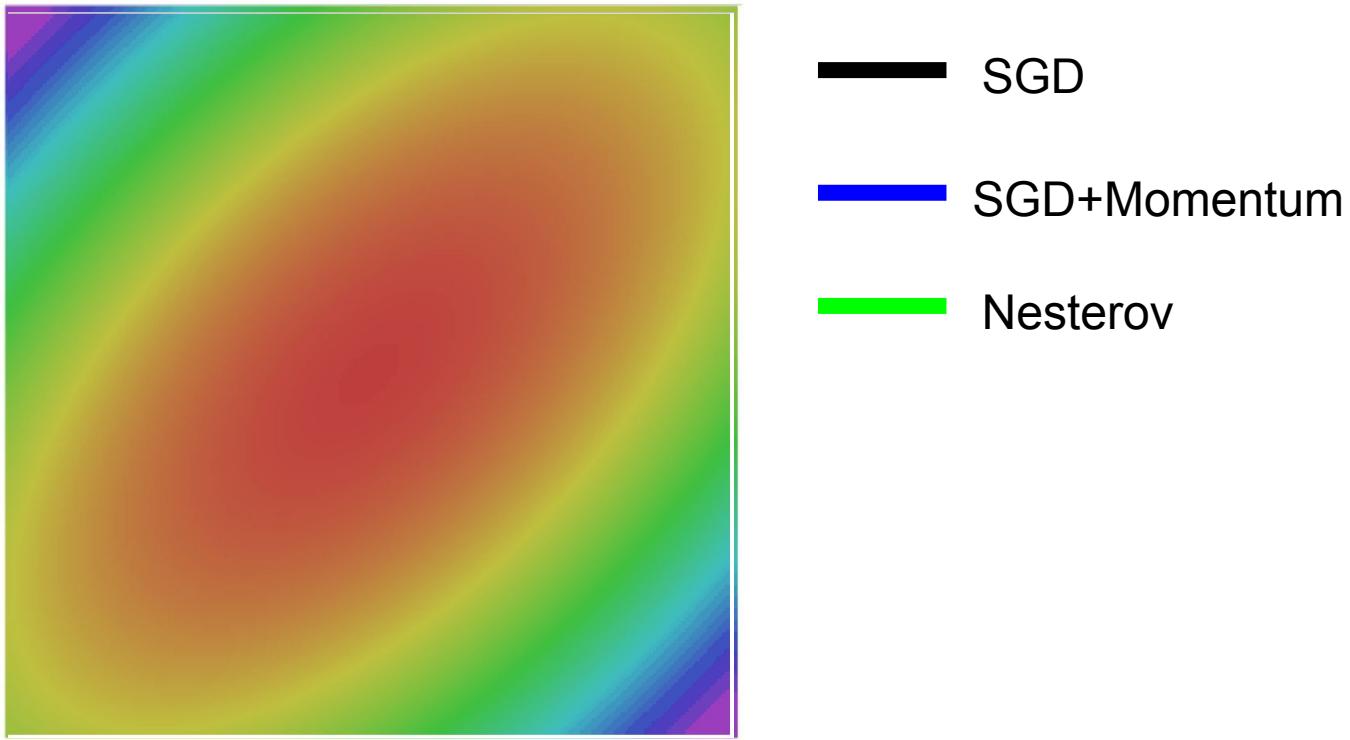
$$\begin{aligned}\tilde{x}_{t+1} &= \tilde{x}_t - \rho v_t + (1 + \rho)v_{t+1} \\ &= \tilde{x}_t + v_{t+1} + \rho(v_{t+1} - v_t)\end{aligned}$$

