Optimisation

ACTL3143 & ACTL5111 Deep Learning for Actuaries

Patrick Laub

Warning

This page is out of date for 2024, and will be updated shortly.

Lecture Outline

- **Dense Layers in Matrices**
- Optimisation
- Loss and derivatives

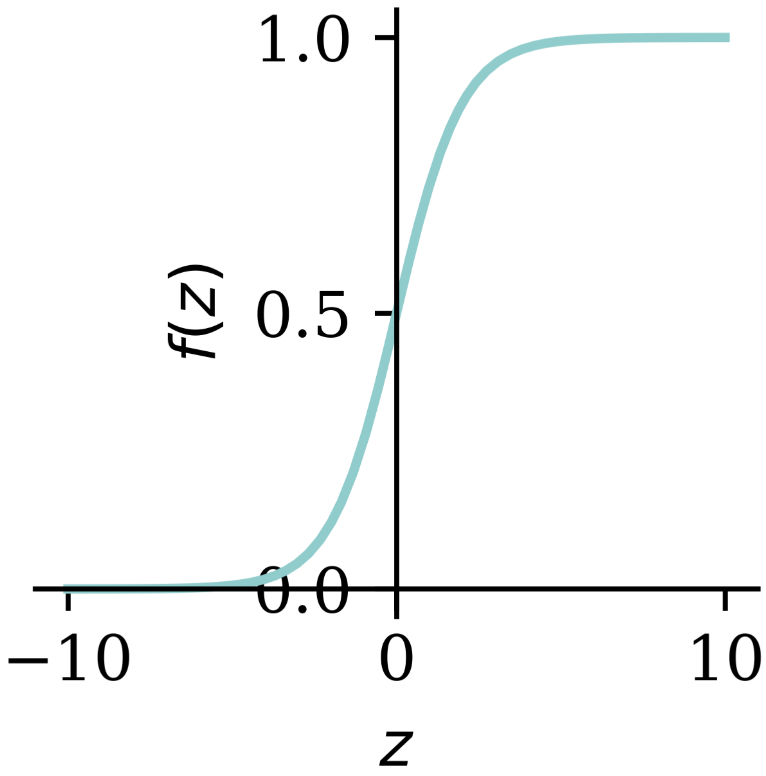
Logistic regression

Observations: $\mathbf{x}_{i,\bullet} \in \mathbb{R}^2$.

Target: $y_i \in \{0, 1\}$.

Predict: $\hat{y}_i = \mathbb{P}(Y_i = 1)$.

```python
import sympy
sympy.plot("1/(1 + exp(-z))");
```



The model

For $\mathbf{x}_{i,\bullet} = (x_{i,1}, x_{i,2})$:

$$z_i = x_{i,1} w_1 + x_{i,2} w_2 + b$$

$$\hat{y}_i = \sigma(z_i) = \frac{1}{1 + \mathrm{e}^{-z_i}}.$$

Multiple observations

```python
data = pd.DataFrame({"x_1": [1, 3, 5], "x_2": [2, 4, 6], "y": [0, 1, 1]})
data
```

	x_1	x_2	y
0	1	2	0
1	3	4	1
2	5	6	1

Let $w_1 = 1$, $w_2 = 2$ and $b = -10$.

```python
w_1 = 1; w_2 = 2; b = -10
data["x_1"] * w_1 + data["x_2"] * w_2 + b
```

```
0   -5
1    1
2    7
dtype: int64
```

Matrix notation

Have $\mathbf{X} \in \mathbb{R}^{3\times 2}$.

```
X_df = data[["x_1", "x_2"]]
X = X_df.to_numpy()
X
```

```
array([[1, 2],
       [3, 4],
       [5, 6]])
```

Let $\mathbf{w} = (w_1, w_2)^\top \in \mathbb{R}^{2\times 1}$.

```
w = np.array([[1], [2]])
w
```

```
array([[1],
       [2]])
```

$$\mathbf{z} = \mathbf{X}\mathbf{w} + b, \quad \mathbf{a} = \sigma(\mathbf{z})$$

```
z = X.dot(w) + b
z
```

```
array([[-5],
       [ 1],
       [ 7]])
```

```
1 / (1 + np.exp(-z))
```

```
array([[0.01],
       [0.73],
       [1.  ]])
```

Using a softmax output

Observations: $\mathbf{x}_{i,\bullet} \in \mathbb{R}^2$. Predict: $\hat{y}_{i,j} = \mathbb{P}(Y_i = j)$.

