Lecture 3:
Regularization and Optimization

Administrative: Assignment 1

Released last week, due **Fri 4/19 at 11:59pm**

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

Administrative: Project proposal + Office Hours

Due **Mon 4/22**

TA expertise + Office Hours are posted on the webpage. Mix of in-person and zoom.

(http://cs231n.stanford.edu/office_hours.html)

Administrative: Ed

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

- 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, send us an email: cs231n-staff-spr24@stanford.edu + cc scpd-exams@stanford.edu

Recap from Last Week

Image Classification: A core task in Computer Vision

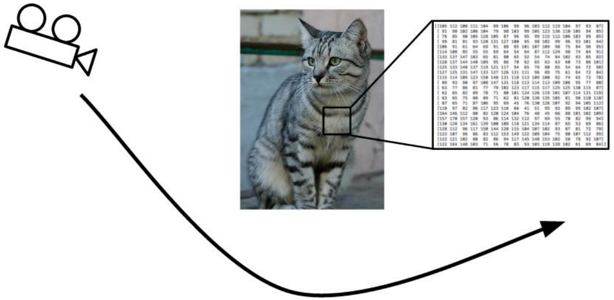
(assume given a set of labels)
{dog, cat, truck, plane, ...}

→

cat
dog
bird
deer
truck

Recall from last time: Challenges of recognition

Viewpoint



Illumination

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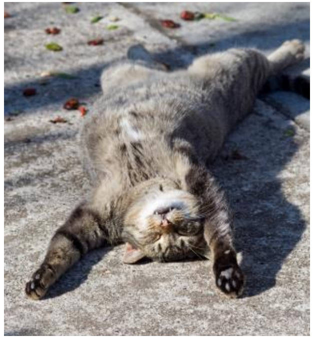
Deformation



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Occlusion

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Clutter

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Intraclass Variation

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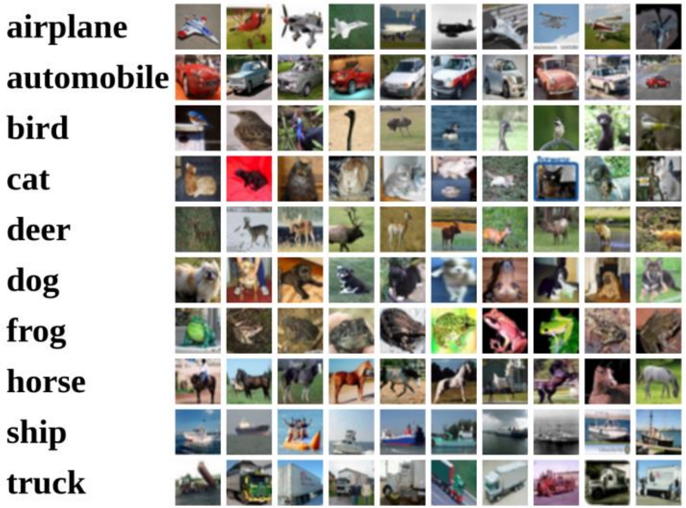
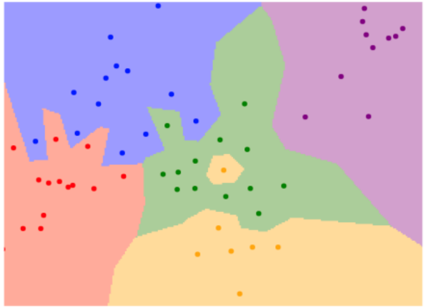
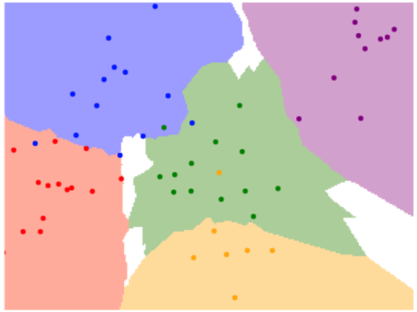
Recall from last time: data-driven approach, kNN



1-NN classifier

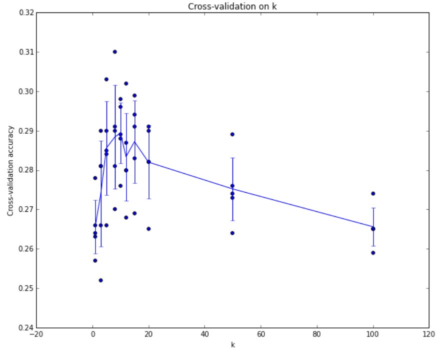


5-NN classifier



train	test

train	validation	test



Recall from last time: Linear Classifier

Image

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

$\rightarrow f(\mathbf{x},\mathbf{W}) \rightarrow$ **10** numbers giving class scores

$\uparrow$

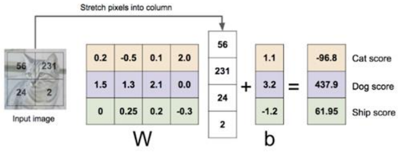
W

parameters or weights

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

<u>Algebraic Viewpoint</u>

$f(x,W) = Wx$

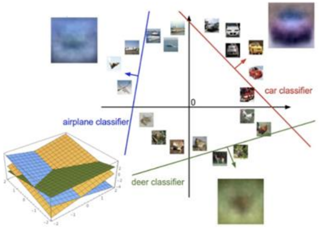


<u>Visual Viewpoint</u>

One template per class

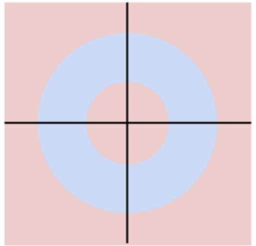
<u>Geometric Viewpoint</u>

Hyperplanes cutting up space



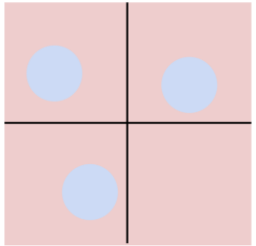
Class 1:
1 <= L2 norm <= 2

Class 2:
Everything else



Class 1:
Three modes

Class 2:
Everything else



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

cat	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**

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

Given a dataset of examples

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

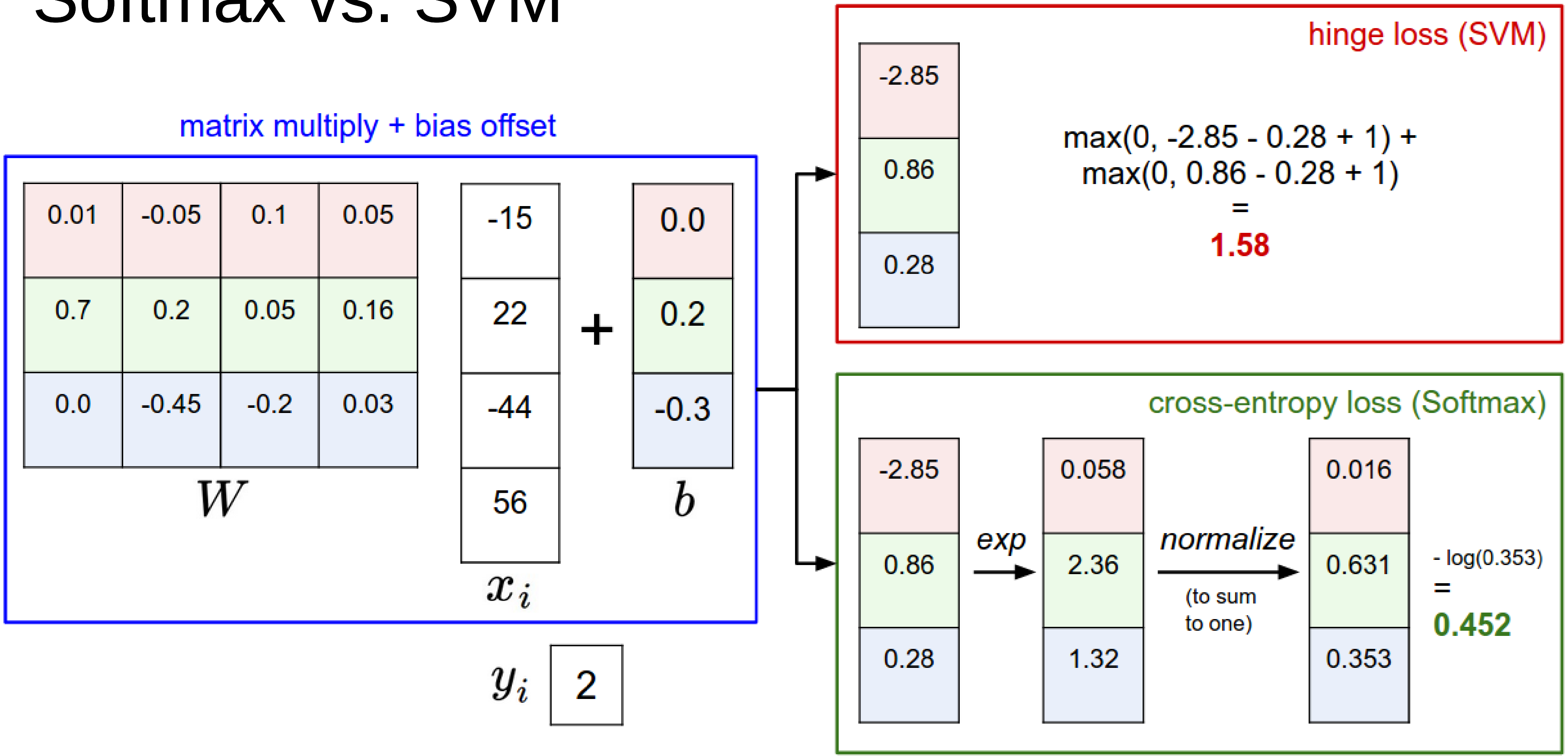
Where x_i is image and y_i is (integer) label

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

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



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

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

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	**3.2**	1.3	2.2
car	5.1	**4.9**	2.5
frog	-1.7	2.0	**-3.1**
Losses:	2.9	0	

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

Before:

= max(0, 1.3 - 4.9 + 1)
+max(0, 2.0 - 4.9 + 1)
= max(0, -2.6) + max(0, -1.9)
= 0 + 0
= 0

With W twice as large:

= max(0, 2.6 - 9.8 + 1)
+max(0, 4.0 - 9.8 + 1)
= max(0, -6.2) + max(0, -4.8)
= 0 + 0
= 0

