深度學習
Deep Learning

常見目標函數

Instructor: 林英嘉 (Ying-Jia Lin)
2025/10/01

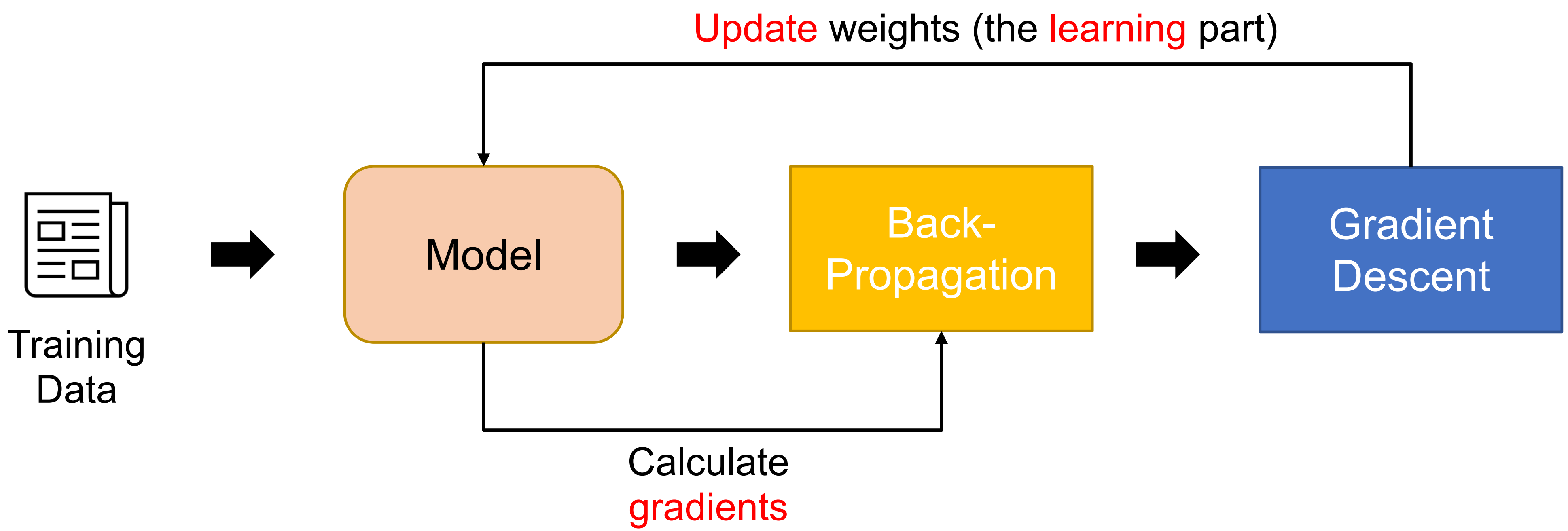
[Course GitHub]

[Slido # DL1001]

Outline

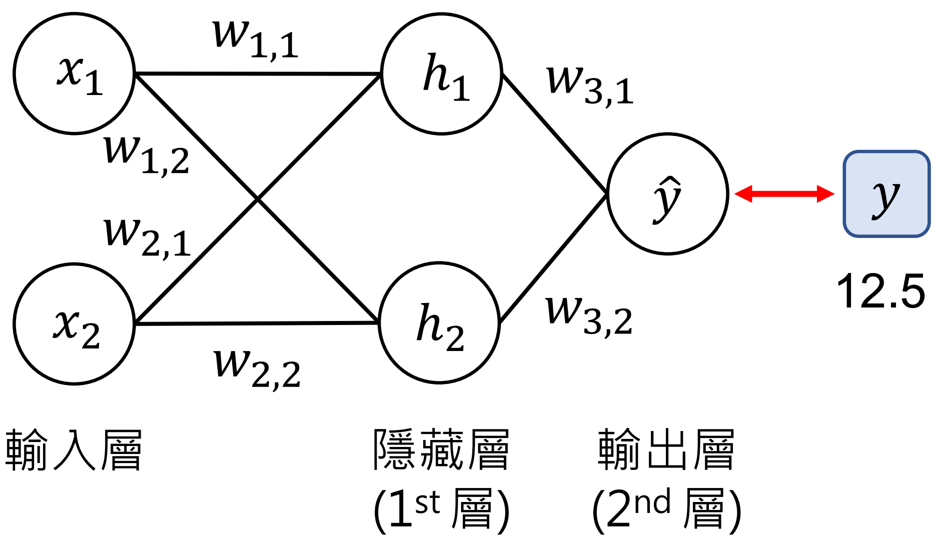
- Common objective functions [60 min]
- PyTorch modeling [60 min]
  - PyTorch modeling code using MNIST
  - PyTorch Gradient Descent code (if we have time)
- Quiz [20 min]

