4. Regularization, Optimization

GEV6135 Deep Learning for Visual Recognition and Applications

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Note on the lecture style

- There might be slides about advanced topics/details we don’t cover.
  - To take account of students with a wide range of background
- Lecture notes and assignments are not exactly aligned.
  - Real-world applications are not that well-designed.
- We generally do not talk about implementation details.
  - We don’t have much time.

Assignment 2

- Due **Monday 9/26, 11:59pm KST**
- K-Nearest Neighbors classification
- If you feel difficult, consider to take **option 2**.
- Please read the instruction carefully!
  - Do **not write or modify any code outside** of the designated blocks.
  - Do **not add or delete cells** from the notebook.
  - Do **not import** additional libraries.
    - + Do not use torch.nn unless instructed.
  - **Run all cells**, and do **not clear out the outputs**, before submitting.
  - Do **not zip by yourself**, run the provided code.

Assignment 3, 4

- A3 will be released around **Tuesday 9/27**
  - Expected due **Monday 10/10**
  - Training linear classifiers (Lec 3) with
    - SVM/softmax loss (Lec 3)
    - SGD (Lec 4, but the code is given)
- A4 will be released around **Tuesday 10/4**
  - Expected due **Monday 10/17**
  - Training two-layer neural networks (Lec 5) with
    - Softmax loss (Lec 3)
    - SGD (Lec 4, but the code is given)
- A5, 6, 7 (, 8) after the midterm

Broadcasting, Vectorization

Elementwise Operations

Python+Numpy (right way):

```
imNew = im**4
```

Python+Numpy (slow way – **why?**):

```
imNew = np.zeros(im.shape)
for y in range(im.shape[0]):
  for x in range(im.shape[1]):
    imNew[y,x] = im[y,x]**4
```

Elementwise Operations

Element-wise power – beware notation

$$(\boldsymbol{A}^p)_{ij} = A_{ij}^p$$

"Hadamard Product" / Element-wise multiplication

$$(\boldsymbol{A} \odot \boldsymbol{B})_{ij} = \boldsymbol{A}_{ij} * \boldsymbol{B}_{ij}$$

Element-wise division

$$(\boldsymbol{A}/\boldsymbol{B})_{ij} = \frac{A_{ij}}{B_{ij}}$$

Sums Across Axes

Let **A** be a matrix of shape (N, 2):

A = np.random.randn(N, 2)

$$\boldsymbol{A} = \begin{bmatrix} x_1 & y_1 \\ \vdots & \vdots \\ x_n & y_n \end{bmatrix}$$

Sum over rows gives vector of shape (2,)

A.sum(axis=0)

$$\Sigma(\boldsymbol{A}, 0) = \left[\sum_{i=1}^{n} x_i \quad , \sum_{i=1}^{n} y_i \right]$$

Sum over columns gives vector of shape (N,)

A.sum(axis=1)

$$\Sigma(\boldsymbol{A}, 1) = \begin{bmatrix} x_1 + y_1 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

Note – libraries distinguish between N-D column vector and Nx1 matrix.

Operations they don't teach

You Probably Saw Matrix Addition

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} + \begin{bmatrix} e & f \\ g & h \end{bmatrix} = \begin{bmatrix} a+e & b+f \\ c+g & d+h \end{bmatrix}$$

What is this? FYI: e is a scalar

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} + e = \begin{bmatrix} a+e & b+e \\ c+e & d+e \end{bmatrix}$$

Broadcasting

If you want to be pedantic and proper, you expand e by multiplying a matrix of 1s (denoted **1**)

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} + e = \begin{bmatrix} a & b \\ c & d \end{bmatrix} + \mathbf{1}_{2\times 2} e$$

$$= \begin{bmatrix} a & b \\ c & d \end{bmatrix} + \begin{bmatrix} e & e \\ e & e \end{bmatrix}$$

Many smart matrix libraries do this automatically.
This is the source of many bugs.

Broadcasting Example

Given: Matrix **P** of shape (N, 2) vector **v** of shape (2, 1)
Want: Difference matrix **D** of shape (N, 2)

$$\boldsymbol{P} = \begin{bmatrix} x_1 & y_1 \\ \vdots & \vdots \\ x_N & y_N \end{bmatrix} \quad \boldsymbol{v} = \begin{bmatrix} a \\ b \end{bmatrix} \quad \boldsymbol{D} = \begin{bmatrix} x_1 - a & y_1 - b \\ \vdots & \vdots \\ x_N - a & y_N - b \end{bmatrix}$$

$$\boldsymbol{P} - \boldsymbol{v}^T = \begin{bmatrix} x_1 & y_1 \\ \vdots & \vdots \\ x_N & y_N \end{bmatrix} - \begin{bmatrix} a & b \\ \vdots & \\ a & b \end{bmatrix}$$

Blue stuff is assumed / broadcast

Broadcasting Rules

Suppose we have numpy arrays x and y.
How will they broadcast?

1. Write down the **shape** of each array as a tuple of integers:
For example: x: (10,) y: (20, 10)

2. If they have different numbers of dimensions, **prepend** with ones until they have the same number of dimensions
For example: x: (10,) y: (20, 10) → x: (1, 10) y: (20, 10)

3. Compare each dimension. There are 3 cases:
   (a) Dimension match. Everything is good
   (b) Dimensions don't match, but one is =1.
      "Duplicate" the smaller array along that axis to match
   (c) Dimensions don't match, neither are =1. Error!

Broadcasting Examples

```
x = np.ones(10, 20)
y = np.ones(20)
z = x + y
print(z.shape)
```

(10,20)

```
x = np.ones(10, 20)
y = np.ones(10)
z = x + y
print(z.shape)
```

ERROR

```
x = np.ones(10, 20)
y = np.ones(10, 1)
z = x + y
print(z.shape)
```

(10,20)

```
x = np.ones(1, 20)
y = np.ones(10, 1)
z = x + y
print(z.shape)
```

(10,20)

Tensors

Scalar: Just one number

Vector: 1D list of numbers

Matrix: 2D grid of numbers

Tensor: N-dimensional grid of numbers
(Lots of other meanings in math, physics)

Broadcasting with Tensors

The same broadcasting rules apply to tensors with any number of dimensions!

```
x = np.ones(30)
y = np.ones(20, 1)
z = np.ones(10, 1, 1)
w = x + y + z
print(w.shape)
```

(10, 20, 30)

Vectorization

Writing code without explicit loops: use broadcasting, matrix multiply, and other (optimized) numpy primitives instead

Vectorization Example

- Suppose I have two sets of (D-dimensional) vectors $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ and $\{\mathbf{y}_1, \ldots, \mathbf{y}_M\}$ and I want to compute all pairwise distances $d_{i,j} = ||x_i - y_j||$
- Identity: $\|\boldsymbol{x} - \boldsymbol{y}\|^2 = \|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 - 2\boldsymbol{x}^T\boldsymbol{y}$
- Or: $\|\boldsymbol{x} - \boldsymbol{y}\| = (\|\boldsymbol{x}\|^2 + \|\boldsymbol{y}\|^2 - 2\boldsymbol{x}^T\boldsymbol{y})^{1/2}$

Vectorization Example

$$\boldsymbol{X} = \begin{bmatrix} - & \boldsymbol{x}_1 & - \\ & \vdots & \\ - & \boldsymbol{x}_N & - \end{bmatrix} \quad \boldsymbol{Y} = \begin{bmatrix} - & \boldsymbol{y}_1 & - \\ & \vdots & \\ - & \boldsymbol{y}_M & - \end{bmatrix} \quad \boldsymbol{Y^T} = \begin{bmatrix} | & & | \\ \boldsymbol{y}_1 & \cdots & \boldsymbol{y}_M \\ | & & | \end{bmatrix}$$

Compute a Nx1 vector of norms
(can also do Mx1)

$$\boldsymbol{\Sigma}(\boldsymbol{X^2}, \boldsymbol{1}) = \begin{bmatrix} \|\boldsymbol{x_1}\|^2 \\ \vdots \\ \|\boldsymbol{x_N}\|^2 \end{bmatrix}$$

Compute a NxM matrix of dot products

$$\left(\boldsymbol{XY^T}\right)_{ij} = \boldsymbol{x_i^T y_j}$$

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X}^2, 1) + \Sigma(\boldsymbol{Y}^2, 1)^T - 2\boldsymbol{X}\boldsymbol{Y}^T\right)^{1/2}$$

$$\begin{bmatrix} \|\boldsymbol{x}_1\|^2 \\ \vdots \\ \|\boldsymbol{x}_N\|^2 \end{bmatrix} + \begin{bmatrix} \|\boldsymbol{y}_1\|^2 & \cdots & \|\boldsymbol{y}_M\|^2 \end{bmatrix}$$

$$\begin{bmatrix} \|\boldsymbol{x}_1\|^2 + \|\boldsymbol{y}_1\|^2 & \cdots & \|\boldsymbol{x}_1\|^2 + \|\boldsymbol{y}_M\|^2 \\ \vdots & \ddots & \vdots \\ \|\boldsymbol{x}_N\|^2 + \|\boldsymbol{y}_1\|^2 & \cdots & \|\boldsymbol{x}_N\|^2 + \|\boldsymbol{y}_M\|^2 \end{bmatrix}$$

Why?

$$(\Sigma(\boldsymbol{X}^2, 1) + \Sigma(\boldsymbol{Y}^2, 1)^T)_{ij} = \|\boldsymbol{x}_i\|^2 + \|\boldsymbol{y}_j\|^2$$

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

$$\mathbf{D}_{ij} = \|\boldsymbol{x}_i\|^2 + \left\|\boldsymbol{y}_j\right\|^2 + 2\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{y}$$

Numpy code:

```
XNorm = np.sum(X**2,axis=1,keepdims=True)
YNorm = np.sum(Y**2,axis=1,keepdims=True)
D = (XNorm+YNorm.T-2*np.dot(X,Y.T))**0.5
```

Get in the habit of thinking about shapes as tuples.
Suppose X is (N, D), Y is (M, D):

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

$$\mathbf{D}_{ij} = \|\boldsymbol{x}_i\|^2 + \|\boldsymbol{y}_j\|^2 + 2\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{y}$$

Numpy code: (N, 1)

```
XNorm = np.sum(X**2,axis=1,keepdims=True)
YNorm = np.sum(Y**2,axis=1,keepdims=True)
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Get in the habit of thinking about shapes as tuples.
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Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

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Numpy code: (N, 1) (M, 1)

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Vectorization Example

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Get in the habit of thinking about shapes as tuples.
Suppose X is (N, D), Y is (M, D):

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

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Numpy code: (N, 1) (M, 1) (N, M) (N, M)

```
XNorm = np.sum(X**2,axis=1,keepdims=True)
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```

Get in the habit of thinking about shapes as tuples.

Suppose X is (N, D), Y is (M, D):

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

$$\mathbf{D}_{ij} = \|\boldsymbol{x}_i\|^2 + \left\|\boldsymbol{y}_j\right\|^2 + 2\boldsymbol{x}^{\boldsymbol{T}}\boldsymbol{y}$$

Numpy code: (N, 1) (M, 1) (N, M) (N, M)

```
XNorm = np.sum(X**2,axis=1,keepdims=True)
YNorm = np.sum(Y**2,axis=1,keepdims=True)
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```

Get in the habit of thinking about shapes as tuples.

Suppose X is (N, D), Y is (M, D):

Vectorization Example

$$\mathbf{D} = \left(\Sigma(\boldsymbol{X^2}, 1) + \Sigma(\boldsymbol{Y^2}, 1)^{\boldsymbol{T}} - 2\boldsymbol{X}\boldsymbol{Y}^{\boldsymbol{T}}\right)^{1/2}$$

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Numpy code: (N, 1) (M, 1) (N, M) (N, M)

```
XNorm = np.sum(X**2,axis=1,keepdims=True)
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```

Get in the habit of thinking about shapes as tuples.