Target: $\mathbf{y}_{i,\bullet} \in \{(1,0),(0,1)\}$.

The model: For $\mathbf{x}_{i,\bullet} = (x_{i,1}, x_{i,2})$

$$
\begin{aligned}
z_{i,1} &= x_{i,1} w_{1,1} + x_{i,2} w_{2,1} + b_1, \\
z_{i,2} &= x_{i,1} w_{1,2} + x_{i,2} w_{2,2} + b_2.
\end{aligned}
$$

$$
\begin{aligned}
\hat{y}_{i,1} &= \text{Softmax}_1(\mathbf{z}_i) = \frac{\mathrm{e}^{z_{i,1}}}{\mathrm{e}^{z_{i,1}} + \mathrm{e}^{z_{i,2}}}, \\
\hat{y}_{i,2} &= \text{Softmax}_2(\mathbf{z}_i) = \frac{\mathrm{e}^{z_{i,2}}}{\mathrm{e}^{z_{i,1}} + \mathrm{e}^{z_{i,2}}}.
\end{aligned}
$$

Multiple observations

```
data
```

	x_1	x_2	y_1	y_2
0	1	2	1	0
1	3	4	0	1
2	5	6	0	1

Choose:

$w_{1,1} = 1$, $w_{2,1} = 2$,

$w_{1,2} = 3$, $w_{2,2} = 4$, and

$b_1 = -10$, $b_2 = -20$.

```
w_11 = 1; w_21 = 2; b_1 = -10
w_12 = 3; w_22 = 4; b_2 = -20
data["x_1"] * w_11 + data["x_2"] * w_21 + b_1
```

```
0   -5
1    1
2    7
dtype: int64
```

Matrix notation

Have $\mathbf{X} \in \mathbb{R}^{3\times 2}$.

```python
X
```

```
array([[1, 2],
       [3, 4],
       [5, 6]])
```

$\mathbf{W} \in \mathbb{R}^{2\times 2}$, $\mathbf{b} \in \mathbb{R}^2$

```python
W = np.array([[1, 3], [2, 4]])
b = np.array([-10, -20])
display(W); b
```

```
array([[1, 3],
       [2, 4]])
```

```
array([-10, -20])
```

$$\mathbf{Z} = \mathbf{X}\mathbf{W} + \mathbf{b}, \quad \mathbf{A} = \text{Softmax}(\mathbf{Z}).$$

```python
Z = X @ W + b
Z
```

```
array([[-5, -9],
       [ 1,  5],
       [ 7, 19]])
```

```python
np.exp(Z) / np.sum(np.exp(Z),
  axis=1, keepdims=True)
```

```
array([[9.82e-01, 1.80e-02],
       [1.80e-02, 9.82e-01],
       [6.14e-06, 1.00e+00]])
```

