Lecture 4: Regularization + Optimization

Reminder: Assignment 1

Was due on Friday!

Assignment 2

- Released last night
- Use SGD to train linear classifiers and fully-connected networks
- After today, can do linear classifiers section
- After Wednesday, can do fully-connected networks
- If you have a hard time computing derivatives, wait for next Monday's lecture on backprop
- Due Friday September 25, 11:59pm EDT

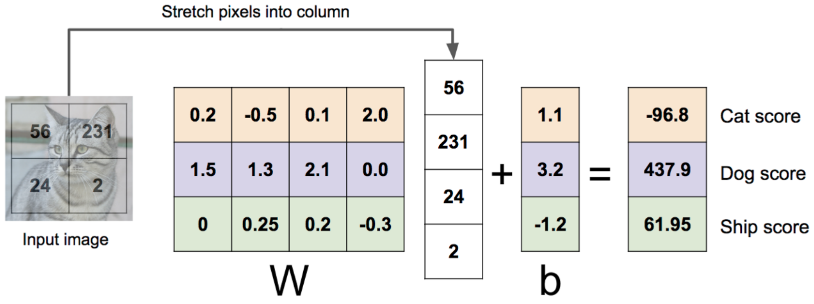
Questions During Lecture

- Lecturing + watching chat is hard!
- I won't actively watch chat constantly – instead I'll go back and address questions on chat when I reach a logical pause point

Last Time: Linear Classifiers

Algebraic Viewpoint

f(x,W) = Wx

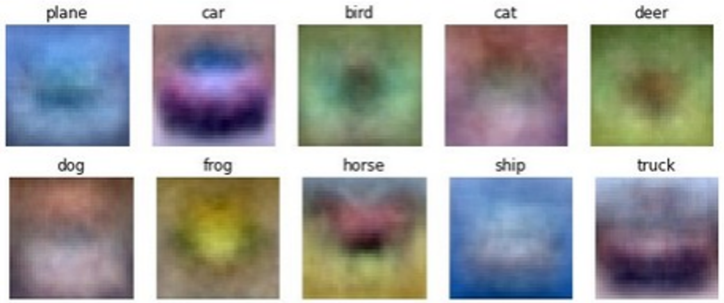


Stretch pixels into column

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

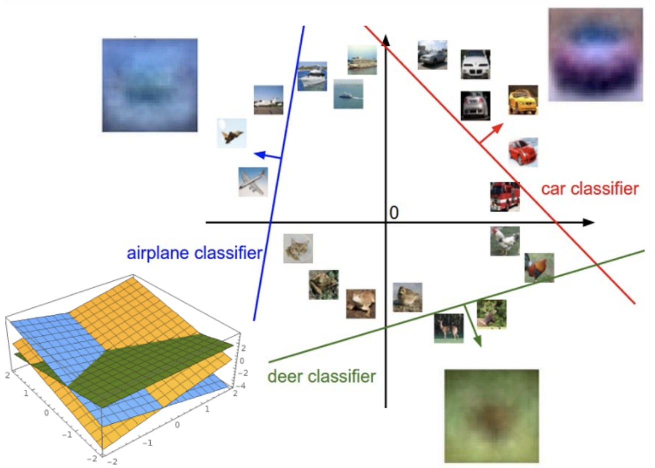
Visual Viewpoint

One template
per class



Geometric Viewpoint

Hyperplanes
cutting up space



Last Time: Loss Functions quantify preferences

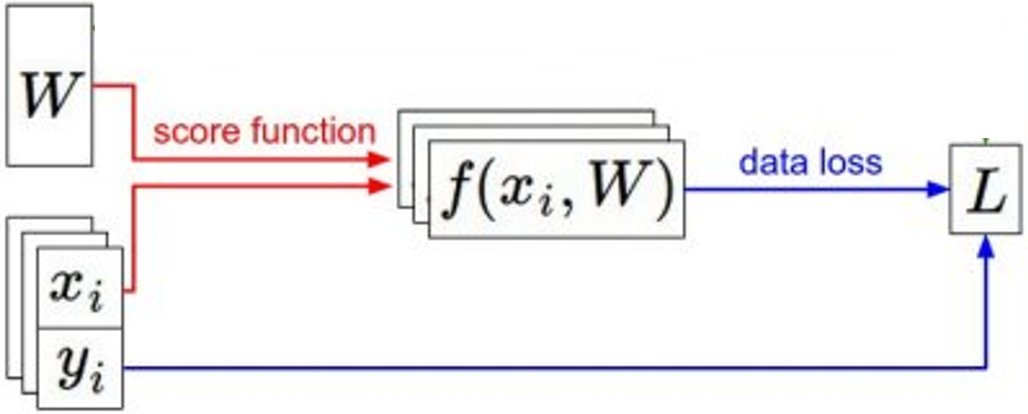
- We have some dataset of (x, y)
- We have a **score function:**
- We have a **loss function**:

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

Linear classifier

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

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



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

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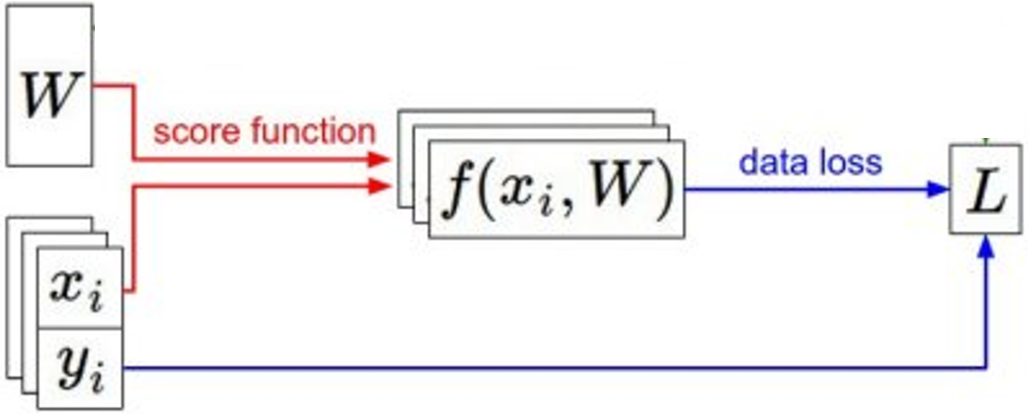

Overfitting

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

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

$$s_i = w_i x + b_i$$

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

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

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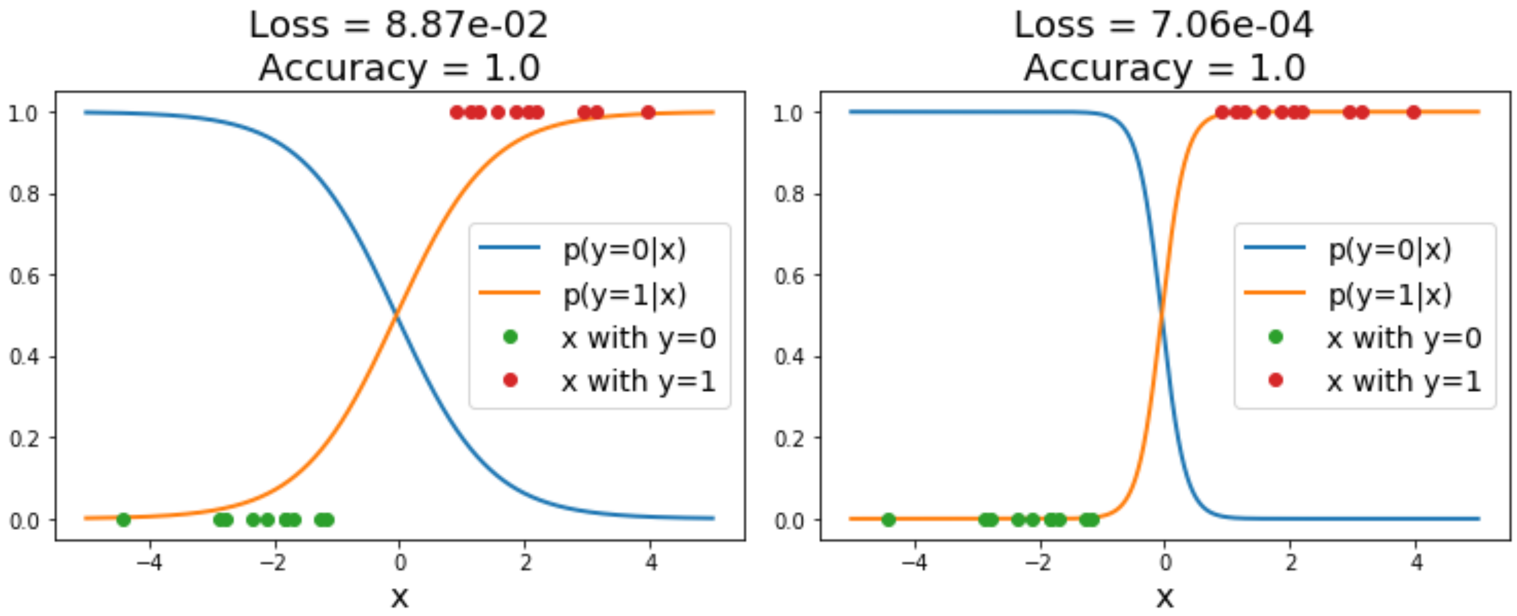

Both models have perfect accuracy on train data!

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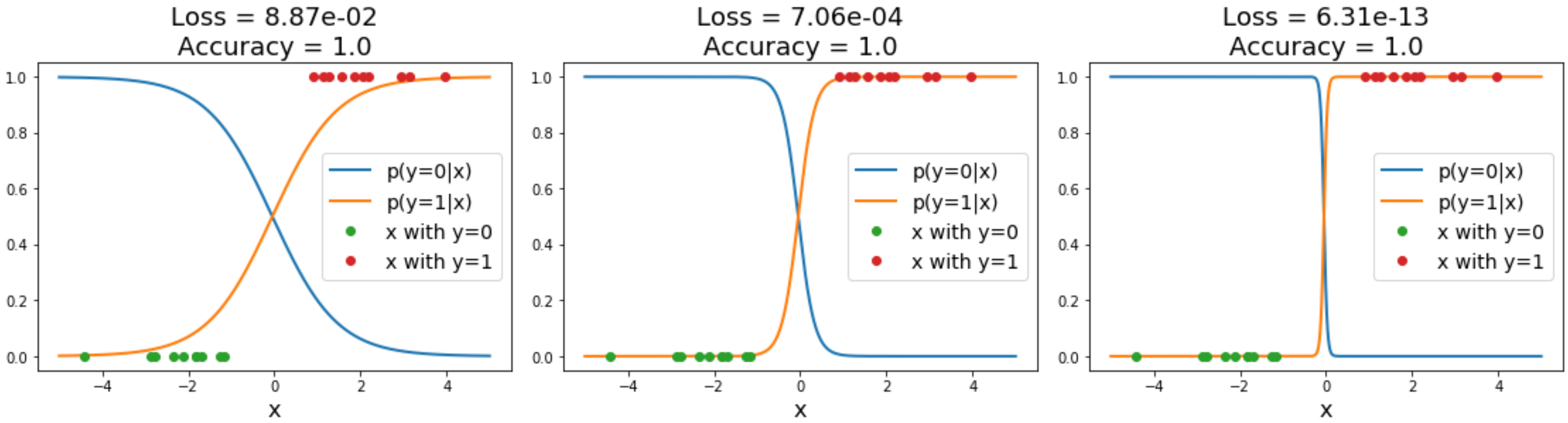

Loss = 8.87e-02
Accuracy = 1.0

Loss = 7.06e-04
Accuracy = 1.0

Loss = 6.31e-13
Accuracy = 1.0

Both models have perfect accuracy on train data!

Low loss, but unnatural "cliff" between training points

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

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

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

Regularization: Beyond Training Error

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λ is a hyperparameter giving regularization strength

Simple examples

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

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

Regularization: Beyond Training Error

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

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

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

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

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

Regularization: Prefer Simpler Models

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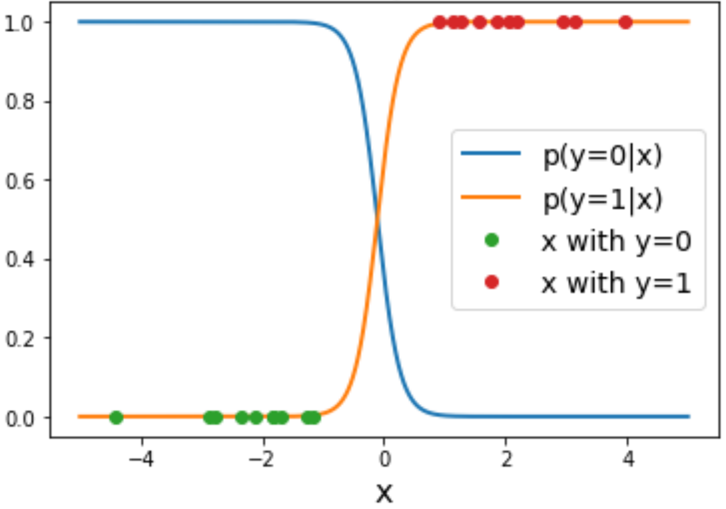
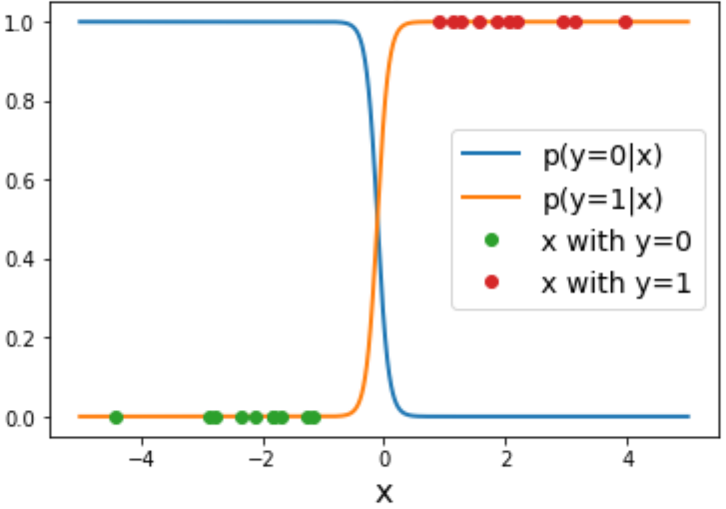
Regularization term causes loss to **increase** for model with sharp cliff

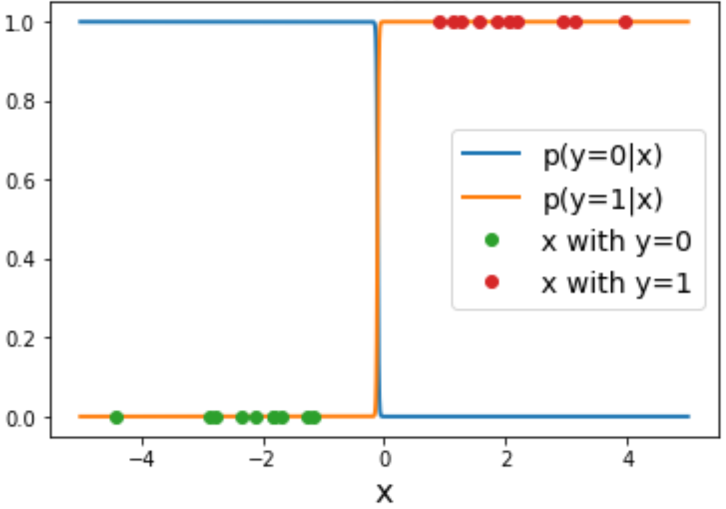
Loss = 2.05e-03
Accuracy = 1.0



Loss = 5.96e-03
Accuracy = 1.0



Loss = 5.95e-01
Accuracy = 1.0



Regularization: Expressing Preferences

L2 Regularization

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

$$x = [1, 1, 1, 1]$$
$$w_1 = [1, 0, 0, 0]$$
$$w_2 = [0.25, 0.25, 0.25, 0.25]$$

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

Same predictions, so data loss will always be the same

Regularization: Expressing Preferences

L2 Regularization

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

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

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

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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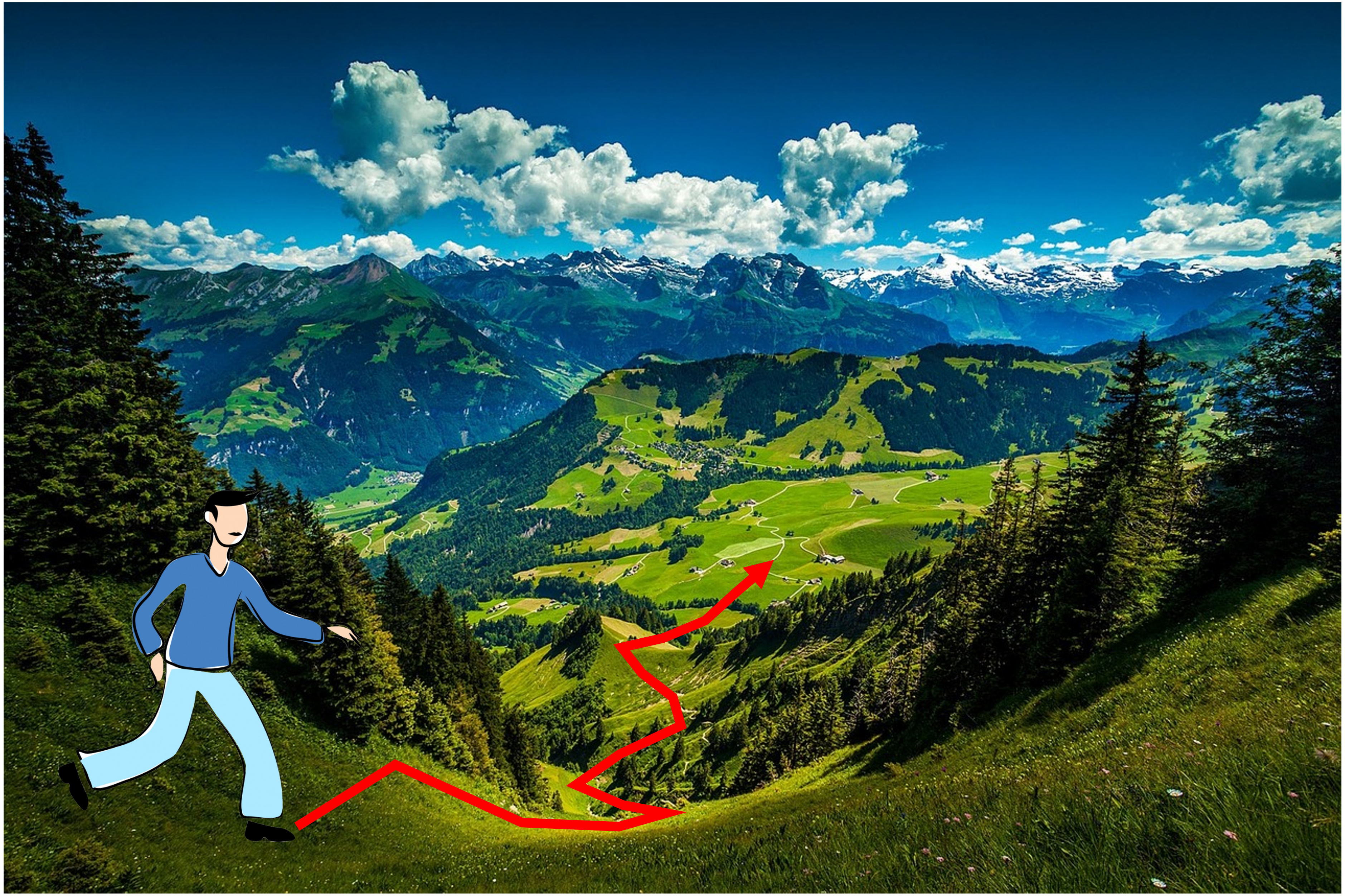