[Recap] 深度學習模型訓練流程



Forward Pass and Objective Function

由輸入層到輸出層進行



迴歸任務：使用 Mean Squared Error (MSE) 作為目標函數

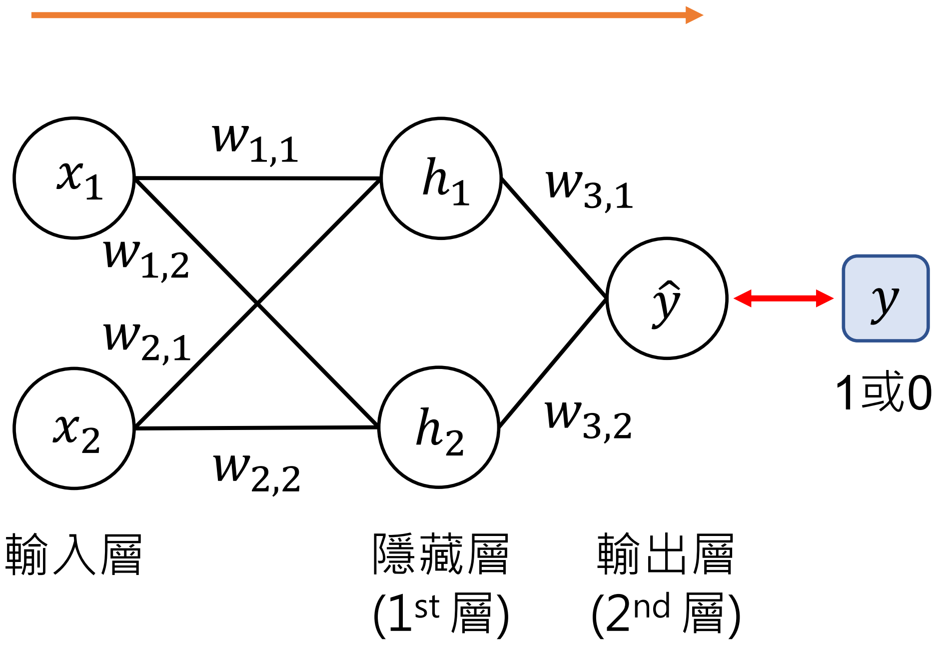
$$h_1 = w_{1,1}x_1 + w_{2,1}x_2 + b_1$$

$$h_2 = w_{1,2}x_1 + w_{2,2}x_2 + b_2$$

$$\hat{y} = w_{3,1}h_1 + w_{3,2}h_2 + b_3$$

Forward Pass and Objective Function

由輸入層到輸出層進行



分類任務：使用 Cross-entropy 作為目標函數

$$h_1 = w_{1,1}x_1 + w_{2,1}x_2 + b_1$$

$$h_2 = w_{1,2}x_1 + w_{2,2}x_2 + b_2$$

$$\hat{y} = w_{3,1}h_1 + w_{3,2}h_2 + b_3$$

Entropy (資訊理論)

- Entropy (熵): 定義為不確定性的量度
- 特性：
  - 越不可能發生的事情，當它發生了，越會提供更多的資訊，entropy 就越高
- Claude Shannon 將熱力學的熵引入到資訊理論 – 夏農熵 (Shannon entropy)