Lecture Outline

- Dense Layers in Matrices
- **Optimisation**
- Loss and derivatives

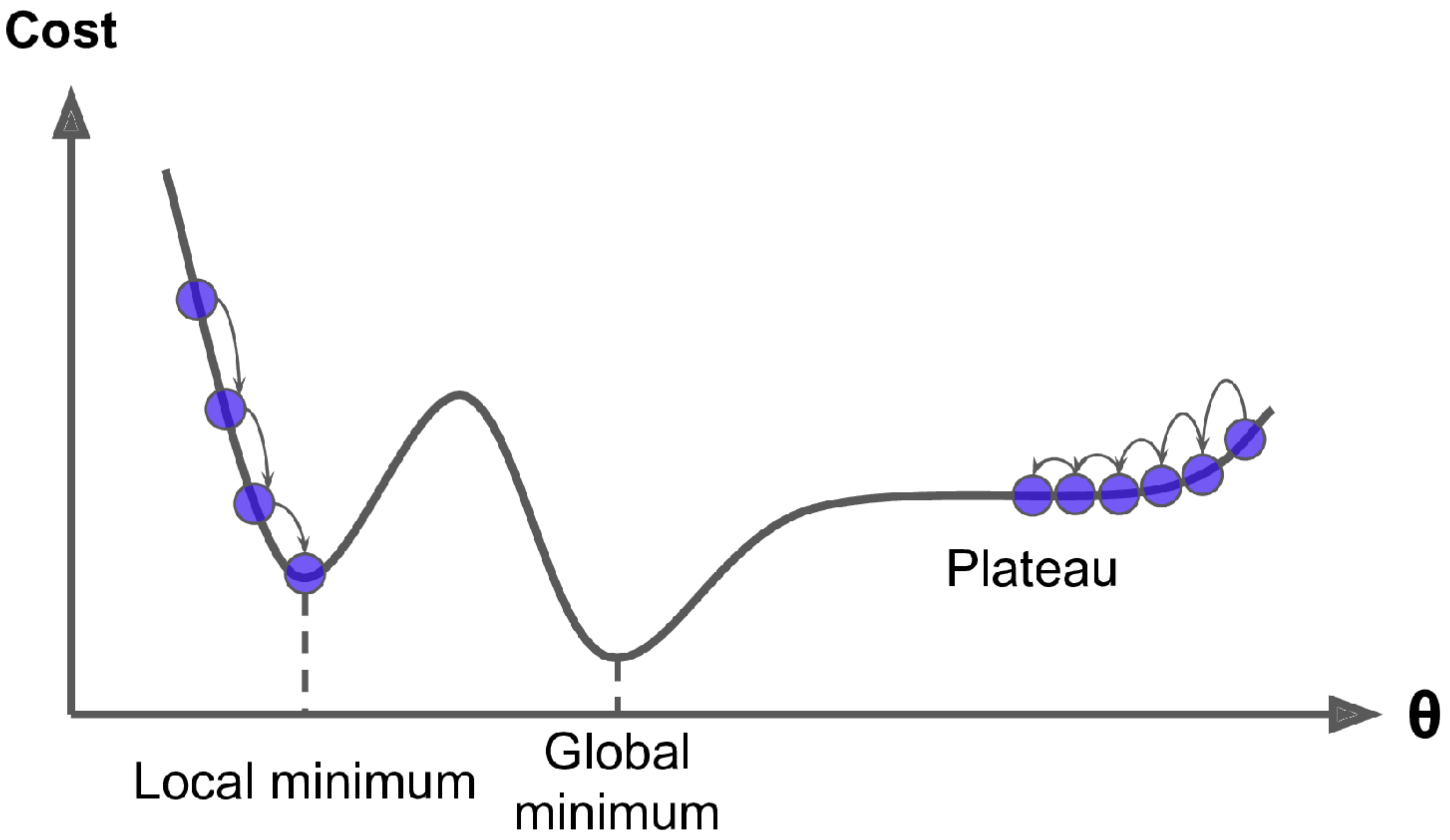
UNSW SYDNEY

Gradient-based learning

Make a guess: 50

Show derivatives: ☐ Reveal function: ☐

Gradient descent pitfalls



Potential problems with gradient descent.

Source: Aurélien Géron (2019), *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, 2nd Edition, Figure 4-6.