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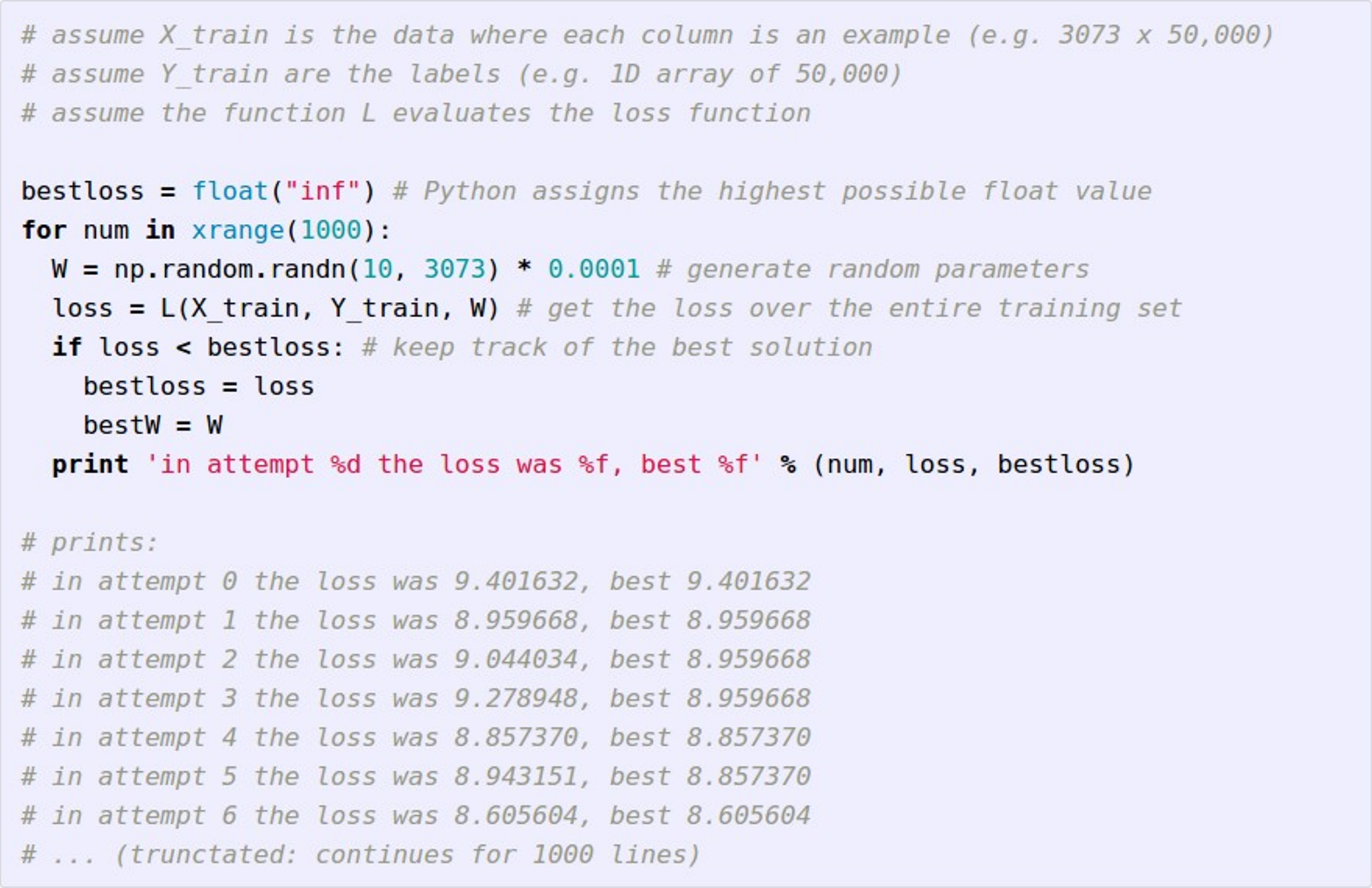
Idea #1: **Random Search** (bad idea!)



```
# 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)
```

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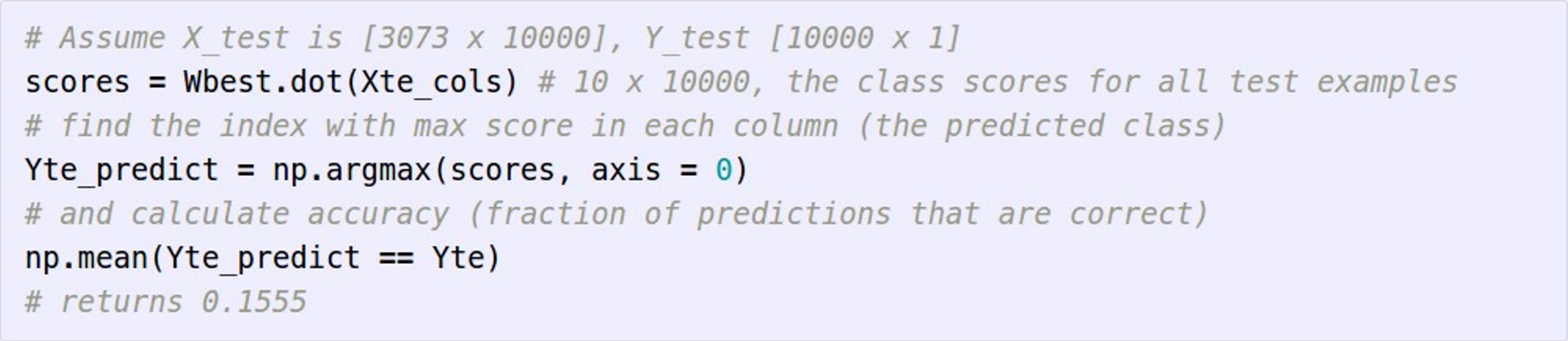

```
# Assume X_test is [3073 x 10000], Y_test [10000 x 1]
scores = Wbest.dot(Xte_cols) # 10 x 10000, the class scores for all test examples
# find the index with max score in each column (the predicted class)
Yte_predict = np.argmax(scores, axis = 0)
# and calculate accuracy (fraction of predictions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

15.5% accuracy! not bad!

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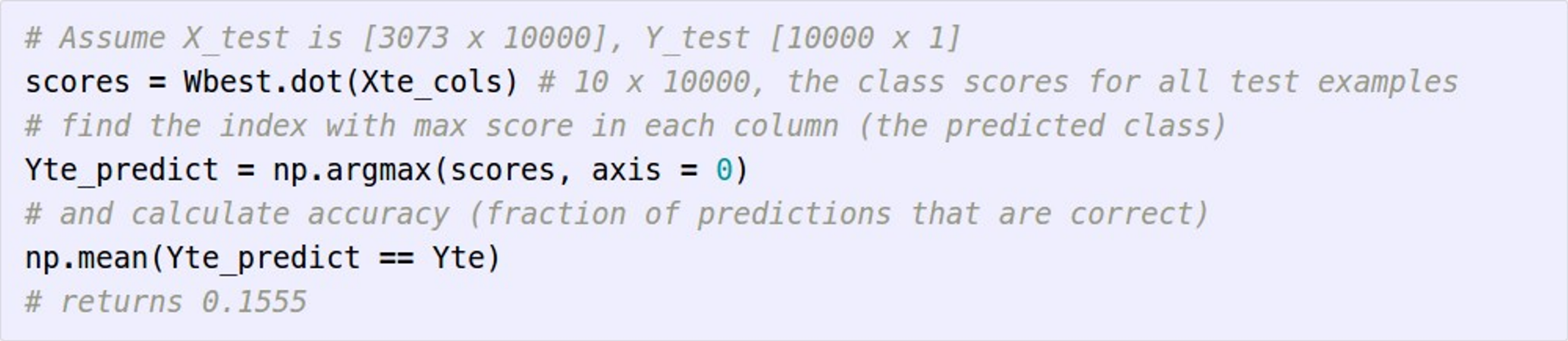

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```

15.5% accuracy! not bad!
(SOTA is ~95%)

Idea #2: **Follow the slope**

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

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

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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

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:

[?,
?,
?,
?,
?,
?,
?,
?,
?,…]

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

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

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 dL/dW:

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

Numeric Gradient:

- Slow: O(#dimensions)
- Approximate

Loss is a function of W

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

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

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

Want $\nabla_W L$

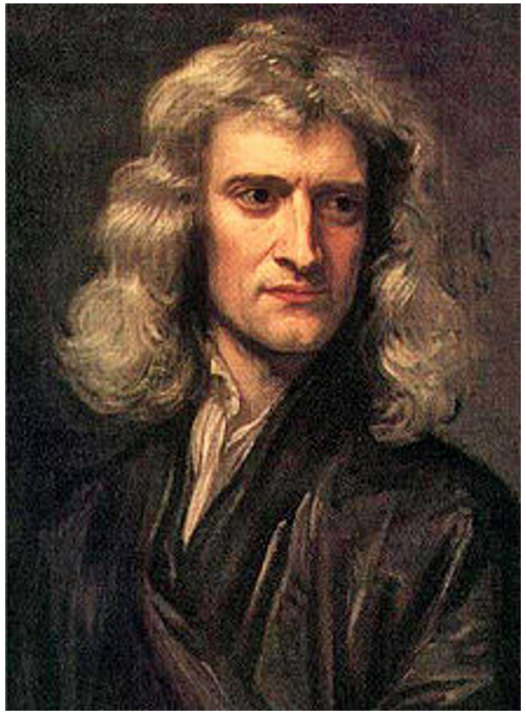
Loss is a function of W: **Analytic Gradient**

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

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

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

Want $\nabla_W L$



This image is in the public domain

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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.**

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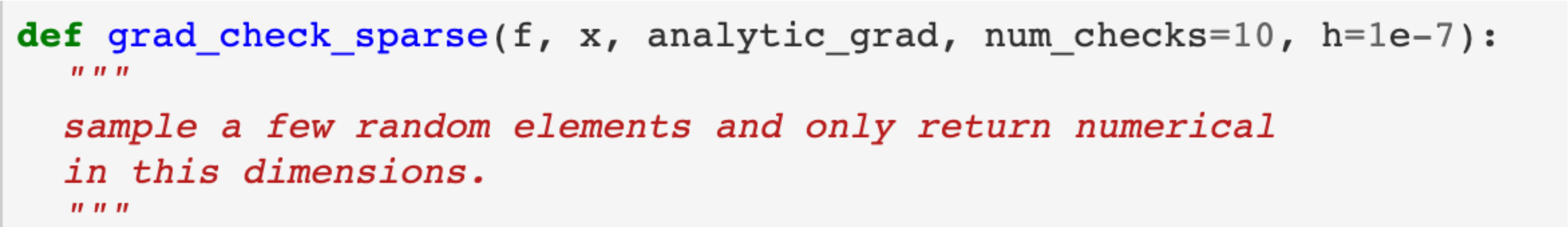
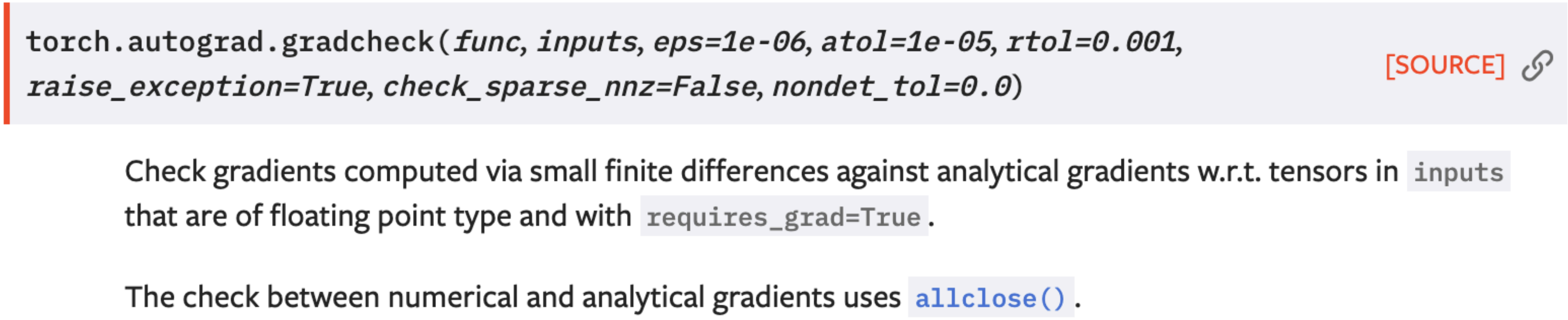