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

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

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 -

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

Data loss: Model predictions should match training data

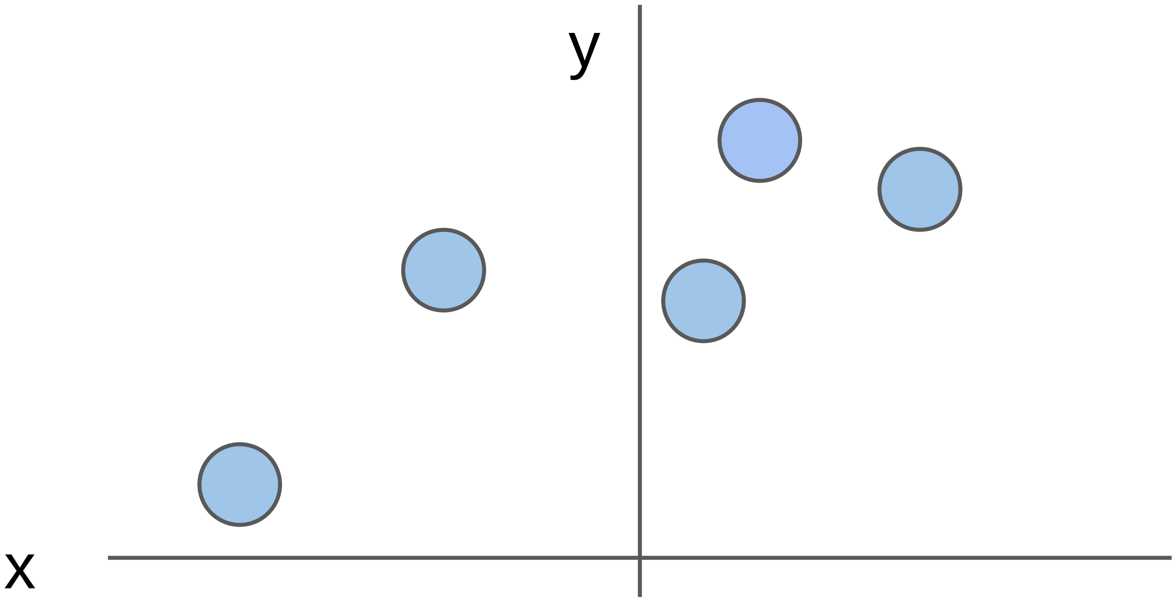
Regularization

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

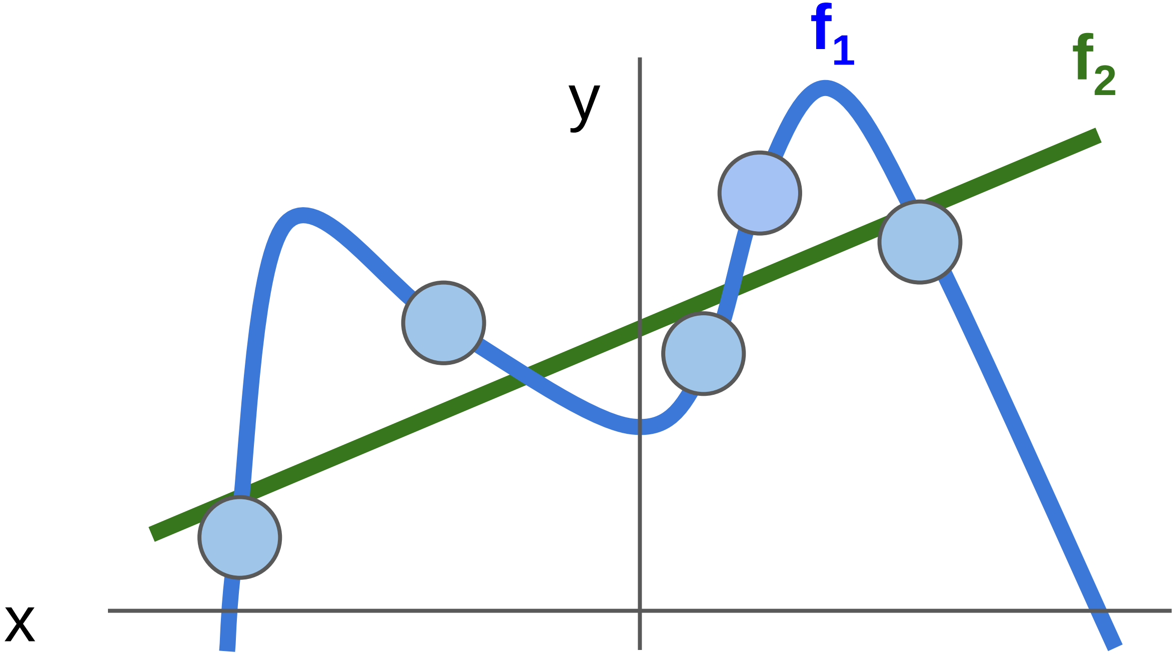
Data loss: Model predictions should match training data

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

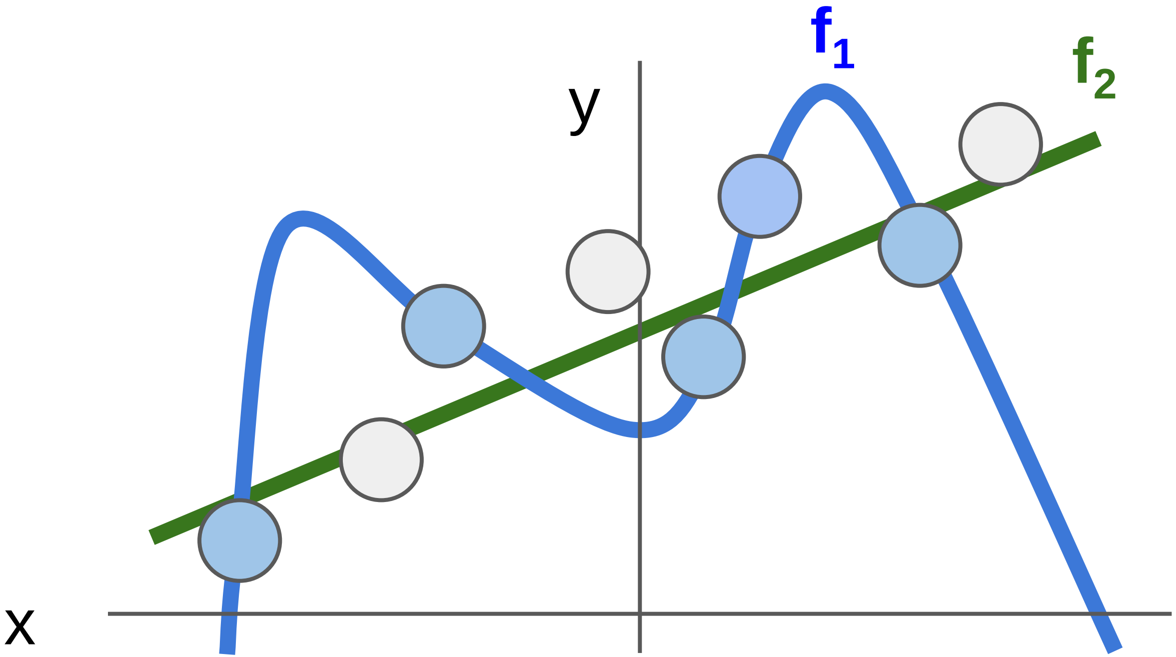
Regularization intuition: toy example training data



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

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

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

λ = regularization strength (hyperparameter)

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

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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

λ = regularization strength (hyperparameter)

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

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

λ = regularization strength (hyperparameter)

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

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

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

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

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

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

L2 Regularization

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

Which of w1 or w2 will
the L2 regularizer prefer?

Regularization: Expressing Preferences

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

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

$$w_2 = \boxed{[0.25, 0.25, 0.25, 0.25]}$$

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

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

Regularization: Expressing Preferences

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

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

$$w_2 = \boxed{[0.25, 0.25, 0.25, 0.25]}$$

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

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

Which one would L1
regularization prefer?

Recap

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

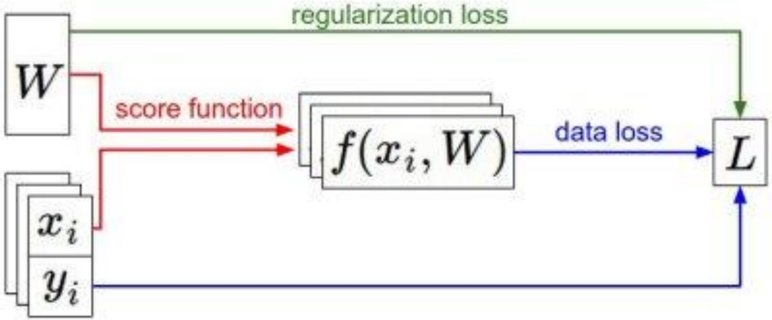
Softmax

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

SVM

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

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



Recap

How do we find the best W?

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

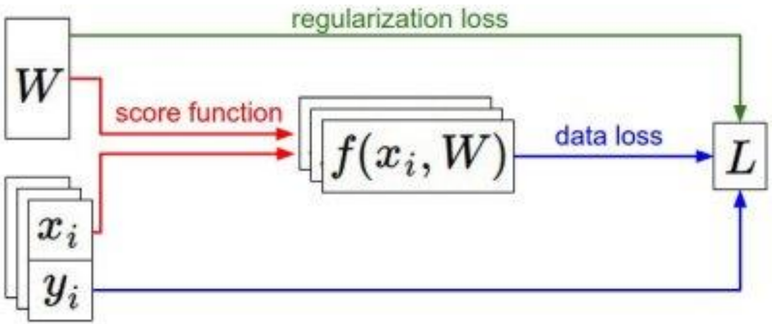
Softmax

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

SVM

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

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



Optimization

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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
# ... (trunctated: 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:

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

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:

[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:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

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**,
?,
?,

(1.25322 - 1.25347)/0.0001
= -2.5

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

?,
?,…]

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 (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,
?,
?,
?,
?,
?,
?,
?,
?,…]

current W:	**W + h** (second dim)**:**	**gradient dW:**
[0.34,	[0.34,	[-2.5,
-1.11,	-1.11 + **0.0001**,	**0.6**,
0.78,	0.78,	?,
0.12,	0.12,	?,
0.55,	0.55,	
2.81,	2.81,	
-3.1,	-3.1,	
-1.5,	-1.5,	
0.33,…]	0.33,…]	?,…]
loss 1.25347	**loss 1.25353**	

(1.25353 - 1.25347)/0.0001
= 0.6

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

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,
?,
?,
?,
?,
?,
?,
?,…]

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,
?,
?,…]

(1.25347 - 1.25347)/0.0001
= 0

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

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:

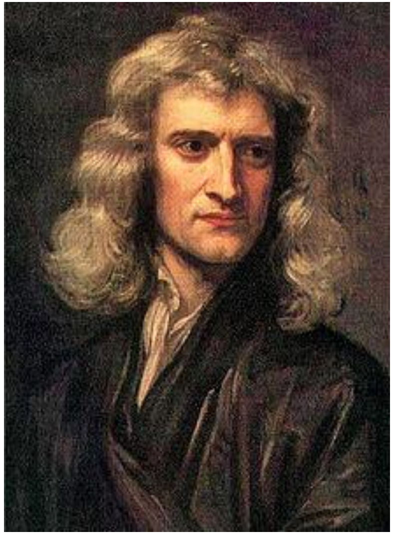
$$L = \frac{1}{N} \sum_{i=1}^{N} L_i + \sum_k W_k^2$$

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

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

want $\nabla_W L$

Use calculus to compute an **analytic gradient**



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current W:

[0.34,
-1.11,
0.78,
0.12,
0.55,
2.81,
-3.1,
-1.5,
0.33,…]
loss 1.25347

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

gradient dW:

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

In summary:

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

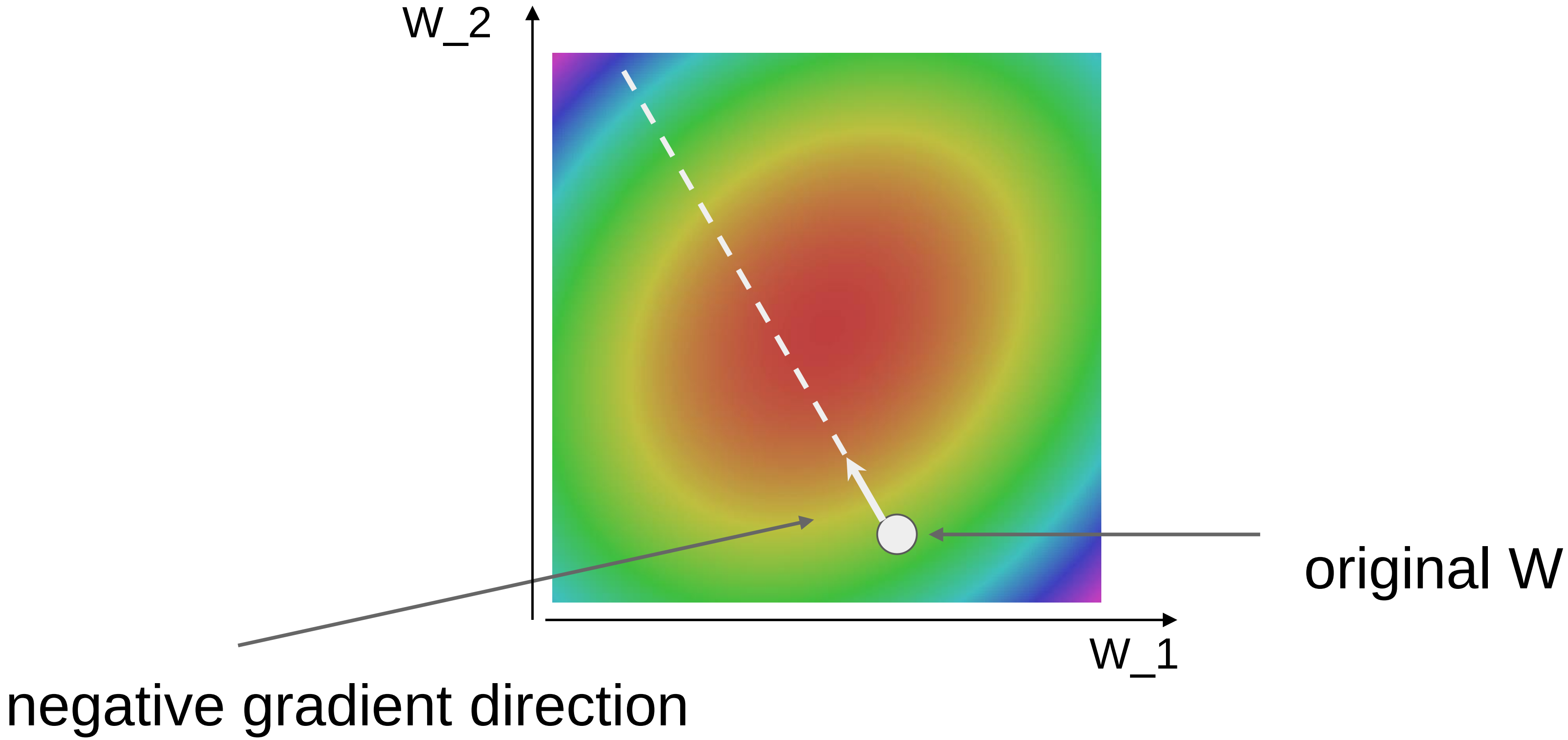
=>

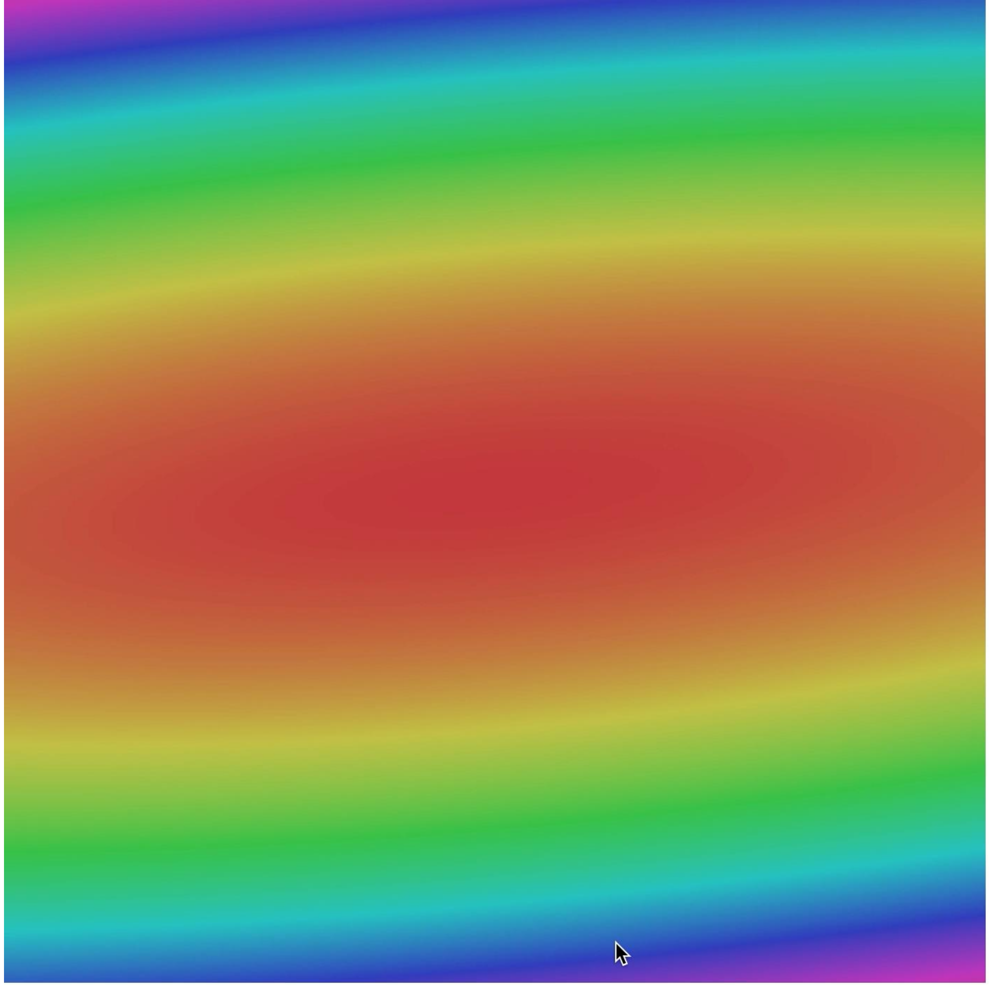
In practice: Always use analytic gradient, but check implementation with numerical gradient. This is called a **gradient check.**

Gradient Descent

```
# Vanilla Gradient Descent

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


W_2
W_1
original W
negative gradient direction



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!

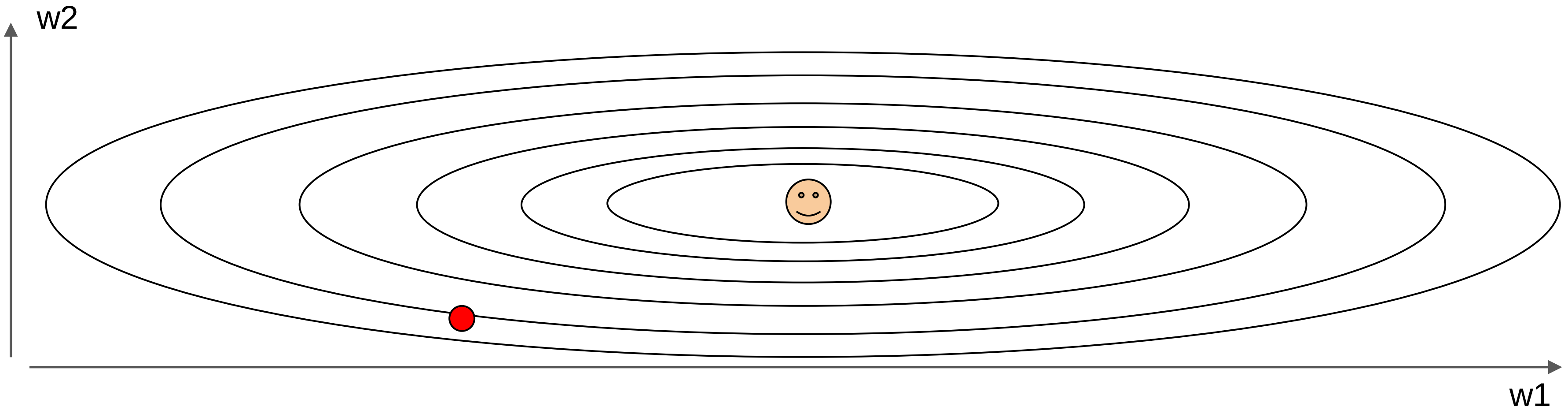
Approximate sum using a **minibatch** of examples
32 / 64 / 128 common