Go over all the training data

Called *batch gradient descent*.

```
for i in range(numEpochs):
  gradient = evaluate_gradient(loss_function, data, weights)
  weights = weights - learningRate * gradient
```

Pick a random training example

Called *stochastic gradient descent*.

```
for i in range(numEpochs):
  rnd.shuffle(data)
  for example in data:
    gradient = evaluate_gradient(loss_function, example, weights)
    weights = weights - learningRate * gradient
```

Take a group of training examples

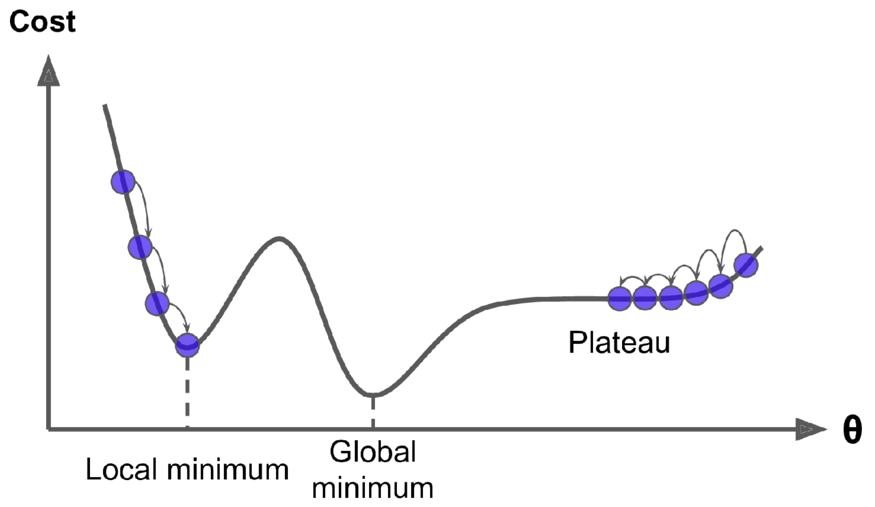
Called *mini-batch gradient descent*.

```python
for i in range(numEpochs):
  rnd.shuffle(data)
  for b in range(numBatches):
    batch = data[b*batchSize:(b+1)*batchSize]
    gradient = evaluate_gradient(loss_function, batch, weights)
    weights = weights - learningRate * gradient
```

Mini-batch gradient descent

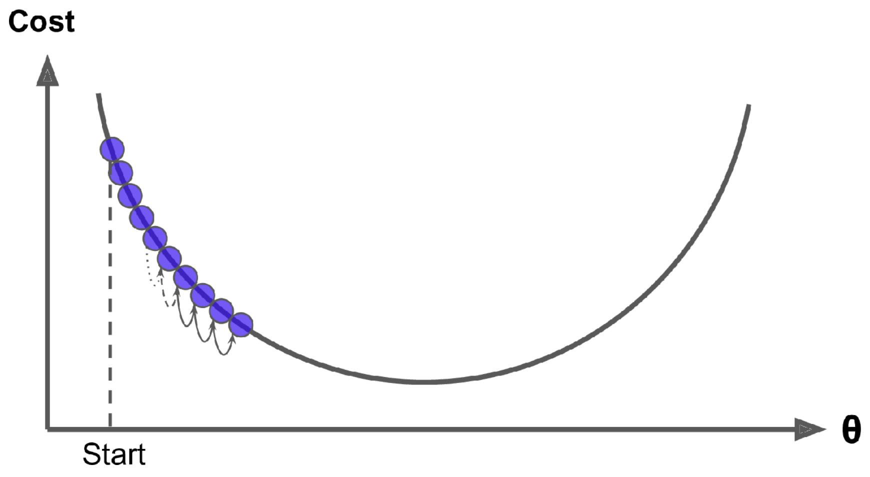
Why?

1. Because we have to (data is too big)
2. Because it is faster (lots of quick noisy steps > a few slow super accurate steps)
3. The noise helps us jump out of local minima