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



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

# Nesterov Momentum



# AdaGrad

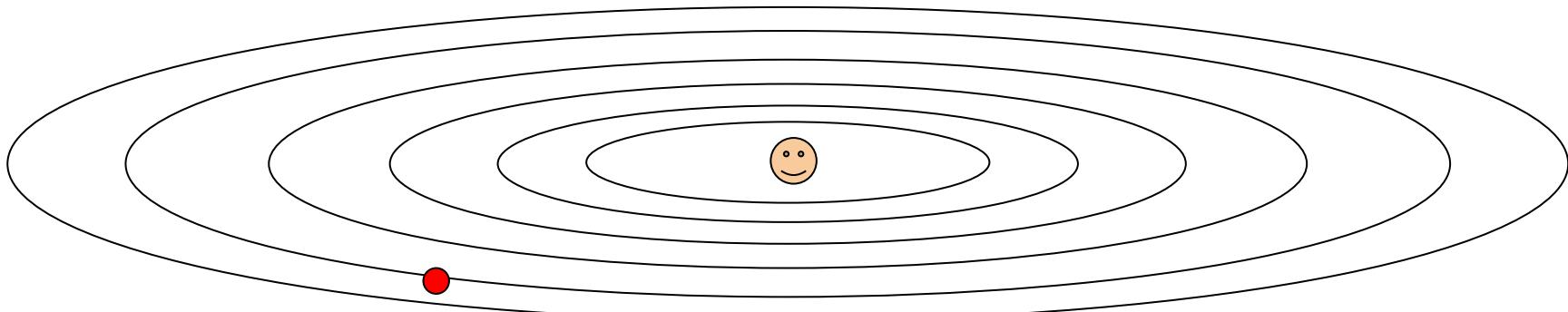
```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

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

“Per-parameter learning rates”  
or “adaptive learning rates”

# AdaGrad

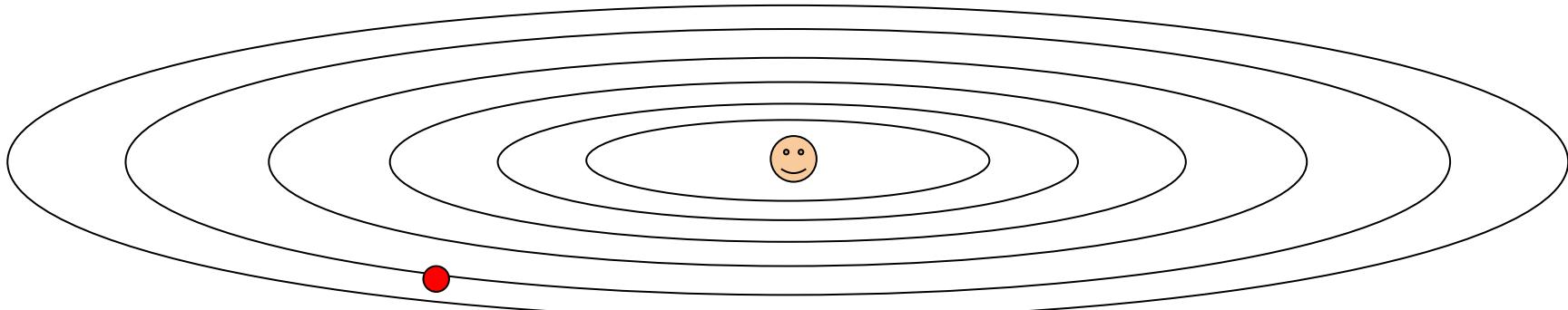
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grad_squared = 0
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```



Q: What happens with AdaGrad?

# AdaGrad

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

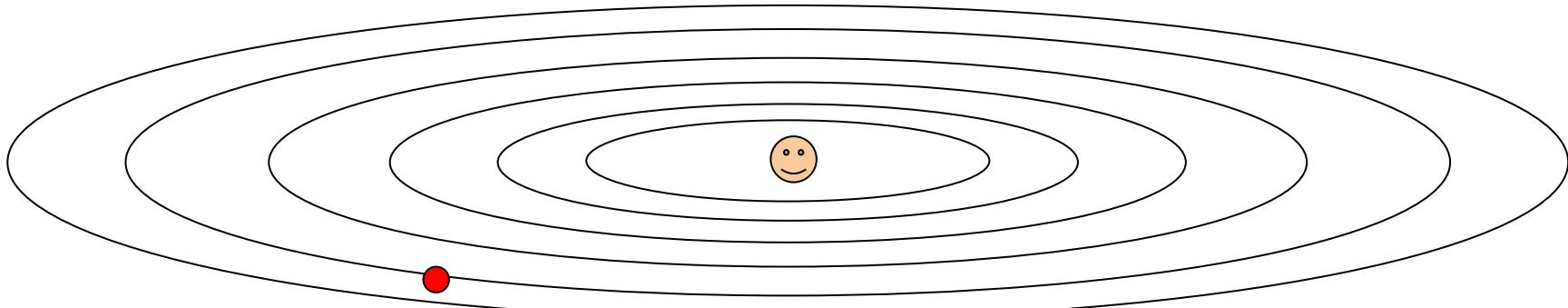


Q: What happens with AdaGrad?

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

# AdaGrad

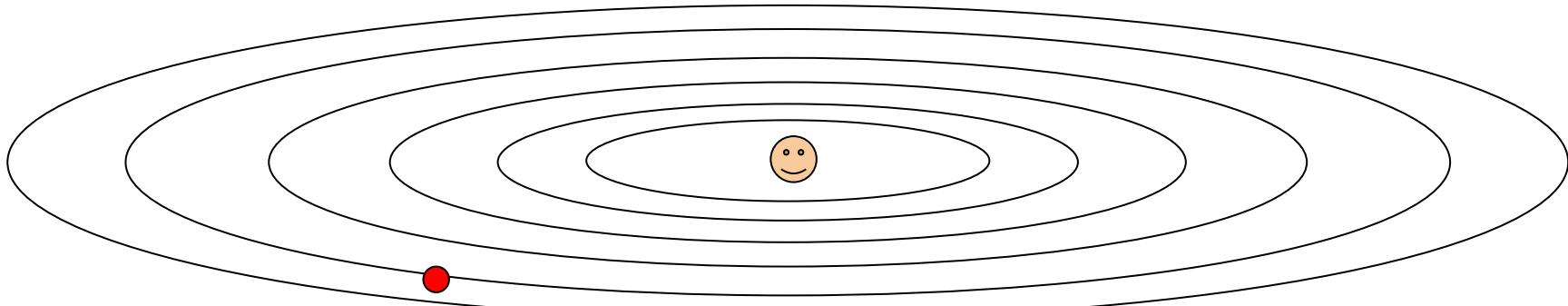
```
grad_squared = 0
while True:
    dx = compute_gradient(x)
    grad_squared += dx * dx
    x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



