Optimisation

ACTL3143 & ACTL5111 Deep Learning for Actuaries

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

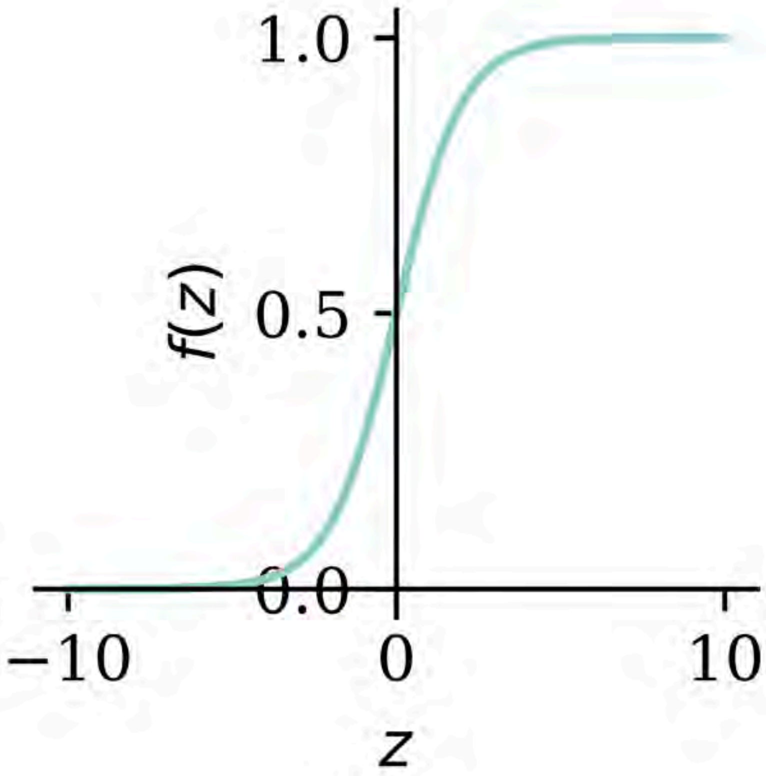
The model

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

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

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

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



Multiple observations

```
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 $b = -10$.

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

$$z_{i,1} = x_{i,1} w_{1,1} + x_{i,2} w_{2,1} + b_1,$$
$$z_{i,2} = x_{i,1} w_{1,2} + x_{i,2} w_{2,2} + b_2.$$

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

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]])
```