```python
def grad_check_sparse(f, x, analytic_grad, num_checks=10, h=1e-7):
  """
  sample a few random elements and only return numerical
  in this dimensions.
  """
```

Computing Gradients

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



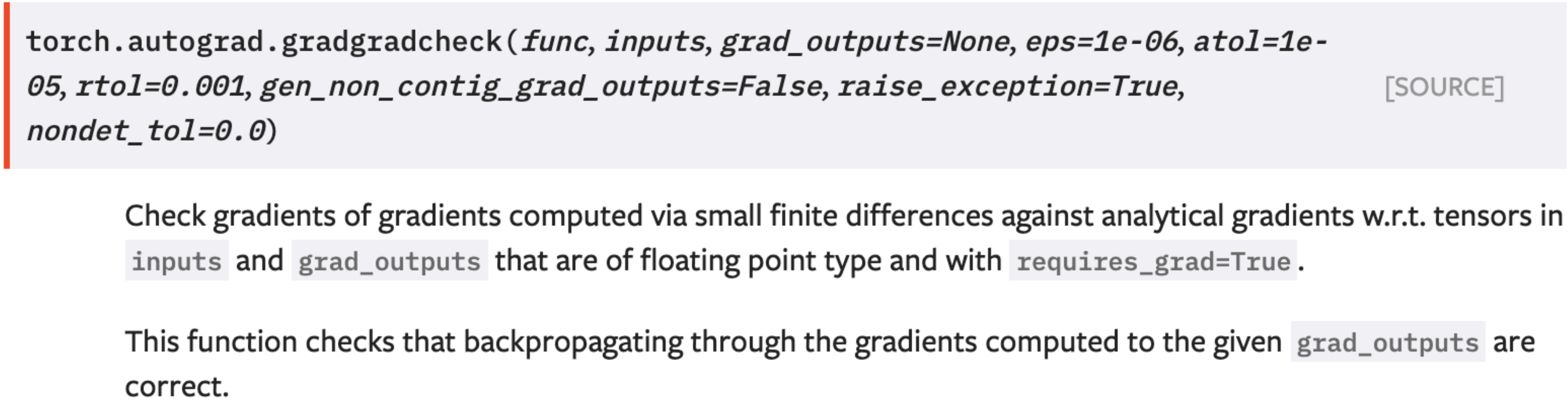
```
torch.autograd.gradcheck(func, inputs, eps=1e-06, atol=1e-05, rtol=0.001,
raise_exception=True, check_sparse_nnz=False, nondet_tol=0.0)
```

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



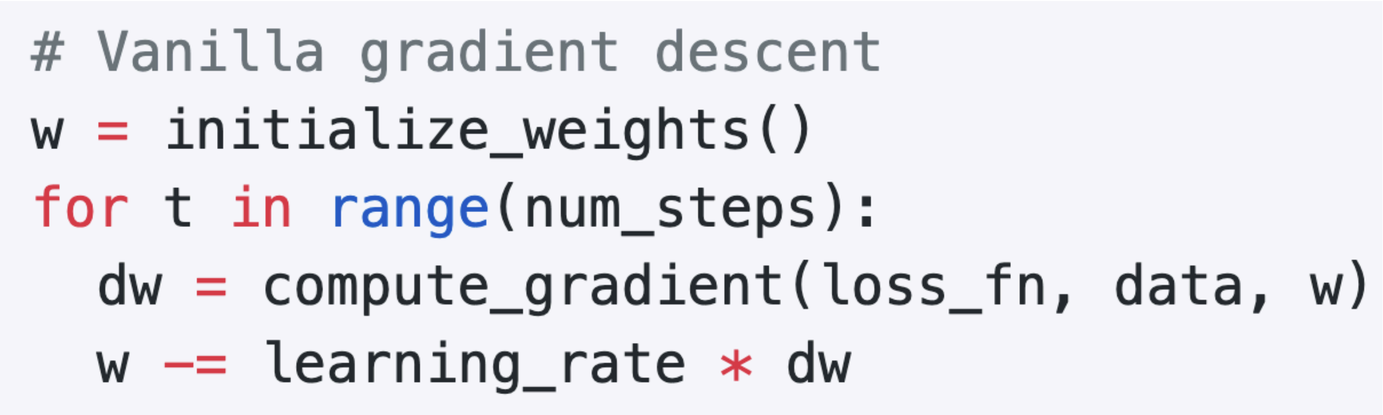
```
torch.autograd.gradgradcheck(func, inputs, grad_outputs=None, eps=1e-06, atol=1e-
05, rtol=0.001, gen_non_contig_grad_outputs=False, raise_exception=True,          [SOURCE]
nondet_tol=0.0)
```

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)



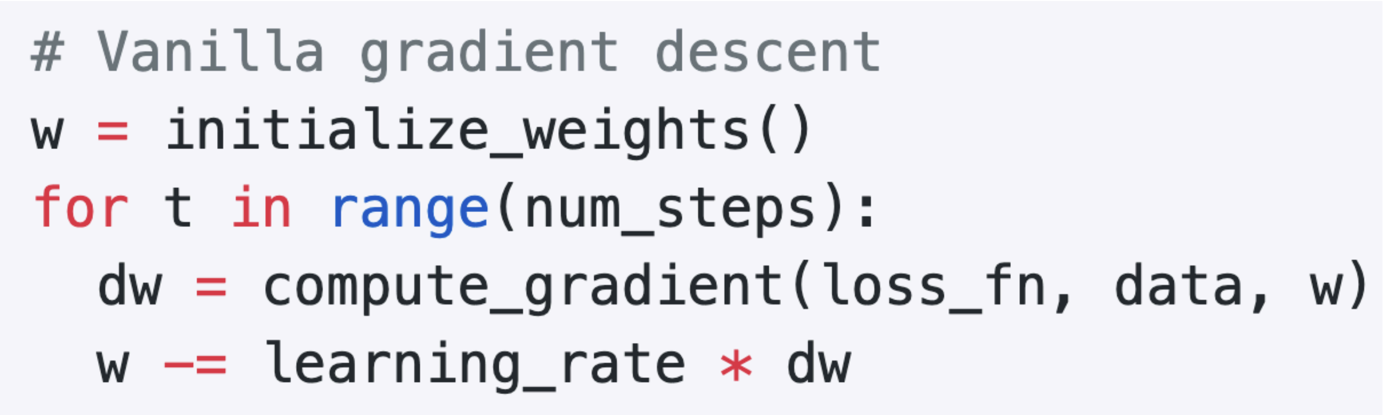
```
# Vanilla gradient descent
w = initialize_weights()
for t in range(num_steps):
  dw = compute_gradient(loss_fn, data, w)
  w -= learning_rate * dw
```

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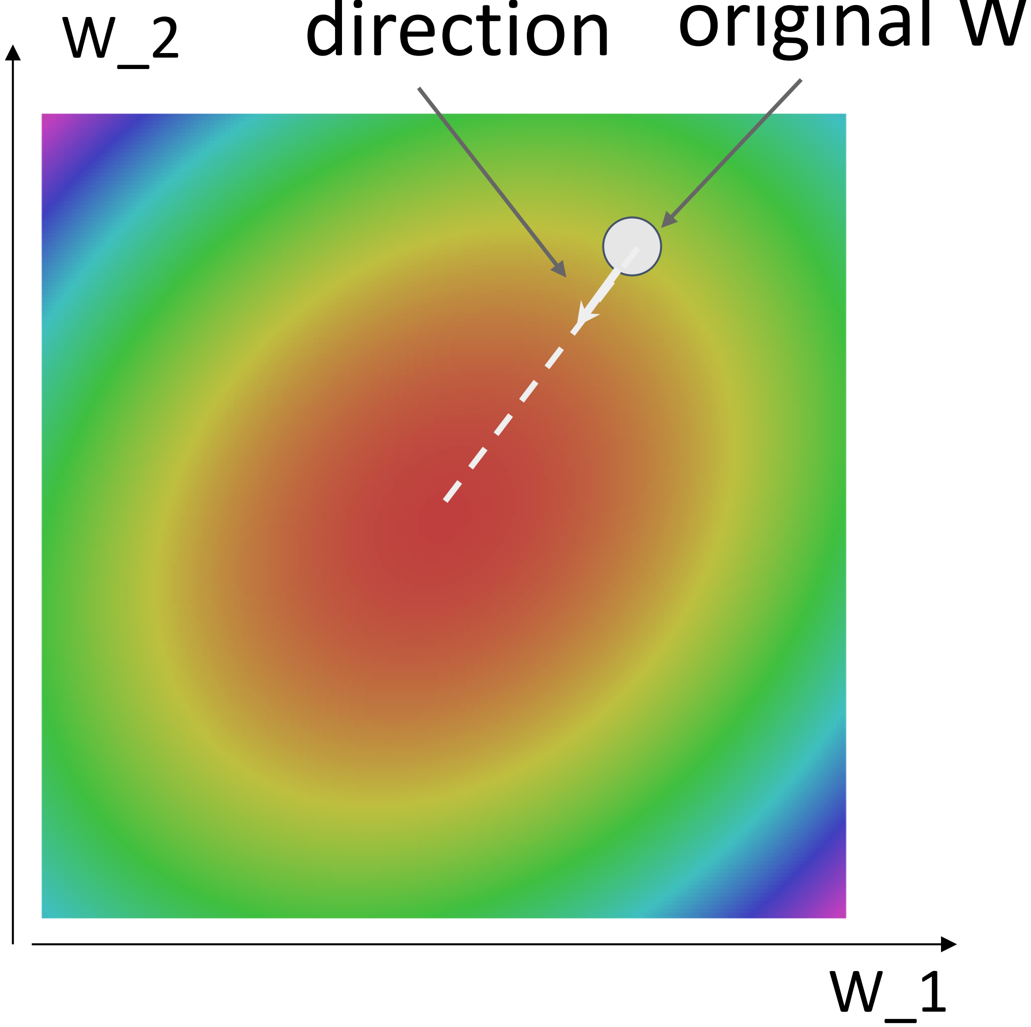

Hyperparameters:

- Weight initialization method
- Number of steps
- Learning rate

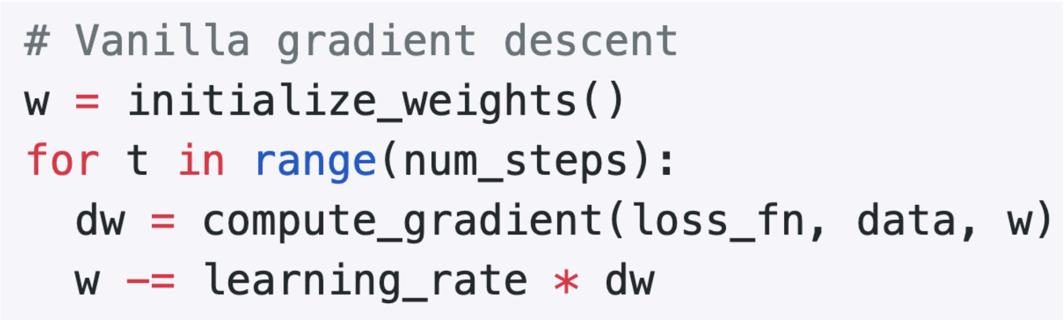


negative gradient direction

original W

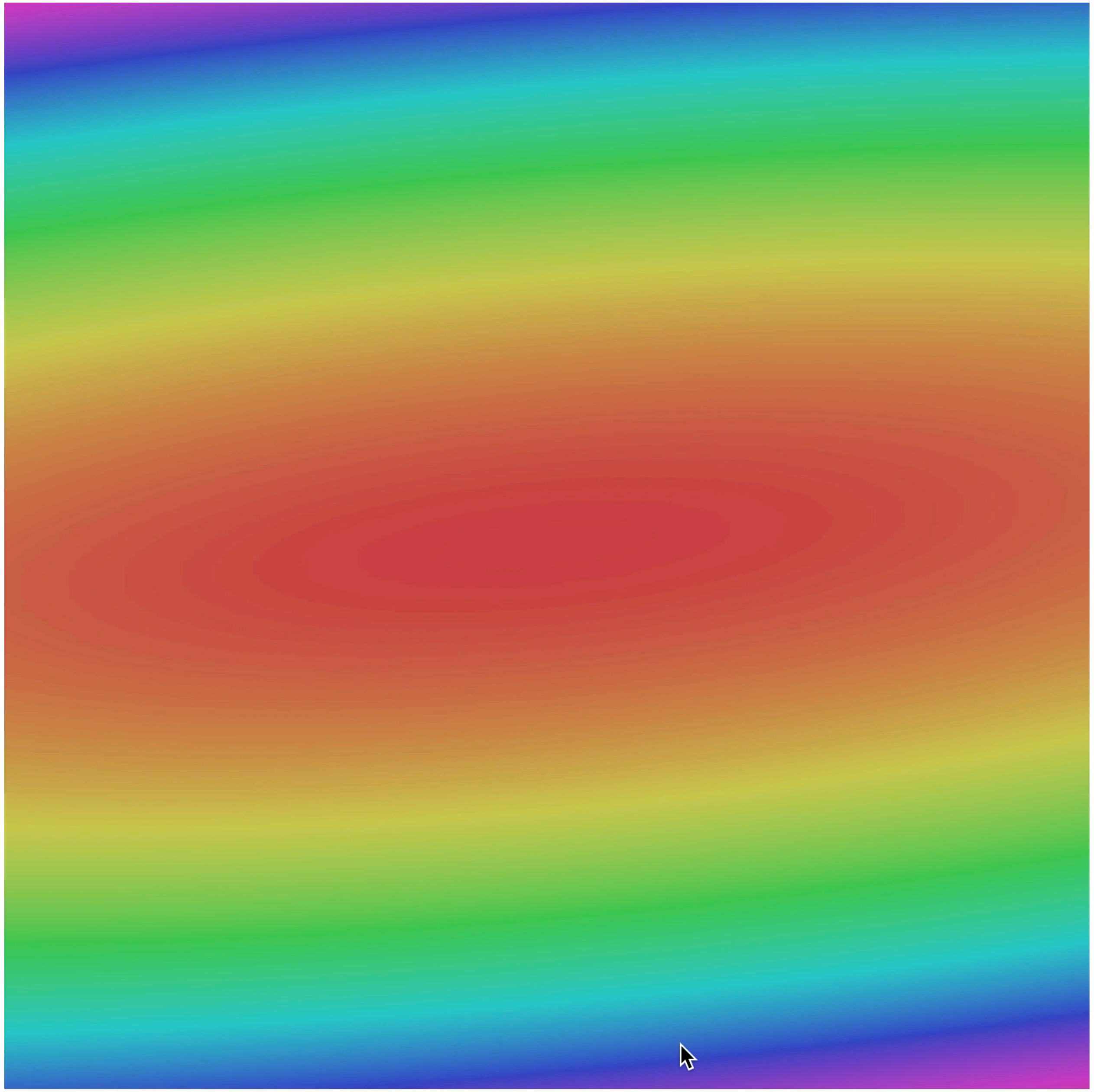
Gradient Descent

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



Batch Gradient Descent

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

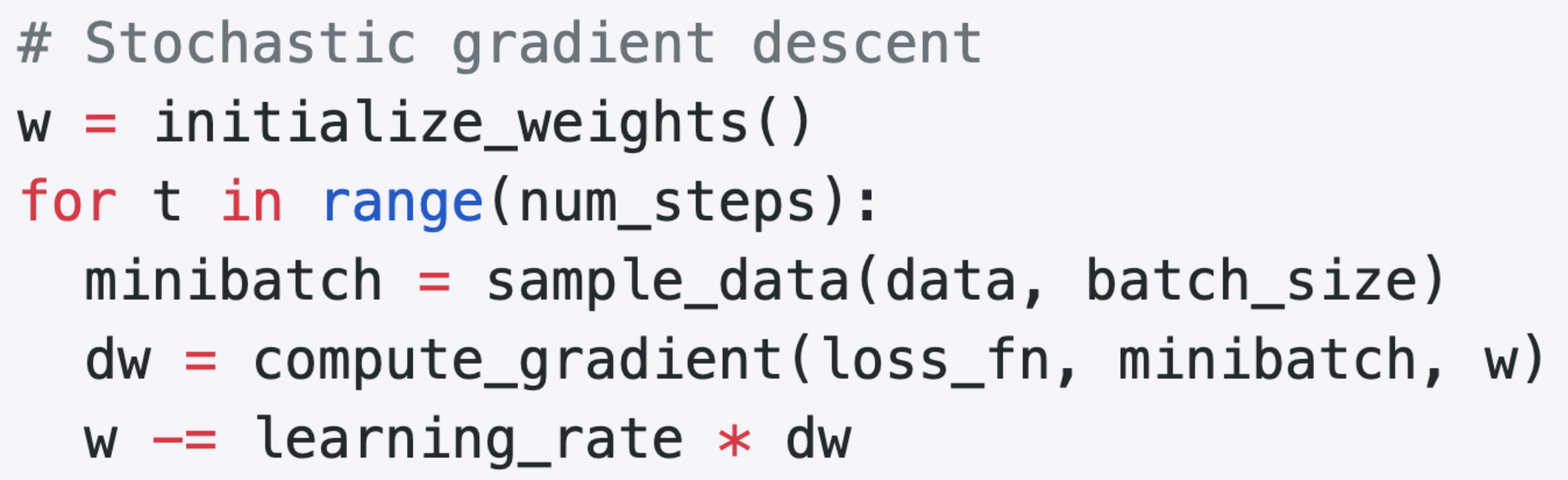
$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Full sum expensive when N is large!

Stochastic Gradient Descent (SGD)

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

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