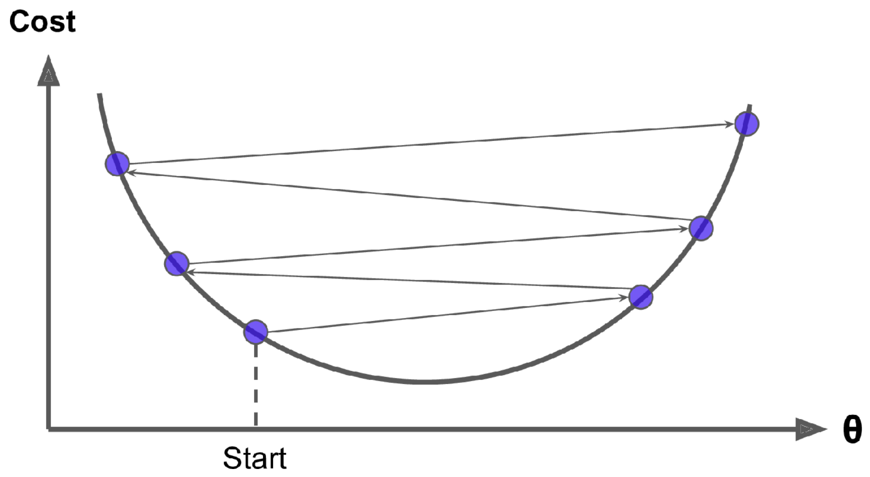


Example of jumping from local minima.

Learning rates



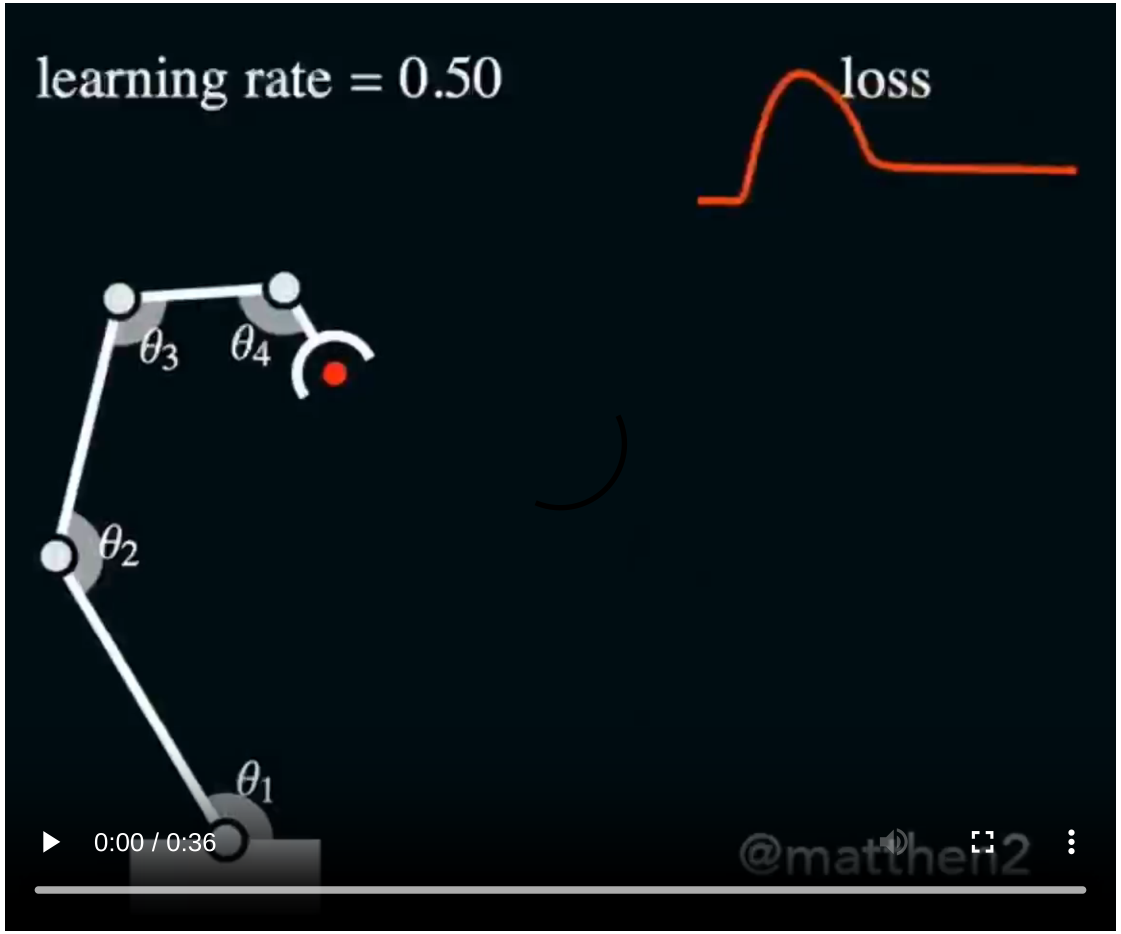
The learning rate is too small



The learning rate is too large

Source: Aurélien Géron (2019), *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, 2nd Edition, Figures 4-4 and 4-5.