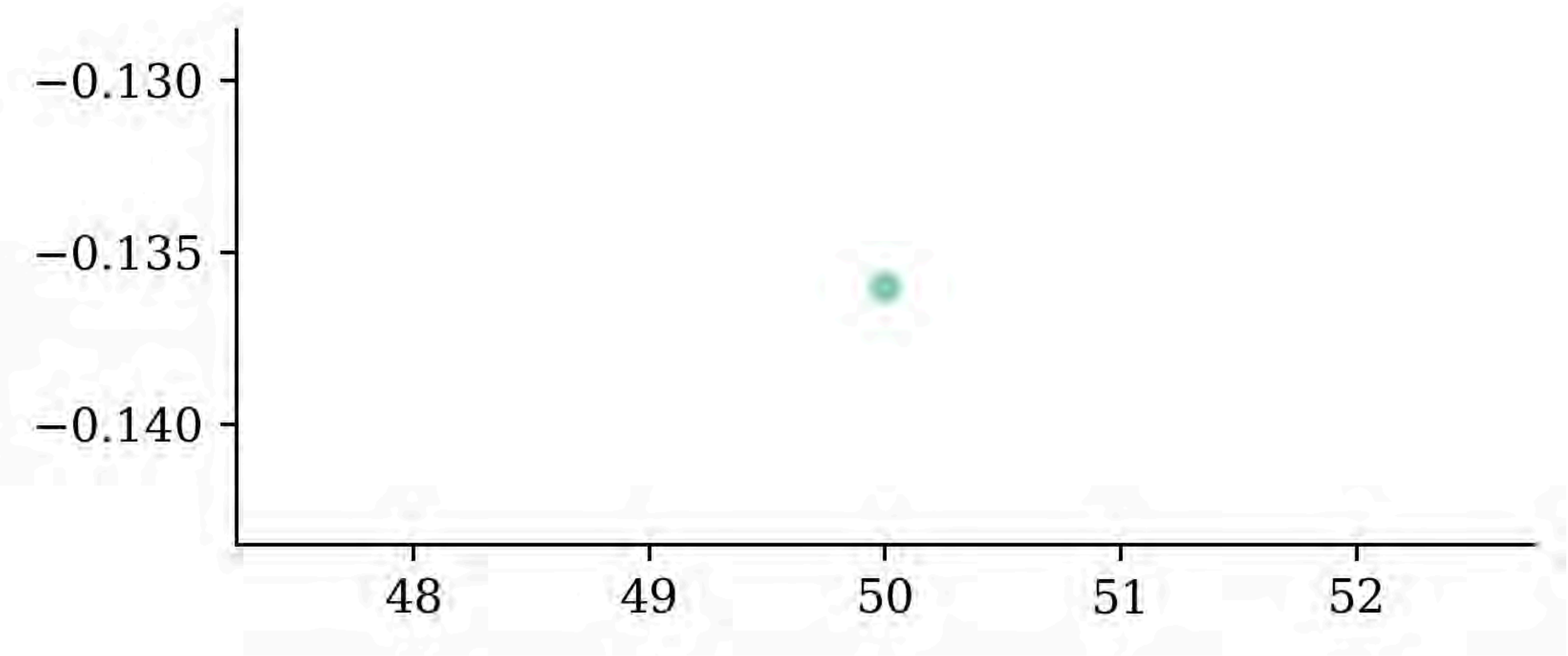
Lecture Outline

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

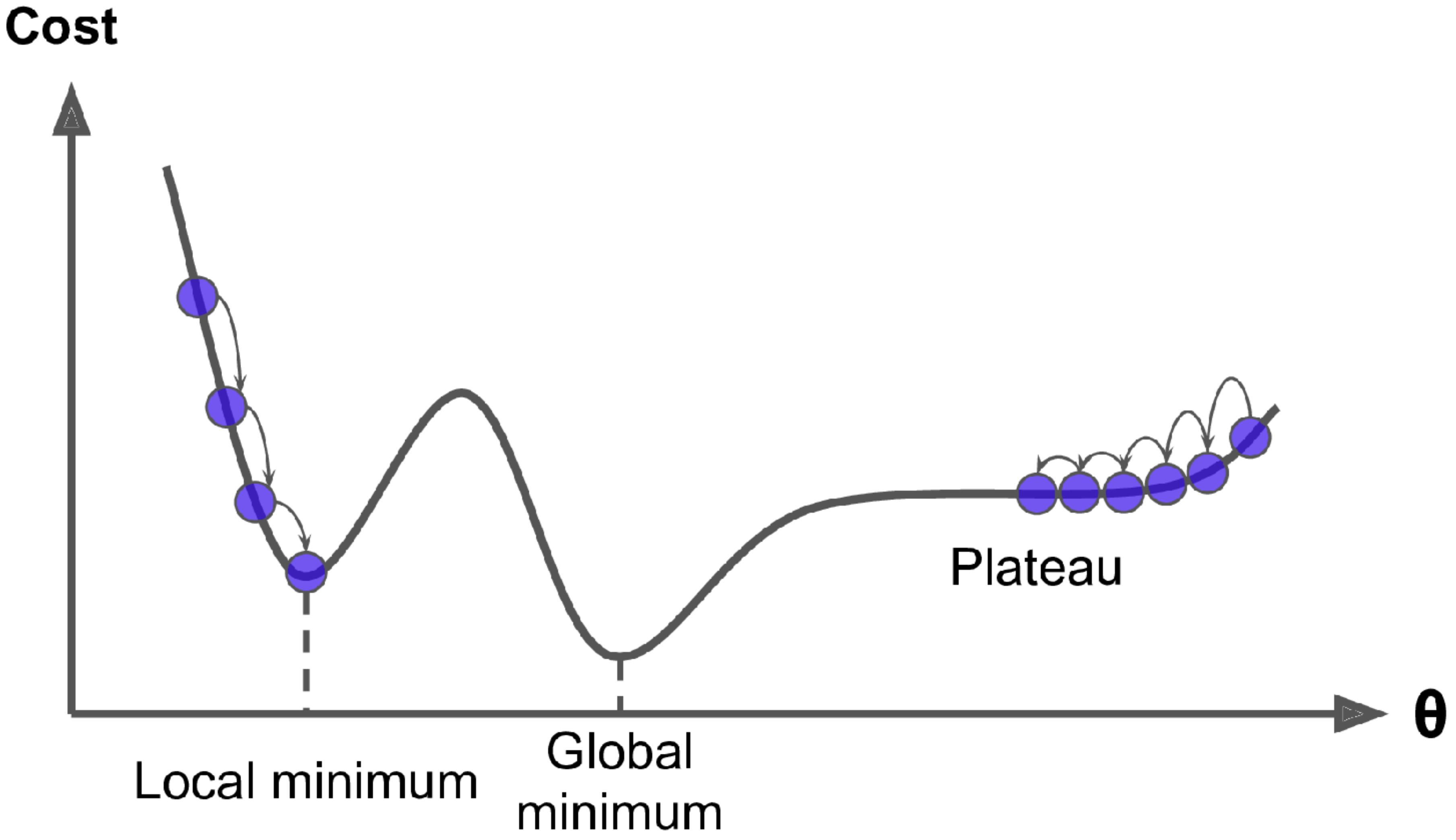
Gradient-based learning

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(num_epochs):
    gradient = evaluate_gradient(loss_function, data, weights)
    weights = weights - learning_rate * gradient
```

Pick a random training example

Called *stochastic gradient descent*.

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

Take a group of training examples

Called *mini-batch gradient descent*.