```
# 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
```

Full sum expensive
when N is large!

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

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$_{\text{data}}$

Approximate expectation via sampling

Stochastic Gradient Descent (SGD)

$$L(W) = \mathbb{E}_{(x,y)\sim p_{data}}[L(x,y,W)] + \lambda R(W)$$
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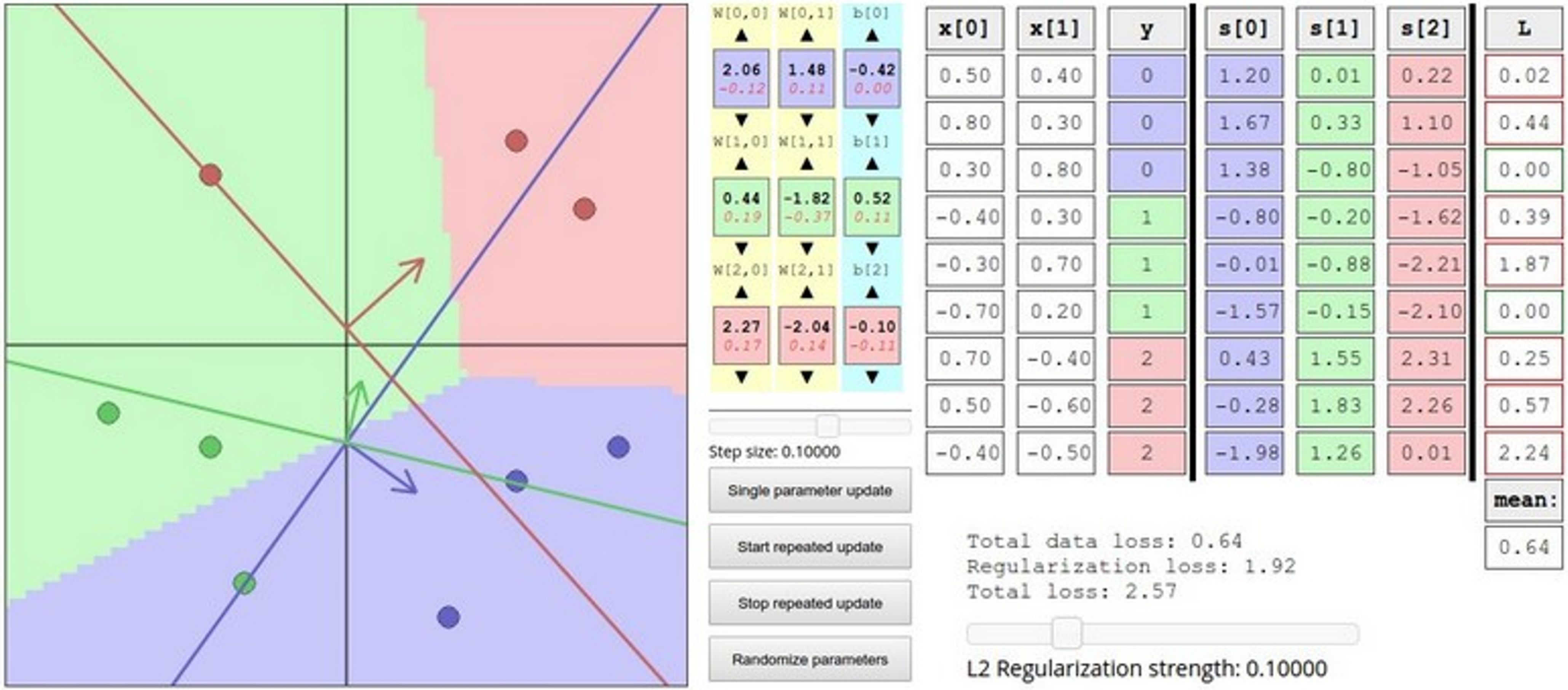
Think of loss as an expectation over the full **data distribution** p$_{\text{data}}$

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



W[0,0]	W[0,1]	b[0]
2.06 -0.12	1.48 0.11	-0.42 0.00
W[1,0]	W[1,1]	b[1]
0.44 0.19	-1.82 -0.37	0.52 0.11
W[2,0]	W[2,1]	b[2]
2.27 0.17	-2.04 0.14	-0.10 -0.11

Step size: 0.10000

x[0]	x[1]	y	s[0]	s[1]	s[2]	L
0.50	0.40	0	1.20	0.01	0.22	0.02
0.80	0.30	0	1.67	0.33	1.10	0.44
0.30	0.80	0	1.38	-0.80	-1.05	0.00
-0.40	0.30	1	-0.80	-0.20	-1.62	0.39
-0.30	0.70	1	-0.01	-0.88	-2.21	1.87
-0.70	0.20	1	-1.57	-0.15	-2.10	0.00
0.70	-0.40	2	0.43	1.55	2.31	0.25
0.50	-0.60	2	-0.28	1.83	2.26	0.57
-0.40	-0.50	2	-1.98	1.26	0.01	2.24
						mean:
						0.64

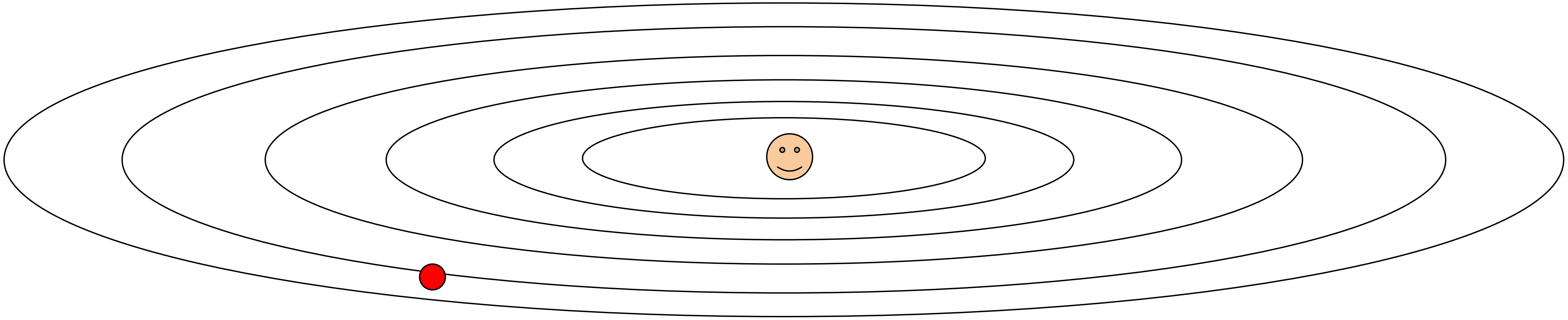
```
Total data loss: 0.64
Regularization loss: 1.92
Total loss: 2.57
```

L2 Regularization strength: 0.10000

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

Problems with SGD

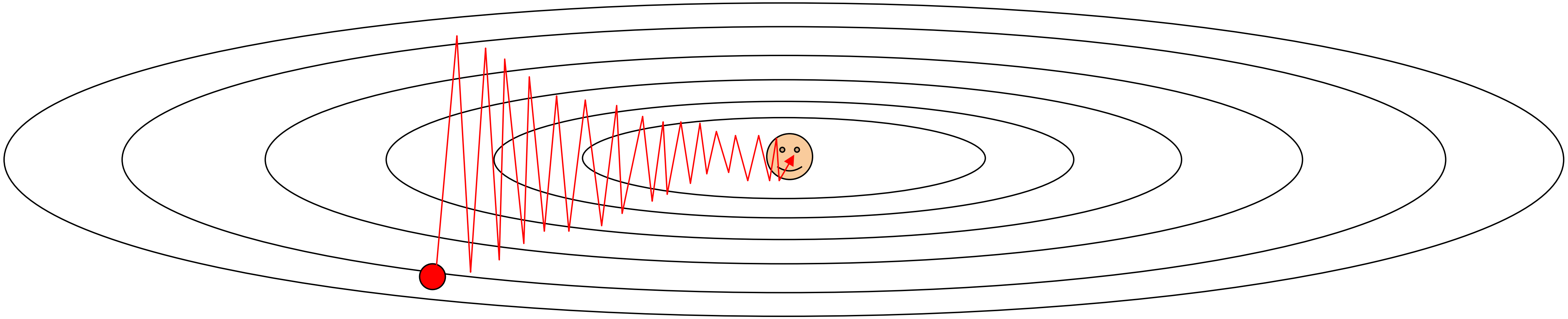
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?



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

Problems with SGD

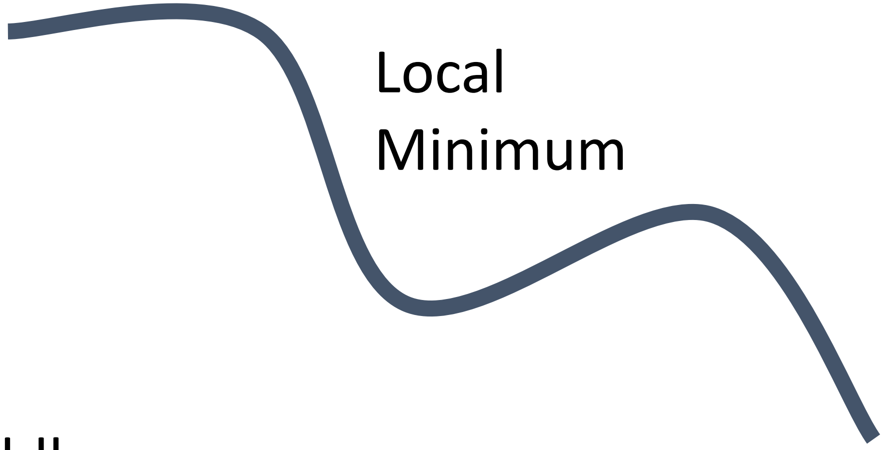
What if loss changes quickly in one direction and slowly in another?
What does gradient descent do?
Very slow progress along shallow dimension, jitter along steep direction



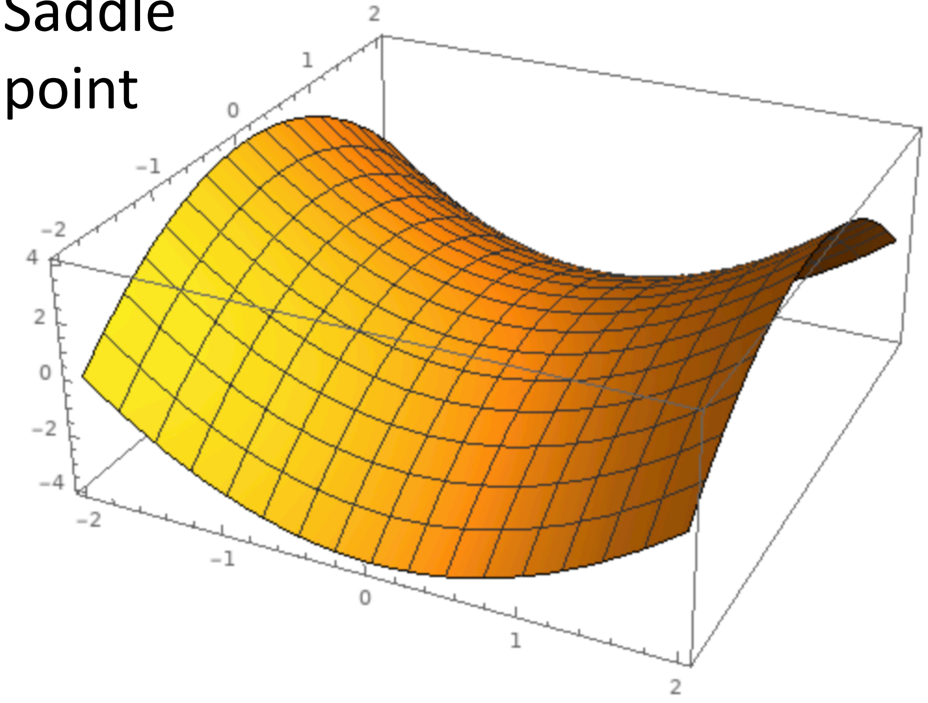
Loss function has high **condition number**: ratio of largest to smallest singular value of the Hessian matrix is large

Problems with SGD

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



Local Minimum

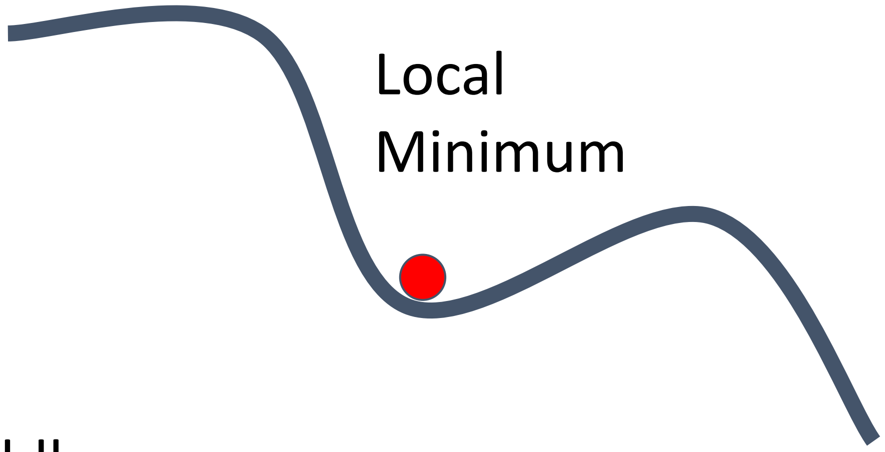


Saddle point

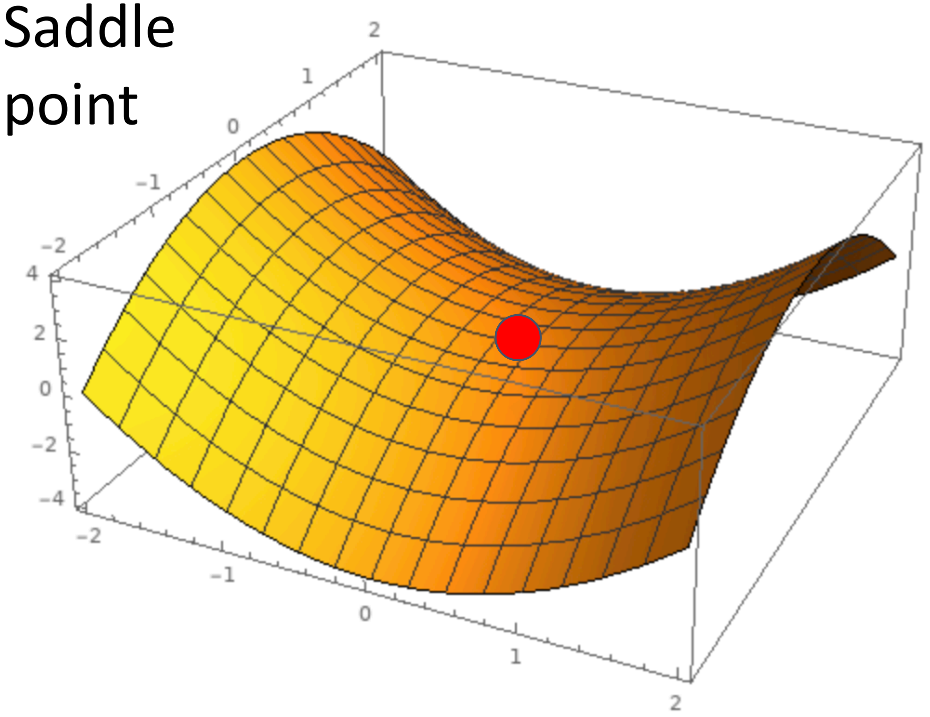
Problems with SGD

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

Zero gradient, gradient descent gets stuck



Local Minimum



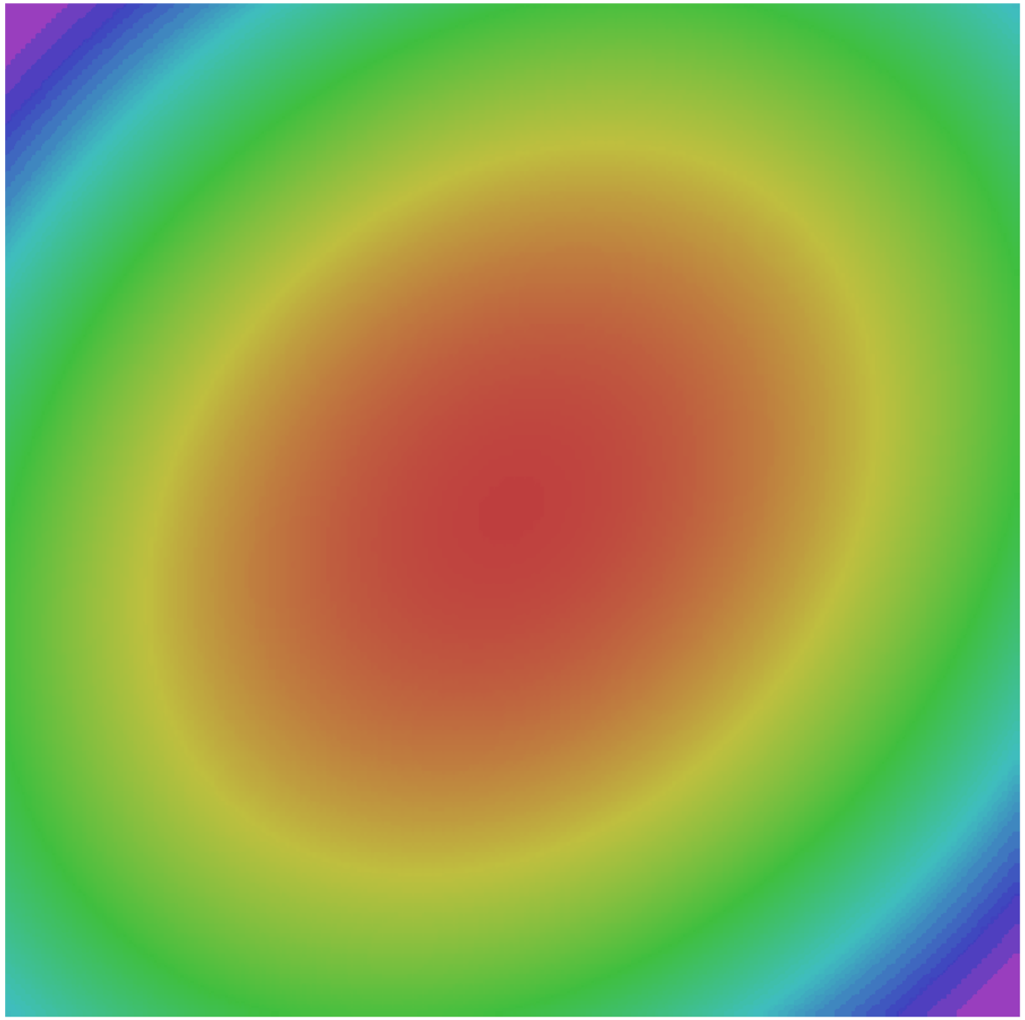
Saddle point

Problems with SGD

Our gradients come from minibatches so they can be noisy!

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

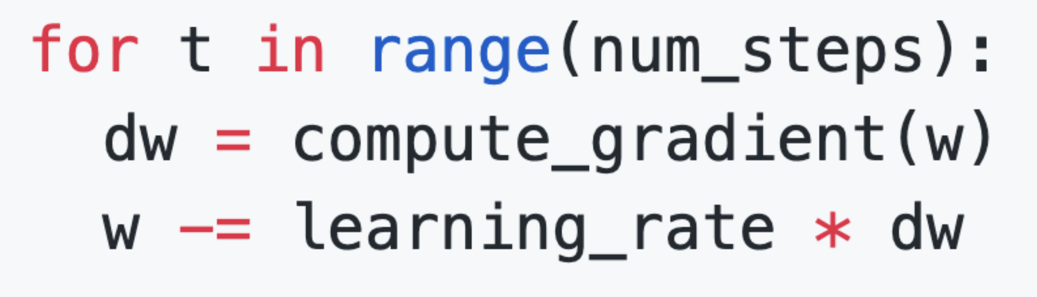
$$\nabla_W L(W) = \frac{1}{N}\sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$



SGD

SGD

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

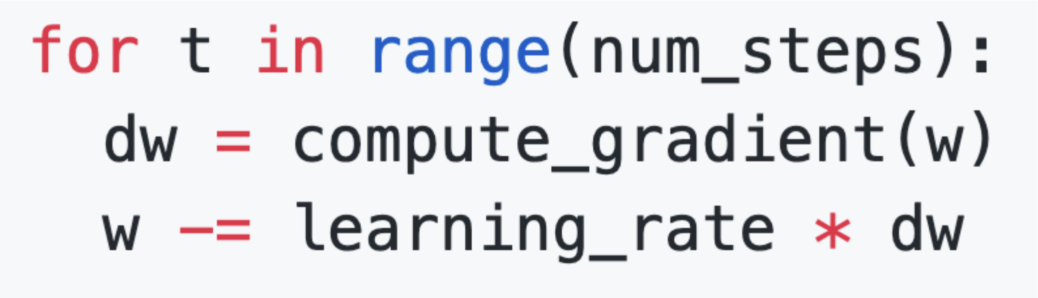


```
for t in range(num_steps):
  dw = compute_gradient(w)
  w -= learning_rate * dw
```

SGD + Momentum

SGD

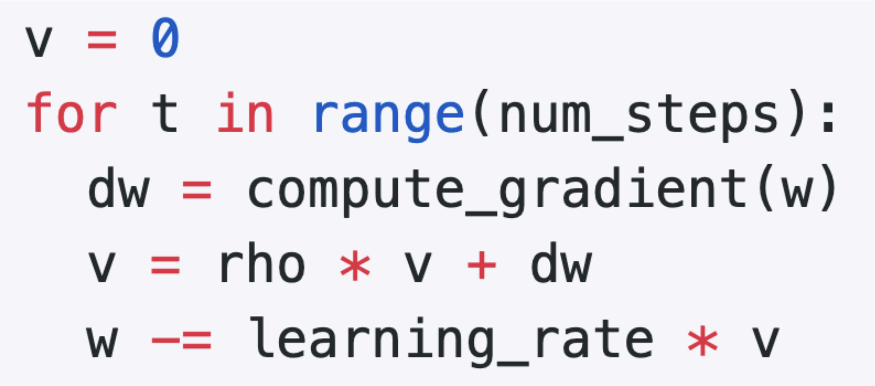
$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$



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

SGD+Momentum

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



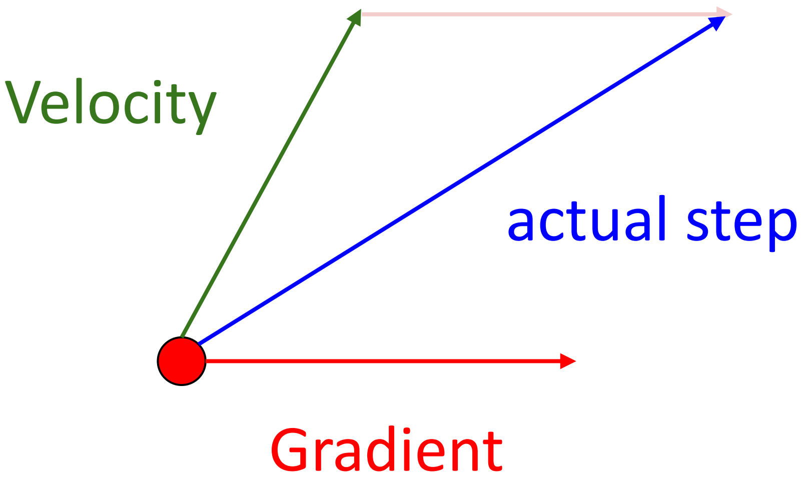
```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

- 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

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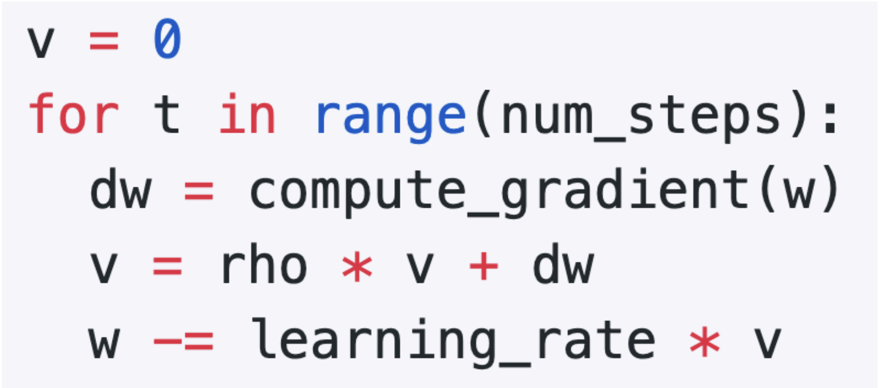

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v = 0
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```

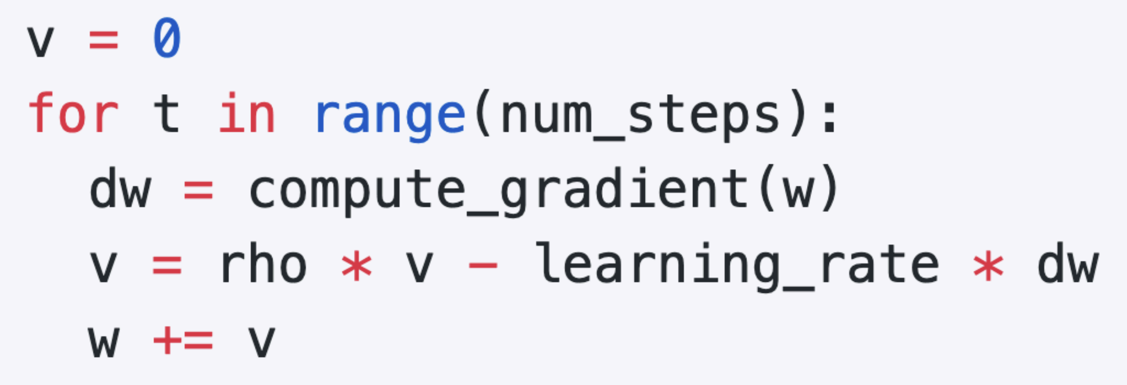
- Build up “velocity” as a running mean of gradients
- Rho gives “friction”; typically rho=0.9 or 0.99

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

SGD + Momentum

SGD+Momentum

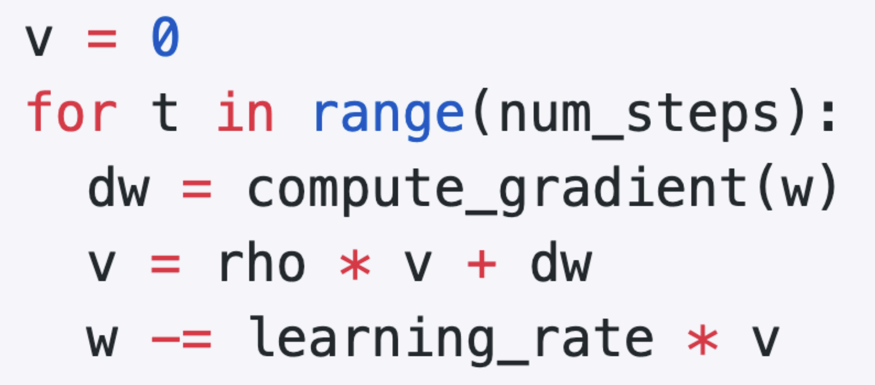
$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t)$$
$$x_{t+1} = x_t + v_{t+1}$$