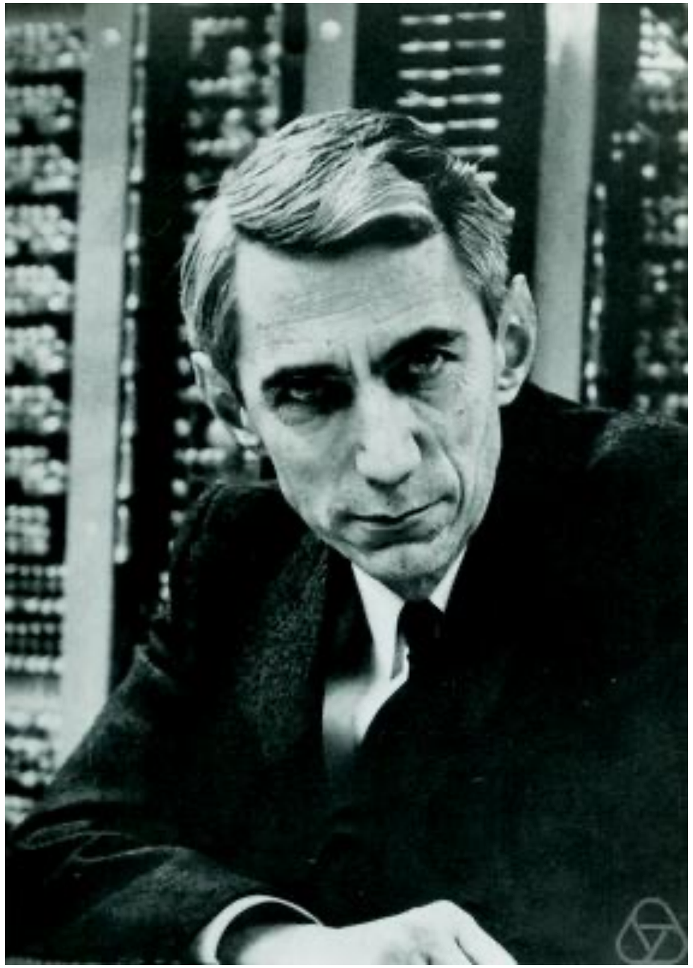
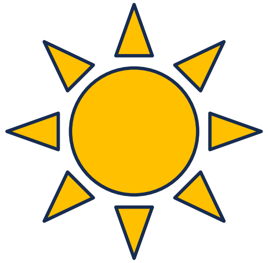
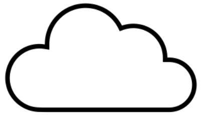