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

# AdaGrad

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



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

# RMSProp: “Leaky AdaGrad”

AdaGrad

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

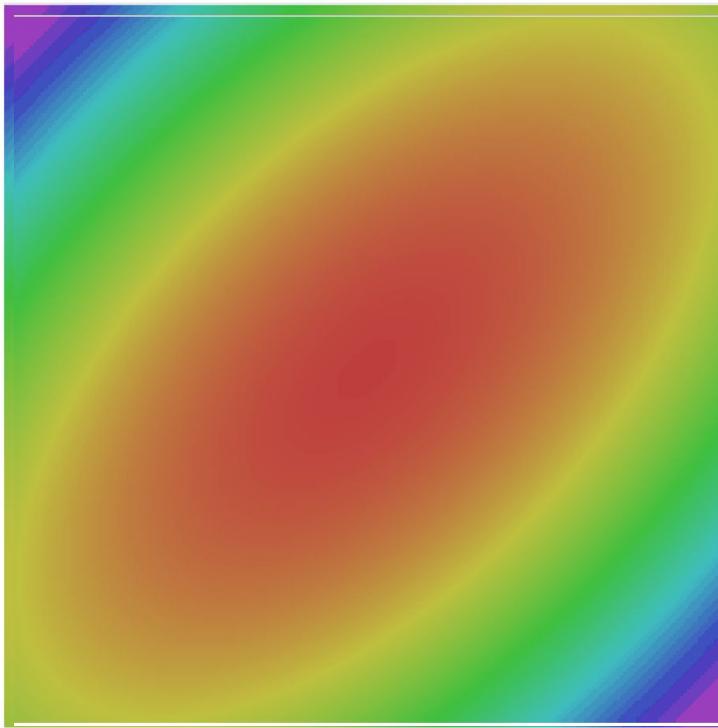


RMSProp

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

Tieleman and Hinton, 2012

# RMSProp



- SGD
- SGD+Momentum
- RMSProp
- AdaGrad  
(stuck due to decaying lr)

# Adam (almost)

```
first_moment = 0
second_moment = 0
while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

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

# Adam (almost)

```
first_moment = 0
second_moment = 0
while True:
    dx = compute_gradient(x)
    first_moment = beta1 * first_moment + (1 - beta1) * dx
    second_moment = beta2 * second_moment + (1 - beta2) * dx * dx
    x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Momentum

AdaGrad / RMSProp

Sort of like RMSProp with momentum

Q: What happens at first timestep?

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

# Adam (full form)

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

Momentum

Bias correction

AdaGrad / RMSProp

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

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

# Adam (full form)

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

Momentum

Bias correction

AdaGrad / RMSProp

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

Adam with  $\text{beta1} = 0.9$ ,  
 $\text{beta2} = 0.999$ , and  $\text{learning\_rate} = 1\text{e-}3$  or  $5\text{e-}4$   
is a great starting point for many models!