Suppose X is (N, D), Y is (M, D):

Vectorization Example

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D = (XNorm+YNorm.T-2*np.dot(X,Y.T))**0.5
```

*May have to make sure this is at least 0 (sometimes roundoff issues happen)

Does Vectorization Matter?

Computing pairwise distances between 300 and 400 128-dimensional vectors

1. for x in X, for y in Y, using native python: 9s
2. for x in X, for y in Y, using numpy to compute distance: 0.8s
3. vectorized: 0.0045s (~2000x faster than 1, 175x faster than 2)

Expressing things in primitives that are optimized is usually faster

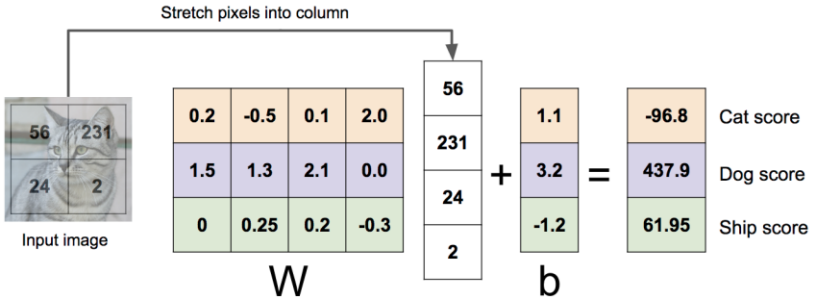
Even more important with special hardware like GPUs or TPUs!

Regularization, Optimization

Recap: Linear Classifiers

Algebraic Viewpoint

$f(x,W) = Wx$

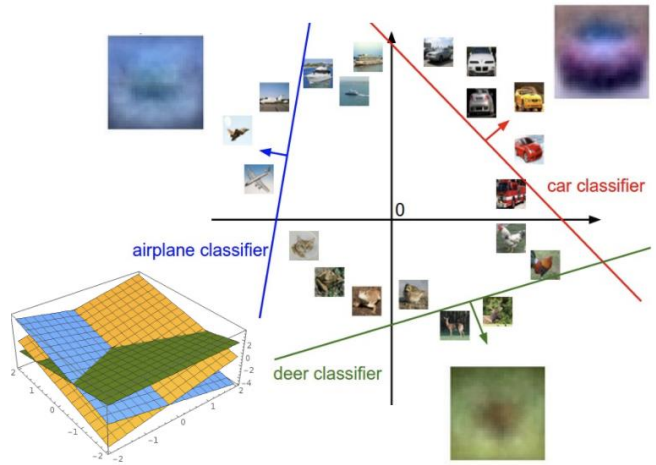


Visual Viewpoint

One template per class

Geometric Viewpoint

Hyperplanes cutting up space



Recap: Loss Functions quantify preferences

- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function**:

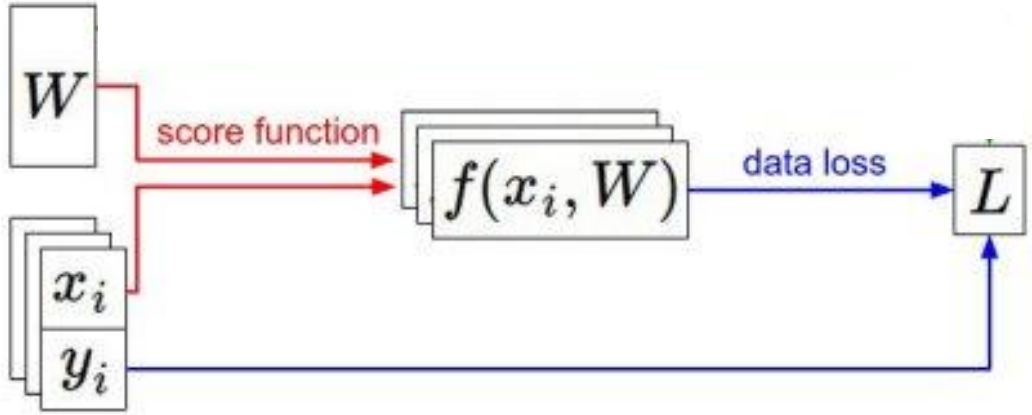
Problem: Loss functions encourage good performance on training data but we really care about test data

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

Linear classifier

Softmax: $L_i = -\log\left(\frac{\exp(s_{y_i})}{\sum_j \exp(s_j)}\right)$

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



Overfitting

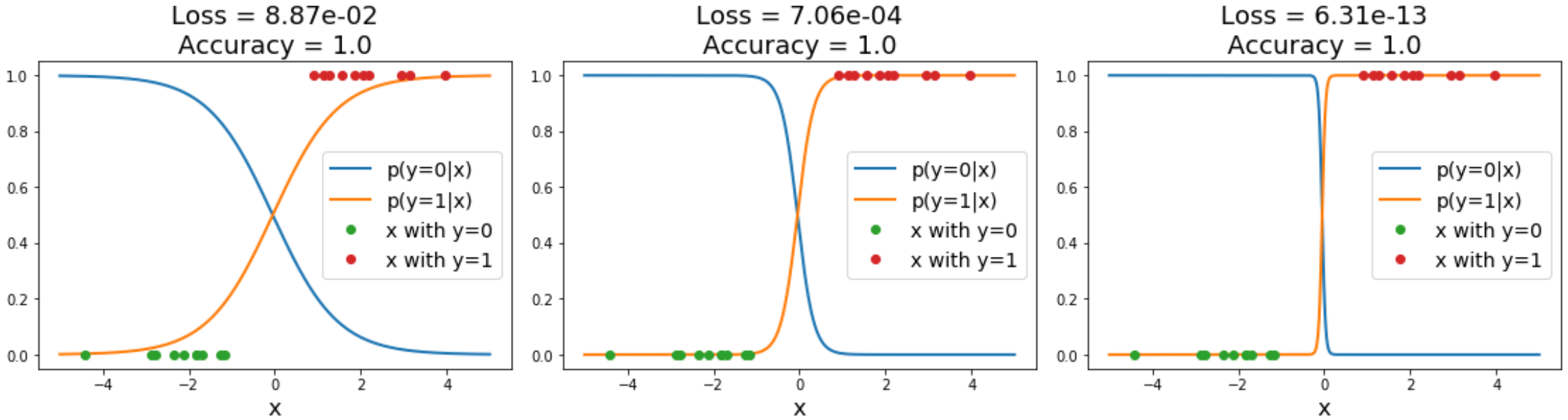
A model is **overfit** when it performs too well on the training data, and has poor performance for unseen data

Example: Linear classifier with 1D inputs, 2 classes, softmax loss

$$s_i = w_i x + b_i$$

$$p_i = \frac{\exp(s_i)}{\exp(s_1) + \exp(s_2)}$$

$$L = -\log(p_y)$$



Both models have perfect accuracy on train data!

Low loss, but unnatural "cliff" between training points

Overfitting

A model is **overfit** when it performs too well on the training data, and has poor performance for unseen data

Example: Linear classifier with 1D inputs, 2 classes, softmax loss

$$s_i = w_i x + b_i$$

$$p_i = \frac{\exp(s_i)}{\exp(s_1) + \exp(s_2)}$$

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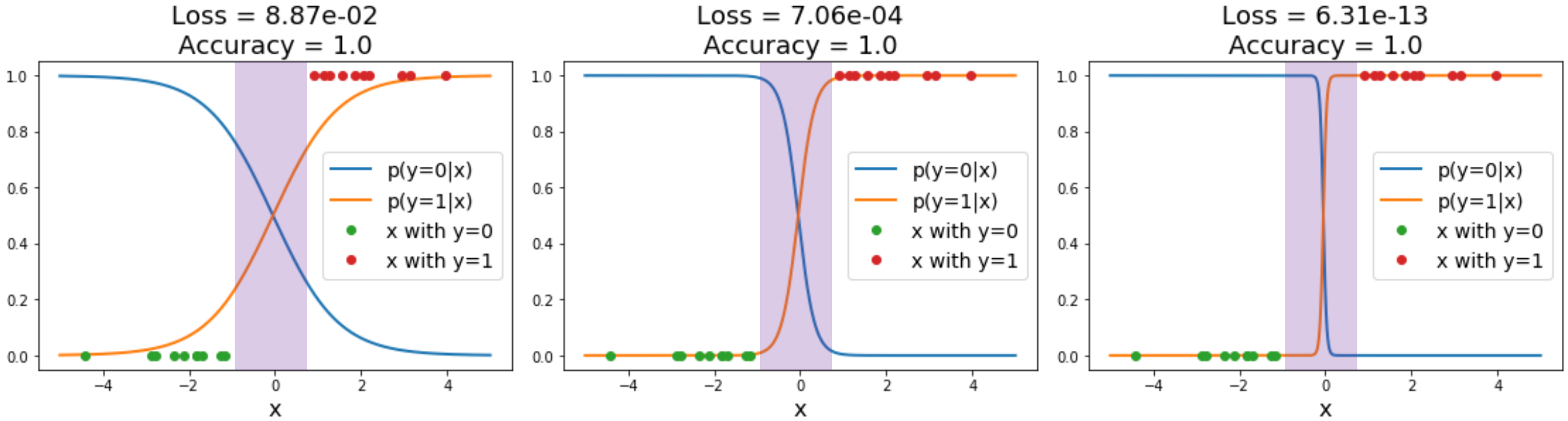


Overconfidence in regions with no training data could give poor generalization

Regularization: Beyond Training Error

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

Data loss: Model predictions should match training data

Regularization: Beyond Training Error

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

λ is a hyperparameter giving regularization strength

Data loss: Model predictions should match training data

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

Simple examples

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

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

More complex:

Dropout

Batch normalization

Cutout, Mixup, Stochastic depth, etc…

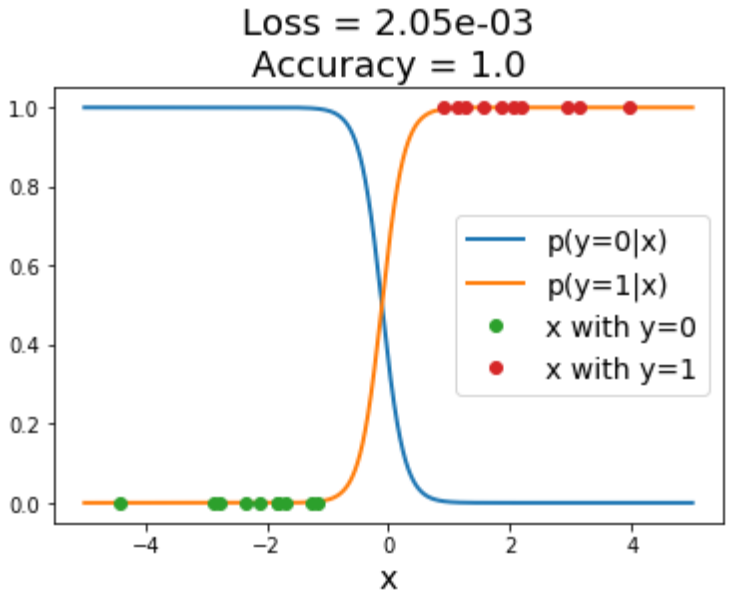
Regularization: Prefer Simpler Models

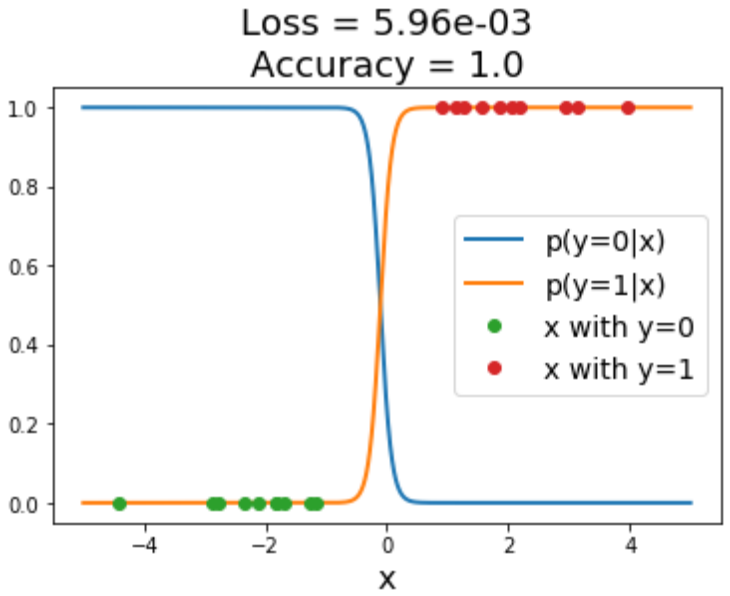
Example: Linear classifier with 1D inputs, 2 classes, softmax loss

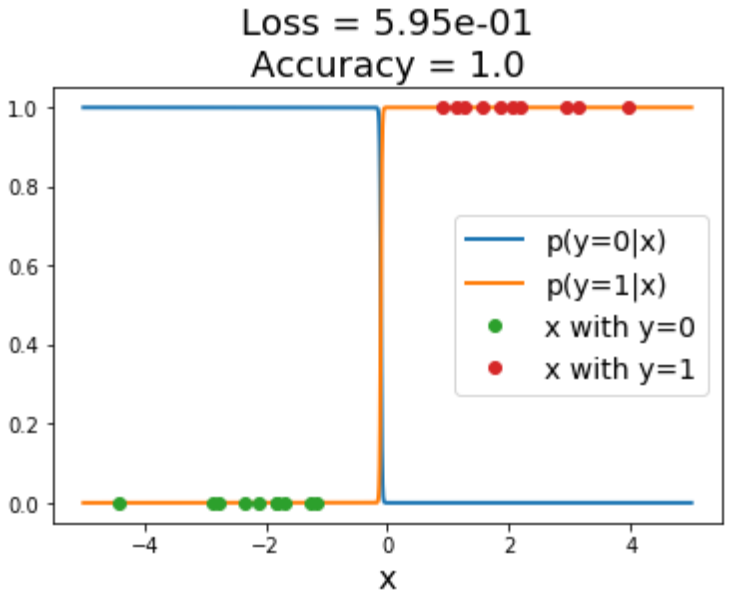
$$s_i = w_i x + b_i \qquad p_i = \frac{\exp(s_i)}{\exp(s_1) + \exp(s_2)}$$

$$L = -\log(p_y) + \lambda \sum_i w_i^2$$

Regularization term causes loss to **increase** for model with sharp cliff







Regularization: Expressing Preferences

L2 Regularization

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

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

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

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

L2 regularization prefers weights to be "spread out"

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

Same predictions, so data loss will always be the same

Finding a good W

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

Loss function consists of **data loss** to fit the training data and **regularization** to prevent overfitting

Optimization

$$w^* = \arg\min_w L(w)$$

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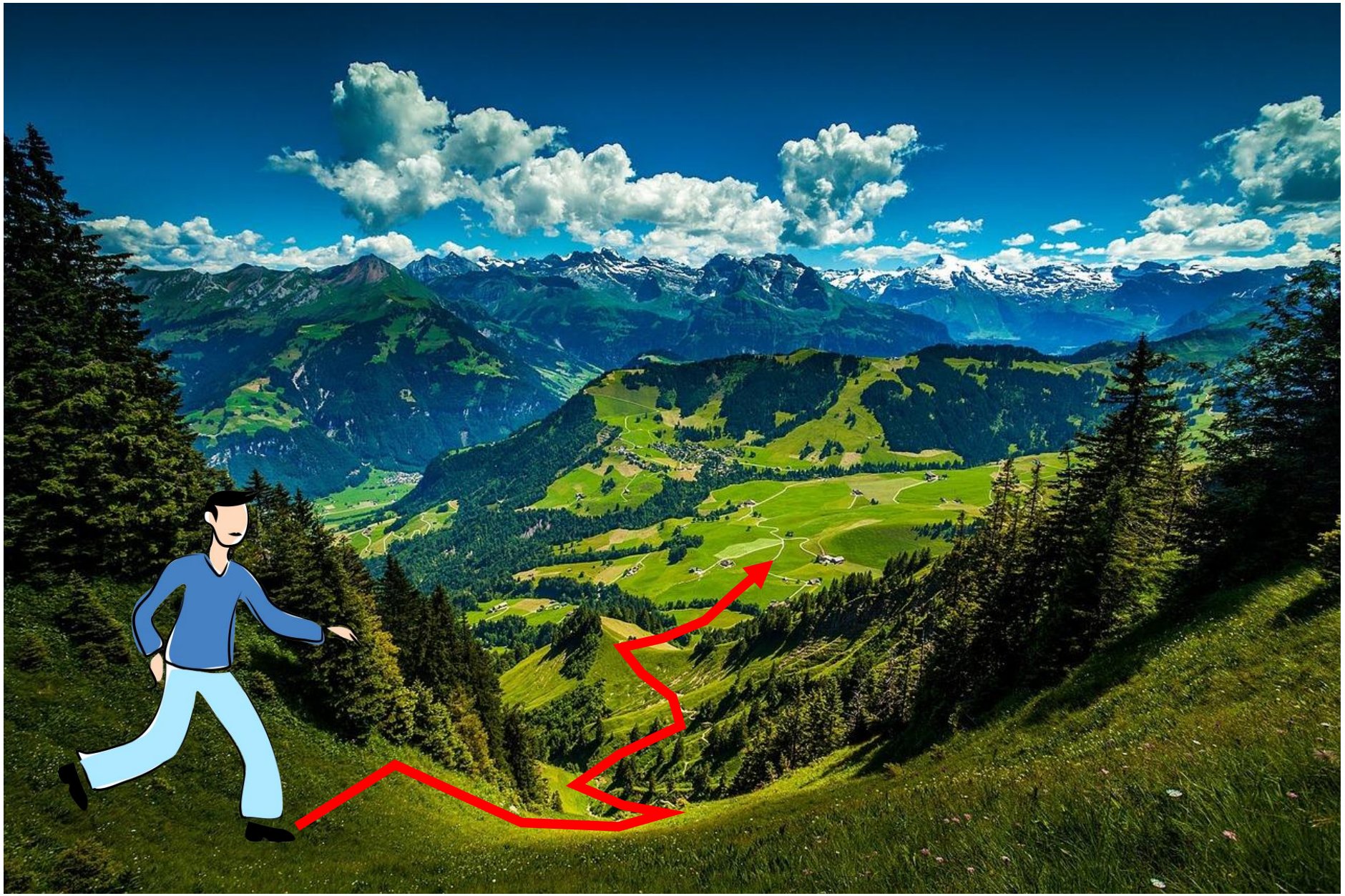
Walking man image is CC0 1.0 public domain



Idea #1: **Random Search** (bad idea!)