```
# 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
```

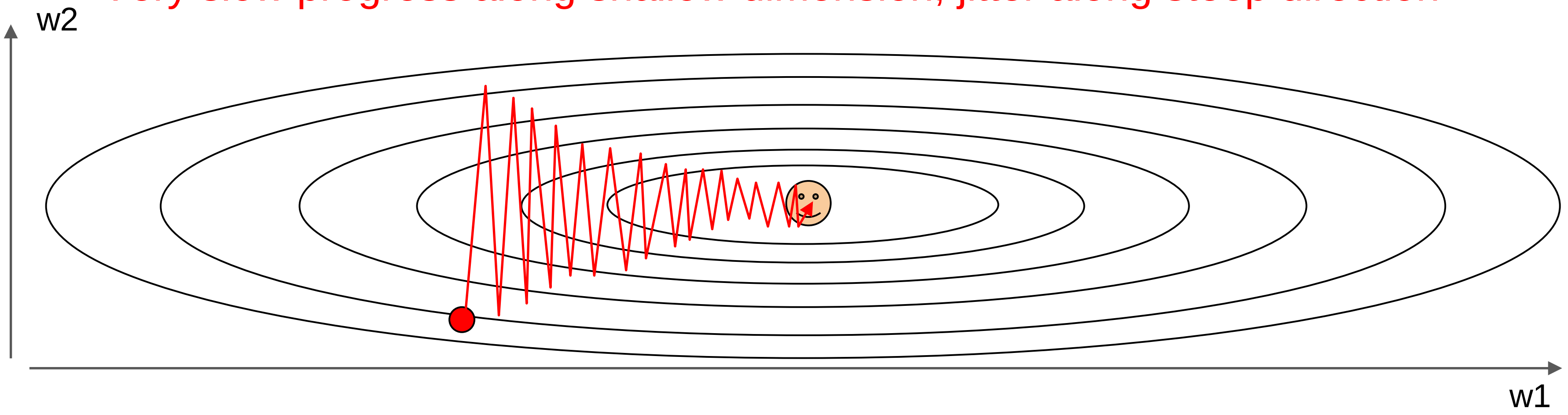
Optimization: Problem #1 with SGD

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



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



Optimization: Problem #1 with SGD

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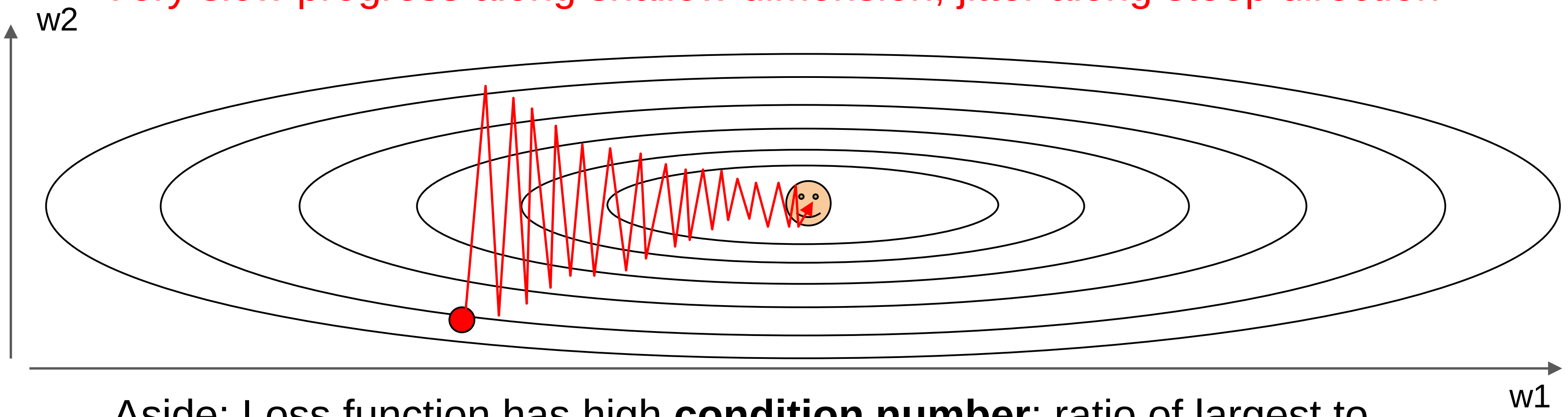
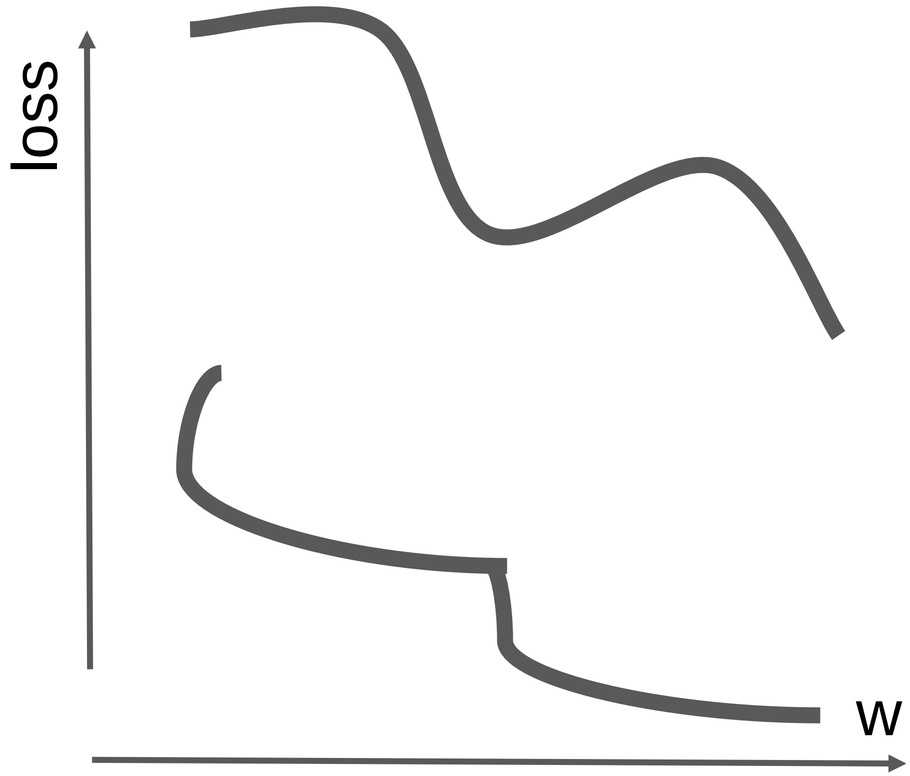


Aside: Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Optimization: Problem #2 with SGD

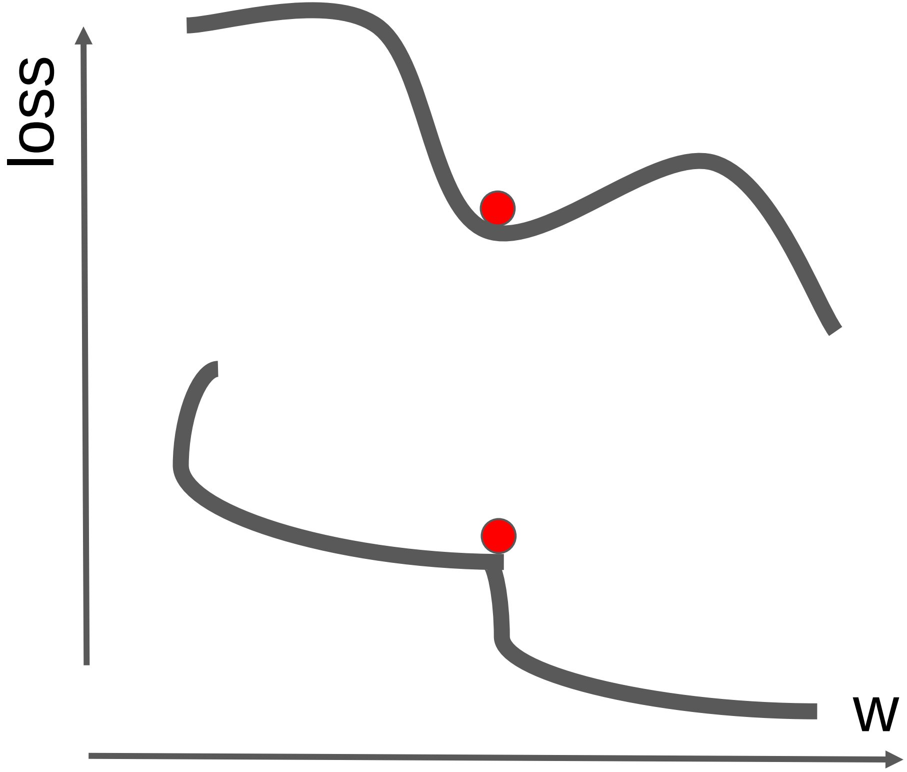
What if the loss function has a **local minima** or **saddle point**?



Optimization: Problem #2 with SGD

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

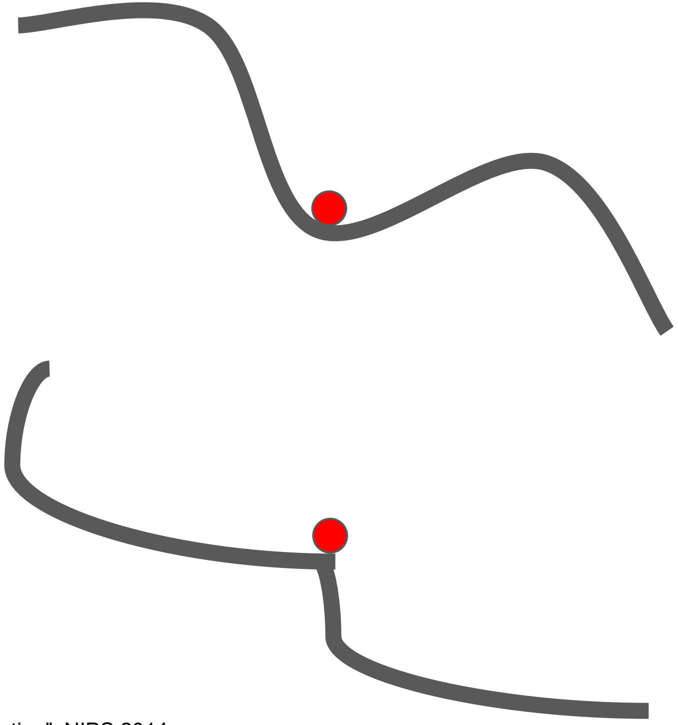
Zero gradient, gradient descent gets stuck



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

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

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

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

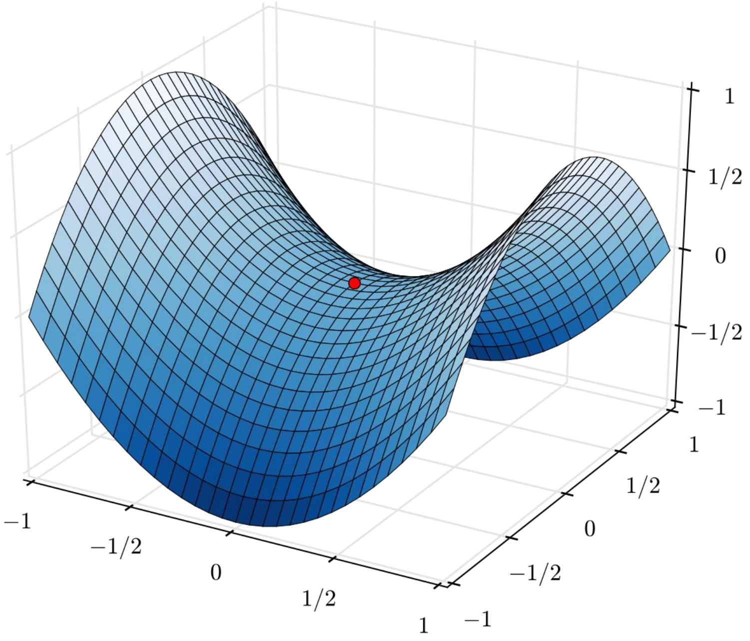


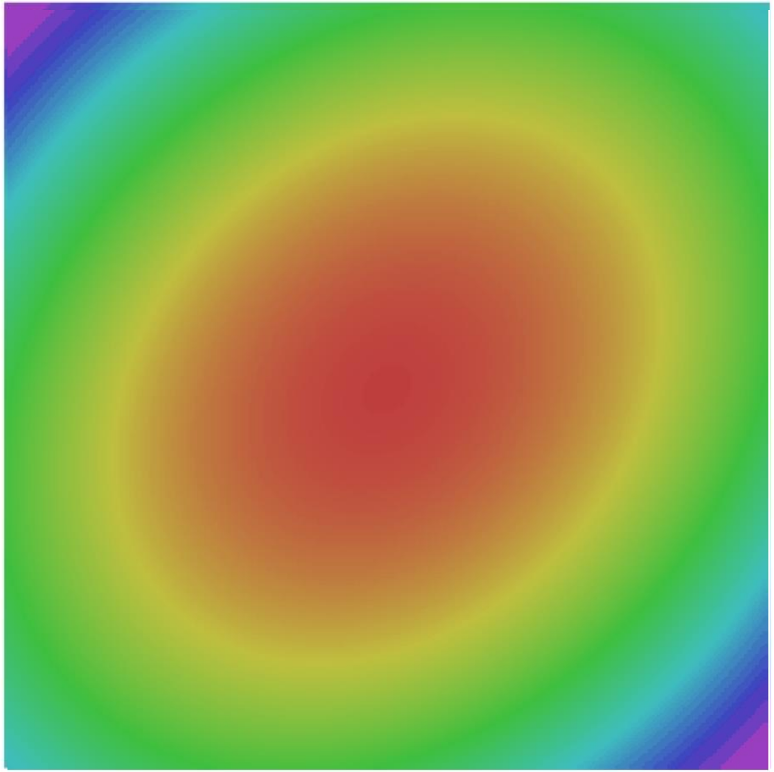
Image source: https://en.wikipedia.org/wiki/Saddle_point

Optimization: Problem #3 with SGD

Our gradients come from minibatches so they can be noisy!

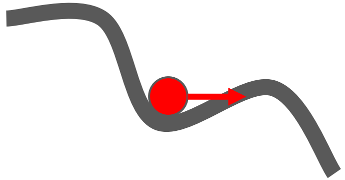
$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

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

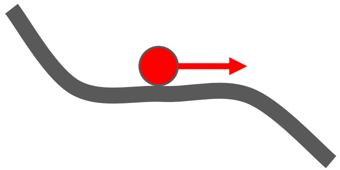


SGD + Momentum

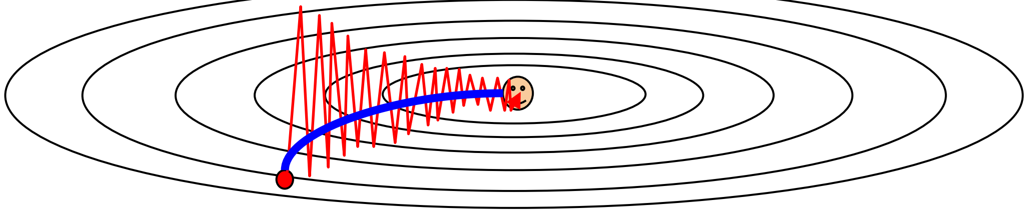
Local Minima



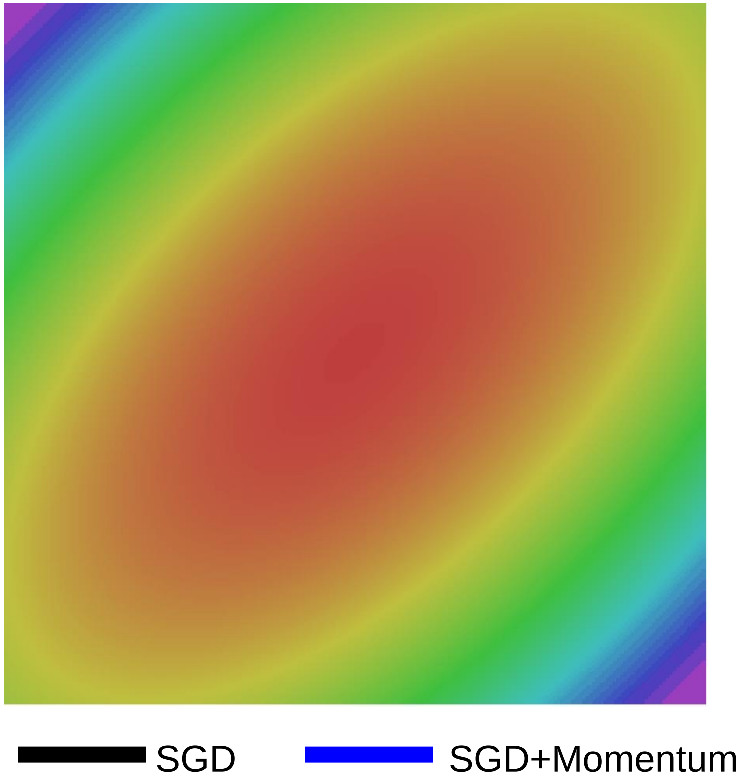
Saddle points



Poor Conditioning



Gradient Noise



SGD: the simple two line update code

SGD

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

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

SGD + Momentum:

continue moving in the general direction as the previous iterations

SGD

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

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

SGD+Momentum

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

- 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

More Complex Optimizers: RMSProp

SGD + Momentum

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

Adds element-wise scaling of the gradient based on the historical sum of squares in each dimension (with decay)

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

More Complex Optimizers: RMSProp

SGD + Momentum

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

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

RMSProp

```
grad_squared = 0
while True:
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  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dx * dx
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Tieleman and Hinton, 2012

RMSProp

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```

Q: What happens with RMSProp?