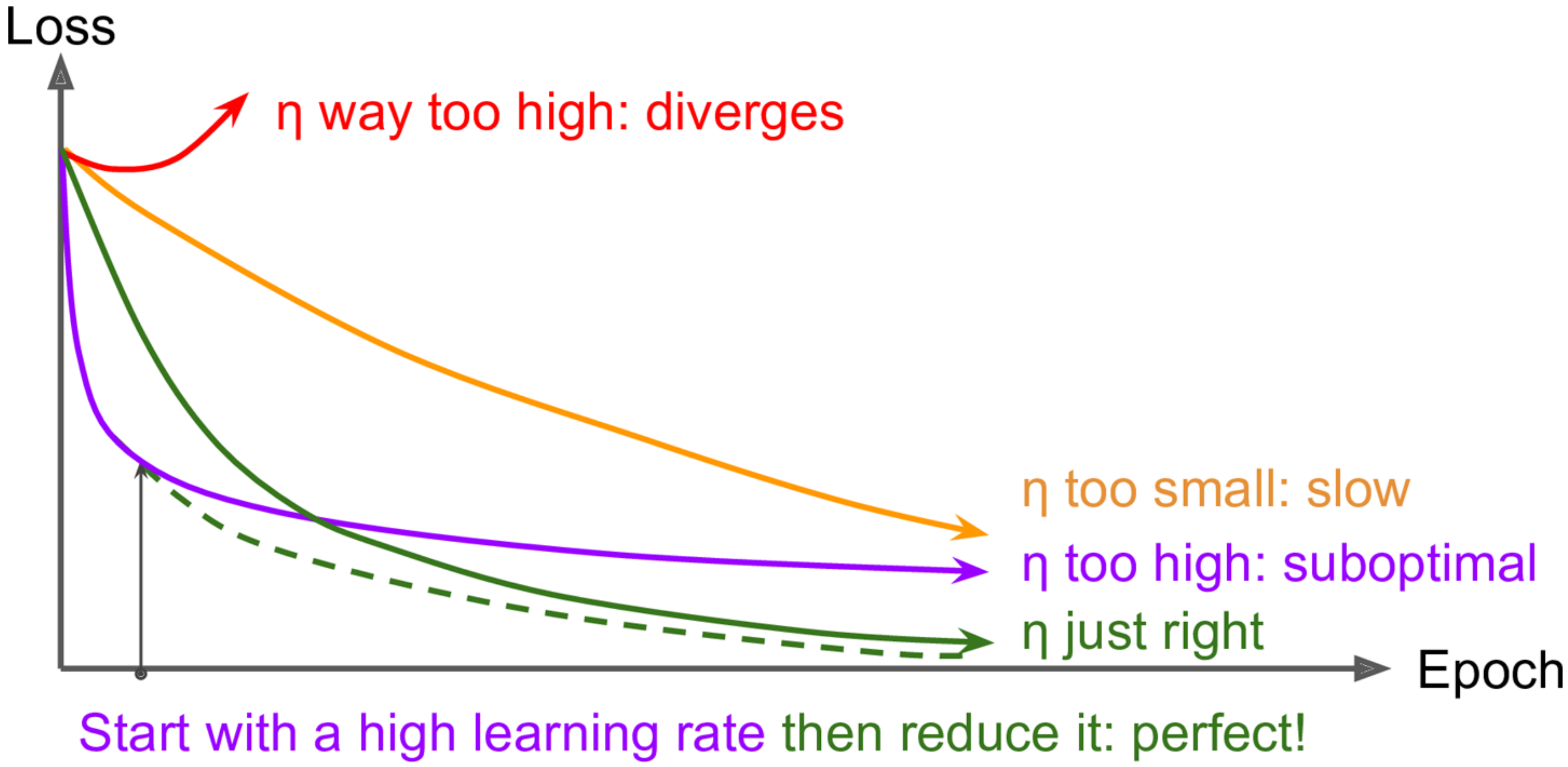
Learning rates #2



Changing the learning rates for a robot arm.