Figure source: https://www.itsoc.org/about/shannon

[定義] 事件發生的機率越低代表資訊量越高

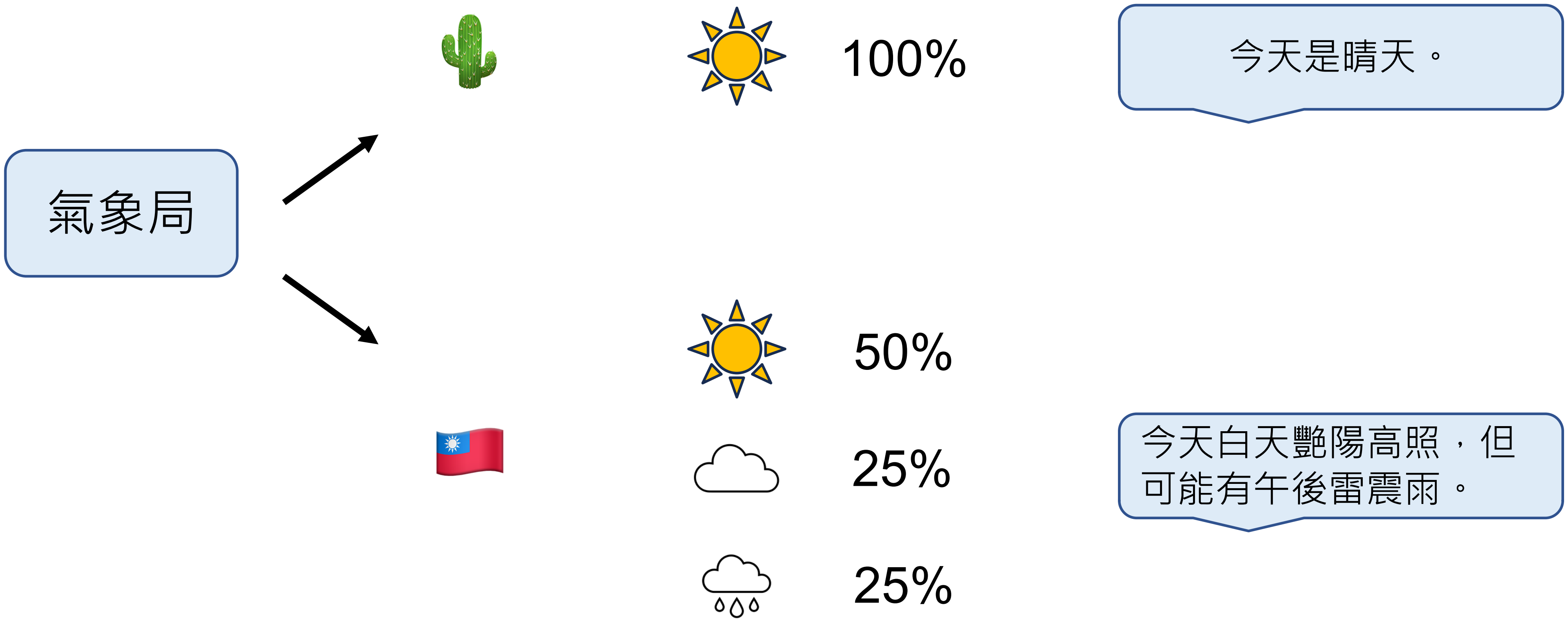
	機率 (P)	資訊量 1 / P
	50%	2
	25%	4
	25%	4

從通訊的角度理解 Entropy

Figure source: https://newsweb.ncc.gov.tw/201910/ch4.html

通訊傳輸

越不驚訝的資訊，傳遞的資訊量越少，可以節省通訊傳輸成本。



Entropy：最低的傳輸成本

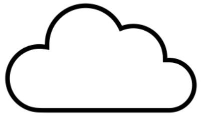
Entropy **=** 每個事件發生的**機率** **x** log(每個事件發生的**資訊量**)

$$= H(P) = P \times \log_2 \frac{1}{P}$$ <- 通常是自然對數，本堂課以2為底數作為範例

$$= -P \times \log_2 P$$

Entropy：最低的傳輸成本 (以🇹🇼為例)

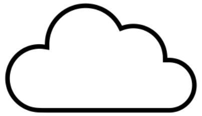
$$\text{Entropy} = H(P) = P \times \log_2 \frac{1}{P}$$

	機率 (P)	**1 / P**	$\log_2 \frac{1}{P}$	**H(P)**
	50%	2	1	0.5
	25%	4	2	0.5
	25%	4	2	0.5

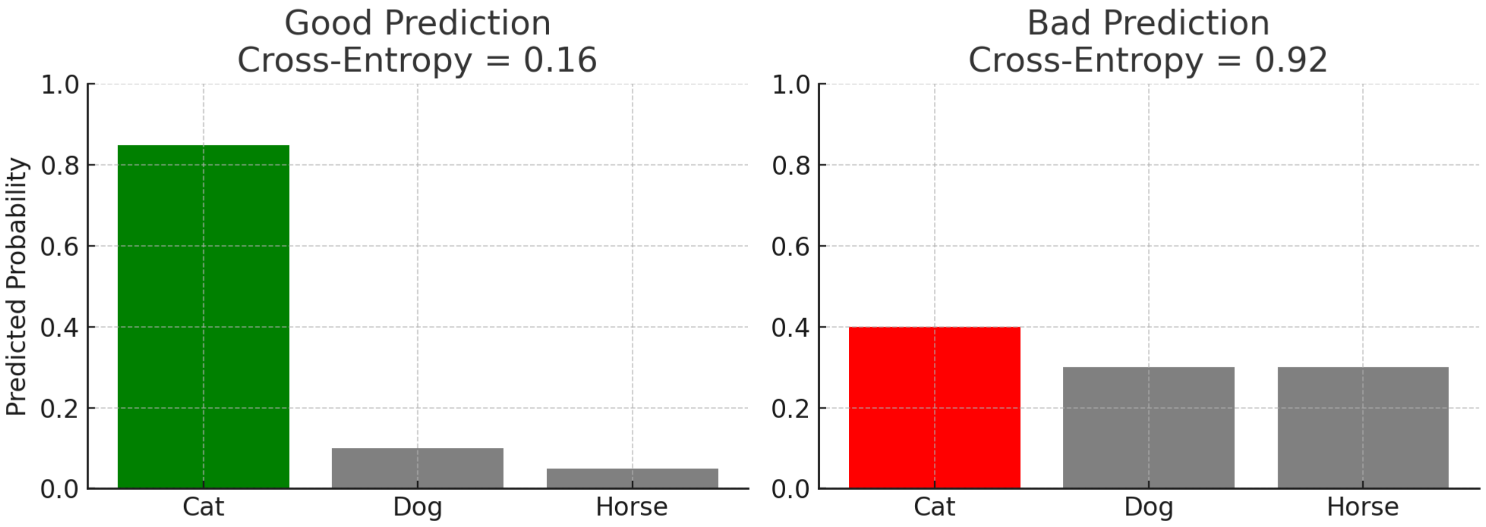
1.5 bits

Entropy：最低的傳輸成本 (以🌵為例)