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

SGD+Momentum

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



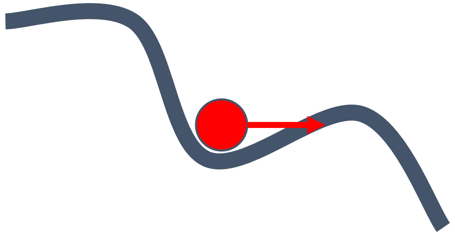
```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

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

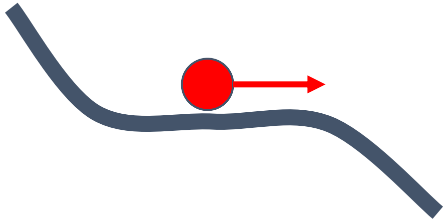
Sutskever et al, “On the importance of initialization and momentum in deep learning”, ICML 2013

SGD + Momentum

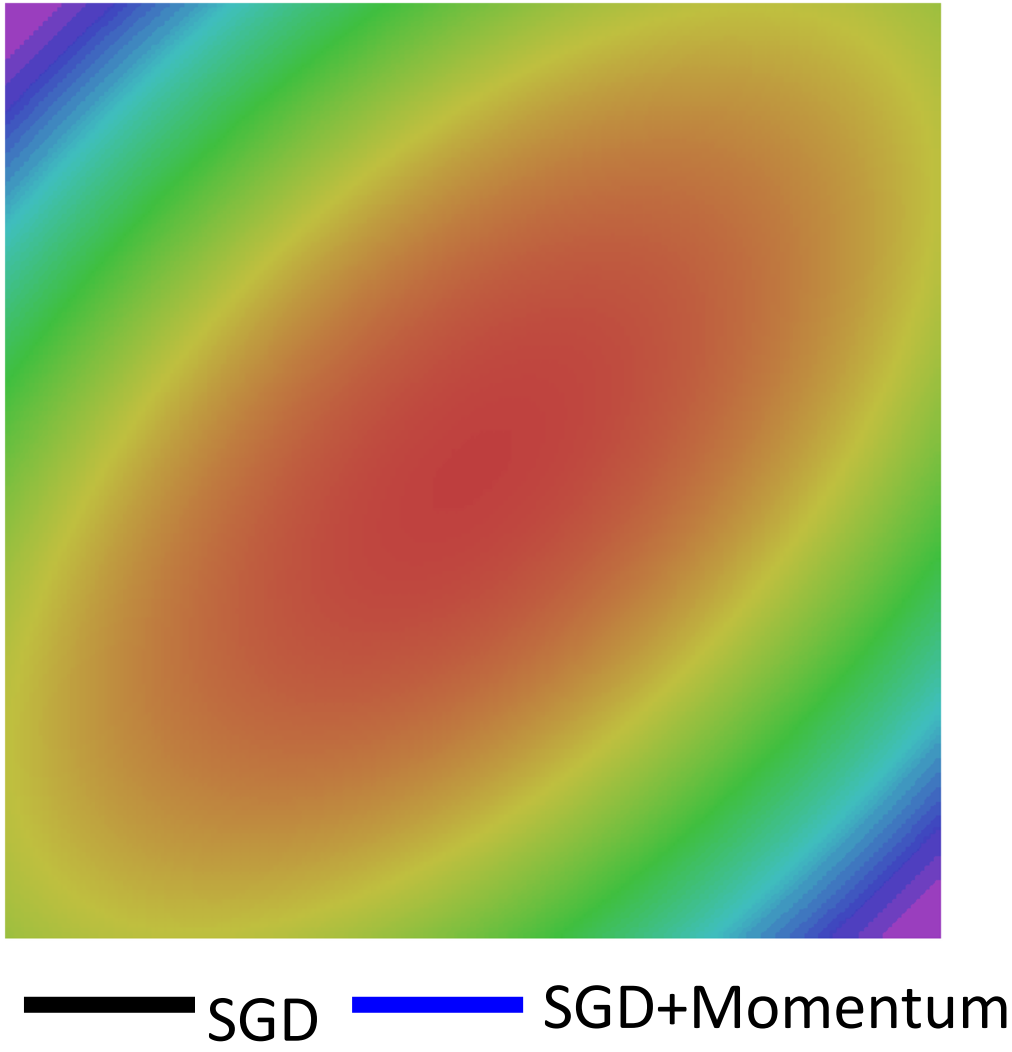
Local Minima



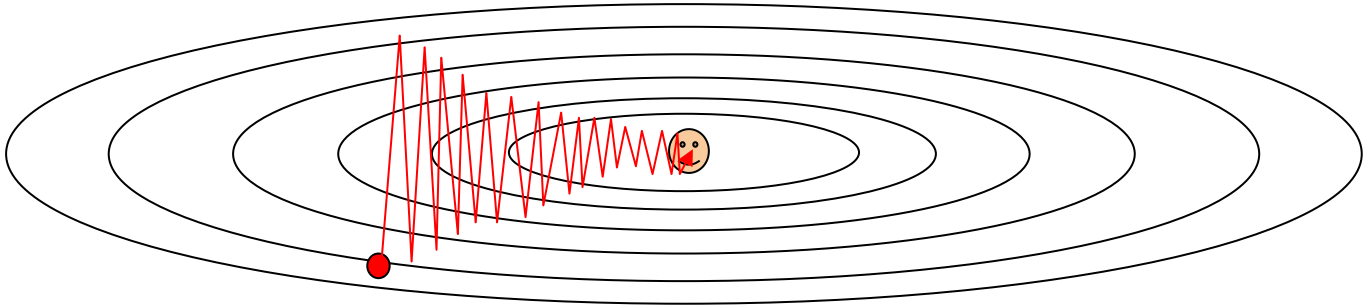
Saddle points



Gradient Noise



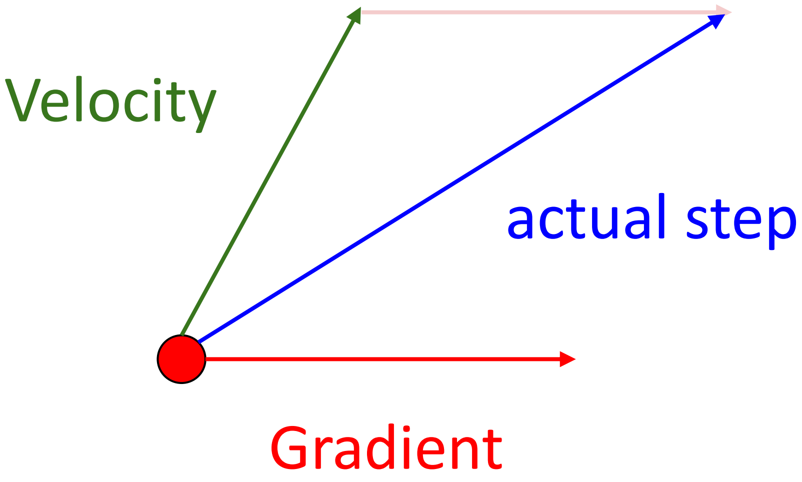
Poor Conditioning



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

SGD + Momentum

Momentum update:

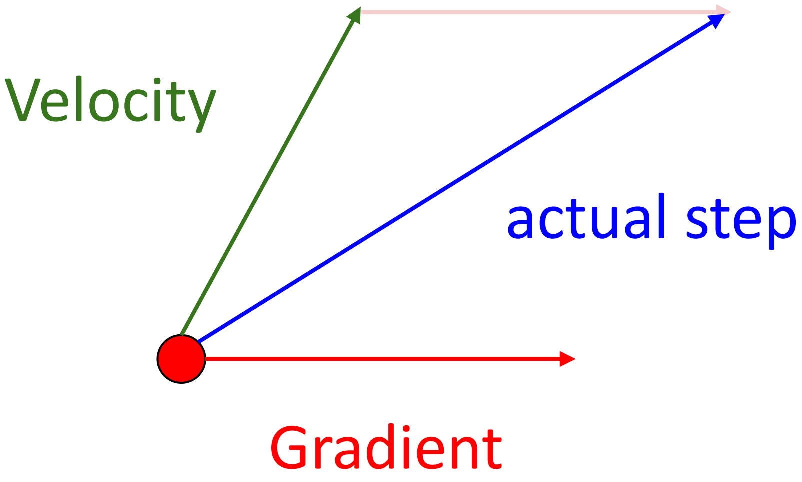


Combine gradient at current point with velocity to get step used to update weights

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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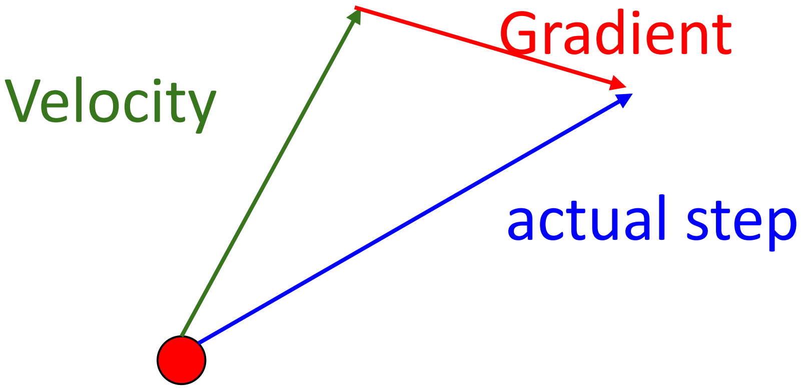
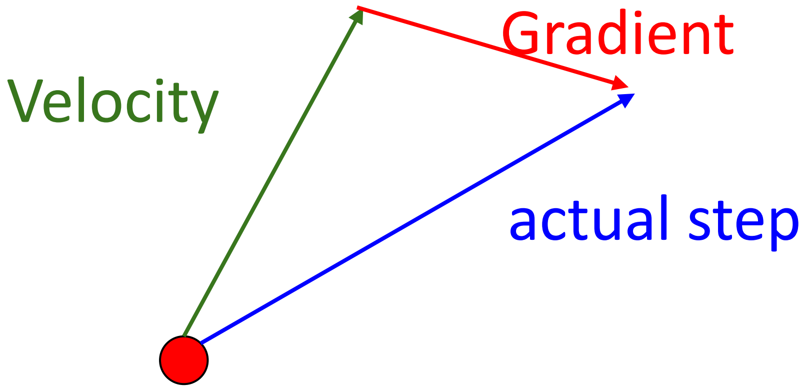


“Look ahead” to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

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

Nesterov Momentum

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



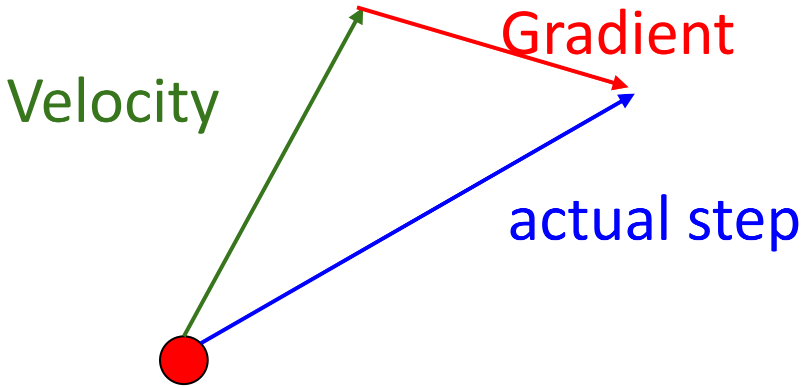
“Look ahead” to the point where updating using velocity would take us; compute gradient there and mix it with velocity to get actual update direction

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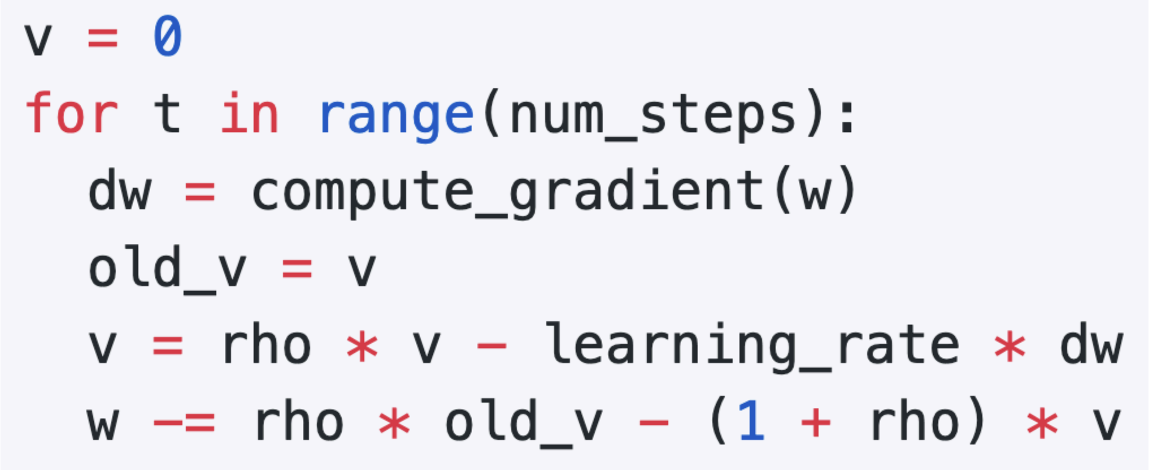
$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
$$x_{t+1} = x_t + v_{t+1}$$

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

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

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



```
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
```

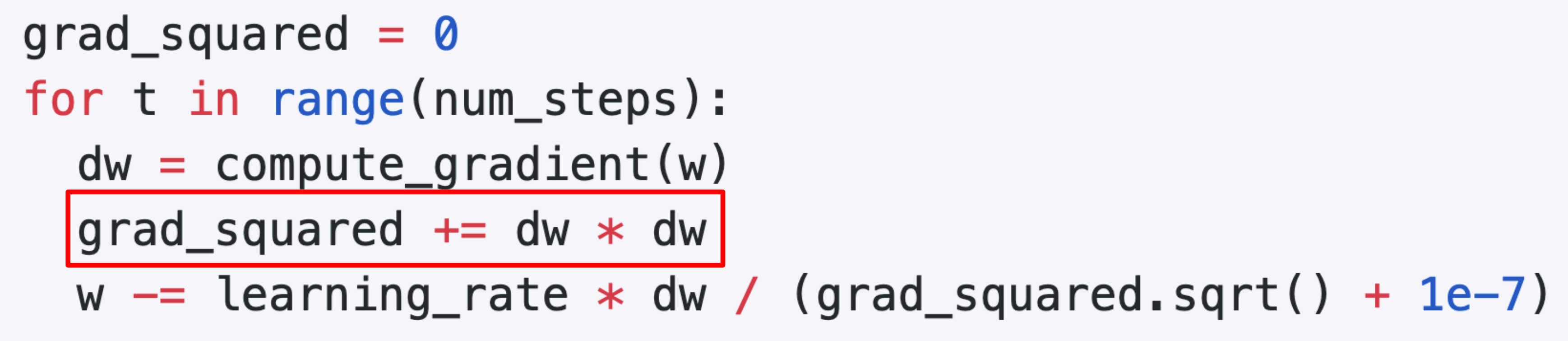
Nesterov Momentum

▬ 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)
```

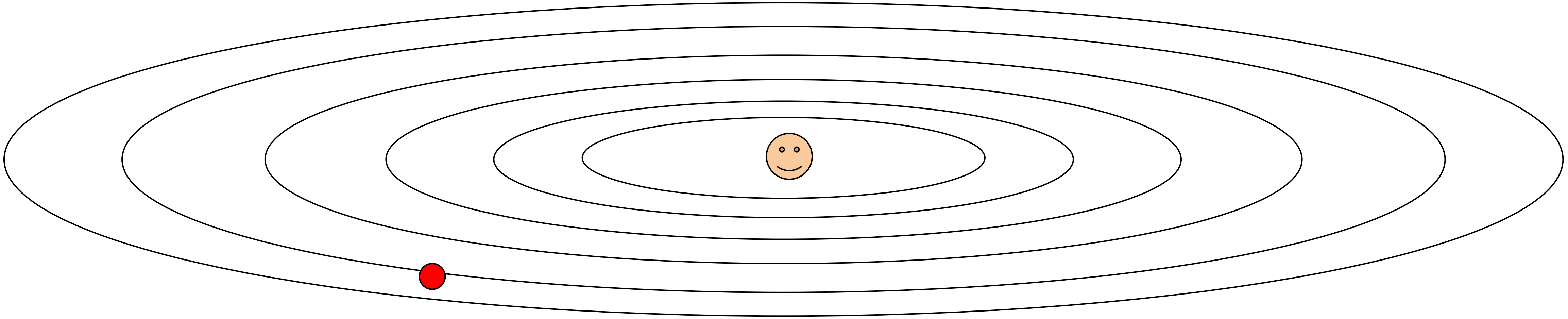
Added element-wise scaling of the gradient based on the historical sum of squares in each dimension

“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)
```



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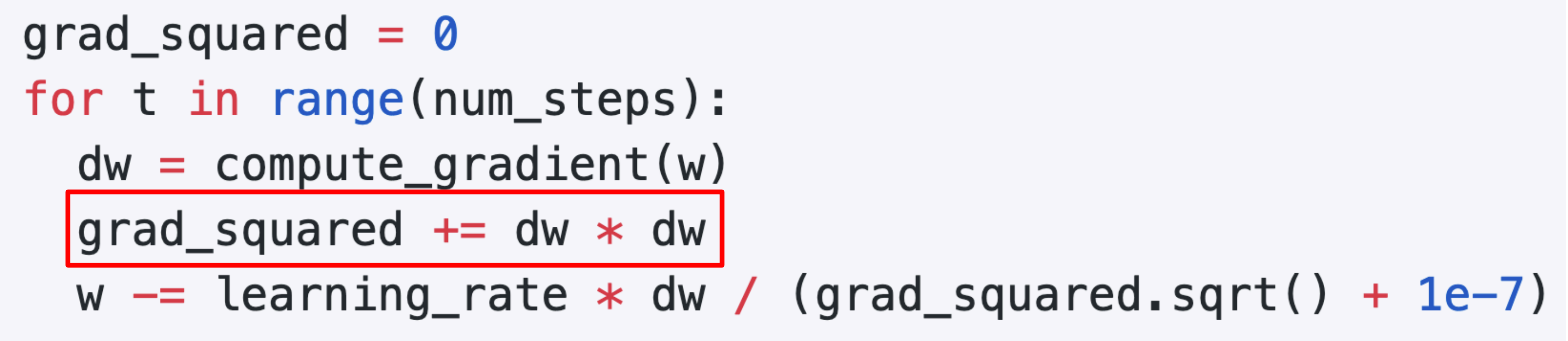
AdaGrad



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for t in range(num_steps):
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```
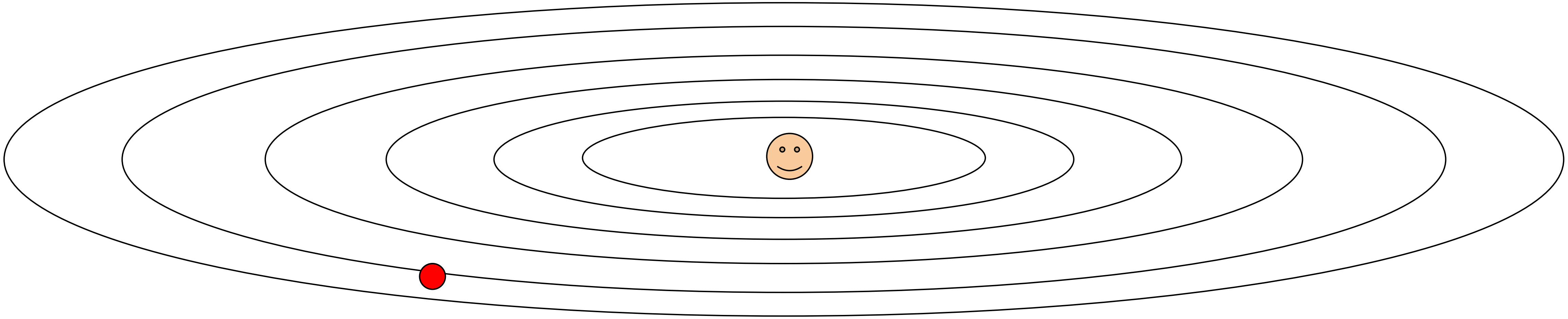
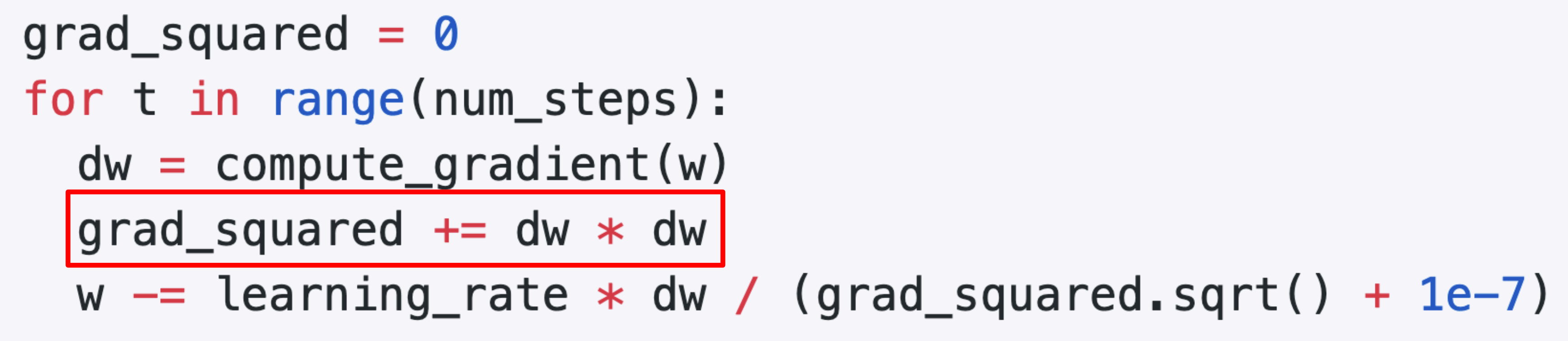



Q: What happens with AdaGrad?

AdaGrad