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

# Adam



- SGD
- SGD+Momentum
- RMSProp
- Adam

# Learning rate schedules

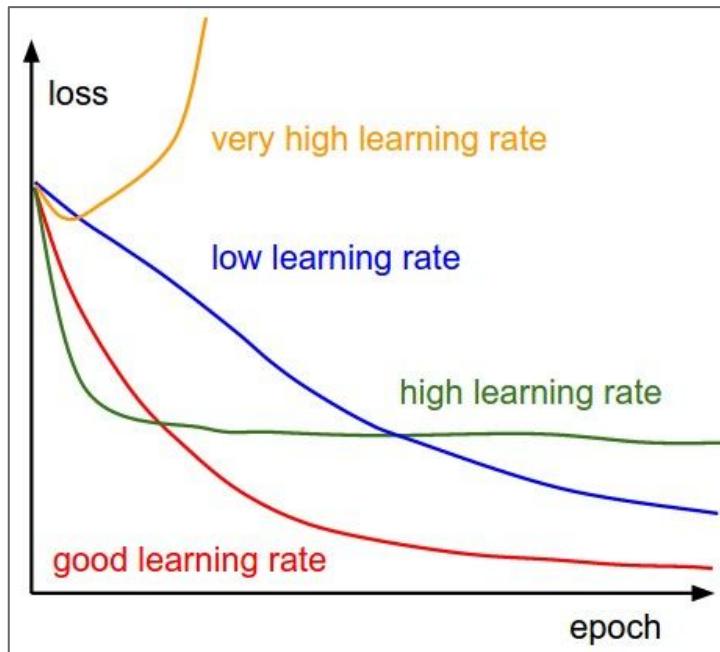
```
# Vanilla Gradient Descent

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



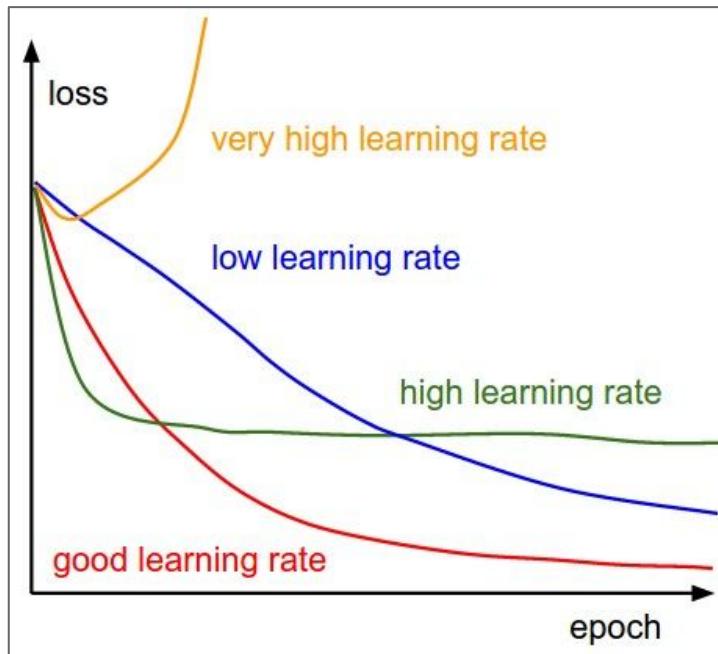
Learning rate

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



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

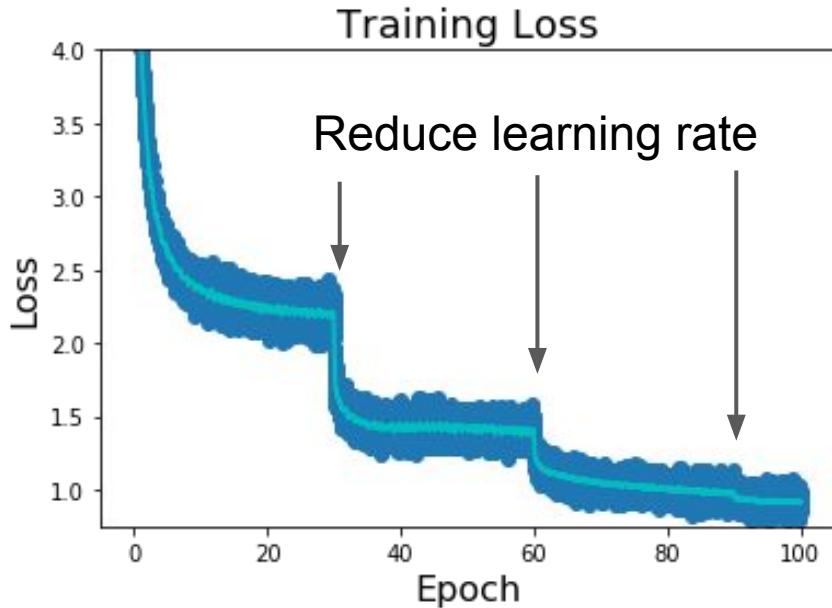
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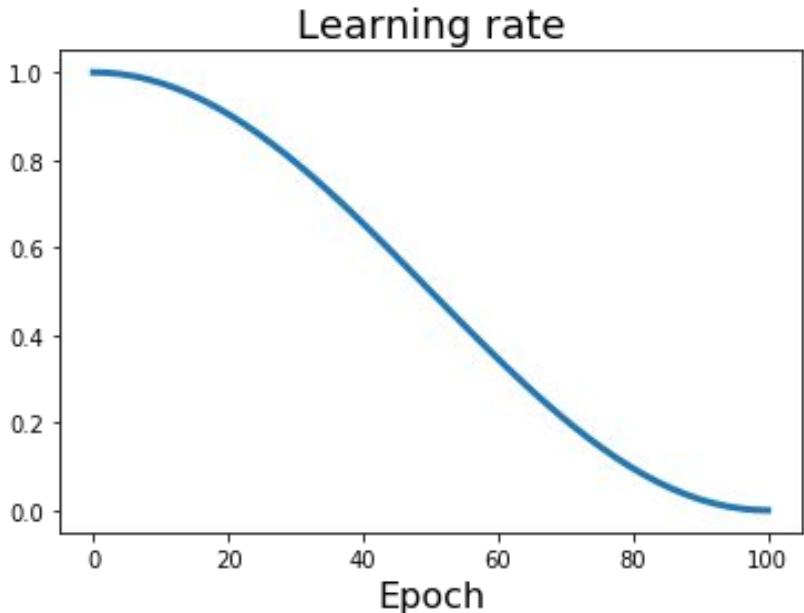
A: In reality, all of these are good learning rates.

# Learning rate decays over time



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

# Learning Rate Decay



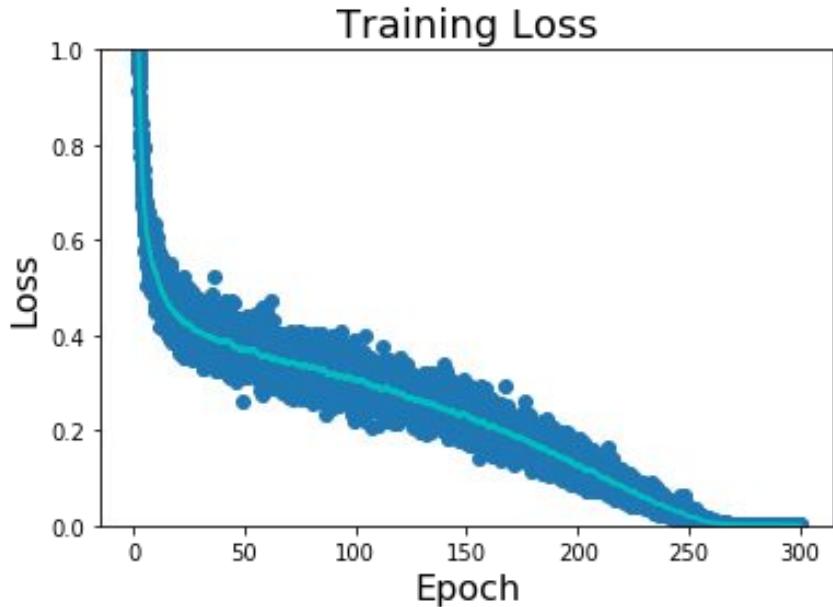