Tieleman and Hinton, 2012

RMSProp

RMSProp

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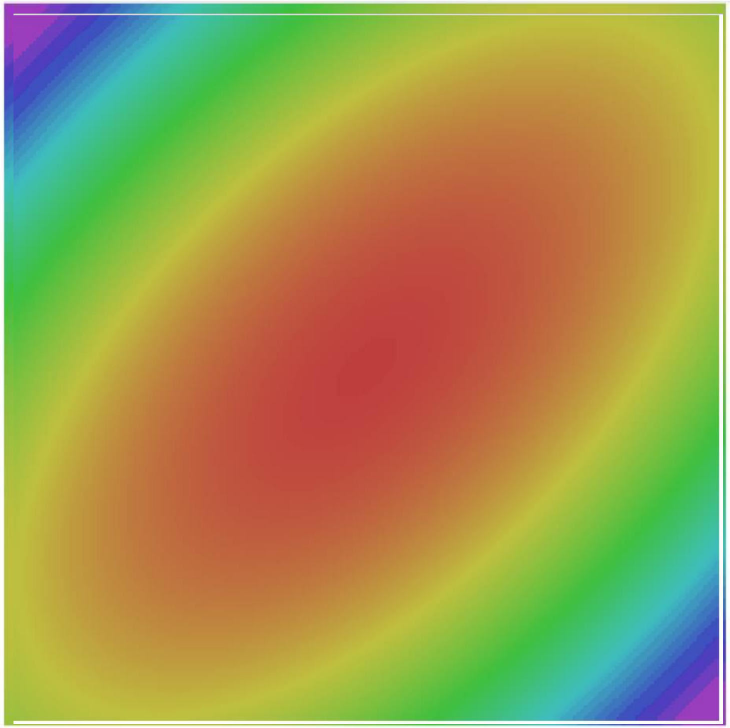
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```

Q: What happens with RMSProp?

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

Tieleman and Hinton, 2012

RMSProp



SGD

SGD+Momentum

RMSProp

Optimizers: 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
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  x -= learning_rate * first_moment / (np.sqrt(second_moment) + 1e-7))
```

Momentum

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)

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

Momentum

Bias correction

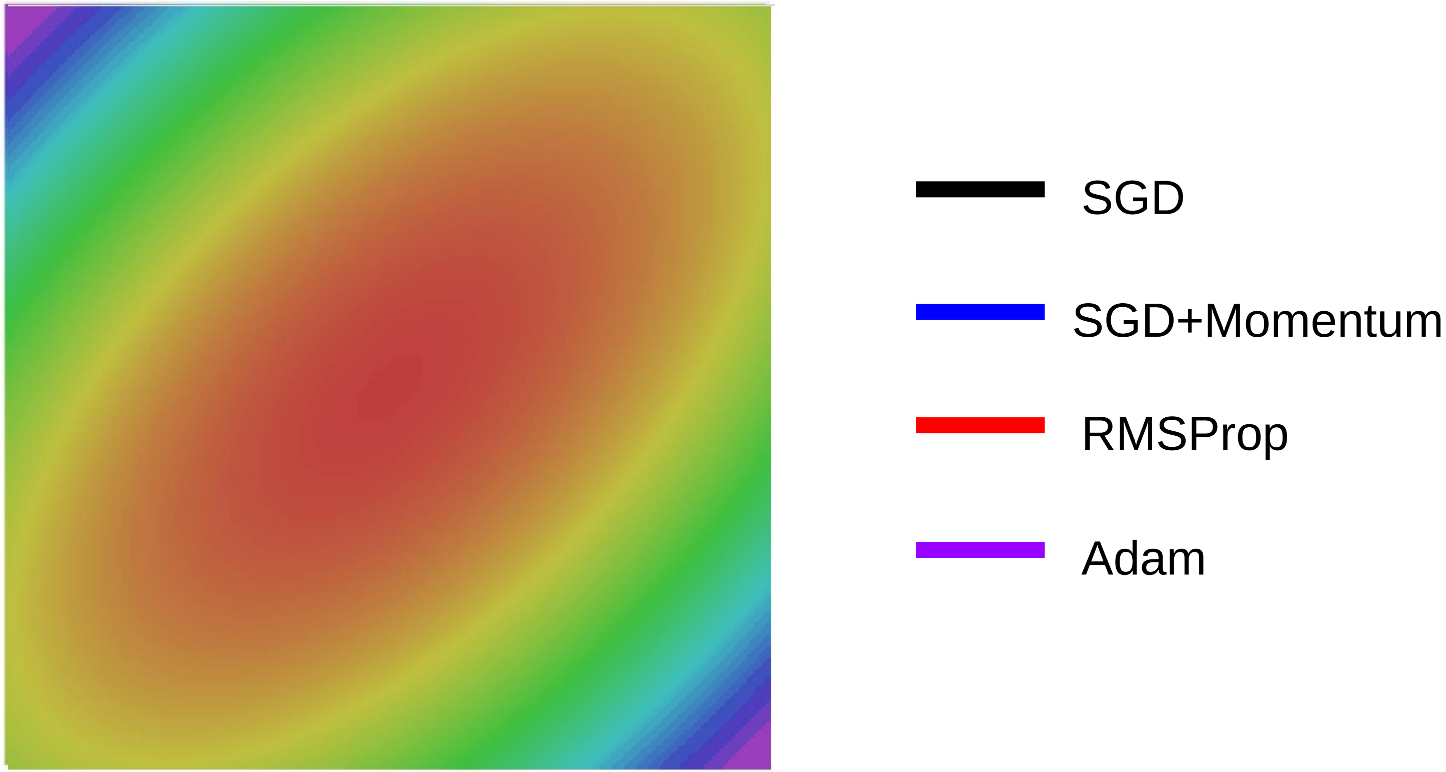
AdaGrad / RMSProp

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

Adam with beta1 = 0.9, beta2 = 0.999, and learning_rate = 1e-3 or 5e-4 is a great starting point for many models!

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

Adam



AdamW: Adam Variant with Weight Decay

Q: How does regularization interact with the optimizer? (e.g., L2)

```
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)
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  second_unbias = second_moment / (1 - beta2 ** t)
  x -= learning_rate * first_unbias / (np.sqrt(second_unbias) + 1e-7))
```

A: It depends!

AdamW: Adam Variant with Weight Decay

Q: How does regularization interact with the optimizer? (e.g., L2)

Standard Adam computes L2 here

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

Used during moment calculations!

AdamW: Adam Variant with Weight Decay

Q: How does regularization interact with the optimizer? (e.g., L2)

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

AdamW (Weight Decay) adds term here

Computed after the moments!

AdamW: Adam Variant with Weight Decay

Q: How does regularization interact with the optimizer? (e.g., L2)

Standard Adam computes L2 here

```
first_moment = 0
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for t in range(1, num_iterations):
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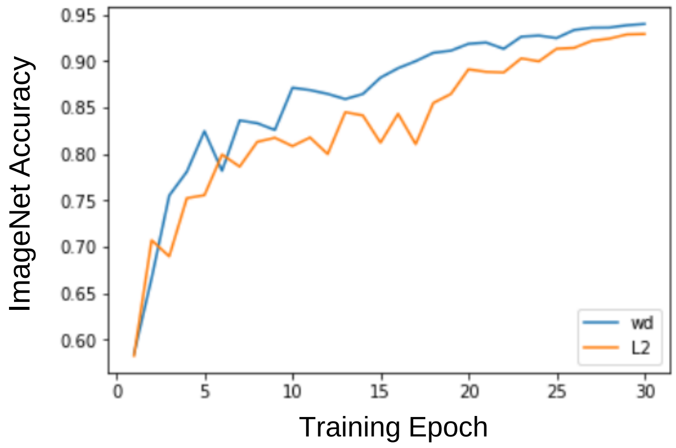
AdamW (Weight Decay) adds term here