```
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  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```
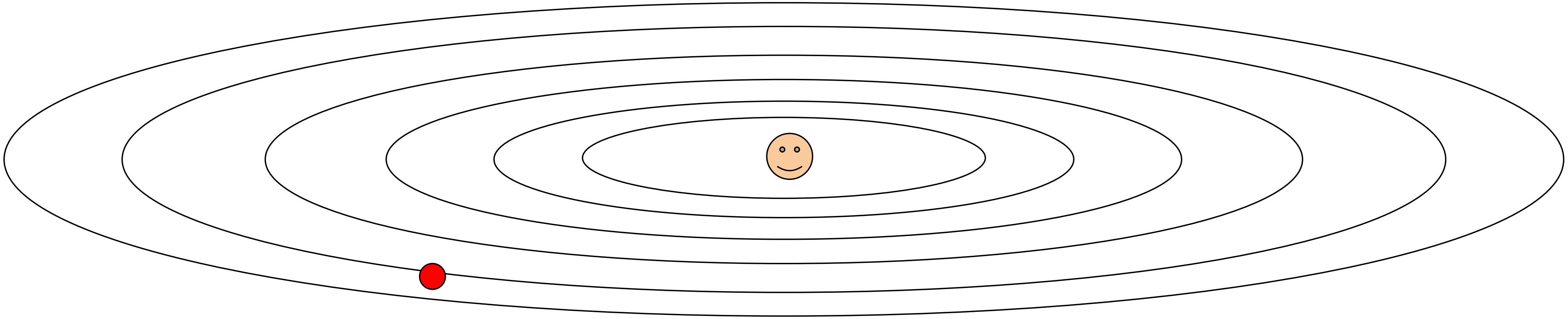
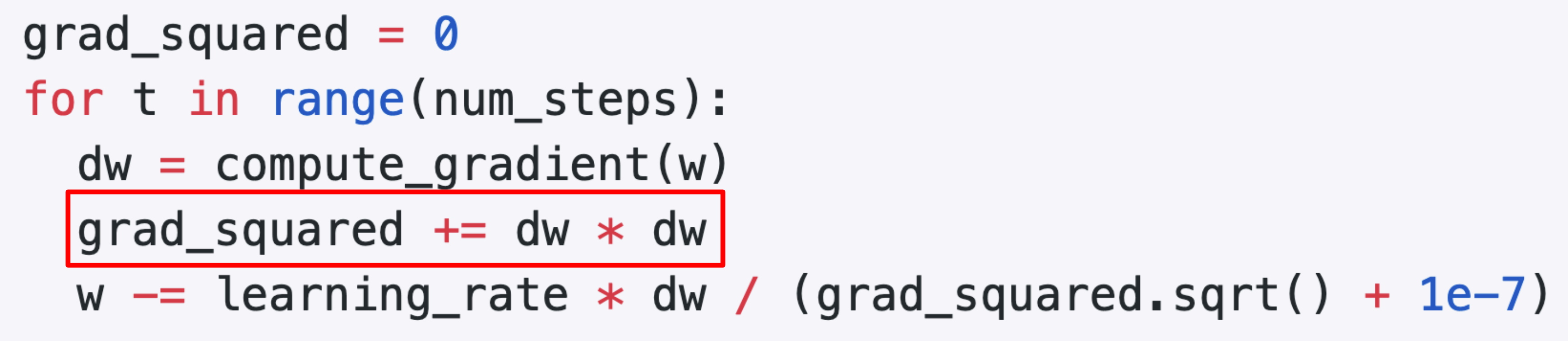



Q: What happens with AdaGrad?

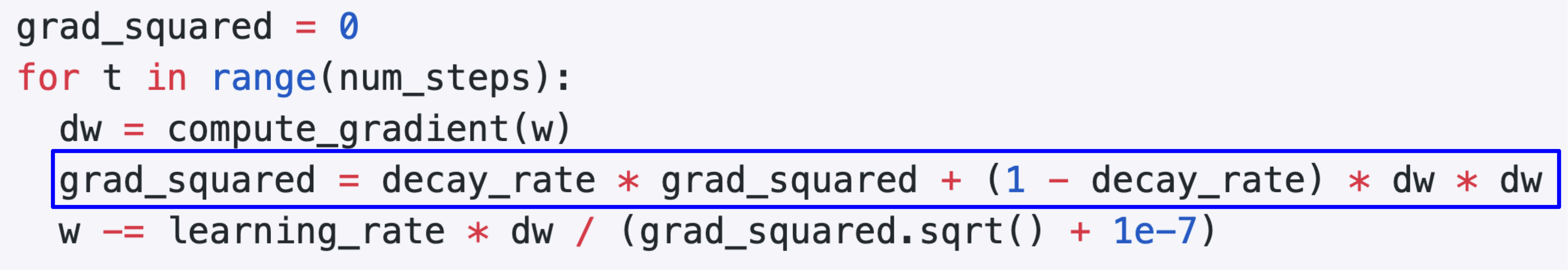
Progress along “steep” directions is damped; progress along “flat” directions is accelerated

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

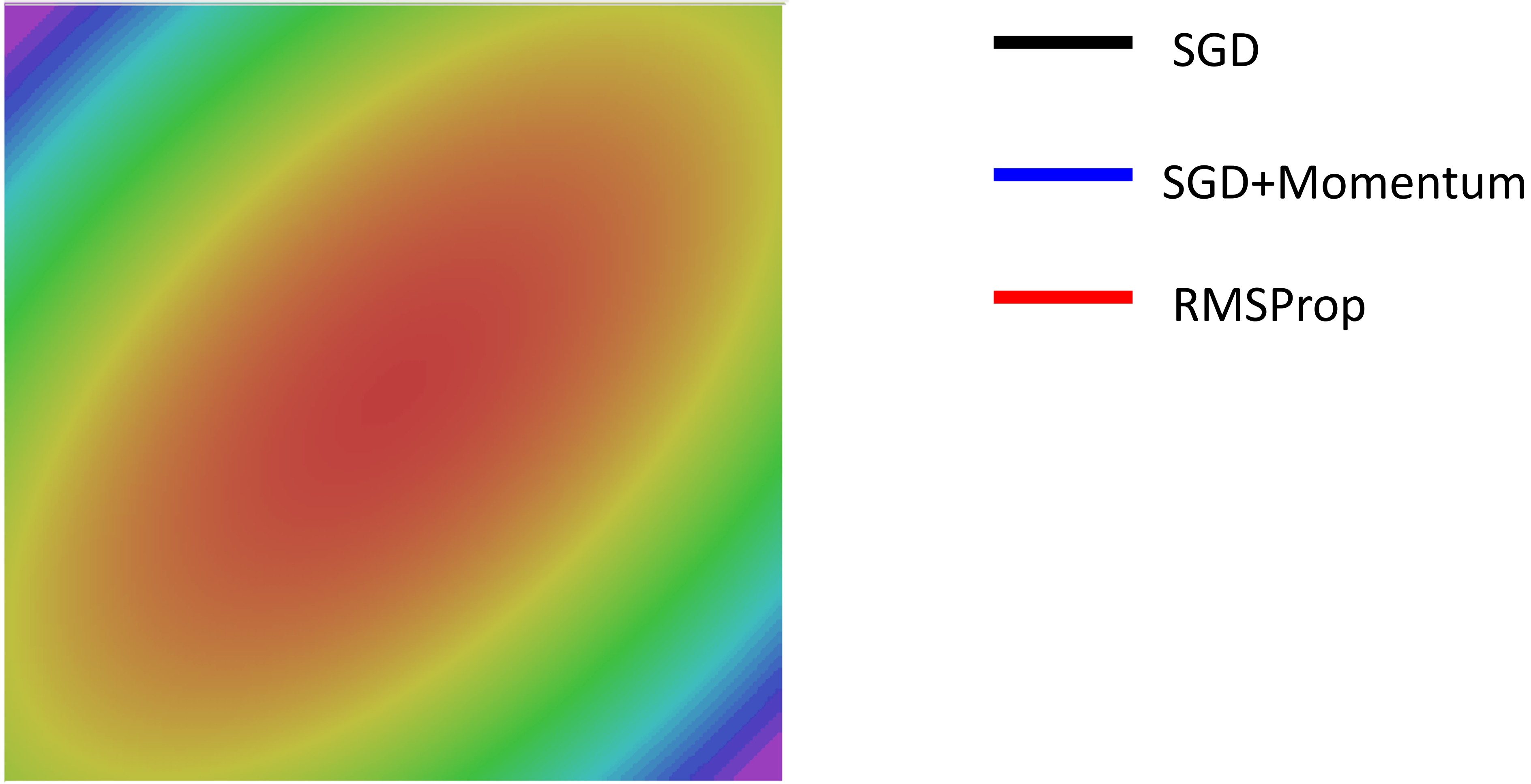


```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

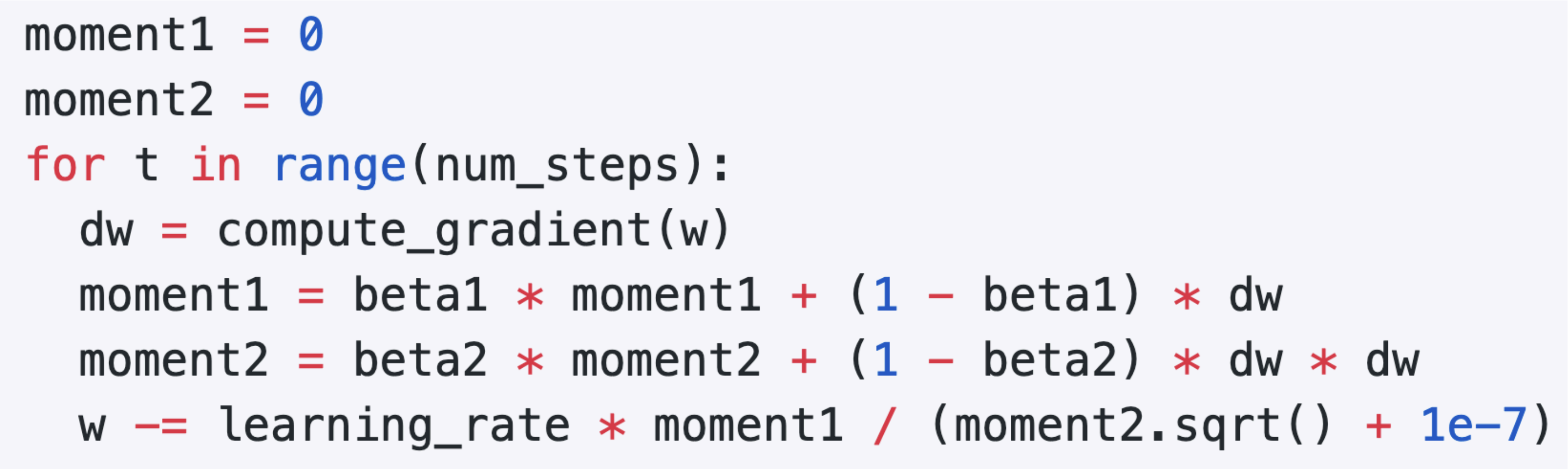
RMSProp

Tieleman and Hinton, 2012

RMSProp



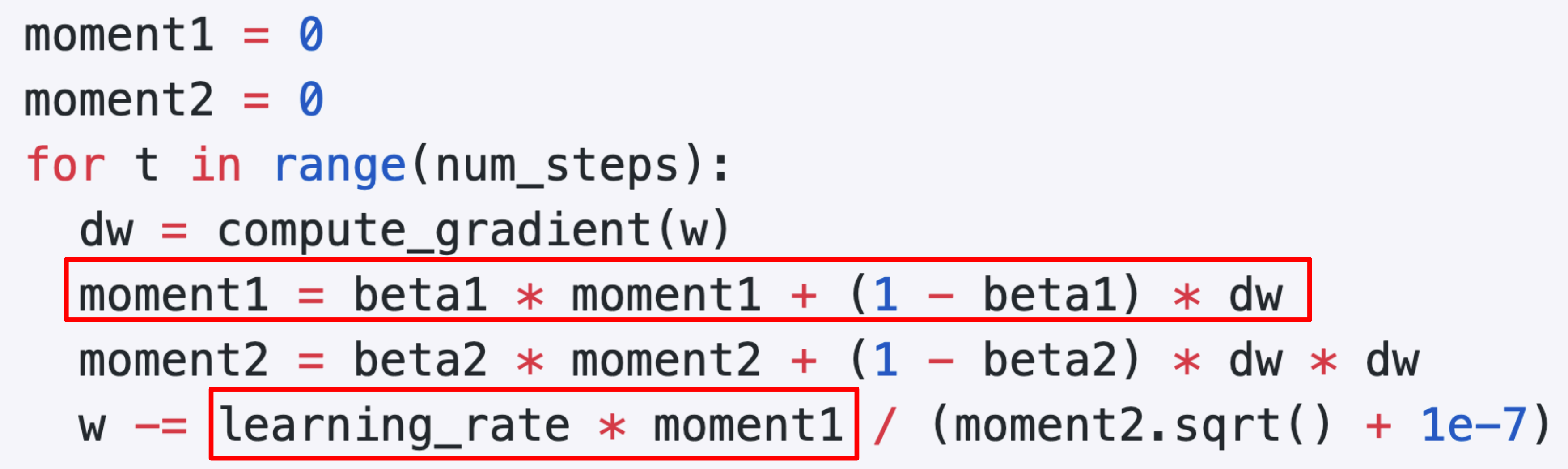
Adam (almost): RMSProp + Momentum



```
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

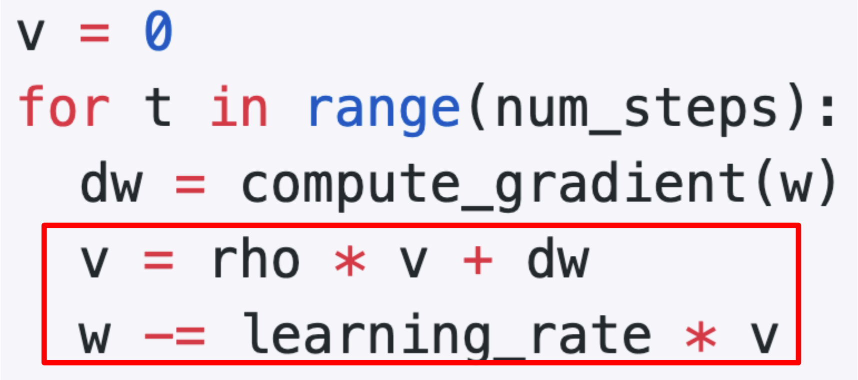
Adam (almost): RMSProp + Momentum



```
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

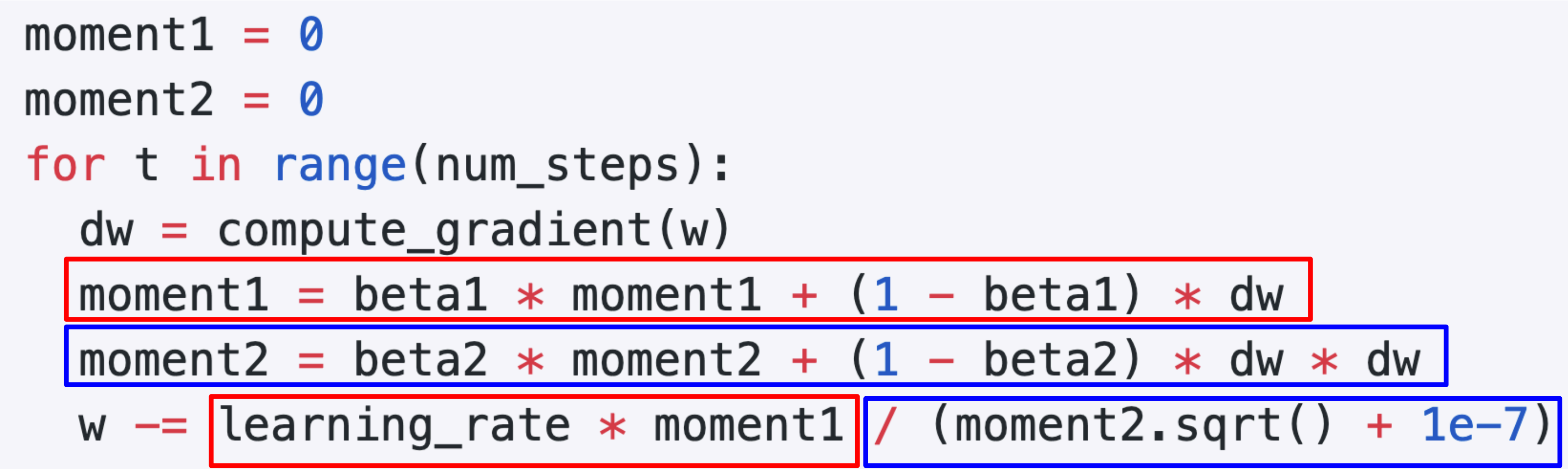


```
v = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  v = rho * v + dw
  w -= learning_rate * v
```

SGD+Momentum

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

Adam (almost): RMSProp + Momentum

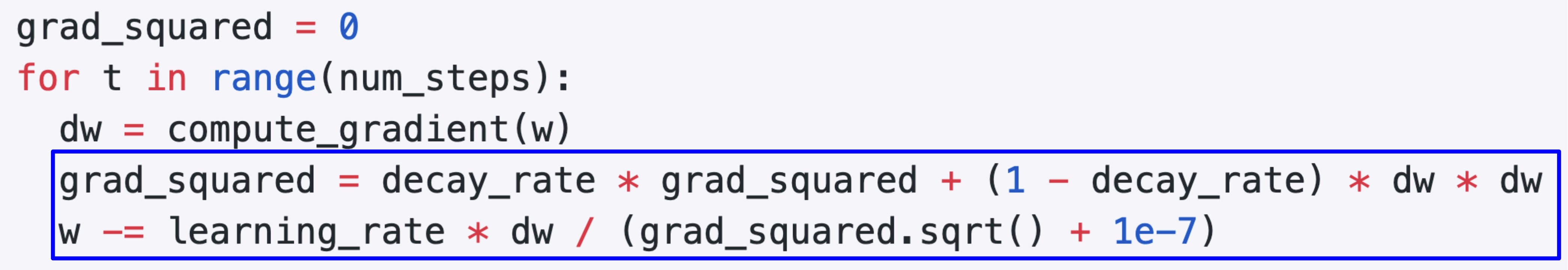


```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  w -= learning_rate * moment1 / (moment2.sqrt() + 1e-7)
```

Adam

Momentum

AdaGrad / RMSProp

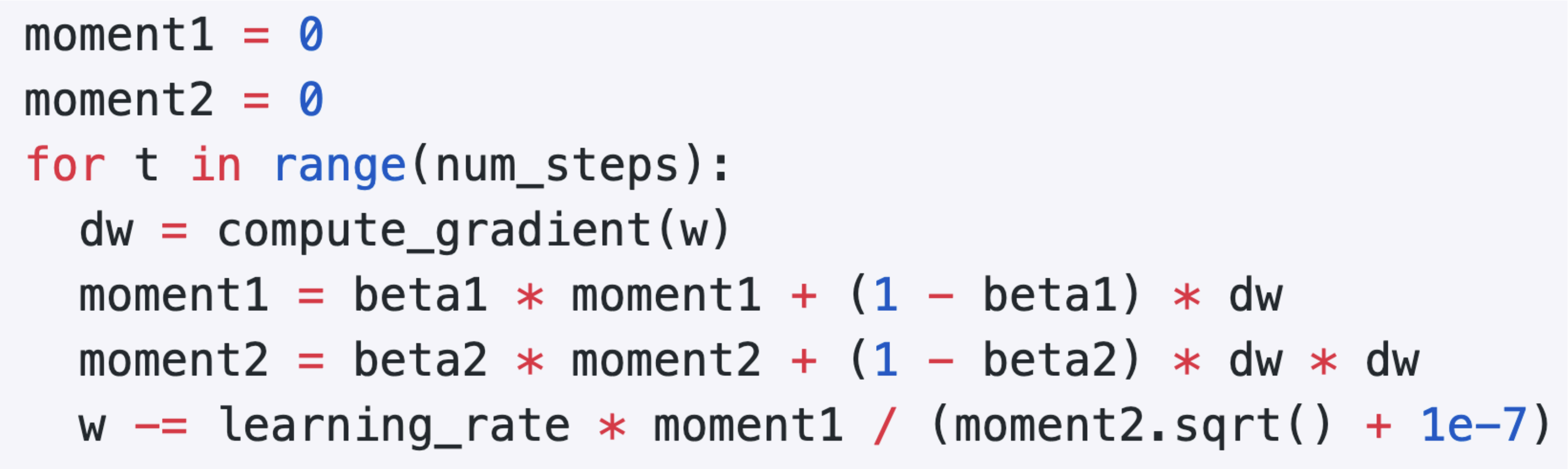