**Step:** Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

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

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

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

# Learning Rate Decay



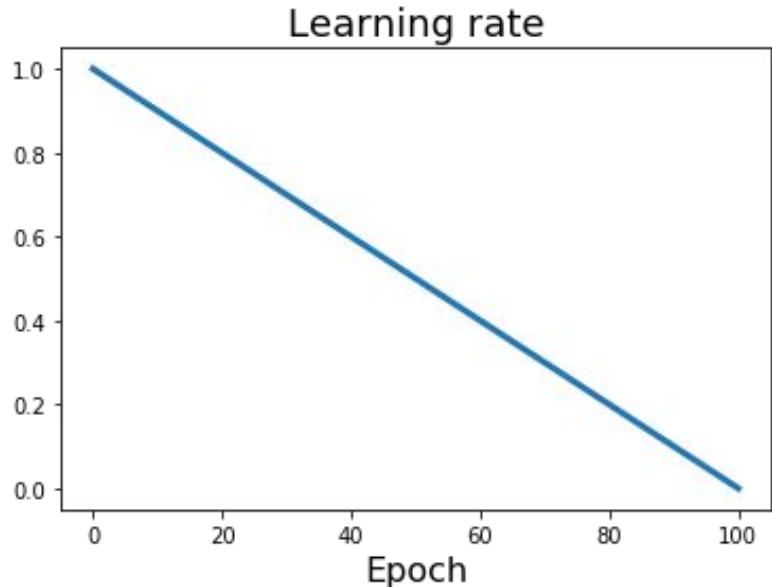
**Step:** Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

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

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

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

# Learning Rate Decay



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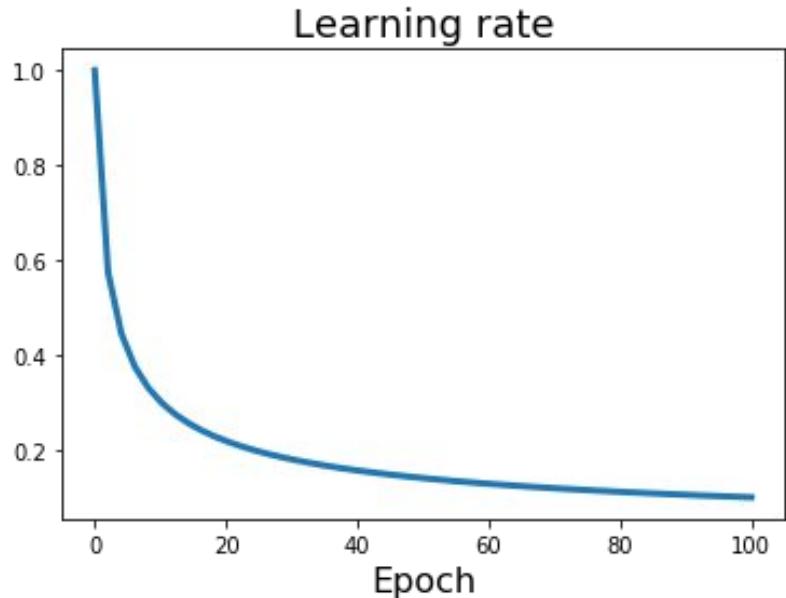
$\alpha_0$  : Initial learning rate

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

# Learning Rate Decay



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

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