```
# 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)
```

Idea #1: **Random Search** (bad idea!)

```
# 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 ~95%)

Idea #2: Follow the slope

Idea #2: Follow the slope

In 1-dimension, the **derivative** of a function gives the slope:

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

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

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 dL/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 dL/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 dL/dW:

[-2.5,
?,
?,
?,
?,
?,
?,
?,
?,…]

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 dL/dW:

[-2.5,
0.6,
?,
?,

(1.25353 - 1.25347)/0.0001
= 0.6

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

?,…]

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 dL/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 dL/dW:

[-2.5,
0.6,
0.0,
?,
?,

(1.25347 - 1.25347)/0.0001
= 0.0

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

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 dL/dW:

[-2.5,
0.6,
0.0,
?,
?,

Numeric Gradient:
- Slow: O(#dimensions)
- Approximate

Loss is a function of W

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

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

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

Want $\nabla_w L$

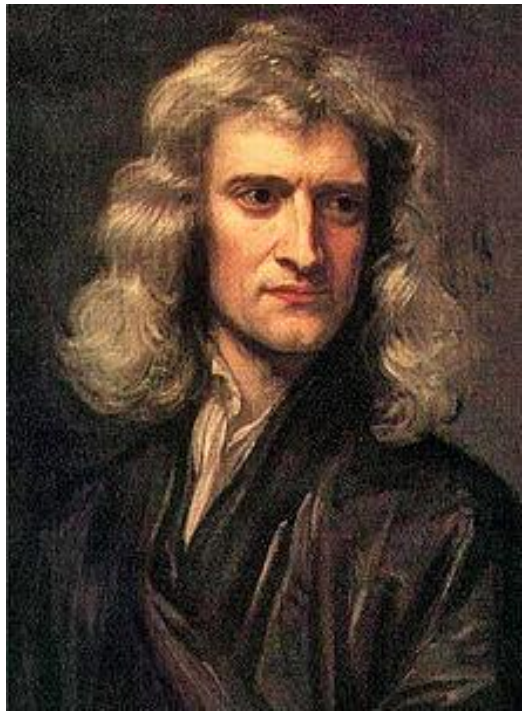
Loss is a function of W: **Analytic Gradient**

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

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

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

Want $\nabla_w L$



This image is in the public domain

This image is in the public domain

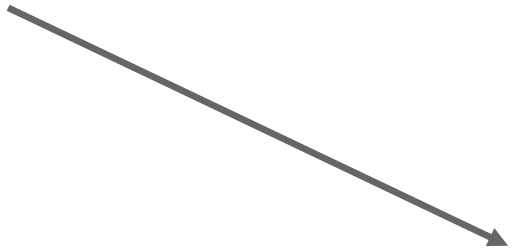
Use calculus to compute an **analytic gradient**

current W:

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

loss 1.25347

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



gradient dL/dW:

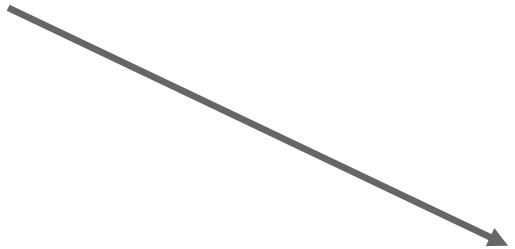
[-2.5,
0.6,
0,
0.2,
0.7,
-0.5,
1.1,
1.3,
-2.1,…]

current W:

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

loss 1.25347

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



(In practice we will compute dL/dW using backpropagation; see Lecture 6)

gradient dL/dW:

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

Computing Gradients

- **Numeric 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.**

```
def grad_check_sparse(f, x, analytic_grad, num_checks=10, h=1e-7):
  """
  sample a few random elements and only return numerical
  in this dimensions.
  """
```

Computing Gradients

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

`torch.autograd.gradcheck(`*`func`*`,` *`inputs`*`,` *`eps=1e-06`*`,` *`atol=1e-05`*`,` *`rtol=0.001`*`,` *`raise_exception=True`*`,` *`check_sparse_nnz=False`*`,` *`nondet_tol=0.0`*`)` [SOURCE]

Check gradients computed via small finite differences against analytical gradients w.r.t. tensors in `inputs` that are of floating point type and with `requires_grad=True`.

The check between numerical and analytical gradients uses `allclose()`.

Computing Gradients

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

`torch.autograd.gradgradcheck(`*`func`*`,` *`inputs`*`,` *`grad_outputs=None`*`,` *`eps=1e-06`*`,` *`atol=1e-05`*`,` *`rtol=0.001`*`,` *`gen_non_contig_grad_outputs=False`*`,` *`raise_exception=True`*`,` *`nondet_tol=0.0`*`)` [SOURCE]

Check gradients of gradients computed via small finite differences against analytical gradients w.r.t. tensors in `inputs` and `grad_outputs` that are of floating point type and with `requires_grad=True`.

This function checks that backpropagating through the gradients computed to the given `grad_outputs` are correct.