```
grad_squared = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  grad_squared = decay_rate * grad_squared + (1 - decay_rate) * dw * dw
  w -= learning_rate * dw / (grad_squared.sqrt() + 1e-7)
```

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

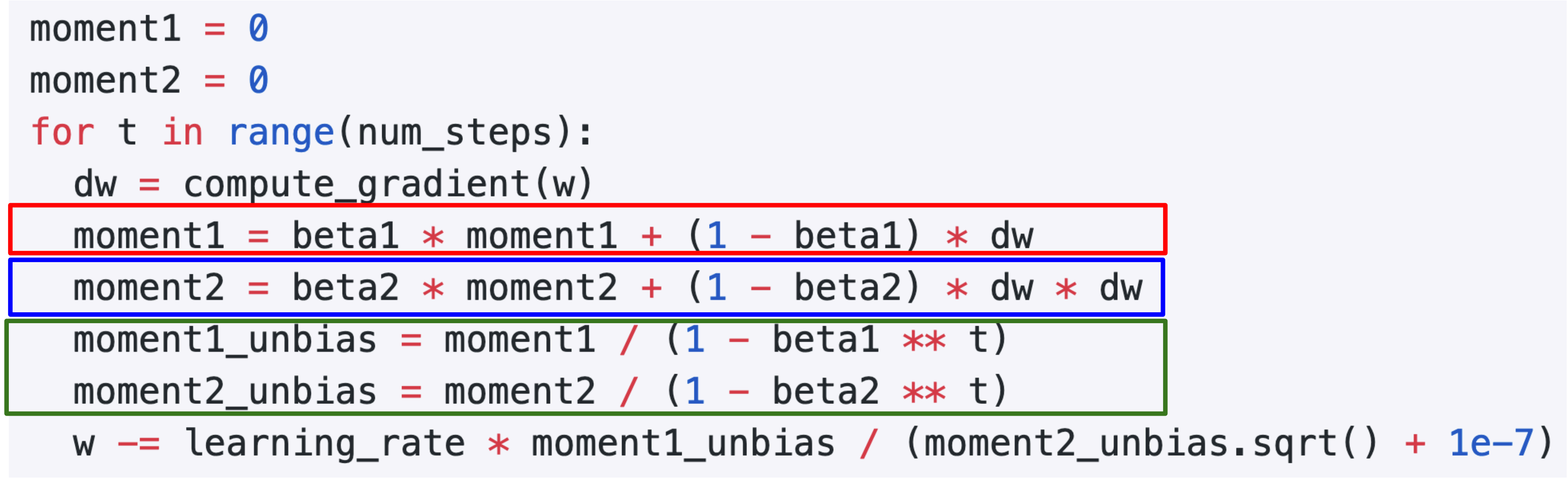
AdaGrad / RMSProp

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(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)
```

Momentum

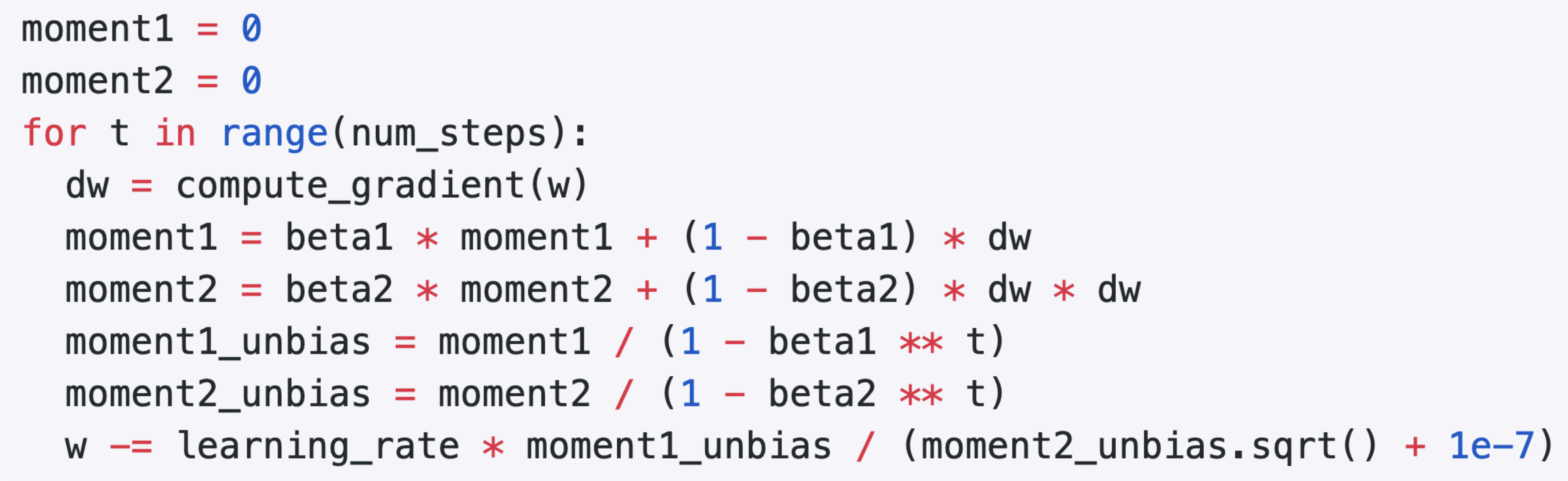
AdaGrad / RMSProp

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



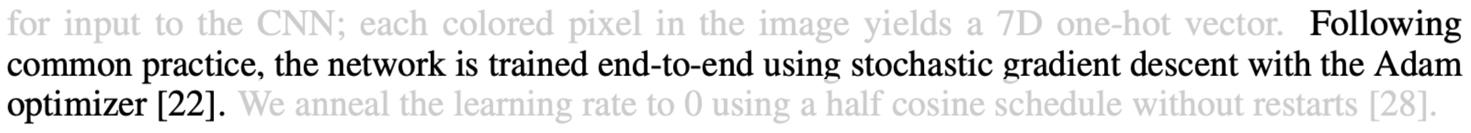
```
moment1 = 0
moment2 = 0
for t in range(num_steps):
  dw = compute_gradient(w)
  moment1 = beta1 * moment1 + (1 - beta1) * dw
  moment2 = beta2 * moment2 + (1 - beta2) * dw * dw
  moment1_unbias = moment1 / (1 - beta1 ** t)
  moment2_unbias = moment2 / (1 - beta2 ** t)
  w -= learning_rate * moment1_unbias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

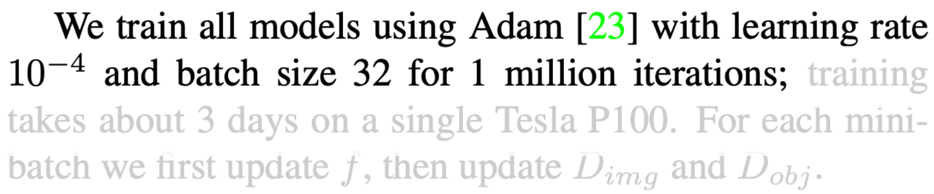
Kingma and Ba, "Adam: A method for stochastic optimization", ICLR 2015

Adam: Very Common in Practice!



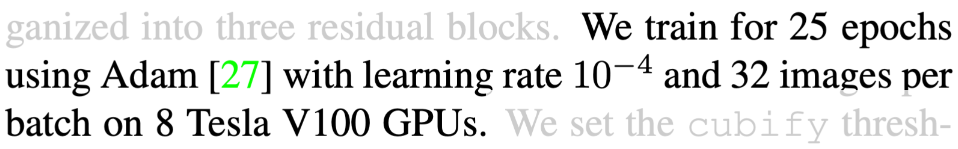
for input to the CNN; each colored pixel in the image yields a 7D one-hot vector. Following common practice, the network is trained end-to-end using stochastic gradient descent with the Adam optimizer [22]. We anneal the learning rate to 0 using a half cosine schedule without restarts [28].

Bakhtin, van der Maaten, Johnson, Gustafson, and Girshick, NeurIPS 2019



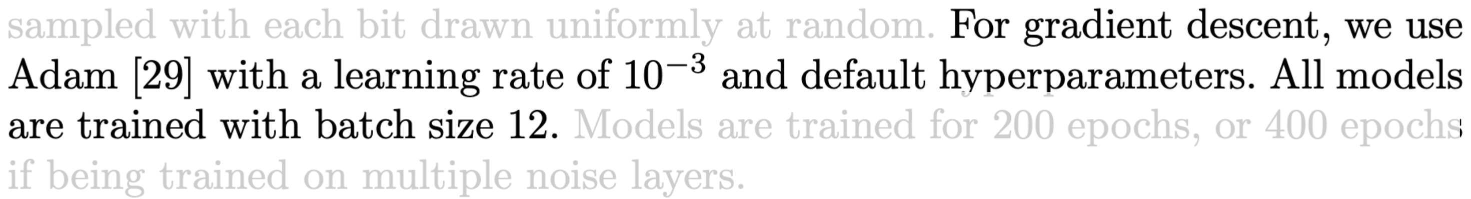
We train all models using Adam [23] with learning rate 10^{-4} and batch size 32 for 1 million iterations; training takes about 3 days on a single Tesla P100. For each minibatch we first update f, then update D_{img} and D_{obj}.

Johnson, Gupta, and Fei-Fei, CVPR 2018



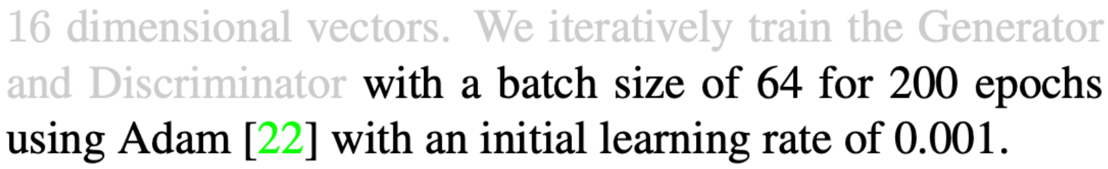
ganized into three residual blocks. We train for 25 epochs using Adam [27] with learning rate 10^{-4} and 32 images per batch on 8 Tesla V100 GPUs. We set the `cubify` thresh-

Gkioxari, Malik, and Johnson, ICCV 2019



sampled with each bit drawn uniformly at random. For gradient descent, we use Adam [29] with a learning rate of 10^{-3} and default hyperparameters. All models are trained with batch size 12. Models are trained for 200 epochs, or 400 epochs if being trained on multiple noise layers.

Zhu, Kaplan, Johnson, and Fei-Fei, ECCV 2018

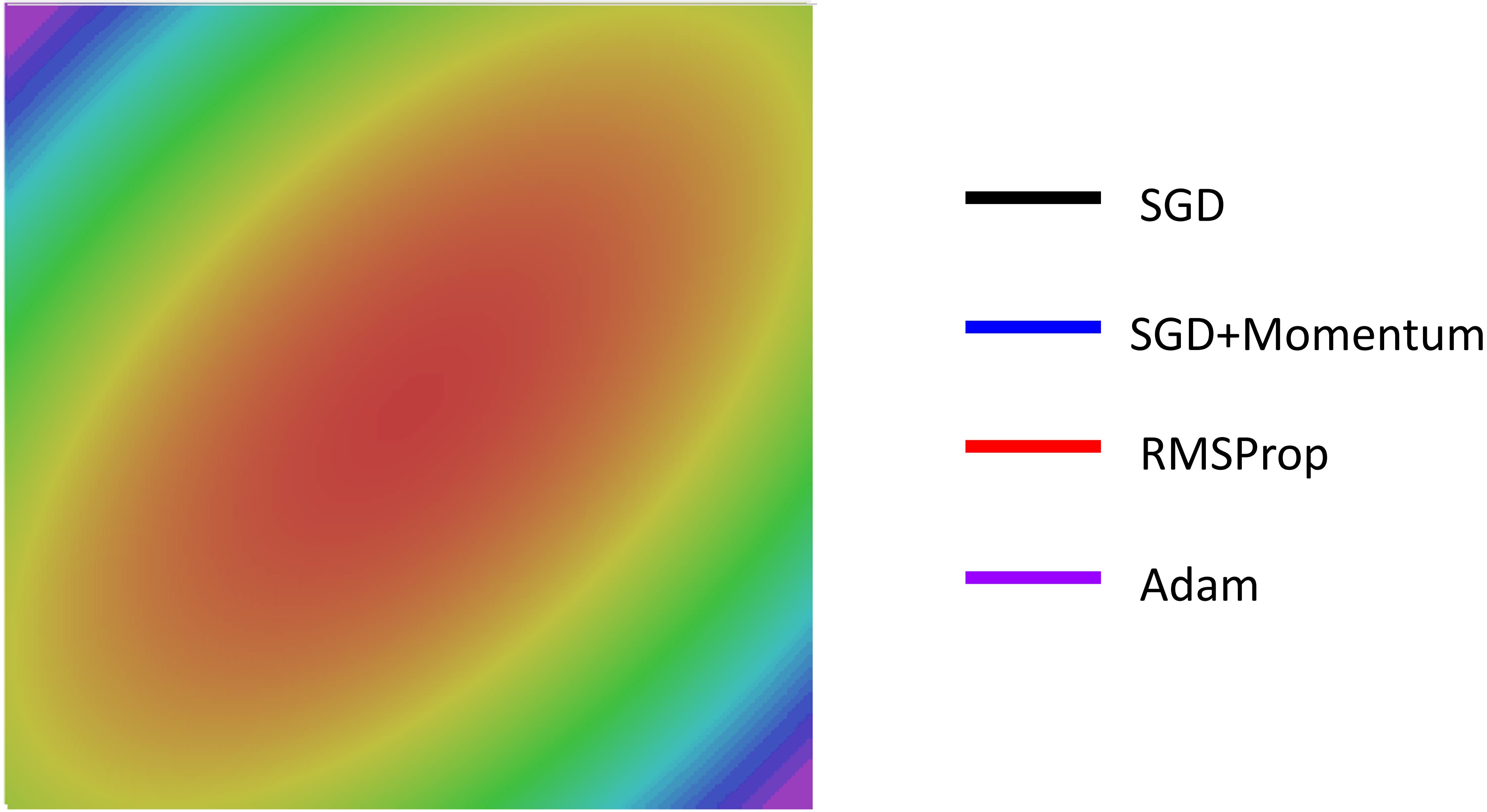


16 dimensional vectors. We iteratively train the Generator and Discriminator with a batch size of 64 for 200 epochs using Adam [22] with an initial learning rate of 0.001.

Gupta, Johnson, et al, CVPR 2018

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!

Adam



Optimization Algorithm Comparison

Algorithm	Tracks first moments (Momentum)	Tracks second moments (Adaptive learning rates)	Leaky second moments	Bias correction for moment estimates
SGD	x	x	x	x
SGD+Momentum	✓	x	x	x
Nesterov	✓	x	x	x
AdaGrad	x	✓	x	x
RMSProp	x	✓	✓	x
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 vs Weight Decay

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L2 Regularization

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

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

$s_t = optimizer(g_t)$

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

Loshchilov and Hutter, “Decoupled Weight Decay Regularization”, ICLR 2019

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L2 Regularization

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

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

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Weight Decay

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

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

L2 Regularization

$$L(w) = L_{data}(w) + \boldsymbol{\lambda |w|^2}$$
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$$s_t = optimizer(g_t)$$
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Weight Decay

$$L(w) = L_{data}(w)$$
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L2 Regularization vs Weight Decay

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Weight Decay

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$$g_t = \nabla L_{data}(w_t)$$
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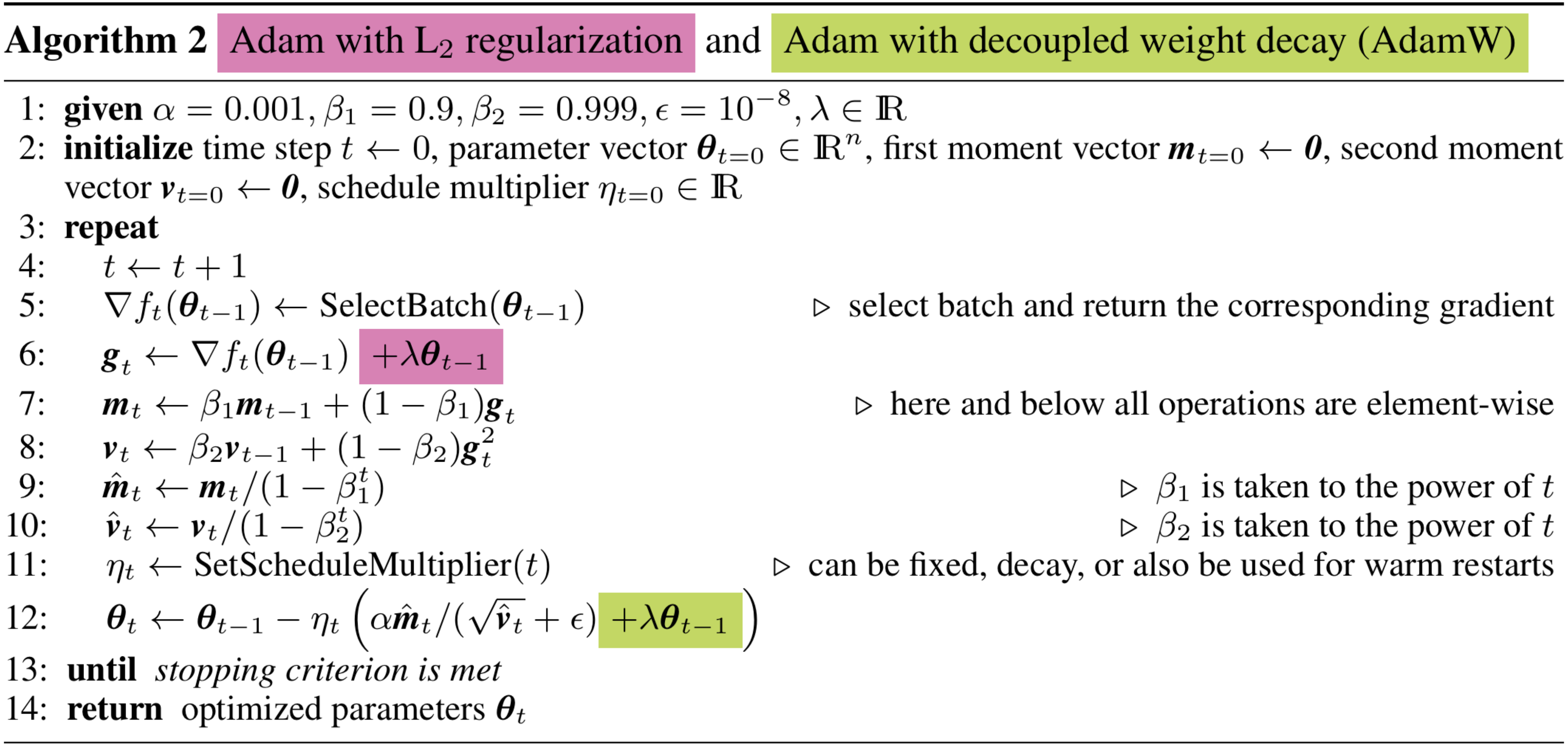
L2 Regularization and Weight Decay are equivalent for SGD, SGD+Momentum so people often use the terms interchangeably!

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

Loshchilov and Hutter, “Decoupled Weight Decay Regularization”, ICLR 2019

AdamW: Decoupled Weight Decay

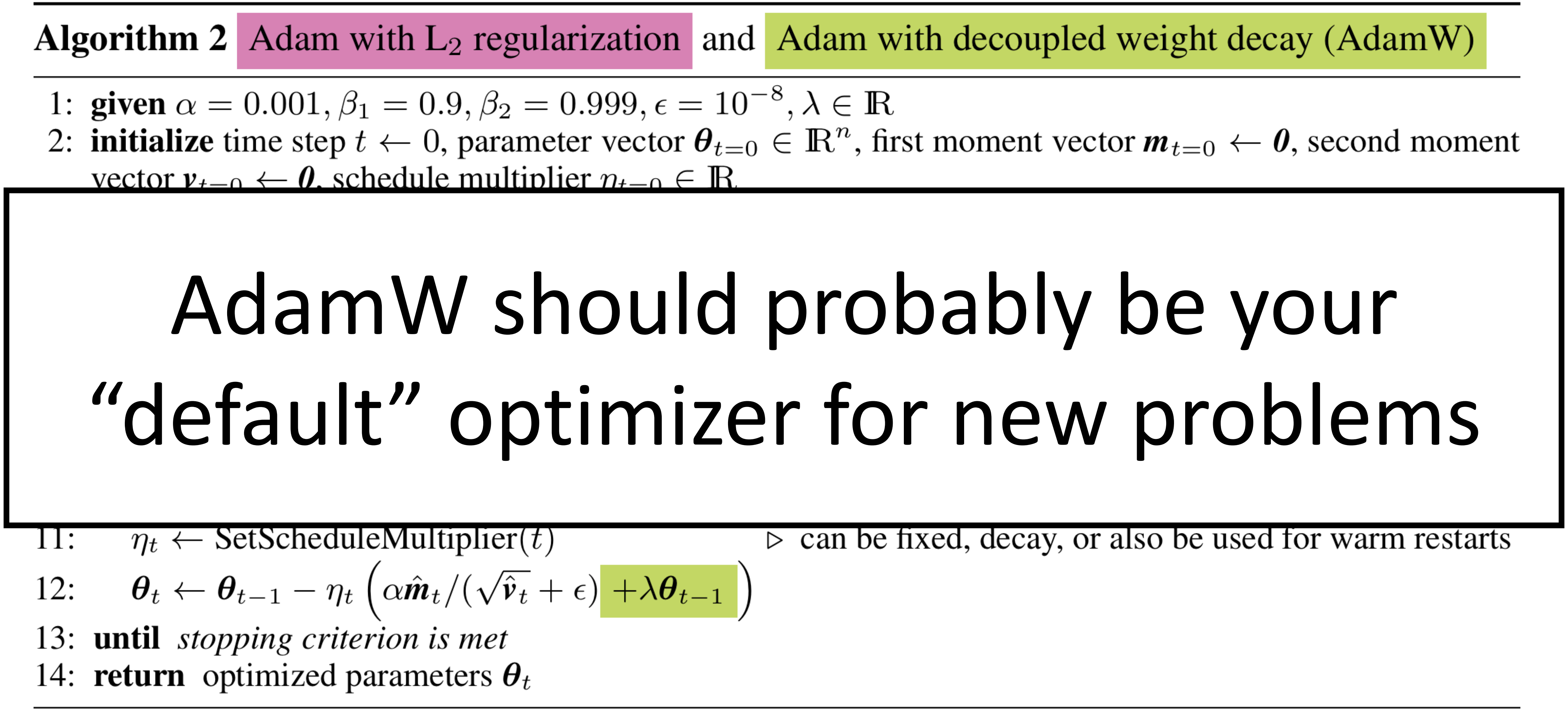


Algorithm 2 Adam with L_2 regularization and Adam with decoupled weight decay (AdamW)