$$\text{Entropy} = H(P) = P \times \log_2 \frac{1}{P}$$

	機率 (P)	1 / P	$\log_2 \frac{1}{P}$	H(P)	
	100%	1	0	0	
	0%	0	0	0	0 bits
	0%	0	0	0	

從ML的角度理解 Cross-Entropy



Cross-Entropy：可能不是最低的傳輸成本

Entropy = 每個事件發生的**機率** x log(每個事件發生的**資訊量**)

Cross-Entropy = 每個事件發生的**機率** x log(預測每個事件發生的**資訊量**)

交叉熵

$$= H(P,Q) = P\times\log_2\frac{1}{Q}$$

<- 通常是自然對數，本堂課以2為底數作為範例

$$= -P\times\log_2 Q$$

<- P 是每個事件發生的機率，
Q 是預測每個事件發生的機率

Cross-entropy (Case1)

$$H(P,Q) = P \times \log_2 \frac{1}{Q}$$

	機率 (P)	機率 (Q)	1 / Q	$\log_2 \frac{1}{Q}$	H(P, Q)
	50%	25%	4	2	1
	25%	25%	4	2	0.5
	25%	50%	2	1	0.25

1.75 bits

Cross-entropy (Case2)

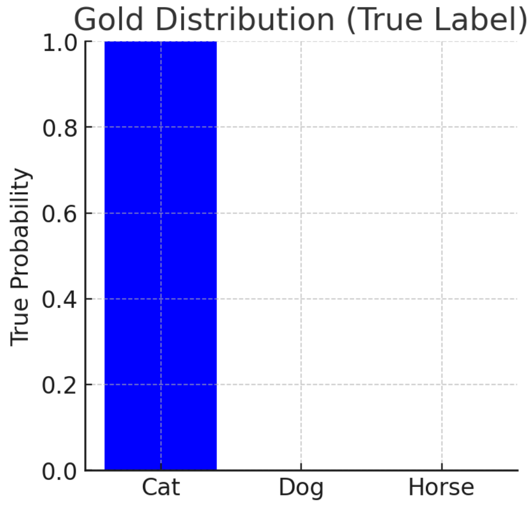
$$H(P, Q) = P \times \log_2 \frac{1}{Q}$$

	機率 (P)	機率 (Q)	1 / Q	$\log_2 \frac{1}{Q}$	H(P, Q)
	50%	60%	1.67	0.74	0.37
	25%	20%	5	2.32	0.58
	25%	20%	5	2.32	0.58