Source: https://www.fast.ai/posts/2018-07-02-adam-weight-decay.html

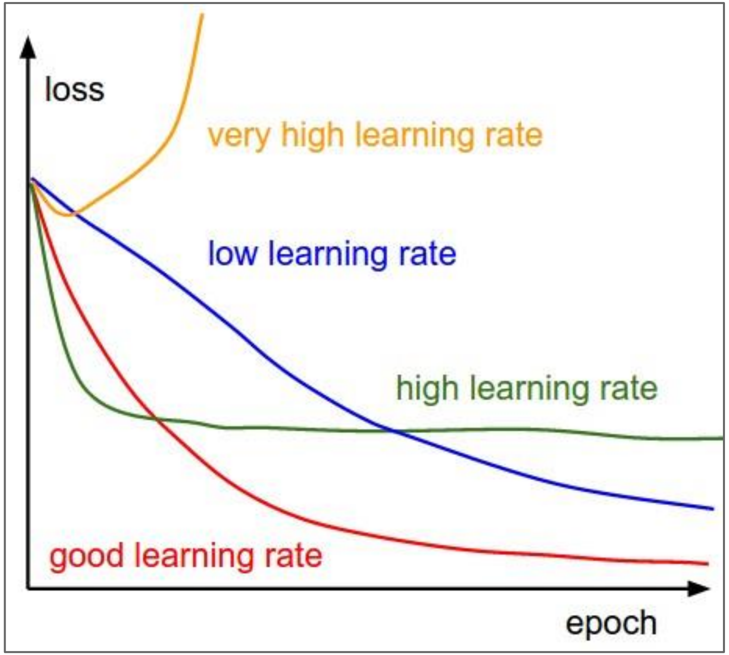
Learning rate schedules

```
# Vanilla Gradient Descent

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

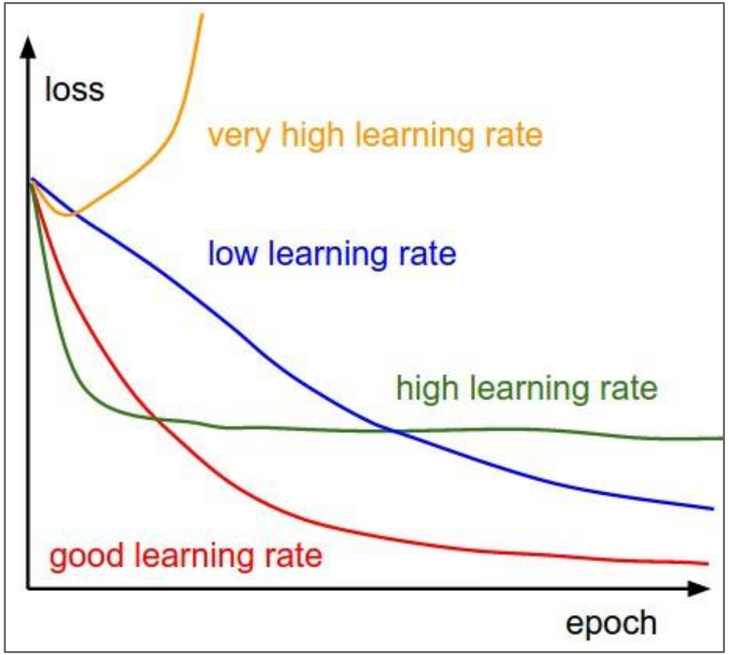
Learning rate

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



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

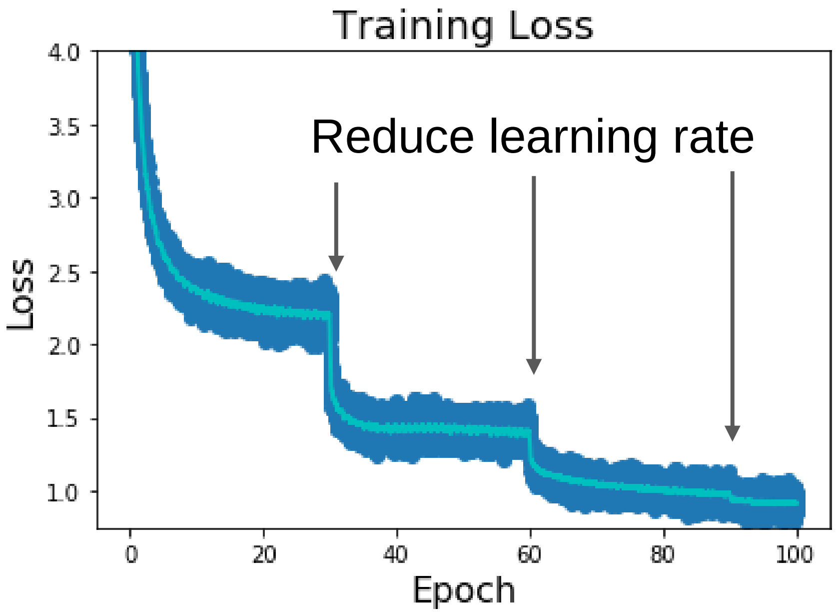
SGD, SGD+Momentum, RMSProp, Adam, AdamW all have **learning rate** as a hyperparameter.



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

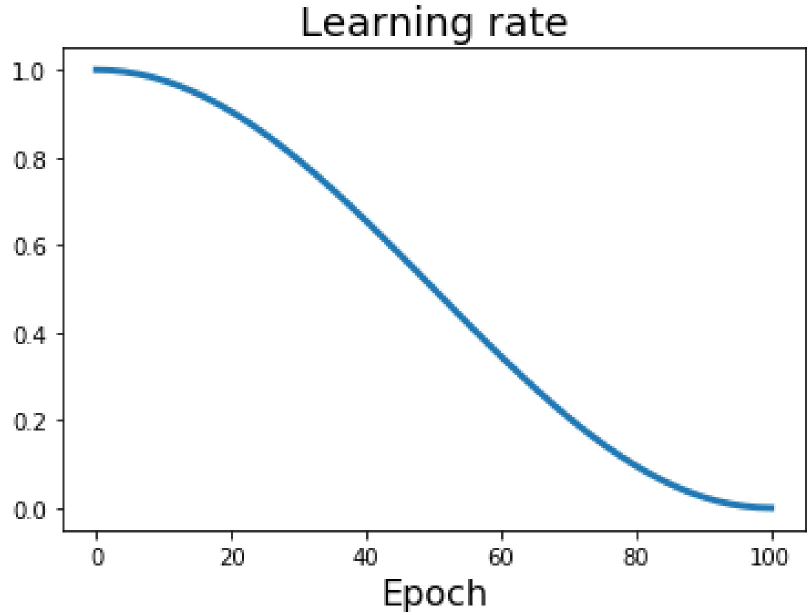
A: In reality, all of these could be good learning rates.

Learning rate decays over time



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

Learning Rate Decay



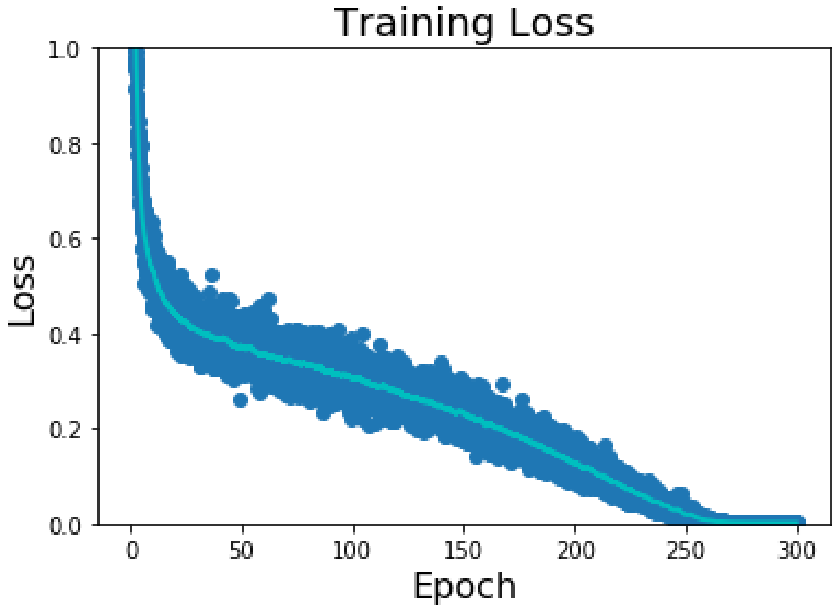
Step: Reduce learning rate at a few fixed points. E.g. for ResNets, multiply LR by 0.1 after epochs 30, 60, and 90.

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

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

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

Learning Rate Decay



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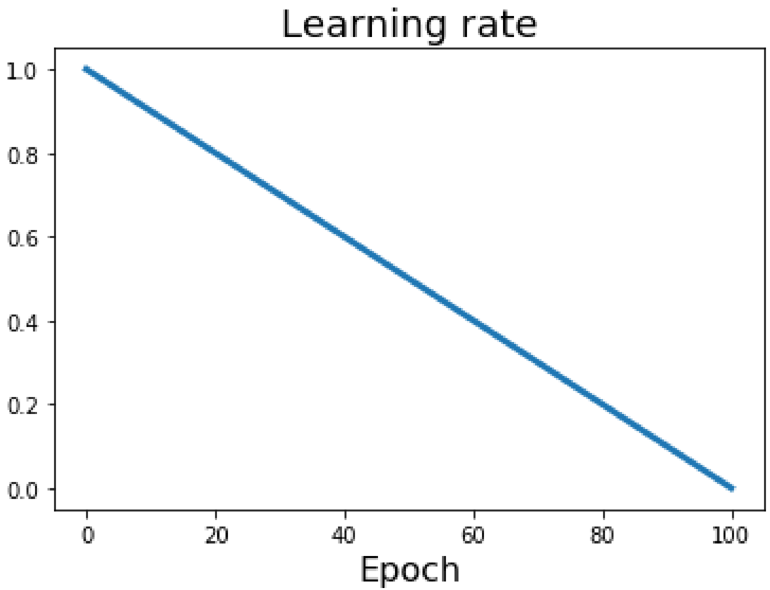
Learning Rate Decay



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

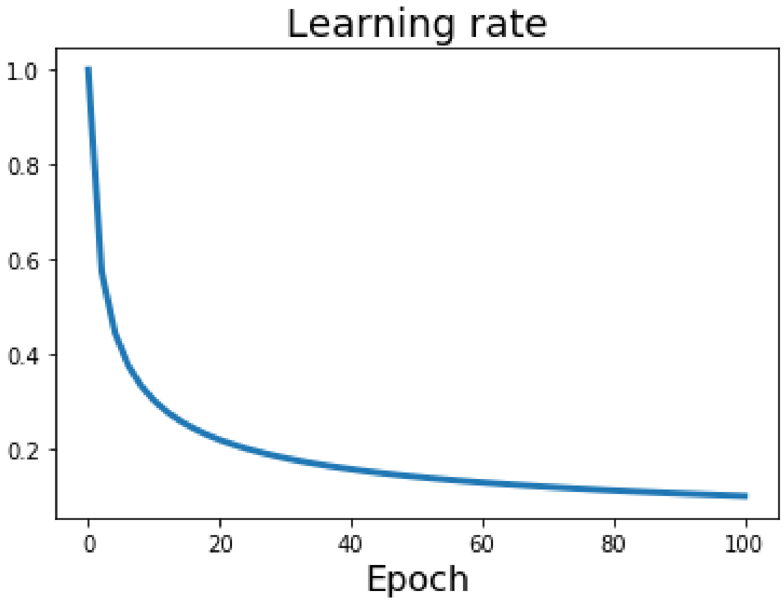
Cosine: $\alpha_t = \frac{1}{2}\alpha_0\left(1 + \cos(t\pi/T)\right)$

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

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

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

Learning Rate Decay



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

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

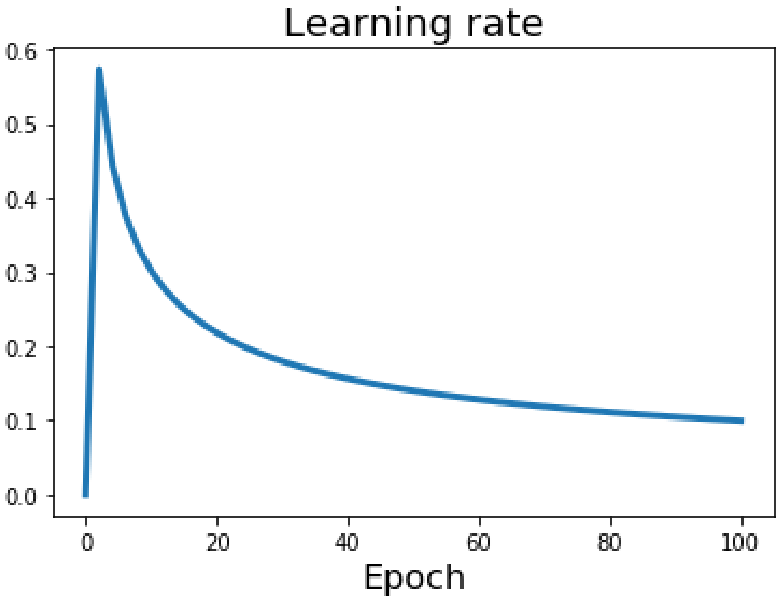
Linear: $\alpha_t = \alpha_0(1 - t/T)$

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

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

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

Learning Rate Decay: Linear Warmup

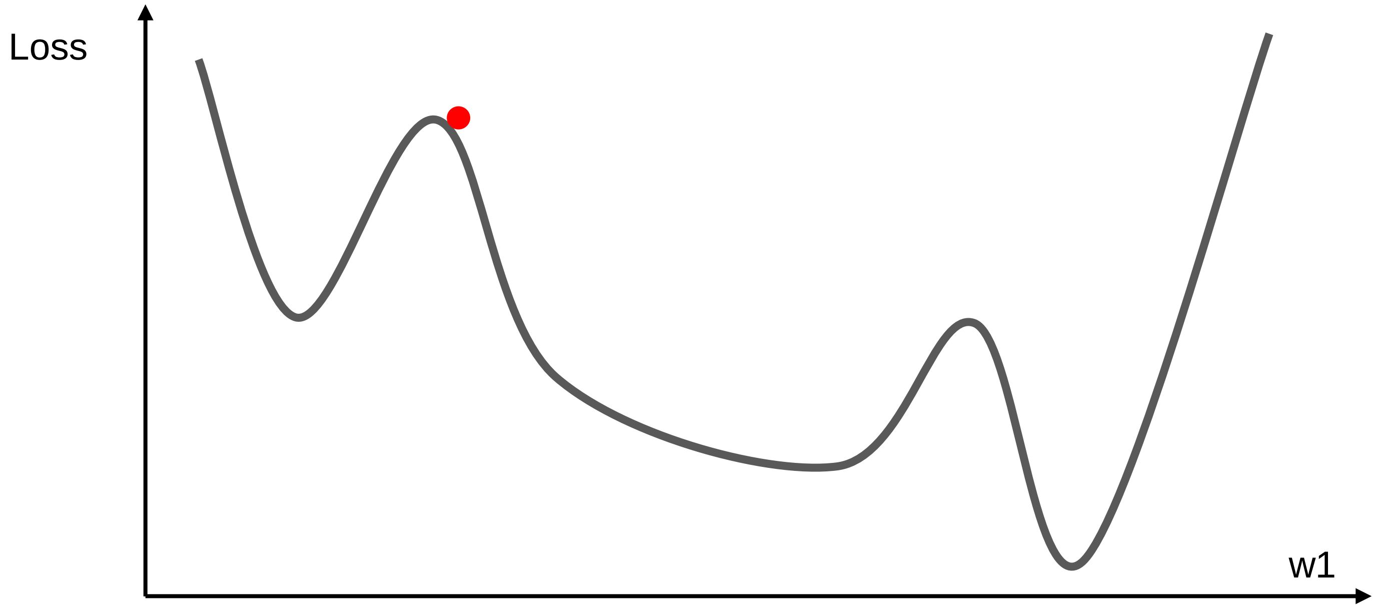


High initial learning rates can make loss explode; linearly increasing learning rate from 0 over the first ~5,000 iterations can prevent this.

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

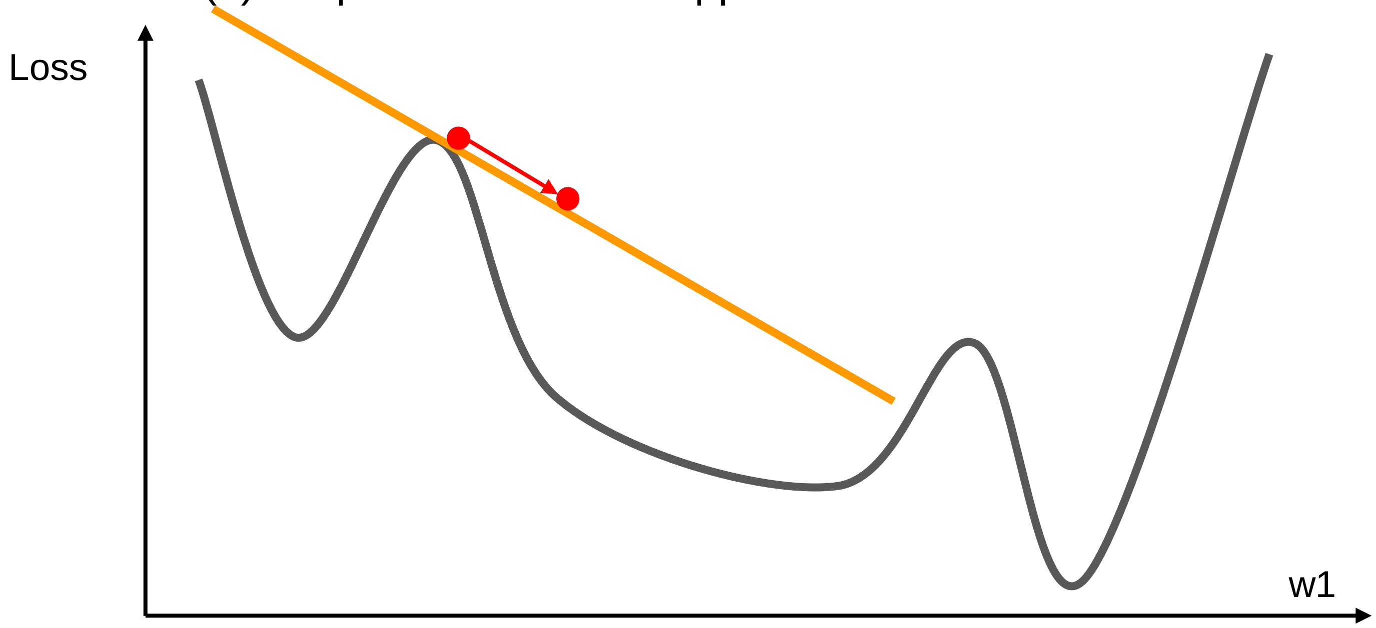
Goyal et al, “Accurate, Large Minibatch SGD: Training ImageNet in 1 Hour”, arXiv 2017

First-Order Optimization



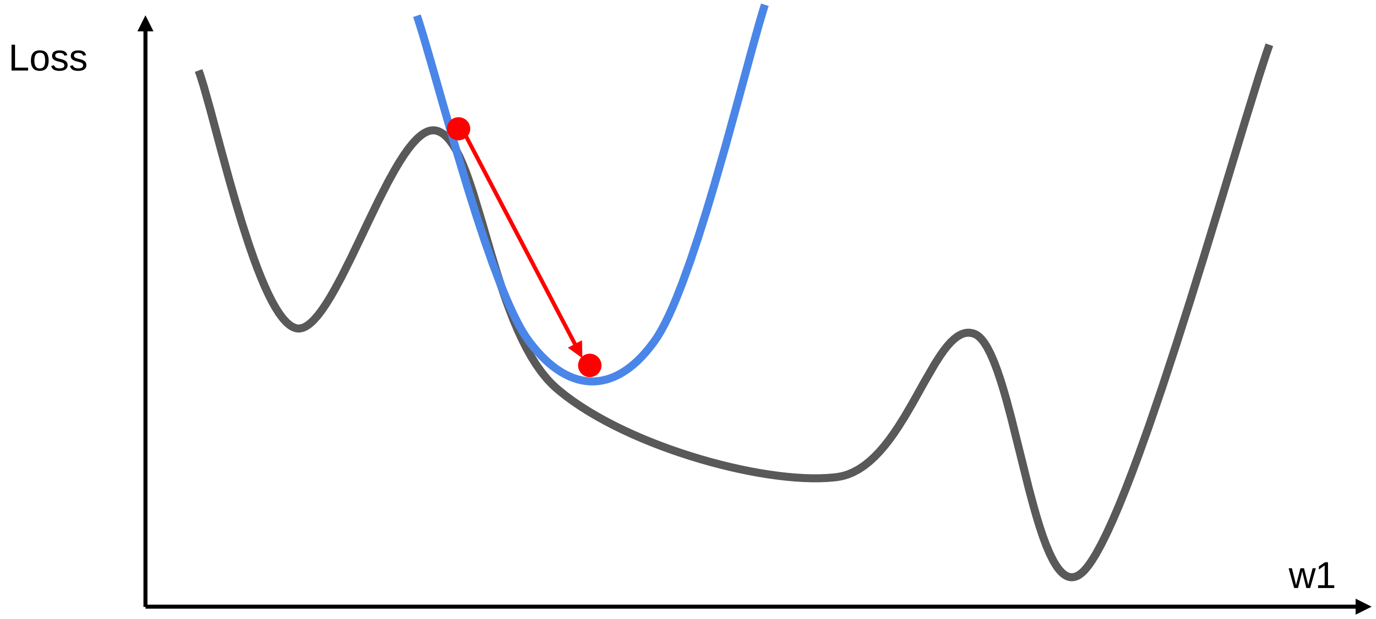
First-Order Optimization

(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:

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

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

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

Q: Why is this bad for deep learning?

Second-Order Optimization

second-order Taylor expansion:

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

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

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

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

Q: Why is this bad for deep learning?

In practice:

- **Adam(W)** 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 look beyond 1st order optimization (**2nd order and beyond**)

Looking Ahead: How to optimize more complex functions?

(Currently) Linear score function: $f = Wx$

$$x \in \mathbb{R}^D, W \in \mathbb{R}^{C \times D}$$

Neural networks: 2 layers

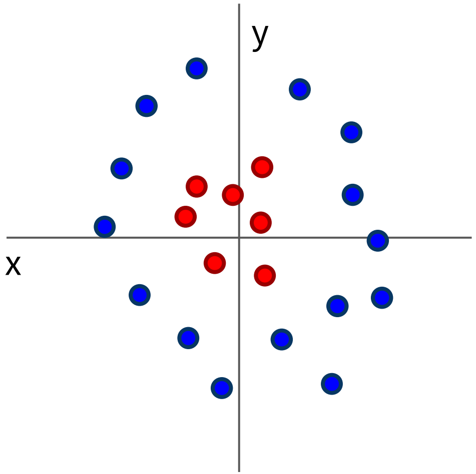
(Currently) Linear score function: $f = Wx$

(Next Class) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

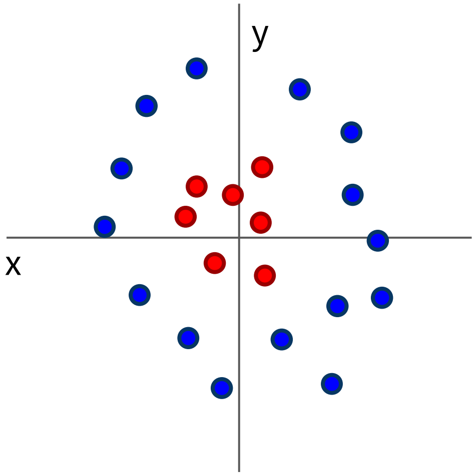
(In practice we will usually add a learnable bias at each layer as well)

Why do we want non-linearity?

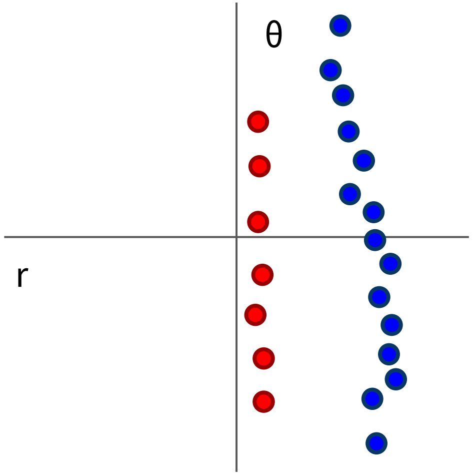


Cannot separate red and blue points with linear classifier

Why do we want non-linearity?



$f(x, y) = (r(x, y), \theta(x, y))$



Cannot separate red and blue points with linear classifier

After applying feature transform, points can be separated by linear classifier

Neural networks: also called fully connected network

(Currently) Linear score function: $f = Wx$

(Next Class) 2-layer Neural Network $f = W_2 \max(0, W_1 x)$

$$x \in \mathbb{R}^D, W_1 \in \mathbb{R}^{H \times D}, W_2 \in \mathbb{R}^{C \times H}$$

“Neural Network” is a very broad term; these are more accurately called “fully-connected networks” or sometimes “multi-layer perceptrons” (MLP)

(In practice we will usually add a learnable bias at each layer as well)

Next time:

Introduction to neural networks

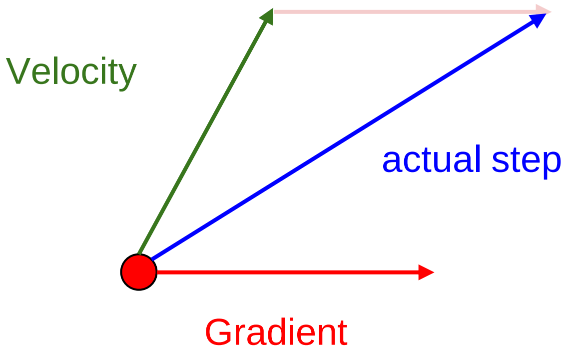
Backpropagation (How do you calculate dx for neural nets?)

Appendix Material

Extraneous content that may be of interest

SGD+Momentum

Momentum update:

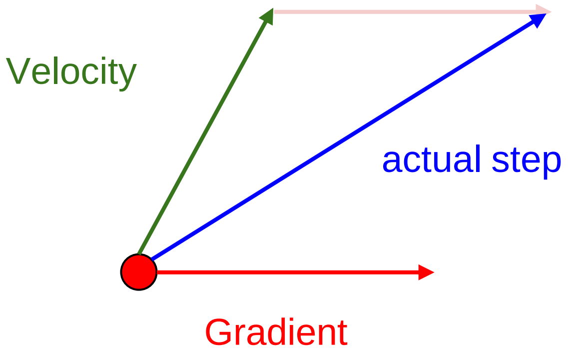


Combine gradient at current point with velocity to get step used to update weights

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

Nesterov Momentum

Momentum update:



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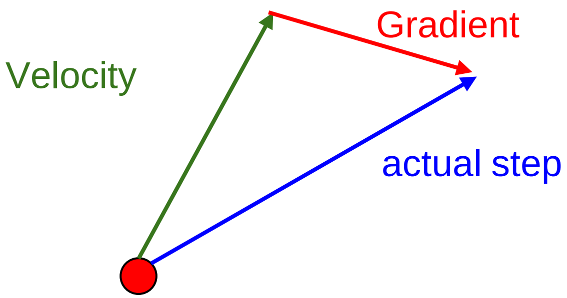