Gradient Descent

Iteratively step in the direction of
the negative gradient
(direction of local steepest descent)

```
# Vanilla gradient descent
w = initialize_weights()
for t in range(num_steps):
  dw = compute_gradient(loss_fn, data, w)
  w -= learning_rate * dw
```

Hyperparameters:

- Weight initialization method
- Number of steps
- Learning rate

Gradient Descent

Iteratively step in the direction of the negative gradient
(direction of local steepest descent)

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```

Hyperparameters:

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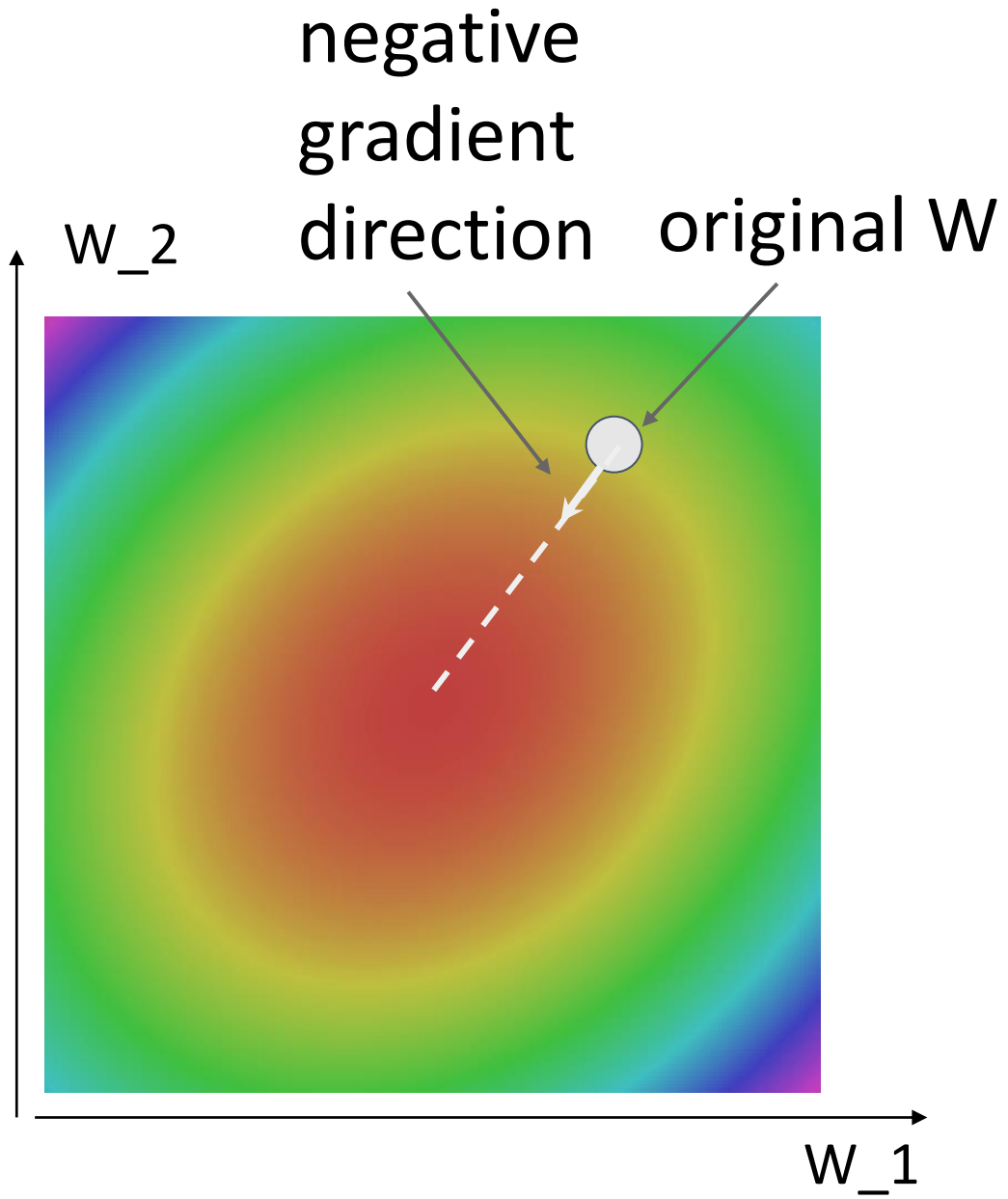
- Number of steps
- Learning rate



Gradient Descent

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```

Hyperparameters:

- Weight initialization method
- Number of steps
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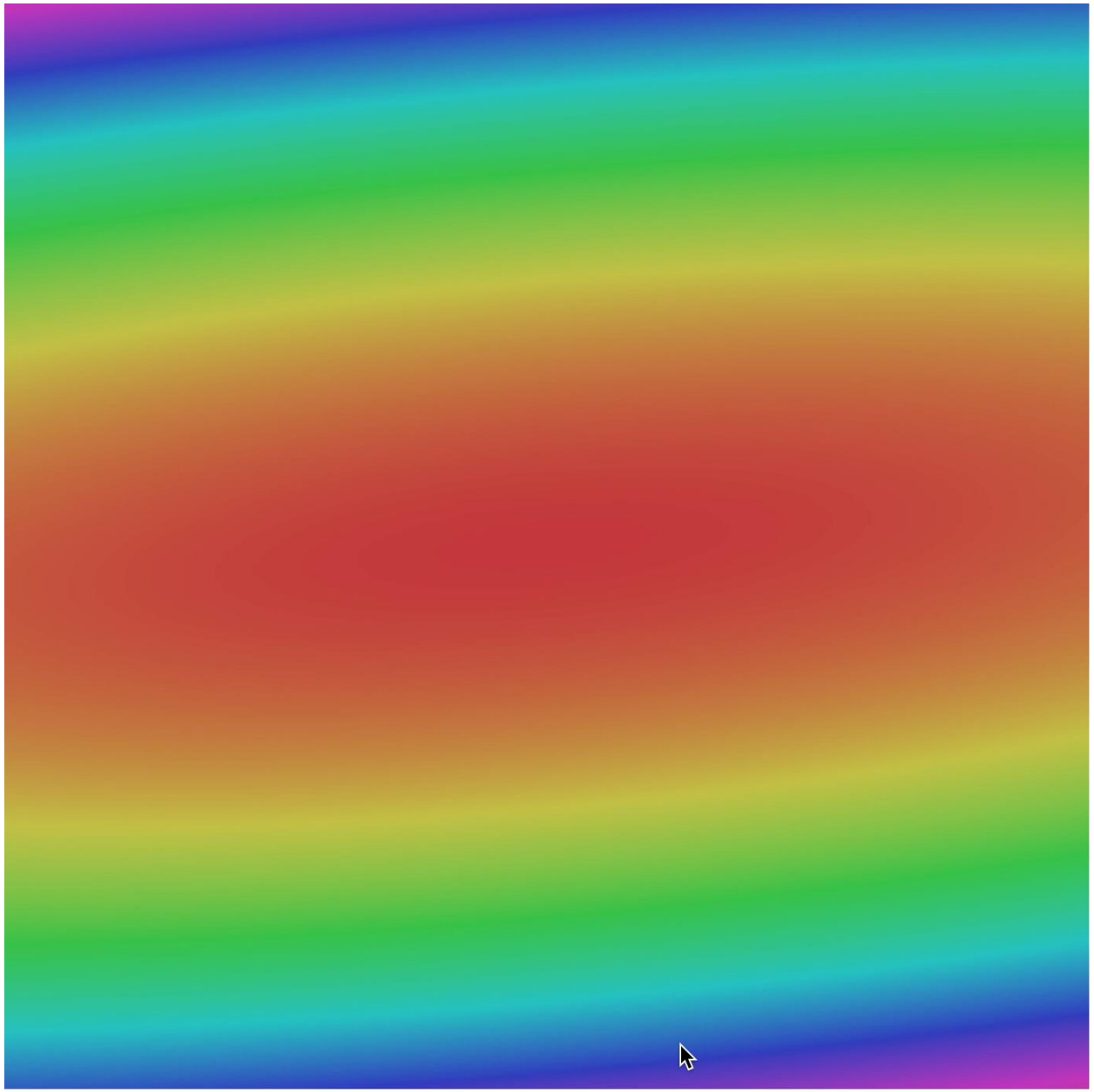


Batch Gradient Descent

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

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

Full sum expensive when N is large!

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

```
# Stochastic gradient descent
w = initialize_weights()
for t in range(num_steps):
  minibatch = sample_data(data, batch_size)
  dw = compute_gradient(loss_fn, minibatch, w)
  w -= learning_rate * dw
```

Hyperparameters:

- Weight initialization
- Number of steps
- Learning rate
- Batch size
- Data sampling

Stochastic Gradient Descent (SGD)

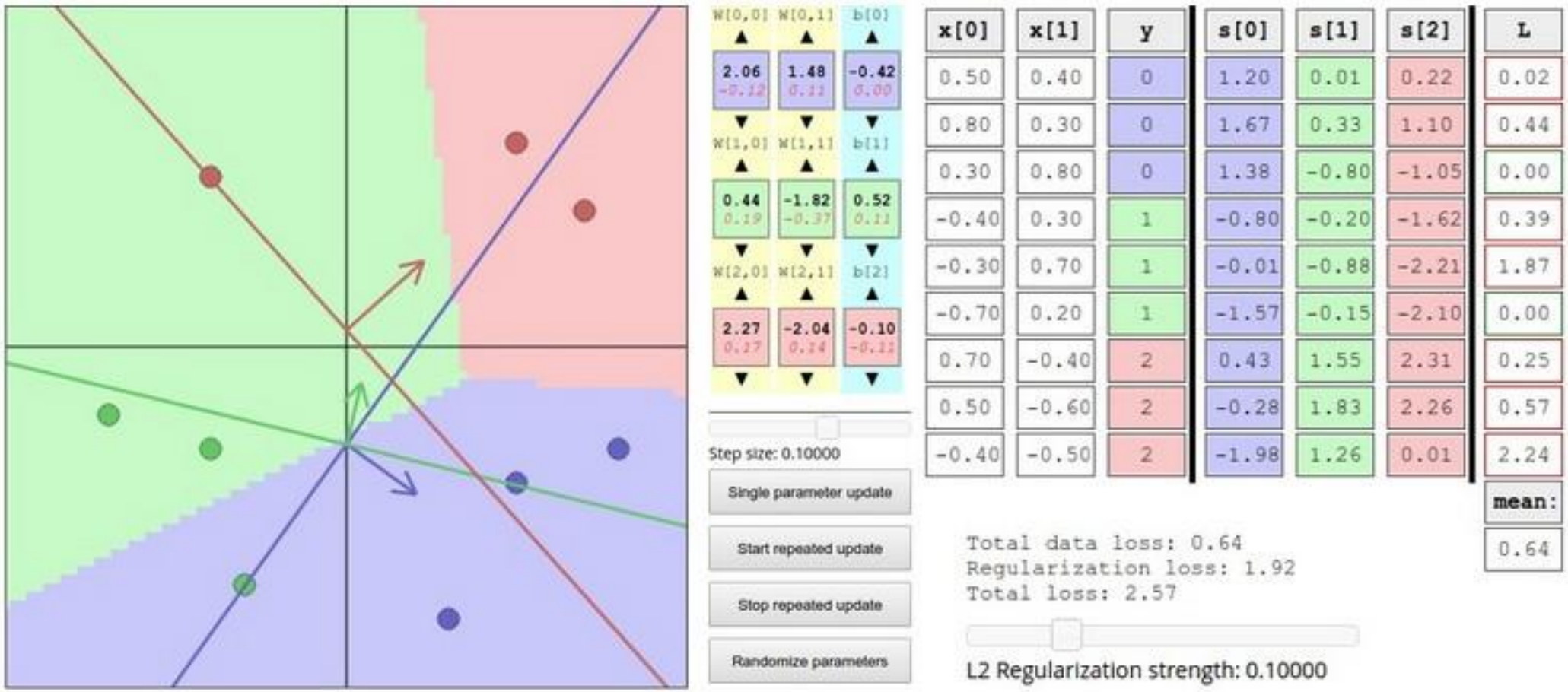
$$L(W) = \mathbb{E}_{(x,y)\sim p_{data}}[L(x, y, W)] + \lambda R(W)$$
$$\approx \frac{1}{N}\sum_{i=1}^{N} L(x_i, y_i, W) + \lambda R(W)$$

Think of loss as an expectation over the full **data distribution** p_{data}

Approximate expectation via sampling

$$\nabla_W L(W) = \nabla_W \mathbb{E}_{(x,y)\sim p_{data}}[L(x, y, W)] + \lambda \nabla_W R(W)$$
$$\approx \sum_{i=1}^{N} \nabla_w L_W(x_i, y_i, W) + \nabla_w R(W)$$