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

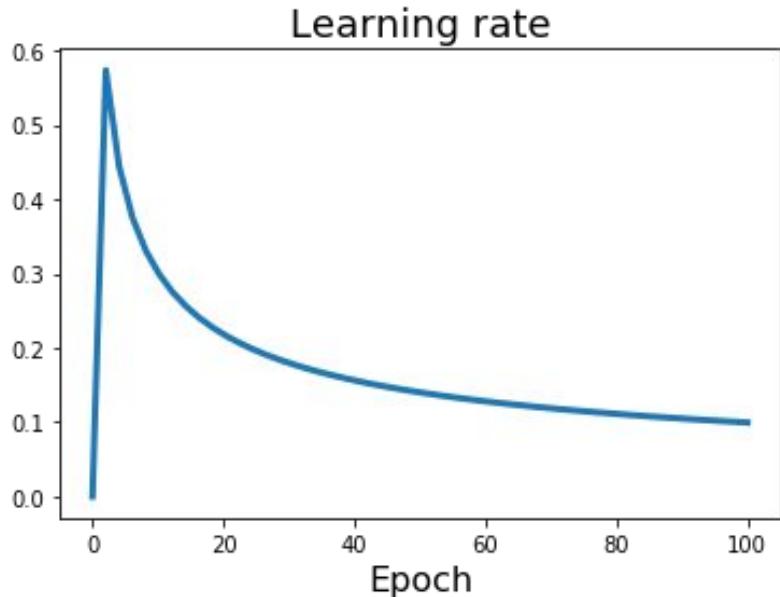
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Vaswani et al, "Attention is all you need", NIPS 2017

# Learning Rate Decay: Linear Warmup

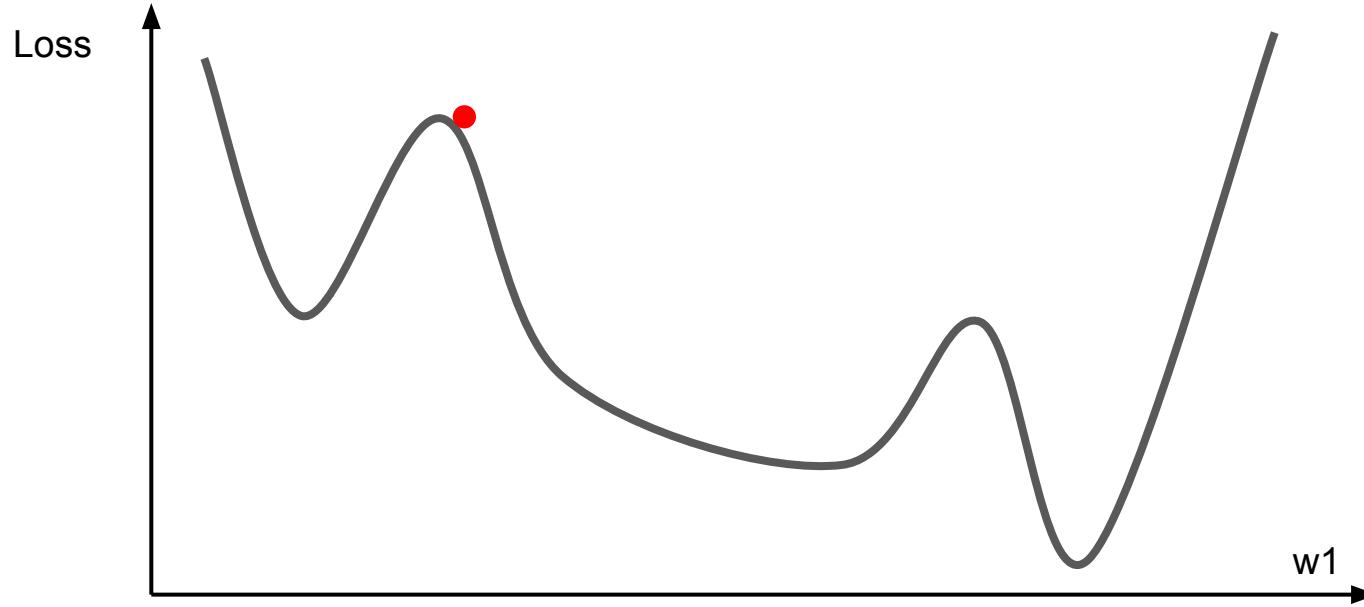


High initial learning rates can make loss explode; linearly increasing learning rate from 0 over the first ~5,000 iterations can prevent this.

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

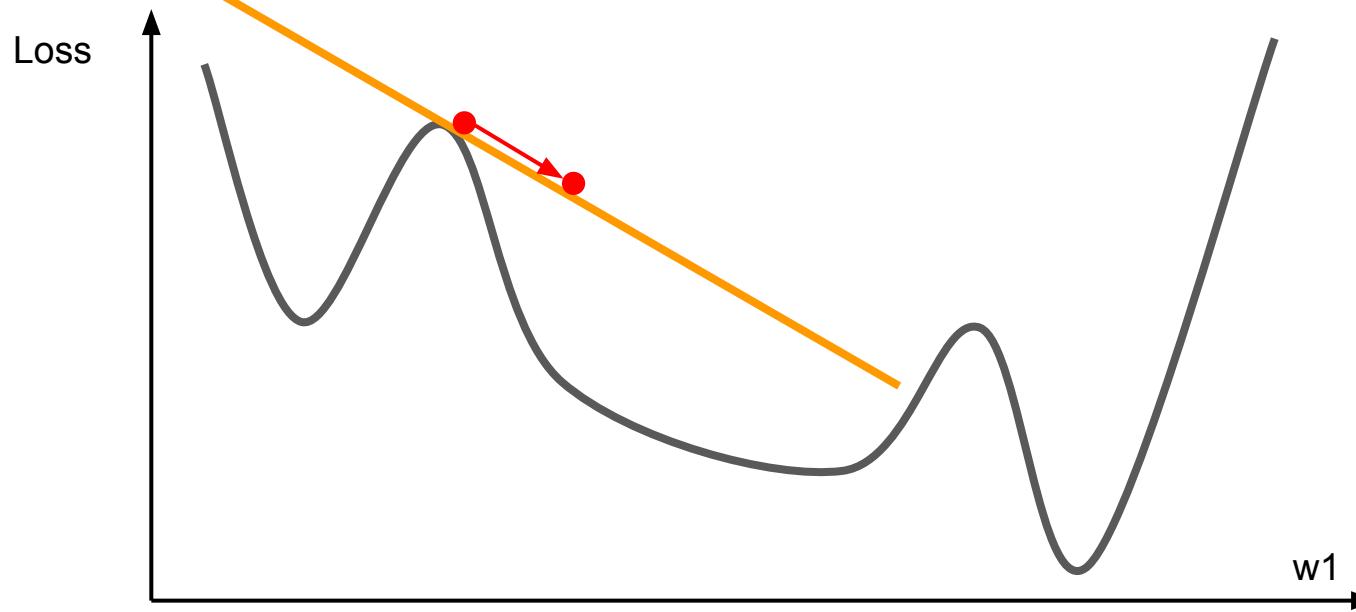
Goyal et al, "Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour", arXiv 2017

# First-Order Optimization



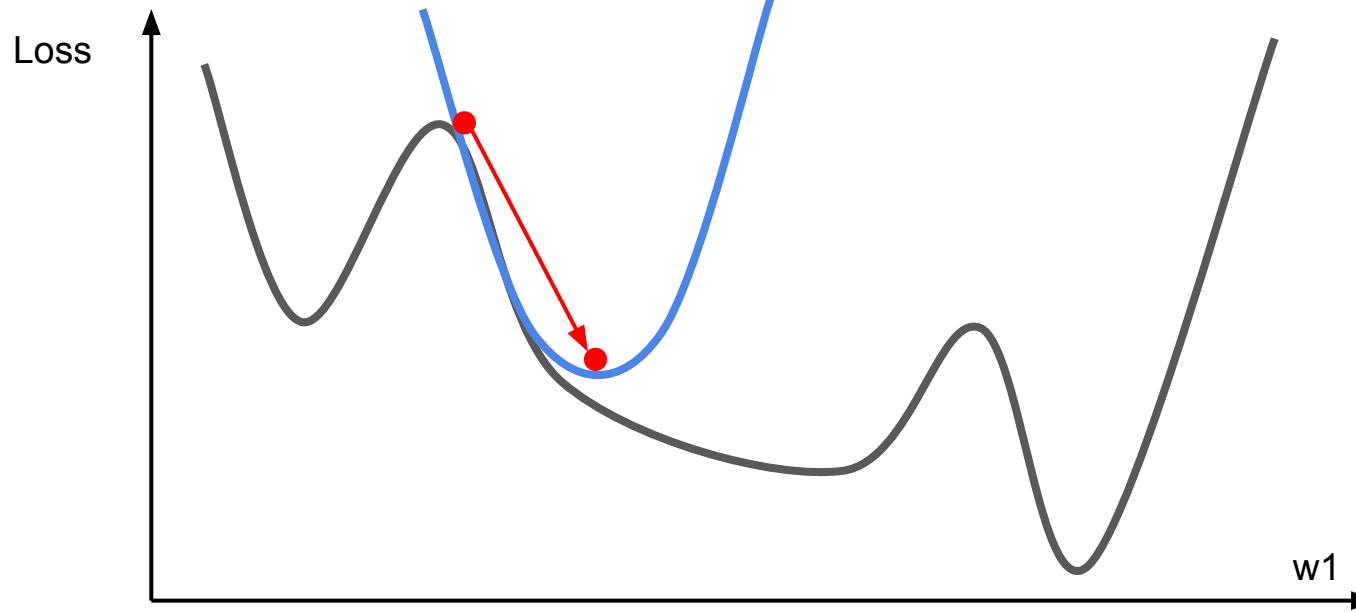
# First-Order Optimization

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



# Second-Order Optimization

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