```
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
    $\boldsymbol{v}_t \leftarrow \beta_2 \boldsymbol{v}_{t-1} + (1 - \beta_2)\boldsymbol{g}_t^2$
    $\hat{\boldsymbol{m}}_t \leftarrow \boldsymbol{m}_t / (1 - \beta_1^t)$    ▷ $\beta_1$ is taken to the power of $t$
    $\hat{\boldsymbol{v}}_t \leftarrow \boldsymbol{v}_t / (1 - \beta_2^t)$    ▷ $\beta_2$ 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

AdamW: Decoupled Weight Decay



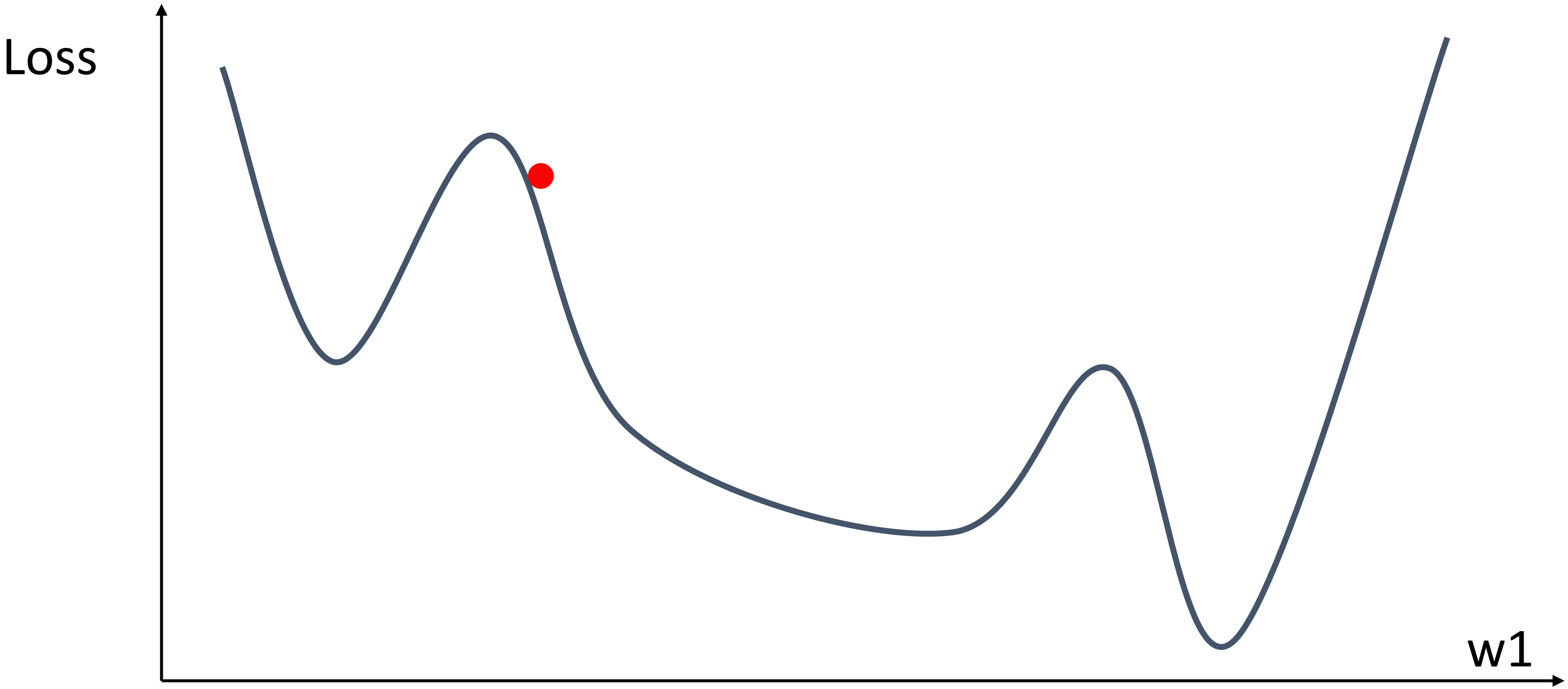
Algorithm 2 Adam with L_2 regularization and Adam with decoupled weight decay (AdamW)

```
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 $\eta_{t=0} \in \mathbb{R}$
    $\eta_t \leftarrow \text{SetScheduleMultiplier}(t)$        ▷ 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 $\boldsymbol{\theta}_t$
```

AdamW should probably be your "default" optimizer for new problems

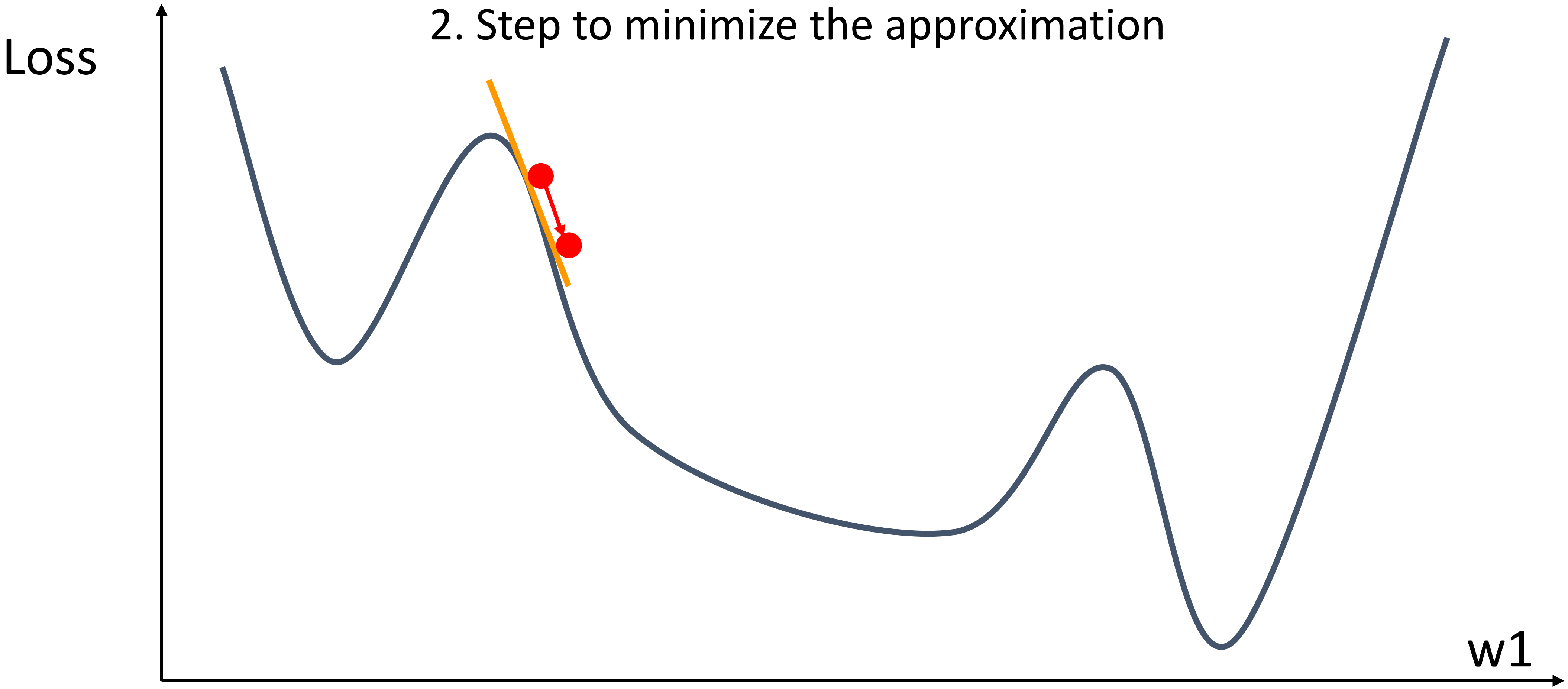
Loshchilov and Hutter, "Decoupled Weight Decay Regularization", ICLR 2019

So far: First-Order Optimization



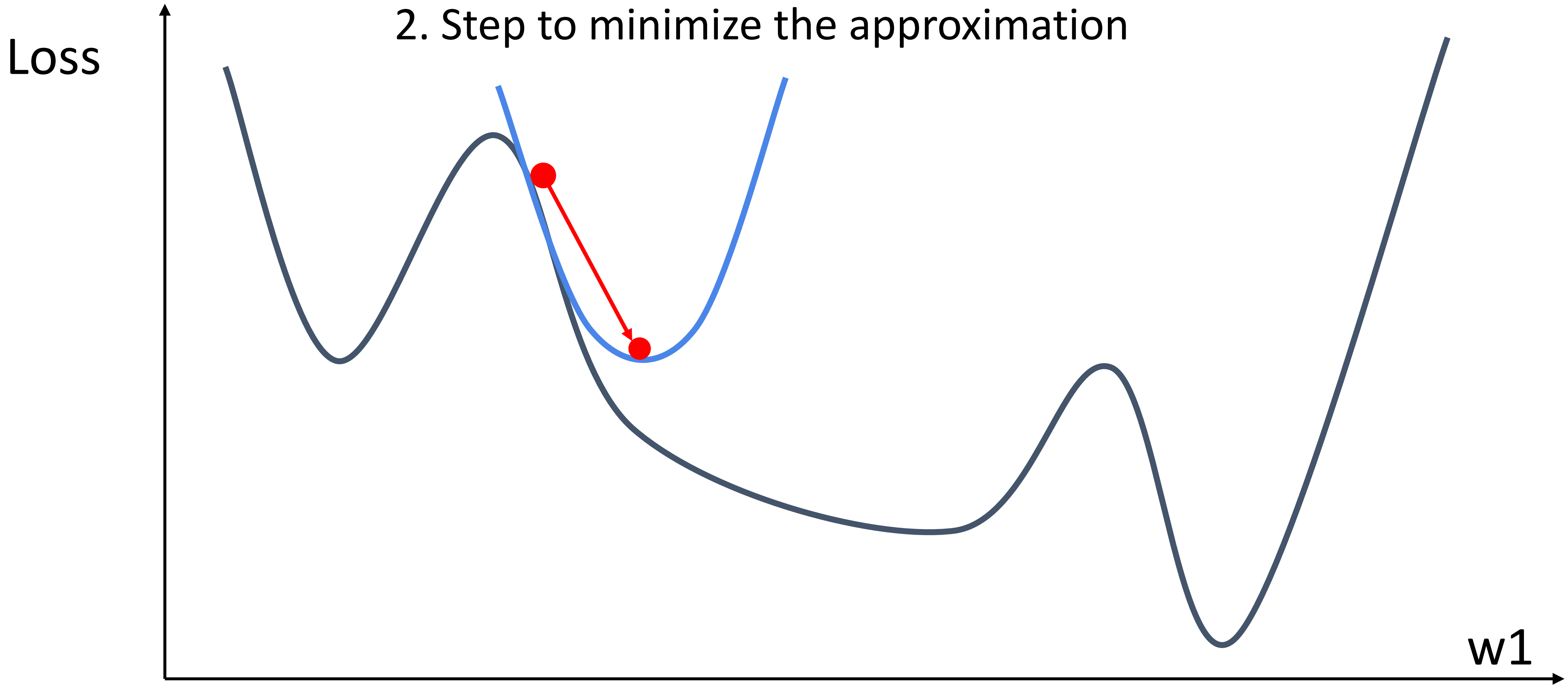
So far: **First-Order** Optimization

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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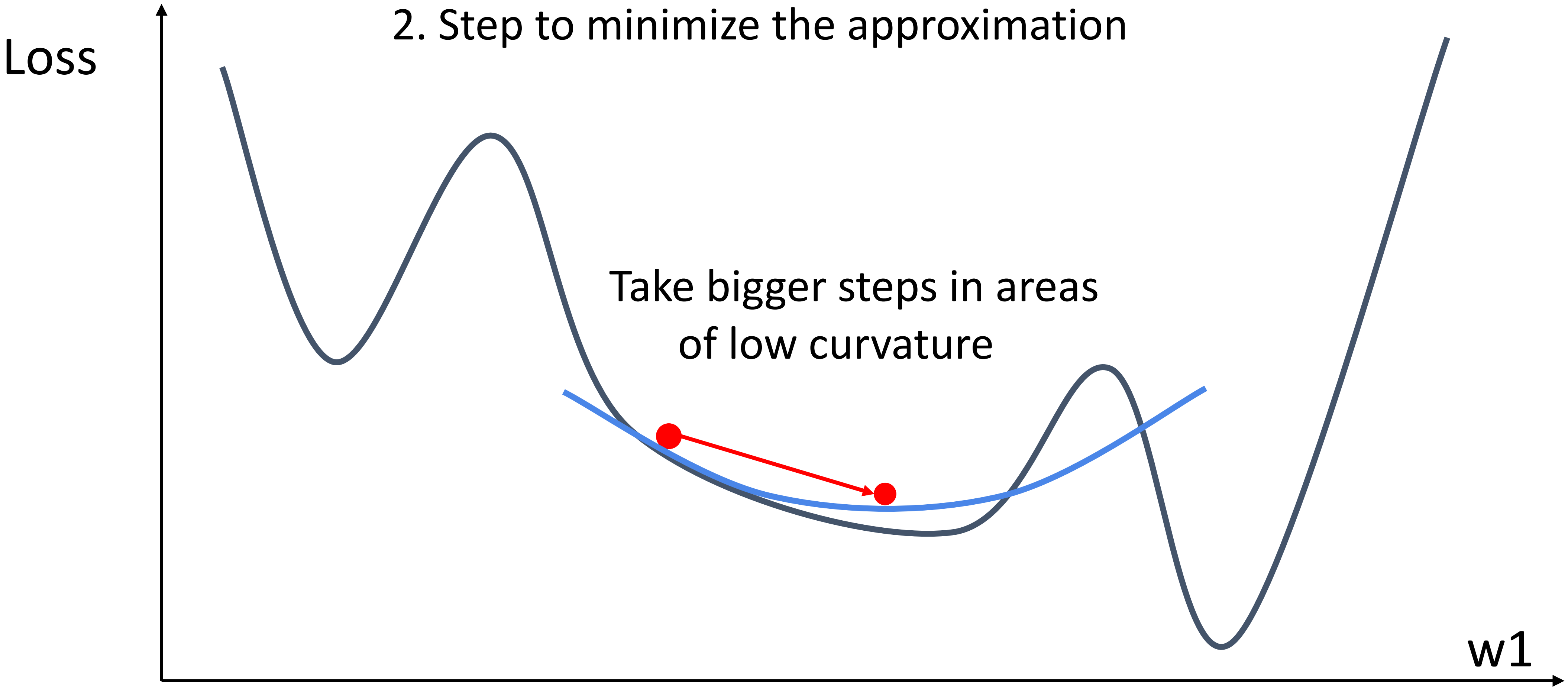

Second-Order Optimization

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:

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

Second-Order Optimization

Second-Order Taylor Expansion:

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Q: Why is this impractical?

Second-Order Optimization

Second-Order Taylor Expansion:

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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.

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

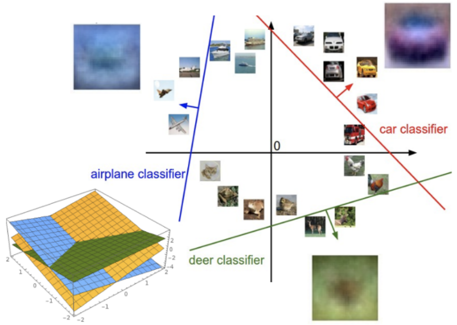
- If you can afford to do full batch updates then try out **L-BFGS** (and don't forget to disable all sources of noise)

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

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

plane
car
bird
cat
deer
dog
frog
horse
ship
truck

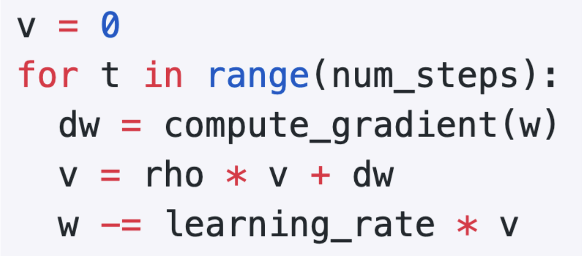


$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$ Softmax

SVM

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

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



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

Next time:
Neural Networks