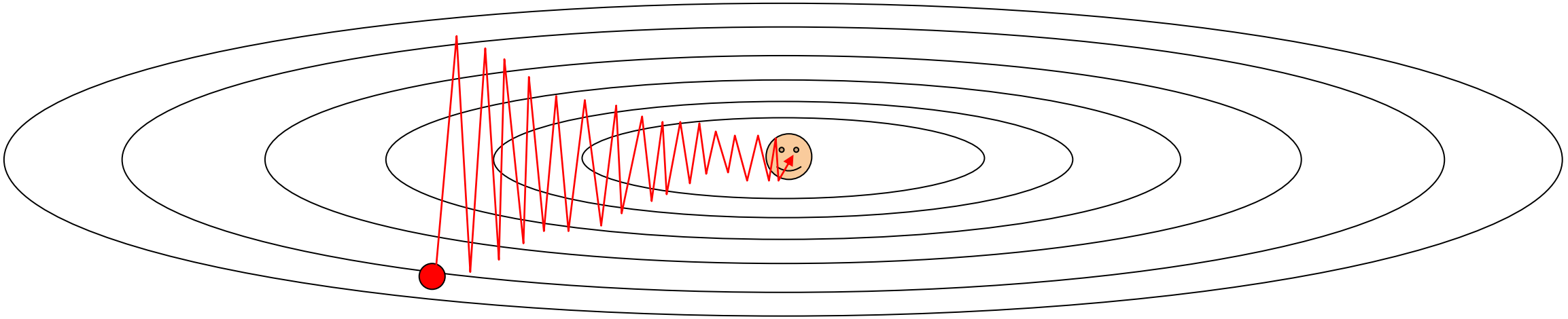
Interactive Web Demo



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

Problems 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

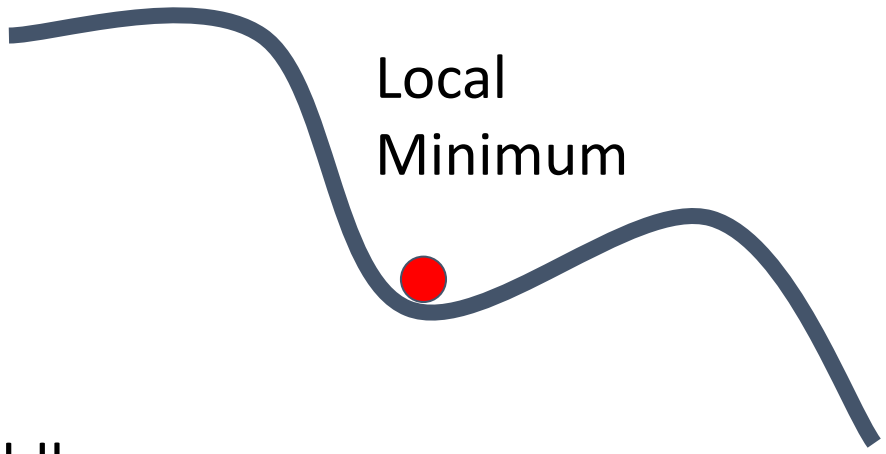


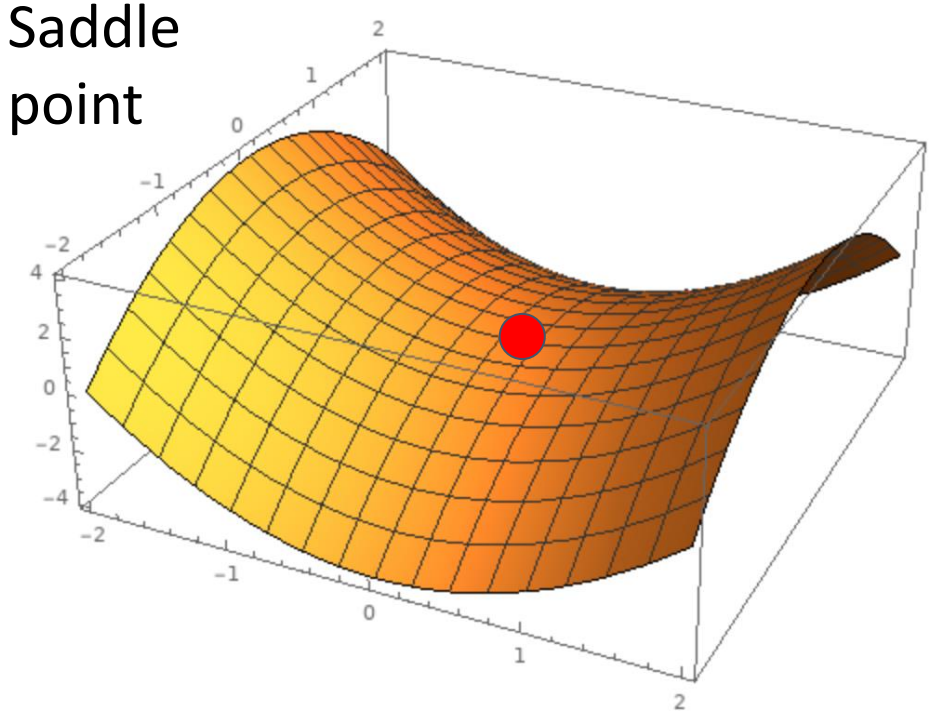
Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Problems with SGD

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

Zero gradient, gradient descent gets stuck



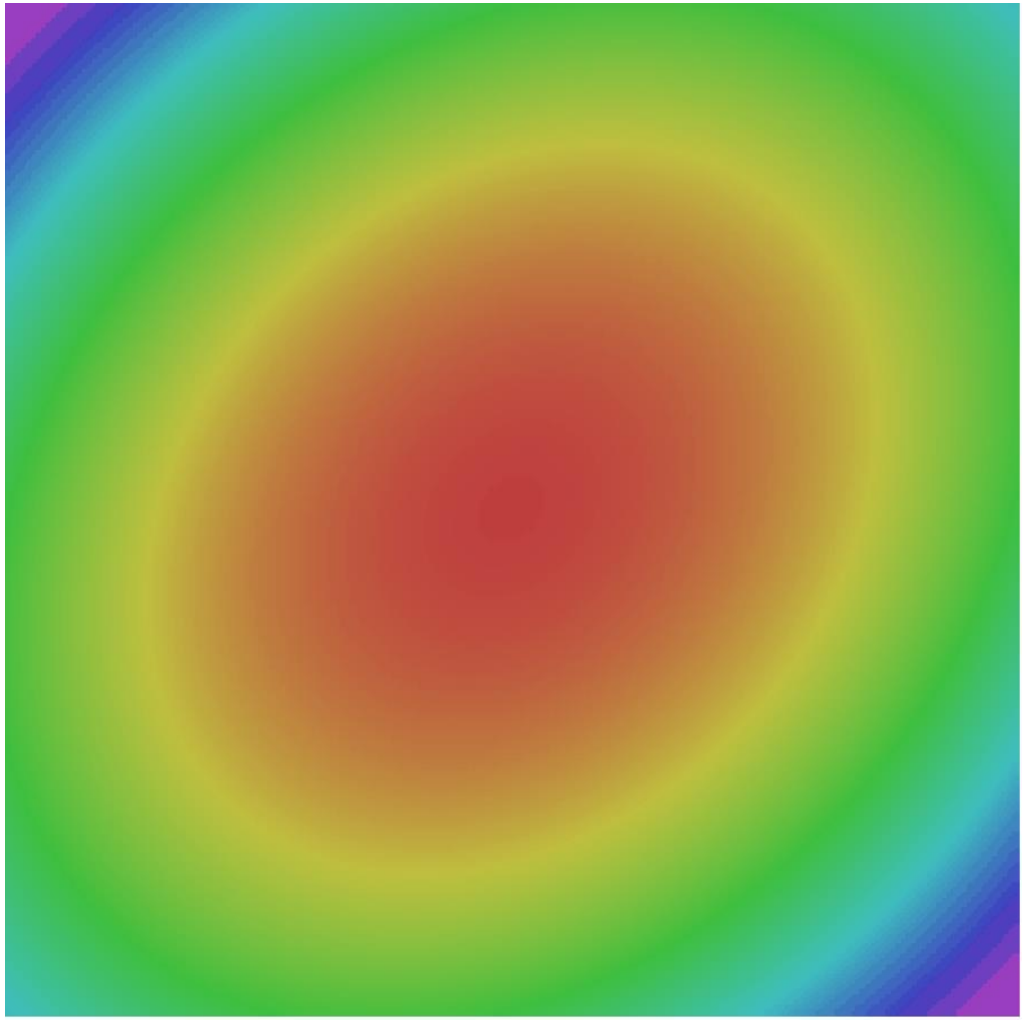


Problems with SGD

Our gradients come from minibatches
so they can be noisy!

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

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



SGD

SGD

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

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD + Momentum

SGD

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

```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD+Momentum

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

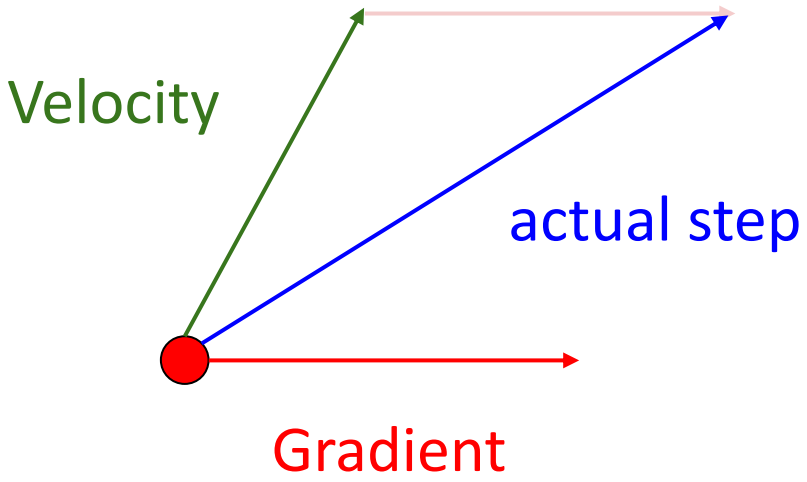
```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

- 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

Momentum update:



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

SGD+Momentum

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

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

- 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

SGD+Momentum

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

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v - learning_rate * dw
  w += v
```

SGD+Momentum

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

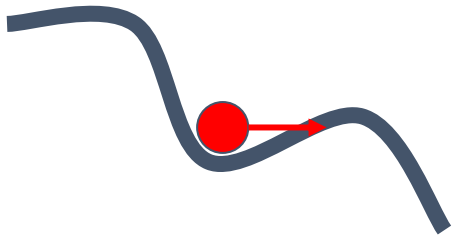
```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

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

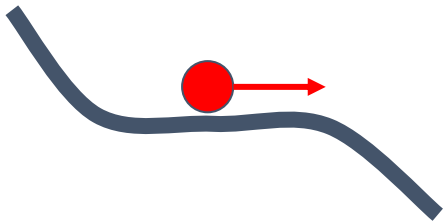
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