```python
for i in range(num_epochs):
    rnd.shuffle(data)
    for b in range(num_batches):
        batch = data[b * batch_size : (b + 1) * batch_size]
        gradient = evaluate_gradient(loss_function, batch, weights)
        weights = weights - learning_rate * gradient
```

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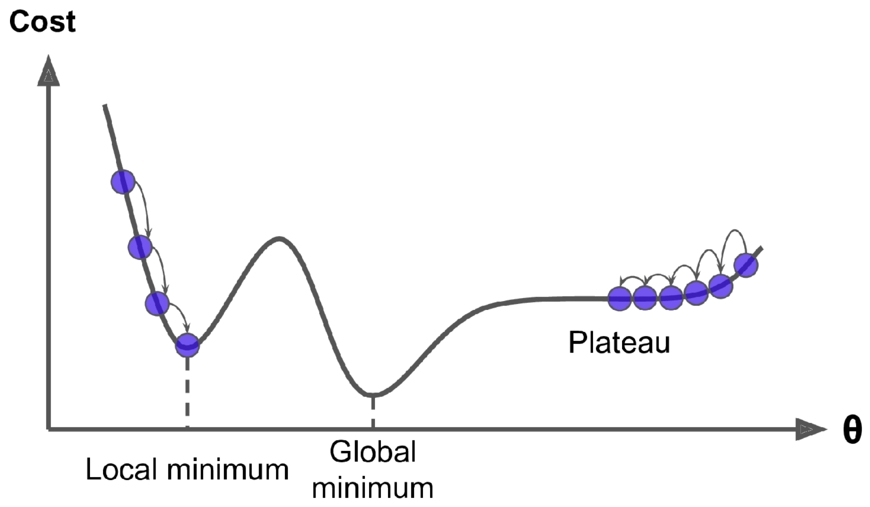
Mini-batch gradient descent

Why?

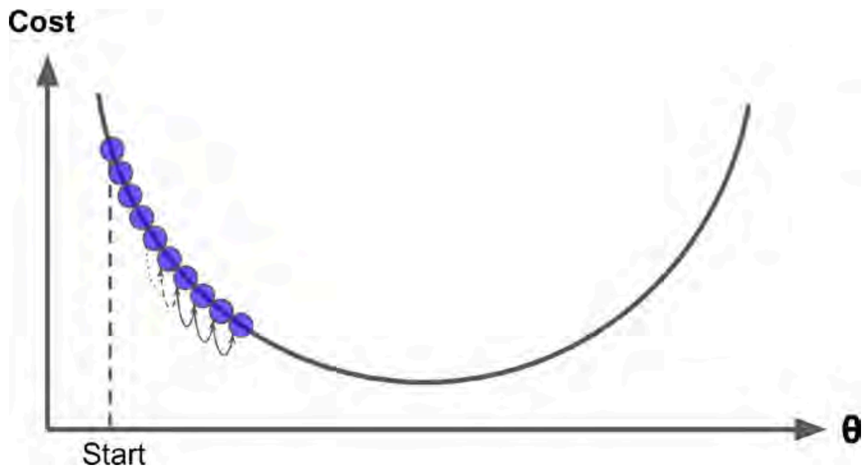
1. Because we have to (data is too big)
2. Because it is faster (lots of quick noisy steps > a few slow super accurate steps)