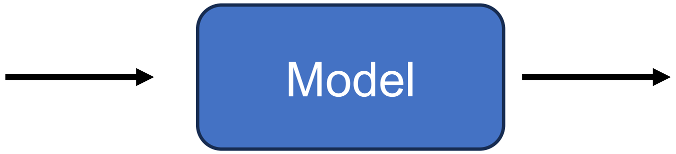
1.53 bits

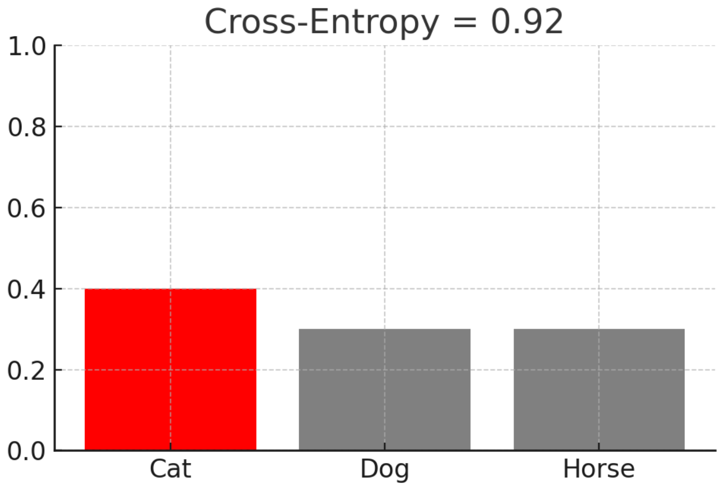
[定義] 機率分佈

機率分佈：機率分佈是指對一個隨機變數的所有可能取值，分別給出它們發生的機率，而這些機率的總和必須為 1。



越接近越好





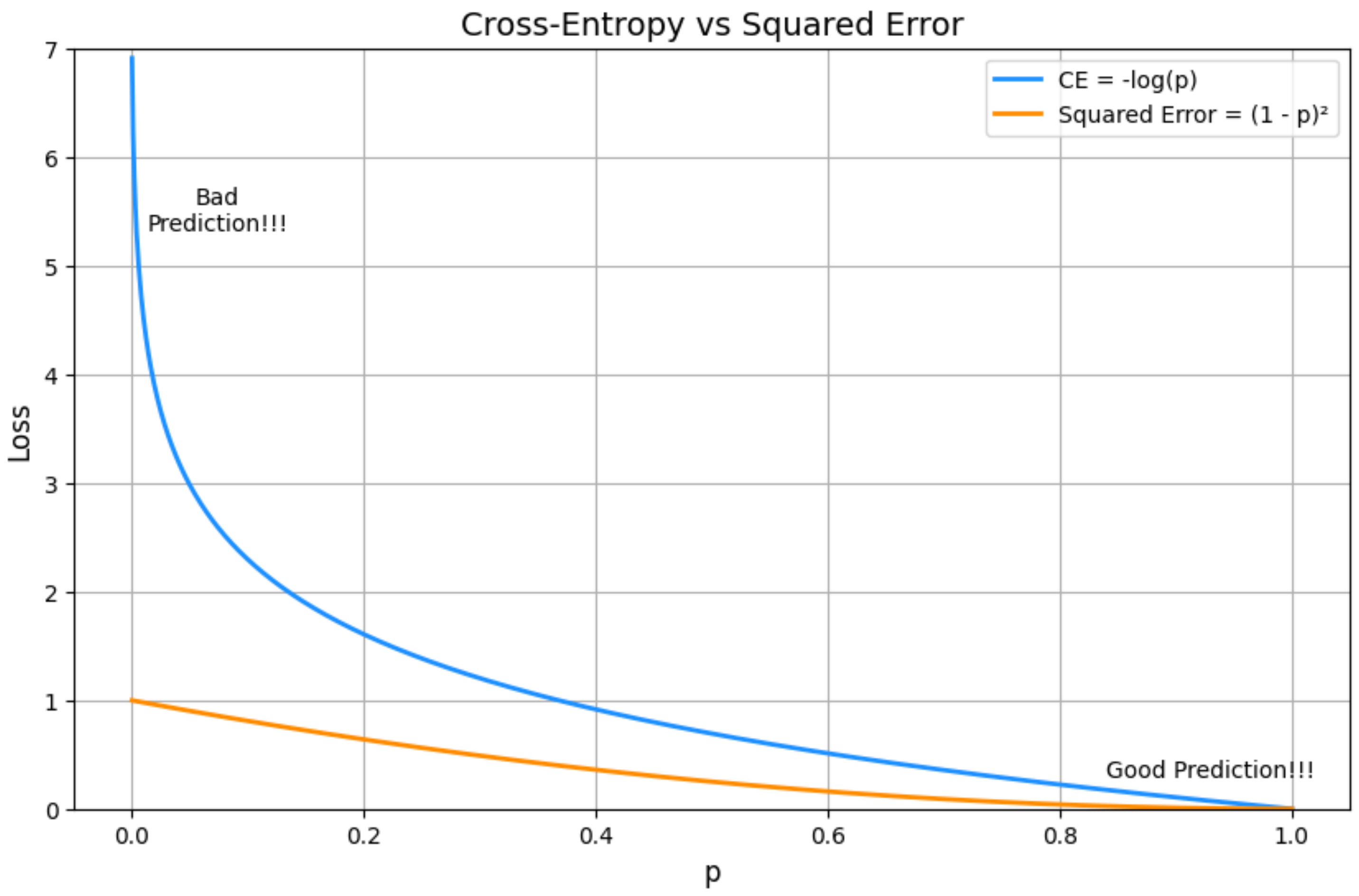
Summary for Cross-entropy

- Entropy 帶來最低的平均傳輸成本
  - 初衷：發生機率高的事件，可以用較低的資訊量進行傳輸
- Cross-entropy 代表用了**錯估的**資訊量後所得到的平均傳輸成本
  - 機器學習就是採用 Cross-entropy 來讓**錯誤的分佈**接近**最佳**的分佈