Source: Matt Henderson (2021), Twitter post

Learning rate schedule



Learning curves for various learning rates η

In training the learning rate may be tweaked manually.

Source: Aurélien Géron (2019), *Hands-On Machine Learning with Scikit-Learn, Keras, and TensorFlow*, 2nd Edition, Figure 11-8.

We need non-zero derivatives

This is why can’t use accuracy as the loss function for classification.

Also why we can have the *dead ReLU* problem.

Lecture Outline

- Dense Layers in Matrices
- Optimisation
- **Loss and derivatives**

Example: linear regression

$$\hat{y}(x) = wx + b$$

For some observation $\{x_i, y_i\}$, the (MSE) loss is

$$\text{Loss}_i = (\hat{y}(x_i) - y_i)^2$$

For a batch of the first n observations the loss is

$$\text{Loss}_{1:n} = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}(x_i) - y_i)^2$$

Derivatives

Since $\hat{y}(x) = wx + b$,

$$\frac{\partial \hat{y}(x)}{\partial w} = x \text{ and } \frac{\partial \hat{y}(x)}{\partial b} = 1.$$

As $\text{Loss}_i = (\hat{y}(x_i) - y_i)^2$, we know

$$\frac{\partial \text{Loss}_i}{\partial \hat{y}(x_i)} = 2(\hat{y}(x_i) - y_i).$$

Chain rule

$$\frac{\partial \text{Loss}_i}{\partial \hat{y}(x_i)} = 2(\hat{y}(x_i) - y_i), \quad \frac{\partial \hat{y}(x)}{\partial w} = x, \quad \text{and} \quad \frac{\partial \hat{y}(x)}{\partial b} = 1.$$

Putting this together, we have

$$\frac{\partial \text{Loss}_i}{\partial w} = \frac{\partial \text{Loss}_i}{\partial \hat{y}(x_i)} \times \frac{\partial \hat{y}(x_i)}{\partial w} = 2(\hat{y}(x_i) - y_i)\, x_i$$

and

$$\frac{\partial \text{Loss}_i}{\partial b} = \frac{\partial \text{Loss}_i}{\partial \hat{y}(x_i)} \times \frac{\partial \hat{y}(x_i)}{\partial b} = 2(\hat{y}(x_i) - y_i).$$

Stochastic gradient descent (SGD)

Start with $\boldsymbol{\theta}_0 = (w, b)^\top = (0, 0)^\top$.

Randomly pick $i = 5$, say $x_i = 5$ and $y_i = 5$.

$$\hat{y}(x_i) = 0 \times 5 + 0 = 0 \Rightarrow \text{Loss}_i = (0 - 5)^2 = 25.$$

The partial derivatives are

$$\begin{aligned}\frac{\partial \text{Loss}_i}{\partial w} &= 2(\hat{y}(x_i) - y_i)\, x_i = 2 \cdot (0 - 5) \cdot 5 = -50, \text{ and}\\ \frac{\partial \text{Loss}_i}{\partial b} &= 2(0 - 5) = -10.\end{aligned}$$

The gradient is $\nabla \text{Loss}_i = (-50, -10)^\top$.

SGD, first iteration

Start with $\boldsymbol{\theta}_0 = (w, b)^\top = (0, 0)^\top$.

Randomly pick $i = 5$, say $x_i = 5$ and $y_i = 5$.

The gradient is $\nabla \text{Loss}_i = (-50, -10)^\top$.