SGD + Momentum

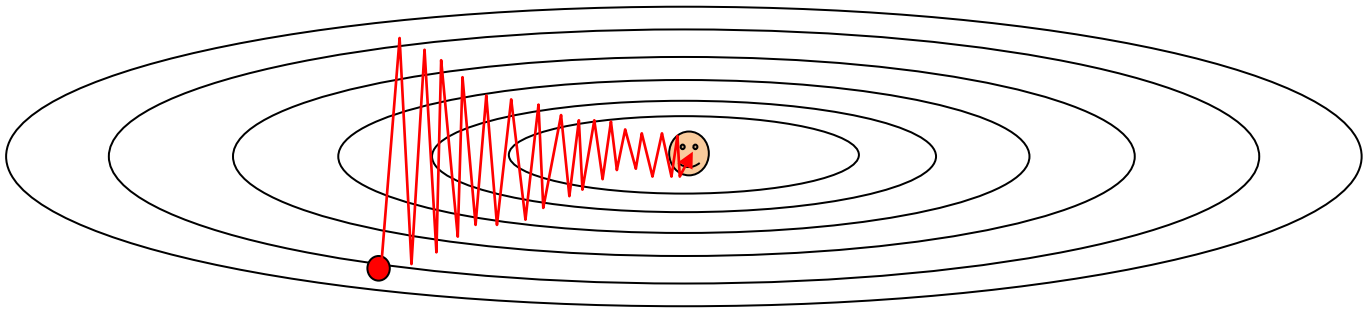
Local Minima



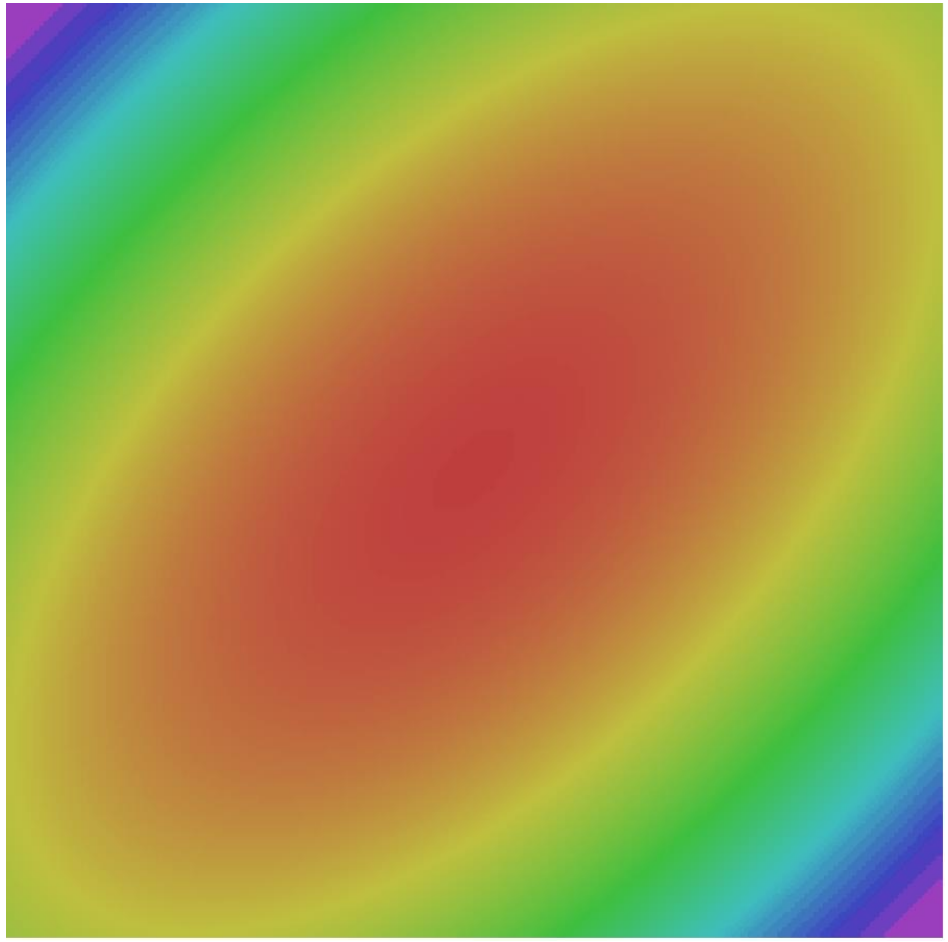
Saddle points



Poor Conditioning



Gradient Noise

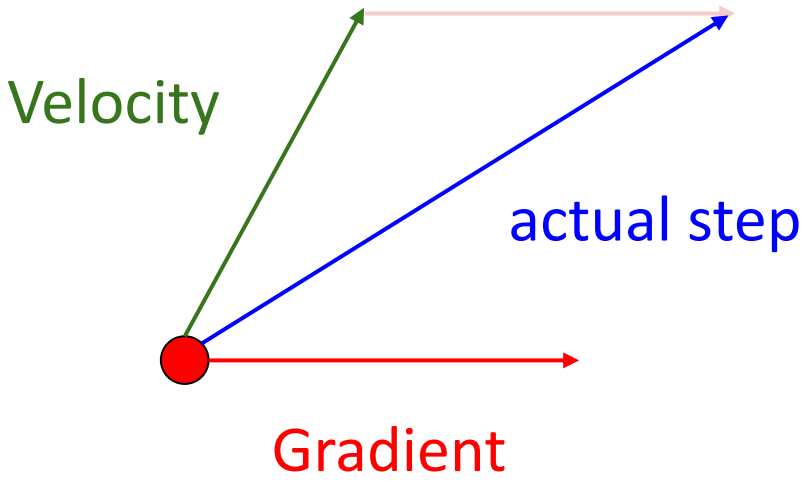


SGD SGD+Momentum

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

SGD + Momentum

Momentum update:

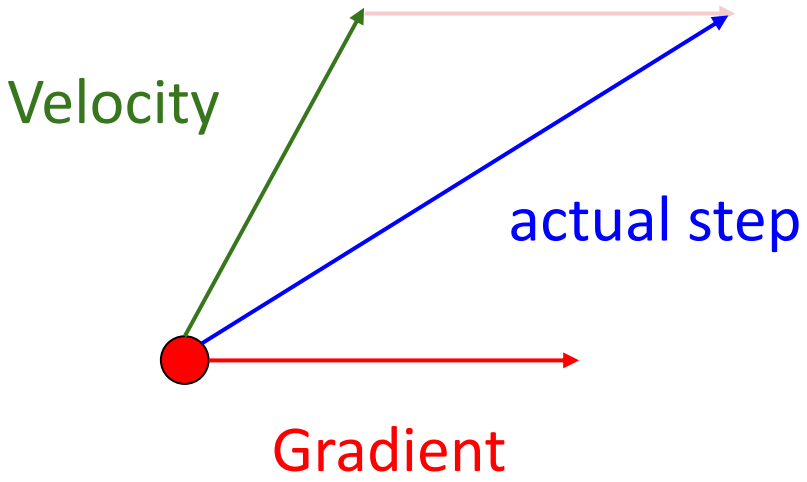


Combine gradient at current point with velocity to get step used to update weights

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

Nesterov Momentum

Momentum update:



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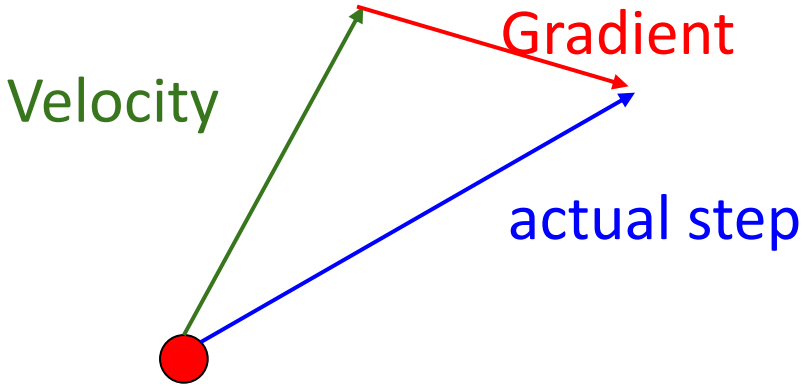
Nesterov Momentum



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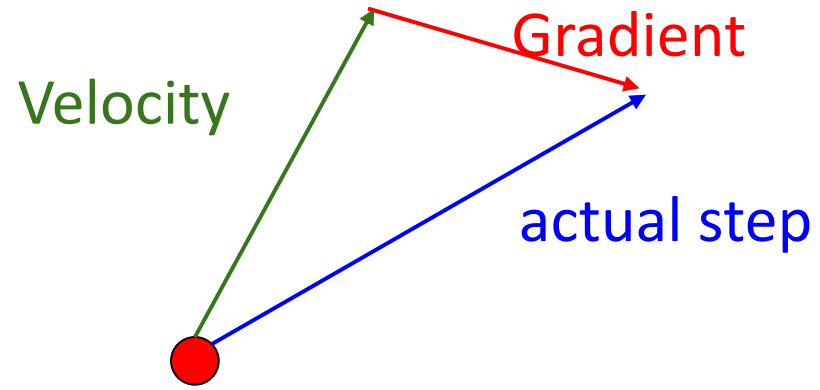
Nesterov Momentum

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

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



"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

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

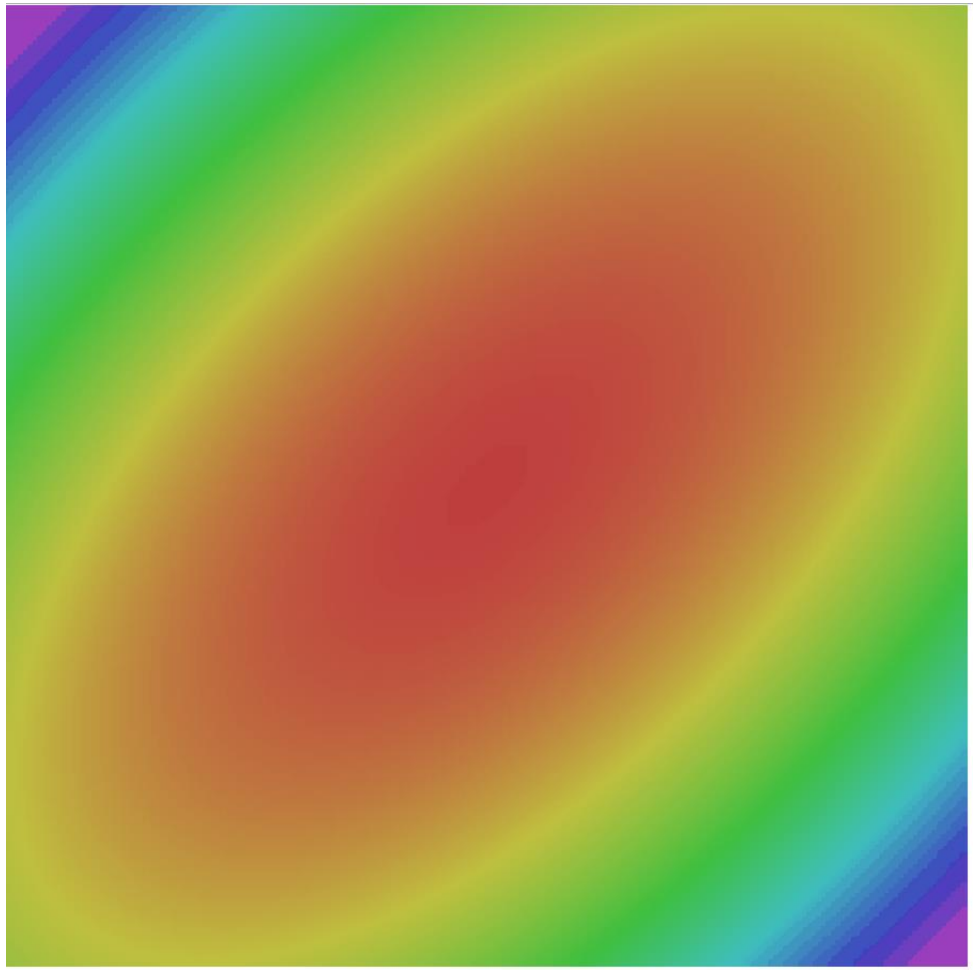
Annoying, usually we want update in terms of $x_t, \nabla f(x_t)$