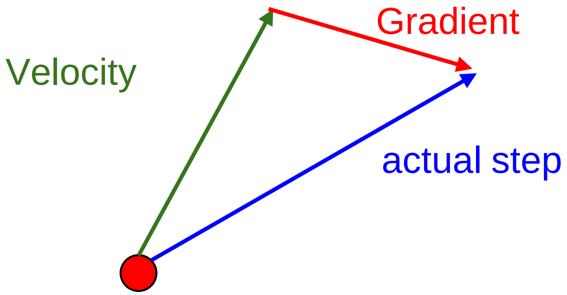
Nesterov Momentum



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

Nesterov Momentum

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



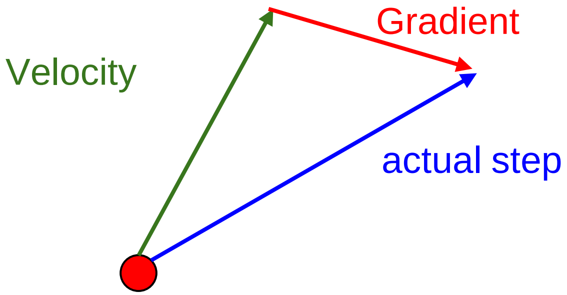
“Look ahead” to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

Nesterov Momentum

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

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

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



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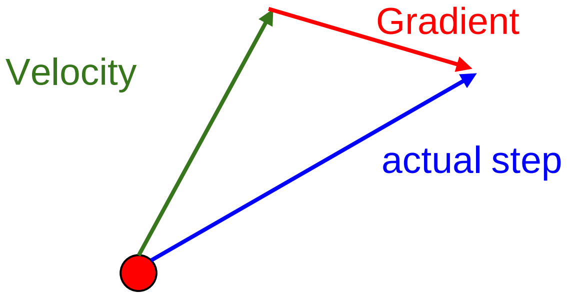
$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
$$x_{t+1} = \boxed{x_t} + v_{t+1}$$

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

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



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

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

Nesterov Momentum

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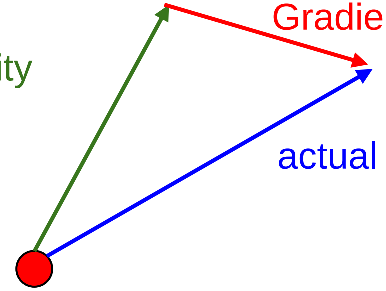


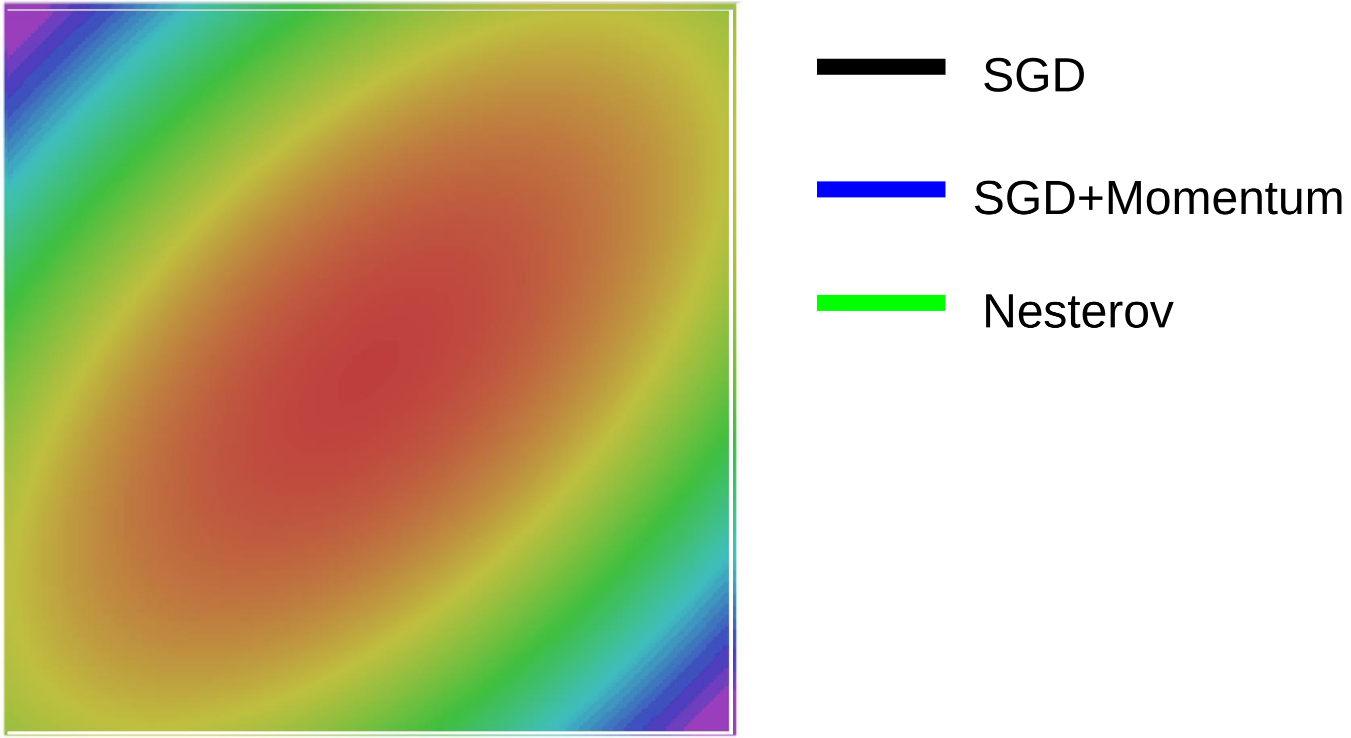
Change of variables $\tilde{x}_t = x_t + \rho v_t$ and rearrange:

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

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

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

Nesterov Momentum



AdaGrad

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

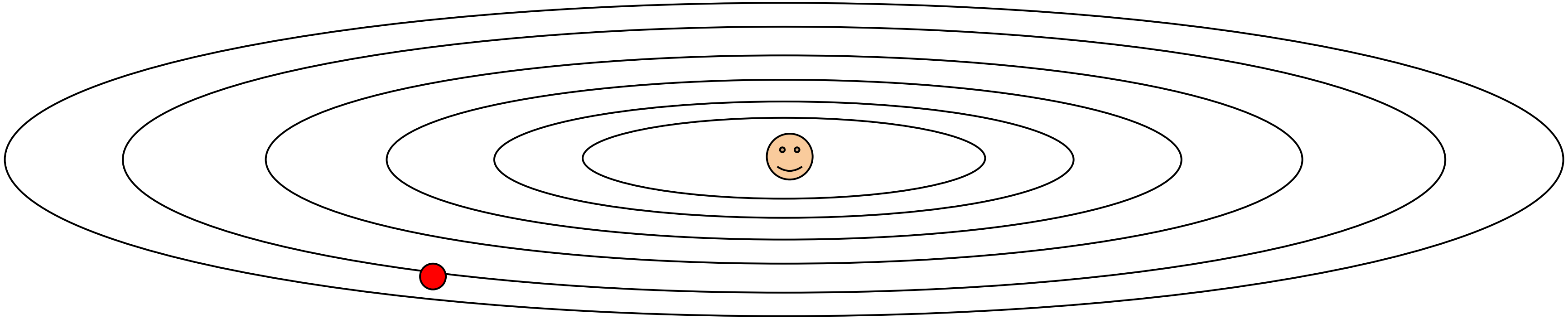
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

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

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

AdaGrad

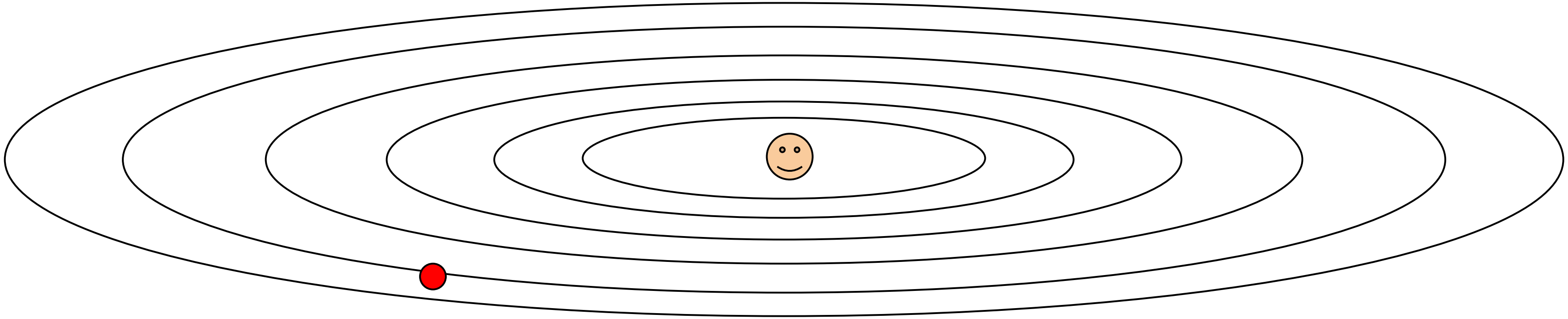
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



Q: What happens with AdaGrad?

AdaGrad

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

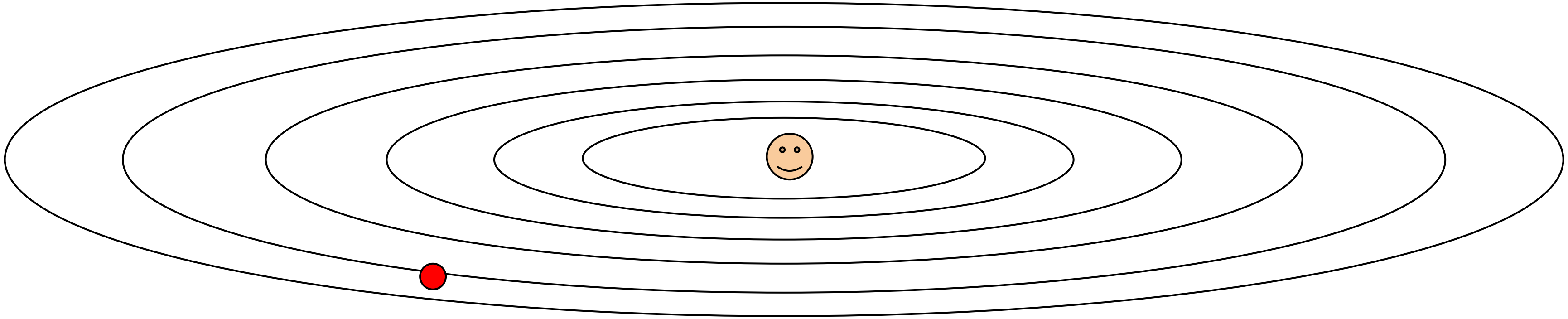


Q: What happens with AdaGrad?

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

AdaGrad

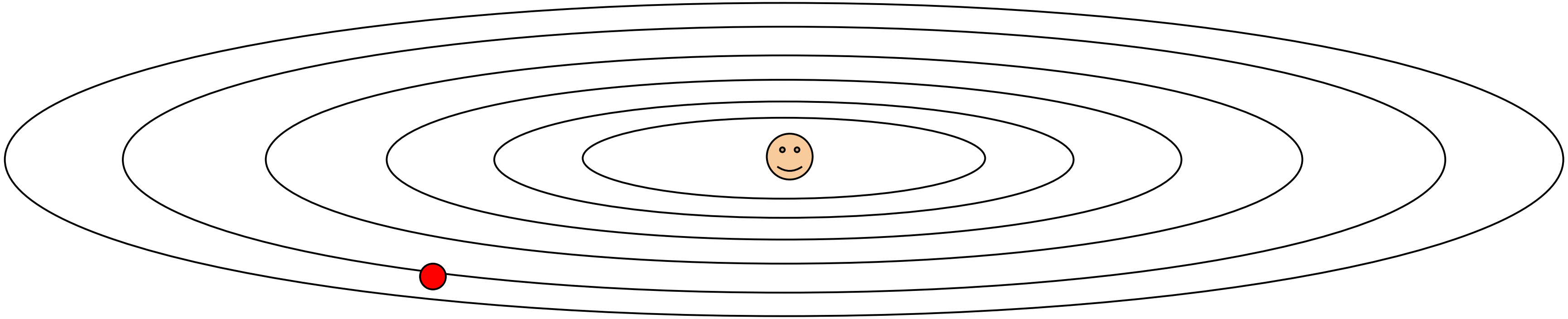
```
grad_squared = 0
while True:
  dx = compute_gradient(x)
  grad_squared += dx * dx
  x -= learning_rate * dx / (np.sqrt(grad_squared) + 1e-7)
```



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

AdaGrad

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



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

RMSProp: “Leaky AdaGrad”

AdaGrad

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

RMSProp

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

Tieleman and Hinton, 2012

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)