# Second-Order Optimization

second-order Taylor expansion:

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

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

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

Q: Why is this bad for deep learning?

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Hessian has  $O(N^2)$  elements  
Inverting takes  $O(N^3)$   
 $N = (\text{Tens or Hundreds of}) \text{ Millions}$

Q: Why is this bad for deep learning?

# Second-Order Optimization

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

- Quasi-Newton methods (**BGFS** most popular):  
*instead of inverting the Hessian ( $O(n^3)$ ), approximate inverse Hessian with rank 1 updates over time ( $O(n^2)$  each).*
- **L-BFGS** (Limited memory BFGS):  
*Does not form/store the full inverse Hessian.*

# L-BFGS

- **Usually works very well in full batch, deterministic mode**  
i.e. if you have a single, deterministic  $f(x)$  then L-BFGS will probably work very nicely
- **Does not transfer very well to mini-batch setting.** Gives bad results. Adapting second-order methods to large-scale, stochastic setting is an active area of research.

Le et al, "On optimization methods for deep learning, ICML 2011"

Ba et al, "Distributed second-order optimization using Kronecker-factored approximations", ICLR 2017

# In practice:

- **Adam** is a good default choice in many cases; it often works ok even with constant learning rate
- **SGD+Momentum** can outperform Adam but may require more tuning of LR and schedule
- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)

# Next time:

Introduction to neural networks

Backpropagation