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

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

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  old_v = v
  v = rho * v - learning_rate * dw
  w -= rho * old_v - (1 + rho) * v
```

Nesterov Momentum



SGD

SGD+Momentum

Nesterov

AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

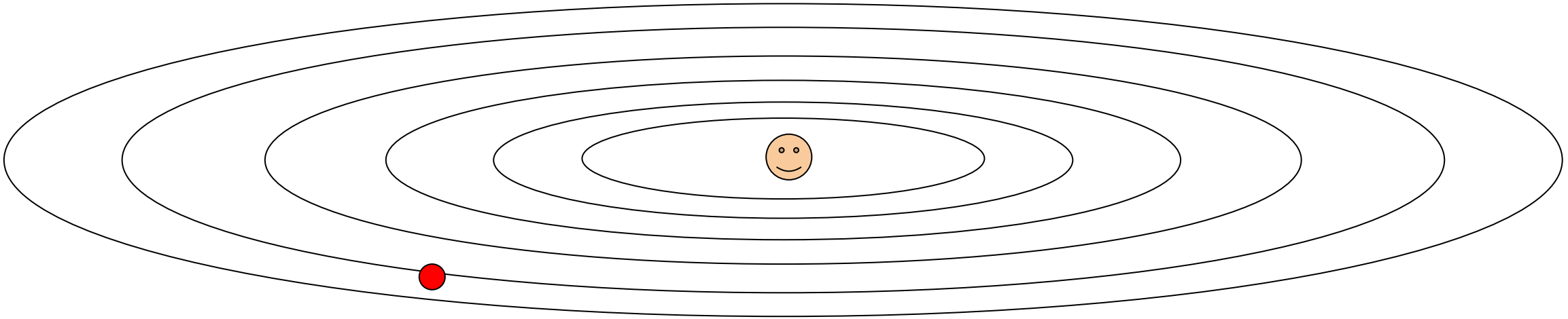
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

"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
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```



Q: What happens with AdaGrad?

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

RMSProp: "Leaky Adagrad"

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared += dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

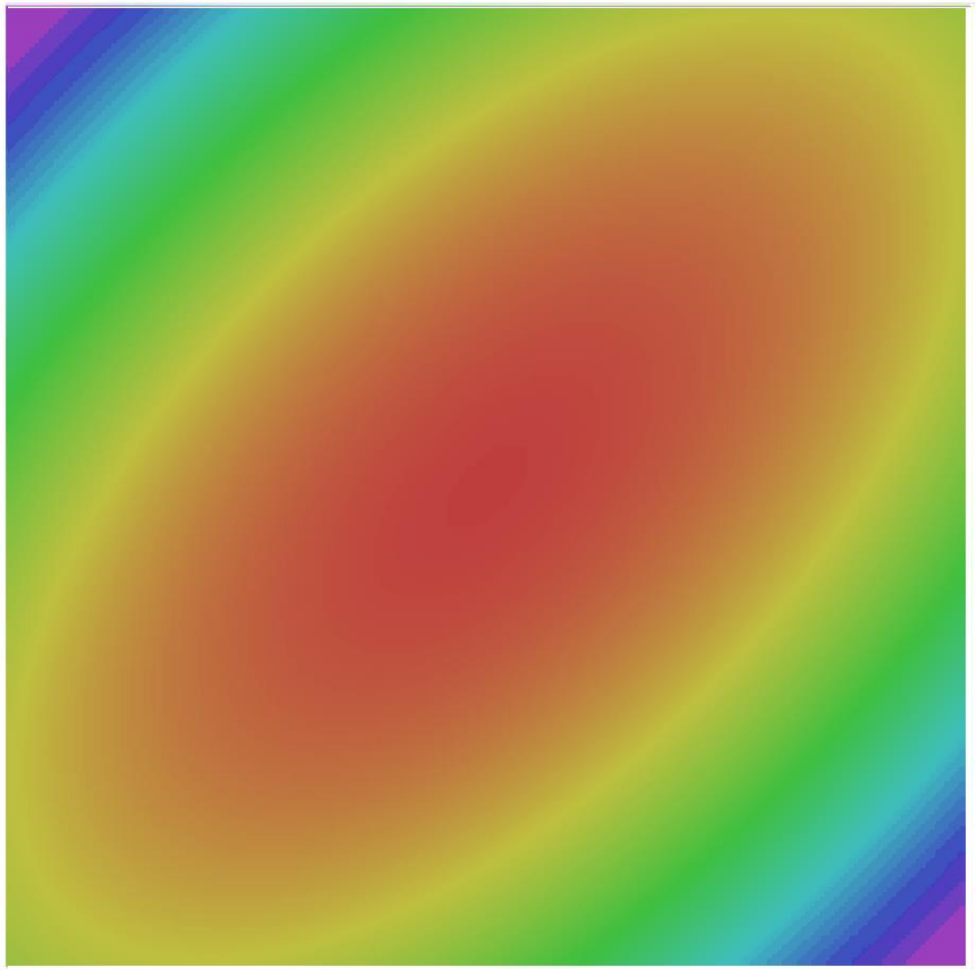
AdaGrad

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

RMSProp

Tieleman and Hinton, 2012

RMSProp



SGD

SGD+Momentum

RMSProp

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

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

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

SGD+Momentum

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

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

AdaGrad / RMSProp

```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

RMSProp

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

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

AdaGrad / RMSProp

Bias correction

Q: What happens at t=0?
(Assume beta2 = 0.999)

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

Adam (almost): RMSProp + Momentum

```
moment1 = 0
moment2 = 0
for t in range(1, num_steps + 1):  # Start at t = 1
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  moment1_unbias = moment1 / (1 - beta1 ** t)
  moment2_unbias = moment2 / (1 - beta2 ** t)
  w -= learning_rate * moment1_unbias / (moment2_unbias.sqrt() + 1e-7)
```

Momentum

AdaGrad / RMSProp

Bias correction

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 (almost): RMSProp + Momentum

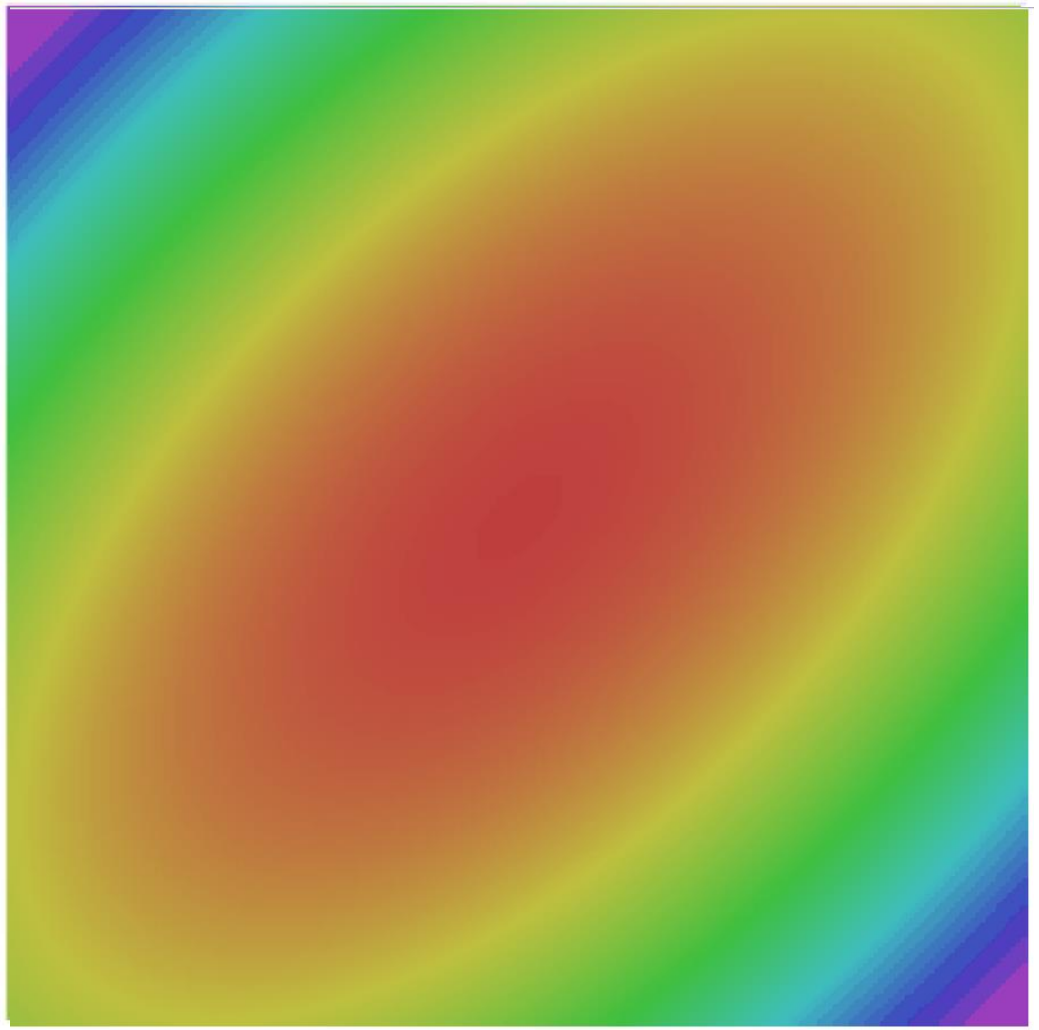
```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  moment1_unbias = moment1 / (1 - beta1 ** t)
  moment2_unbias = moment2 / (1 - beta2 ** t)
  w -= learning_rate * moment1_unbias / (moment2_unbias.sqrt() + 1e-7)
```

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, 5e-4, 1e-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

Optimization Algorithm Comparison

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

L2 Regularization vs Weight Decay

Optimization Algorithm

$$L(w) = L_{data}(w) + L_{reg}(w)$$
$$g_t = \nabla L(w_t)$$
$$s_t = optimizer(g_t)$$
$$w_{t+1} = w_t - \alpha s_t$$

L2 Regularization

$$L(w) = L_{data}(w) + \boldsymbol{\lambda |w|^2}$$
$$g_t = \nabla L(w_t) = \nabla L_{data}(w_t) + \boldsymbol{2\lambda w_t}$$
$$s_t = optimizer(g_t)$$
$$w_{t+1} = w_t - \alpha s_t$$

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

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

Weight Decay

$$L(w) = L_{data}(w)$$
$$g_t = \nabla L_{data}(w_t)$$
$$s_t = optimizer(g_t) + \boldsymbol{2\lambda w_t}$$
$$w_{t+1} = w_t - \alpha s_t$$

Loshchilov and Hutter, "Decoupled Weight Decay Regularization", ICLR 2019

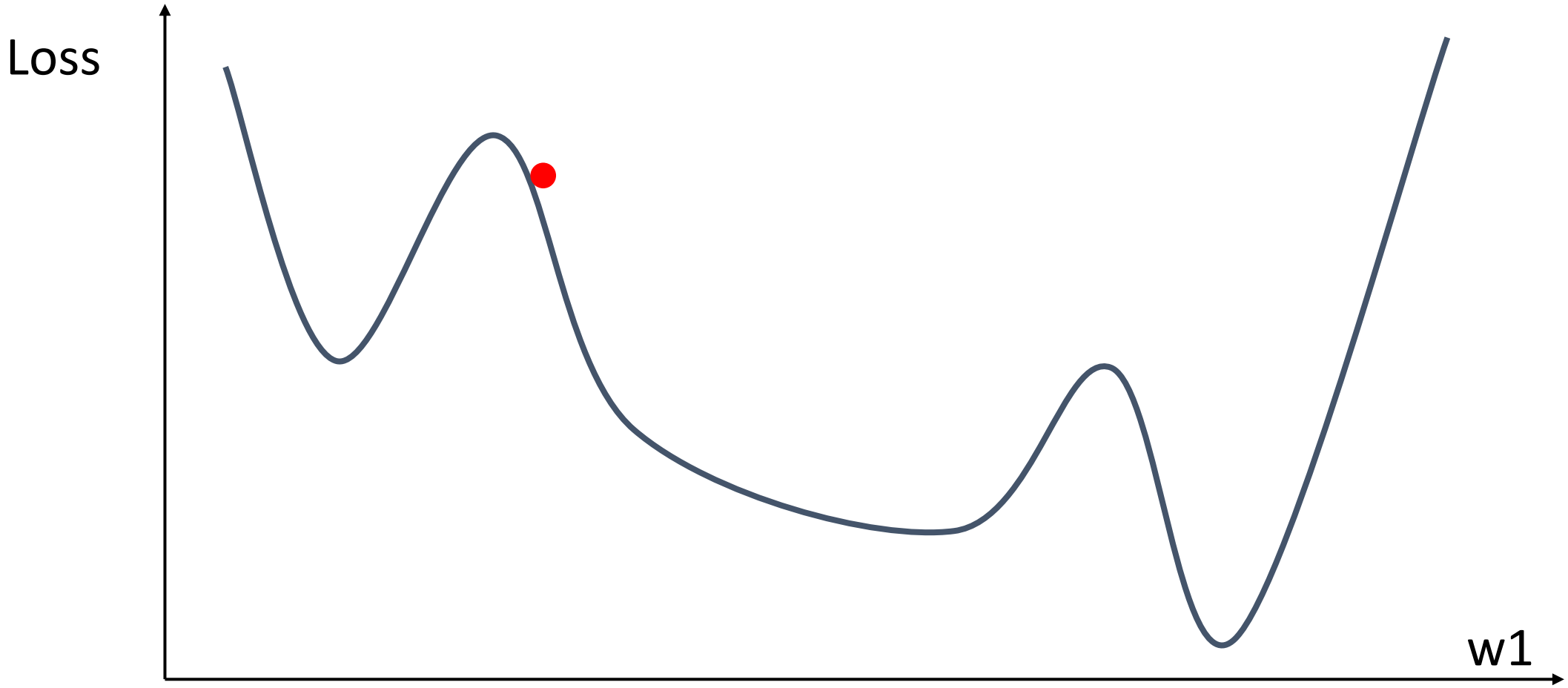
AdamW: Decoupled Weight Decay

Algorithm 2 Adam with L_2 regularization and Adam with decoupled weight decay (AdamW)