3. The noise helps us jump out of local minima



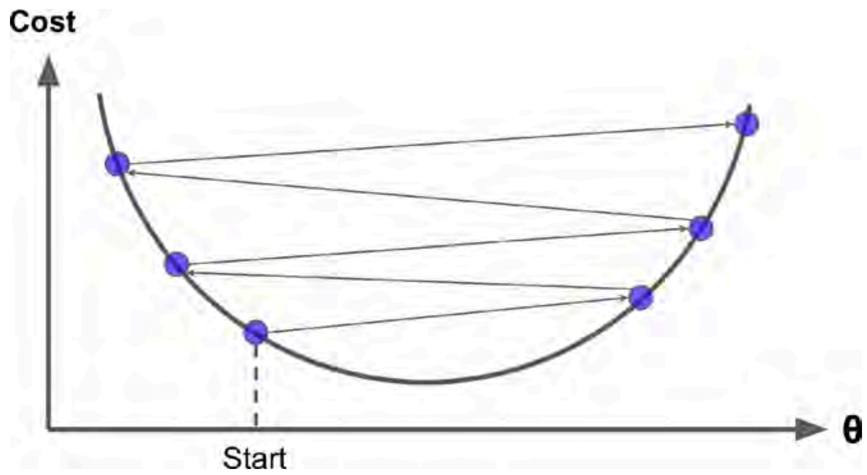
Example of jumping from local minima.

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

Learning rates



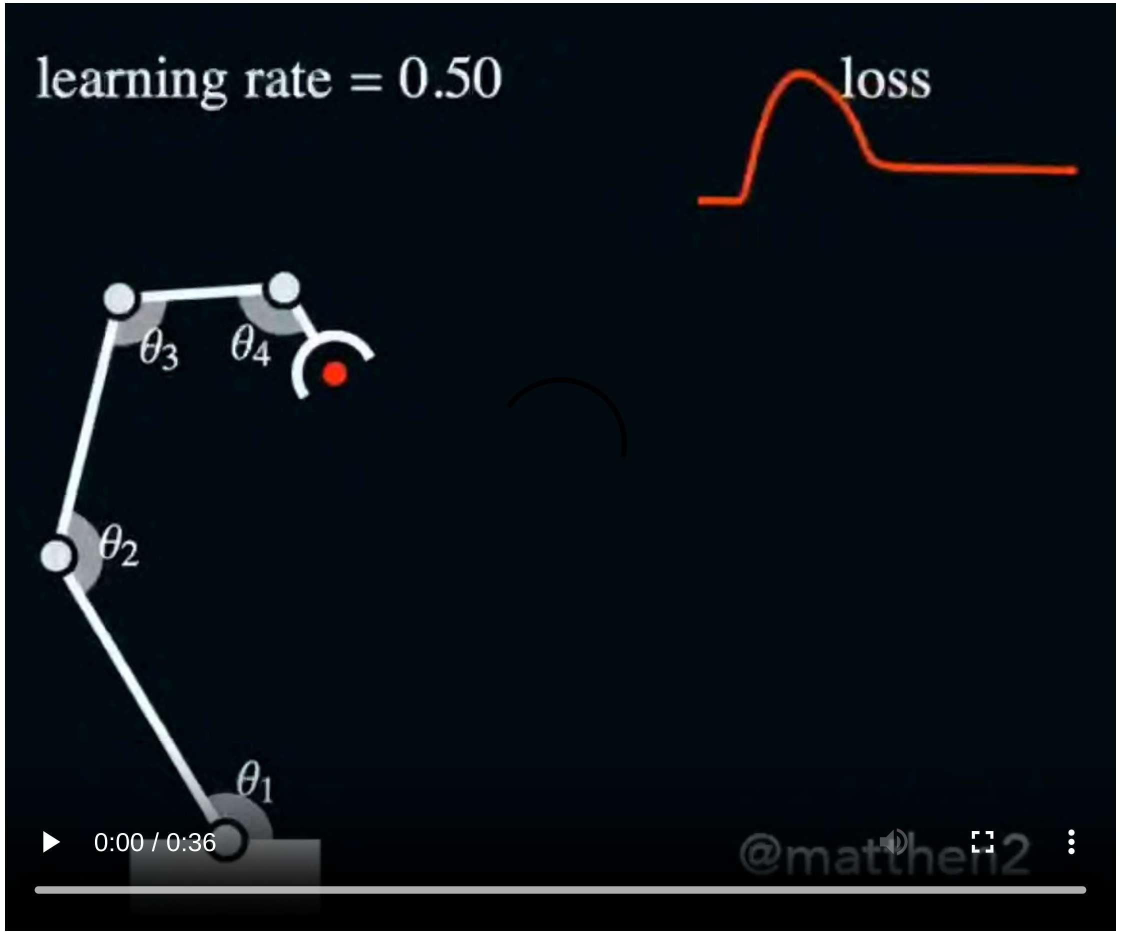
The learning rate is too small



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.

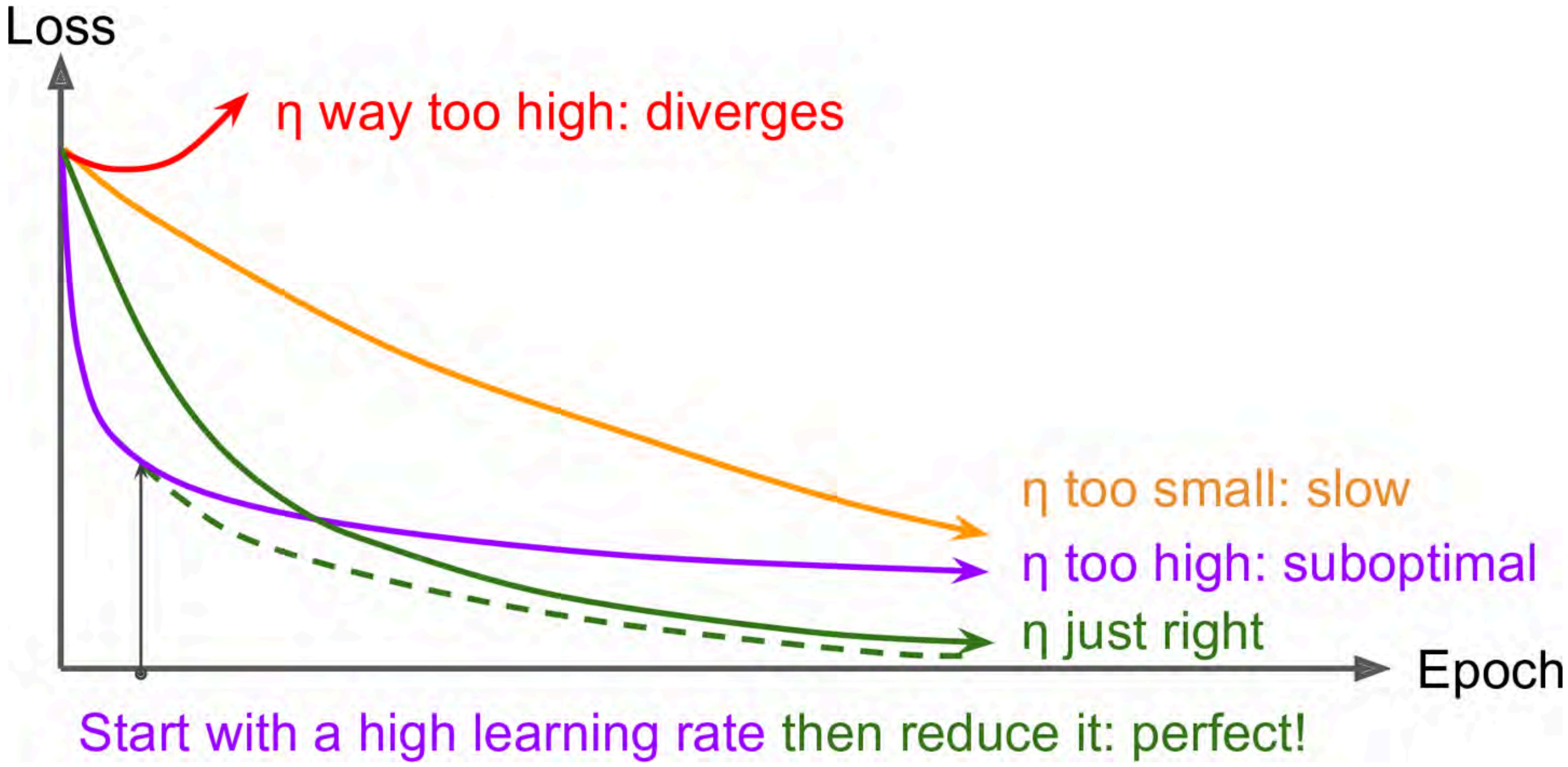
Learning rates #2



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

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

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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

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

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Stochastic gradient descent (SGD)

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

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

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

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

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

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])
```

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Glossary

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