Use learning rate $\eta = 0.01$ to update

$$
\begin{aligned}
\boldsymbol{\theta}_1 &= \boldsymbol{\theta}_0 - \eta \nabla \text{Loss}_i \\
&= \begin{pmatrix} 0 \\ 0 \end{pmatrix} - 0.01 \begin{pmatrix} -50 \\ -10 \end{pmatrix} \\
&= \begin{pmatrix} 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 0.5 \\ 0.1 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.1 \end{pmatrix}.
\end{aligned}
$$

SGD, second iteration

Start with $\boldsymbol{\theta}_1 = (w, b)^\top = (0.5, 0.1)^\top$.

Randomly pick $i = 9$, say $x_i = 9$ and $y_i = 17$.

The gradient is $\nabla \text{Loss}_i = (-223.2, -24.8)^\top$.

Use learning rate $\eta = 0.01$ to update

$$\begin{aligned}
\boldsymbol{\theta}_2 &= \boldsymbol{\theta}_1 - \eta \nabla \text{Loss}_i \\
&= \begin{pmatrix} 0.5 \\ 0.1 \end{pmatrix} - 0.01 \begin{pmatrix} -223.2 \\ -24.8 \end{pmatrix} \\
&= \begin{pmatrix} 0.5 \\ 0.1 \end{pmatrix} + \begin{pmatrix} 2.232 \\ 0.248 \end{pmatrix} = \begin{pmatrix} 2.732 \\ 0.348 \end{pmatrix}.
\end{aligned}$$

Batch gradient descent (BGD)

For the first n observations $\text{Loss}_{1:n} = \frac{1}{n}\sum_{i=1}^{n}\text{Loss}_i$ so

$$\begin{aligned}\frac{\partial \text{Loss}_{1:n}}{\partial w} &= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial \text{Loss}_i}{\partial w} = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial \text{Loss}_i}{\hat{y}(x_i)}\frac{\partial \hat{y}(x_i)}{\partial w} \\ &= \frac{1}{n}\sum_{i=1}^{n} 2(\hat{y}(x_i) - y_i)\, x_i .\end{aligned}$$

$$\begin{aligned}\frac{\partial \text{Loss}_{1:n}}{\partial b} &= \frac{1}{n}\sum_{i=1}^{n}\frac{\partial \text{Loss}_i}{\partial b} = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial \text{Loss}_i}{\hat{y}(x_i)}\frac{\partial \hat{y}(x_i)}{\partial b} \\ &= \frac{1}{n}\sum_{i=1}^{n} 2(\hat{y}(x_i) - y_i).\end{aligned}$$

BGD, first iteration ($\boldsymbol{\theta}_0 = \mathbf{0}$)

	x	y	y_hat	loss	dL/dw	dL/db
0	1	0.99	0	0.98	-1.98	-1.98
1	2	3.00	0	9.02	-12.02	-6.01
2	3	5.01	0	25.15	-30.09	-10.03

So $\nabla \text{Loss}_{1:3}$ is

```
nabla = np.array([df["dL/dw"].mean(), df["dL/db"].mean()])
nabla
```

```
array([-14.69,  -6.  ])
```

so with $\eta = 0.1$ then $\boldsymbol{\theta}_1$ becomes

```
theta_1 = theta_0 - 0.1 * nabla
theta_1
```

```
array([1.47, 0.6 ])
```

BGD, second iteration

	x	y	y_hat	loss	dL/dw	dL/db
0	1	0.99	2.07	1.17	2.16	2.16
1	2	3.00	3.54	0.29	2.14	1.07
2	3	5.01	5.01	0.00	-0.04	-0.01

So $\nabla \text{Loss}_{1:3}$ is

```
nabla = np.array([df["dL/dw"].mean(), df["dL/db"].mean()])
nabla
```

```
array([1.42, 1.07])
```

so with $\eta = 0.1$ then $\boldsymbol{\theta}_2$ becomes

```
theta_2 = theta_1 - 0.1 * nabla
theta_2
```

```
array([1.33, 0.49])
```

Glossary

- batches, batch size
- gradient-based learning, hill-climbing
- metrics
- stochastic (mini-batch) gradient descent