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

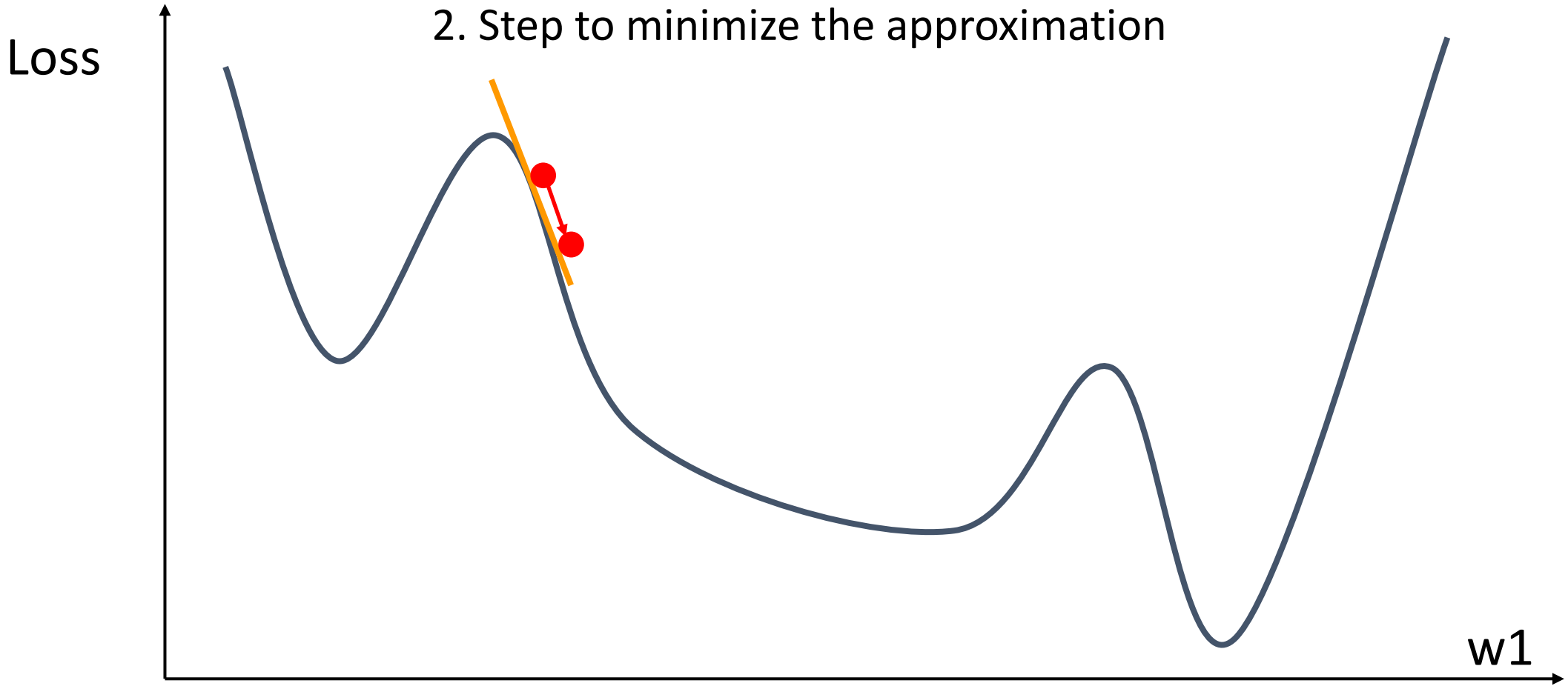
Loshchilov and Hutter, "Decoupled Weight Decay Regularization", ICLR 2019

So far: First-Order Optimization



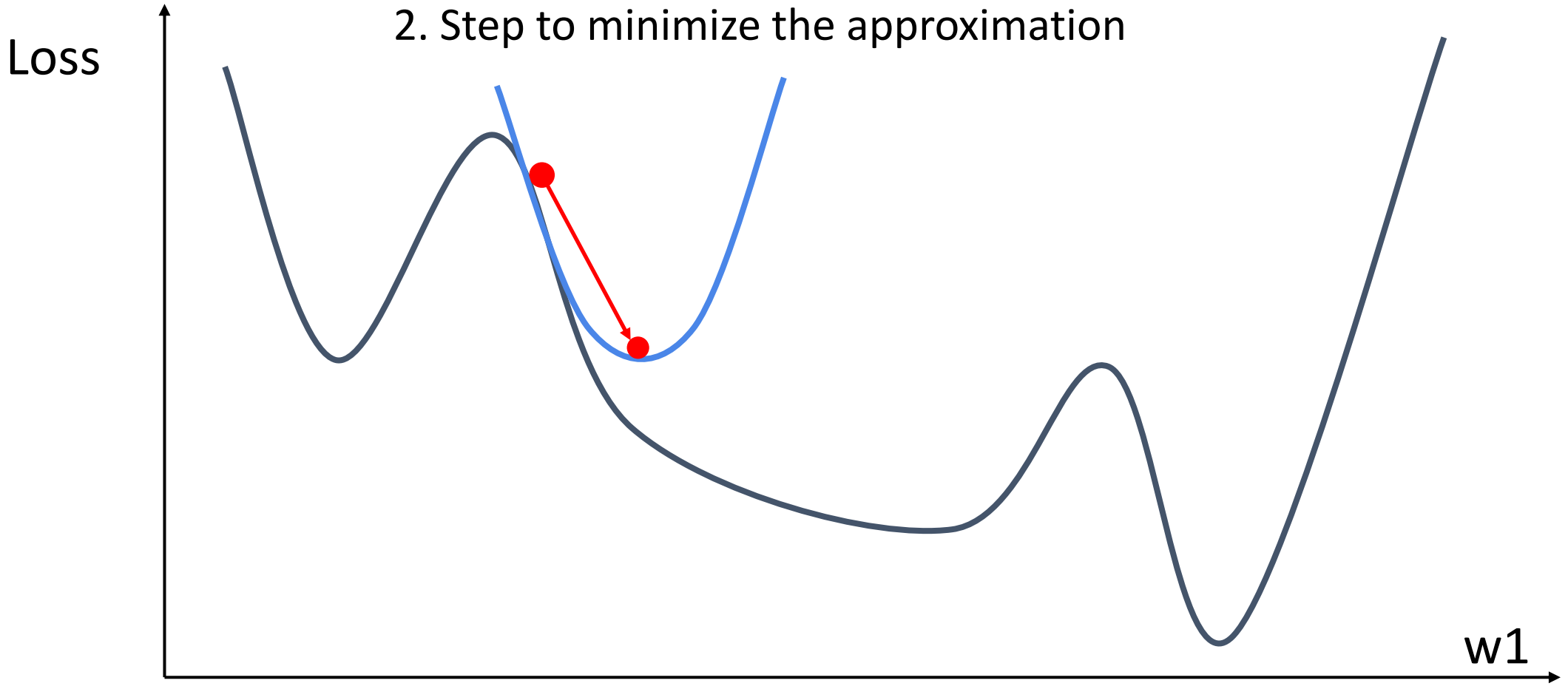
So far: **First-Order** Optimization

1. Use gradient to make linear approximation
2. Step to minimize the approximation



Second-Order Optimization

1. Use gradient and Hessian to make quadratic approximation
2. Step to minimize the approximation



Second-Order Optimization

1. Use gradient and Hessian to make quadratic approximation
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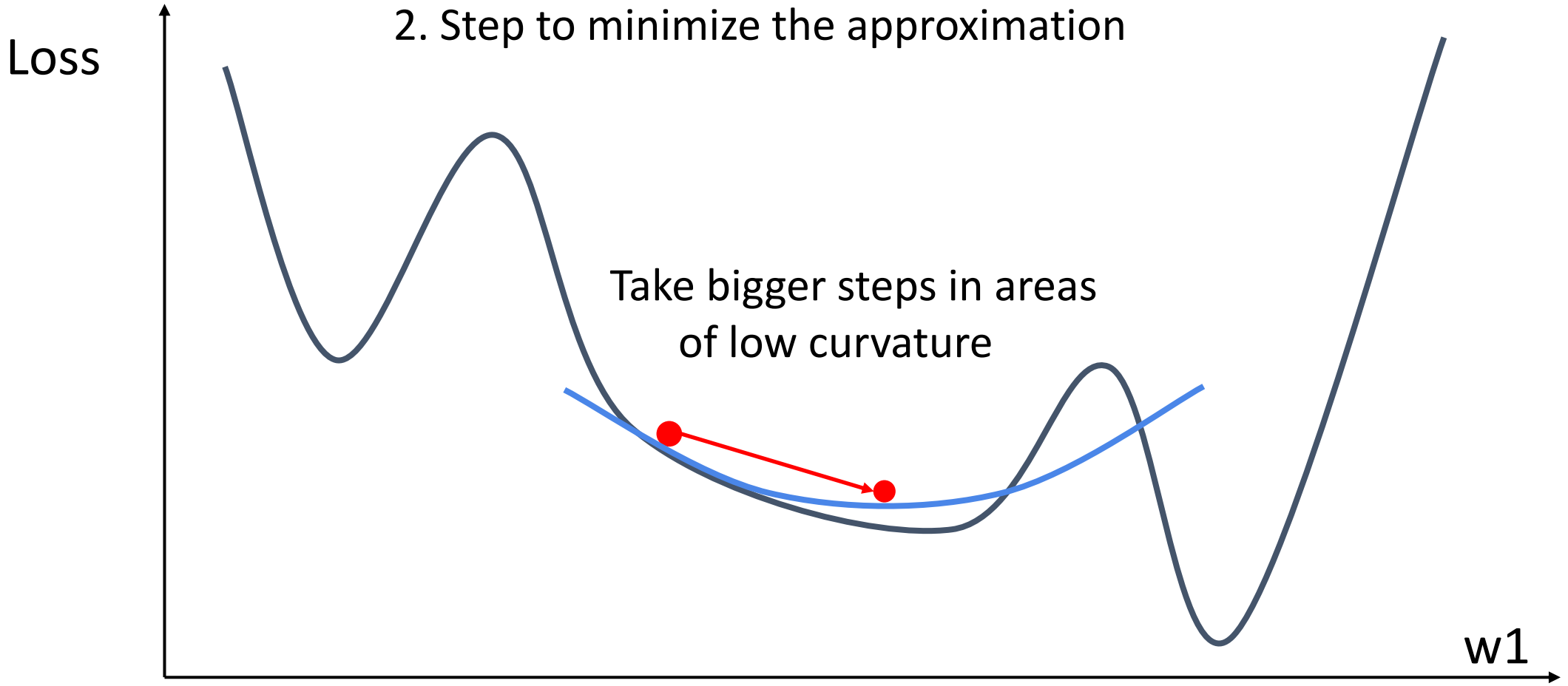


Second-Order Optimization

Second-Order Taylor Expansion:

$$L(w) \approx L(w_0) + (w - w_0)^\intercal \nabla_w L(w_0) + \frac{1}{2}(w - w_0)^\intercal \mathbf{H}_w L(w_0)(w - w_0)$$

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

$$w^* = w_0 - \mathbf{H}_w L(w_0)^{-1} \nabla_w L(w_0)$$

Q: Why is this impractical?

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

Second-Order Optimization

$$w^* = w_0 - \mathbf{H}_w L(w_0)^{-1} \nabla_w L(w_0)$$

- 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 but only a few vectors.

Second-Order Optimization: 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:

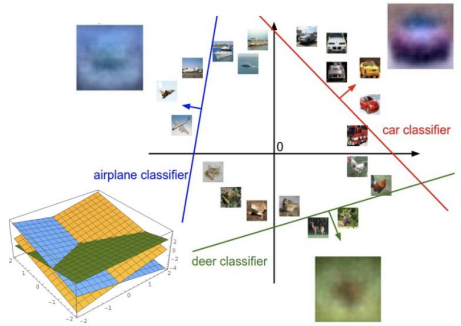
- **Adam** is a good default choice in many cases
  SGD+Momentum can outperform Adam but may require more tuning

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

Summary

1. Use **Linear Models** for image classification problems
2. Use **Loss Functions** to express preferences over different choices of weights
3. Use **Regularization** to prevent overfitting to training data
4. Use **Stochastic Gradient Descent** to minimize our loss functions and train the model

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

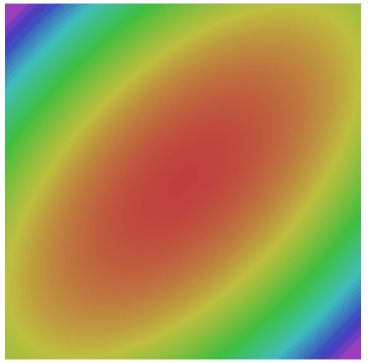


$$L_i = -\log\left(\frac{e^{sy_i}}{\sum_j e^{s_j}}\right)$$ Softmax

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

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

```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```



Next: Neural Networks