為什麼分類任務不用 MSE?

code/w5_plot_loss.py

- Ans: 在分類任務上使用 Cross-entropy，能夠在模型預測差時帶來更大的梯度 -> 模型能有更大的幅度更新參數



實作細節

Cross-entropy in ML

- 對於多數的機器學習分類任務來說，我們目標讓模型學會正確的類別

🐈 Cat

$$H(P,Q) = \underset{1}{P} \times \ln \frac{1}{Q} = -\ln Q$$

🐶 Dog

$$H(P,Q) = \underset{0}{P} \times \ln \frac{1}{Q} = 0$$

🍎 Apple

$$H(P,Q) = \underset{0}{P} \times \ln \frac{1}{Q} = 0$$

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Cross-entropy in ML

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$$H(P,Q) = \underset{0}{P} \times \ln\frac{1}{Q} = 0$$

🍎 **Apple**

$$H(P,Q) = \underset{1}{P} \times \ln\frac{1}{Q} = -\ln Q$$

Cross-entropy 公式

$$H(P,Q) = -P\times\log_2 Q$$

所有類別的 cross-entropy 加總

Cross-entropy: $\mathcal{L}_i = -\sum_j \underline{y_j} \log \underline{P(\hat{y}_j|x_i)}$

模型看到 x_i 預測 $\hat{y}_j$ 的機率值 (Q)

y_j 發生的機率值 (P)

x_i: 資料集中第 i 筆資料

y_j: label，在此範例中 $j = 1,2,3$

x_i

→ Model →

	Model output (logits)	Softmax $P(\hat{y}_j|x_i)$	label (y_j)	Cross-entropy
y_1 Cat	0.5	0.225	1	$-\log 0.225$
y_2 Dog	0.7	0.275	0	0
y_3 Apple	1.3	0.500	0	0

各類別加總：$\mathcal{L}_i = -\log 0.225$

如何把模型輸出變成機率值 (0~1)？

Class_0	Class_1	Class_2
50	**25**	**25**

$$\longrightarrow \quad \frac{\mathrm{x}}{\sum_{\mathrm{j}} \mathrm{x_j}} = [0.5,0.25,0.25]$$

- **Softmax** function，採用 exponential -> 大的數值更大，小的數值更小
  - 有助於梯度下降

$$\text{Softmax}(x_i) = \frac{e_i^x}{\sum_j e^{x_j}} = [0.665,0.244,0.090]$$

注意！Softmax 有考慮到類別總和

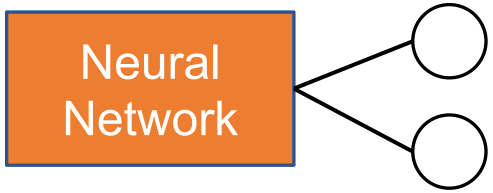
兩種方法來做 Binary Classification

多類別分類任務

對兩個模型輸出值取機率值，
且機率值總和為1

是貓

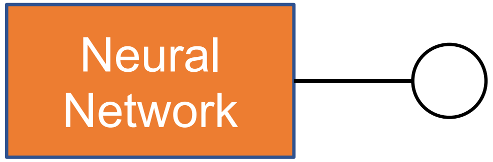
不是貓



二元分類任務

對一個模型輸出值取機率值

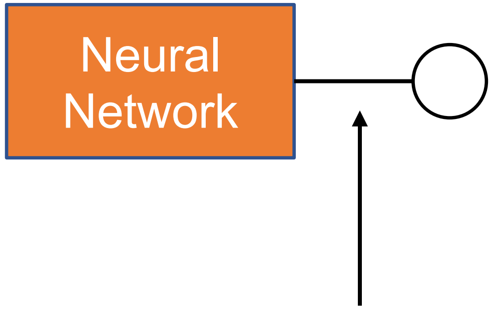
> 0.5 是貓，否則不是貓



實作上採用 BinaryCrossEntropy

如何對一個模型輸出值取機率值 (0~1)？

- **Sigmoid** function:



假設閾值為0.5

> 0.5 是貓，
否則不是貓

$$\mathrm{Sigmoid}(x) = \frac{1}{1 + e^{-x}}$$

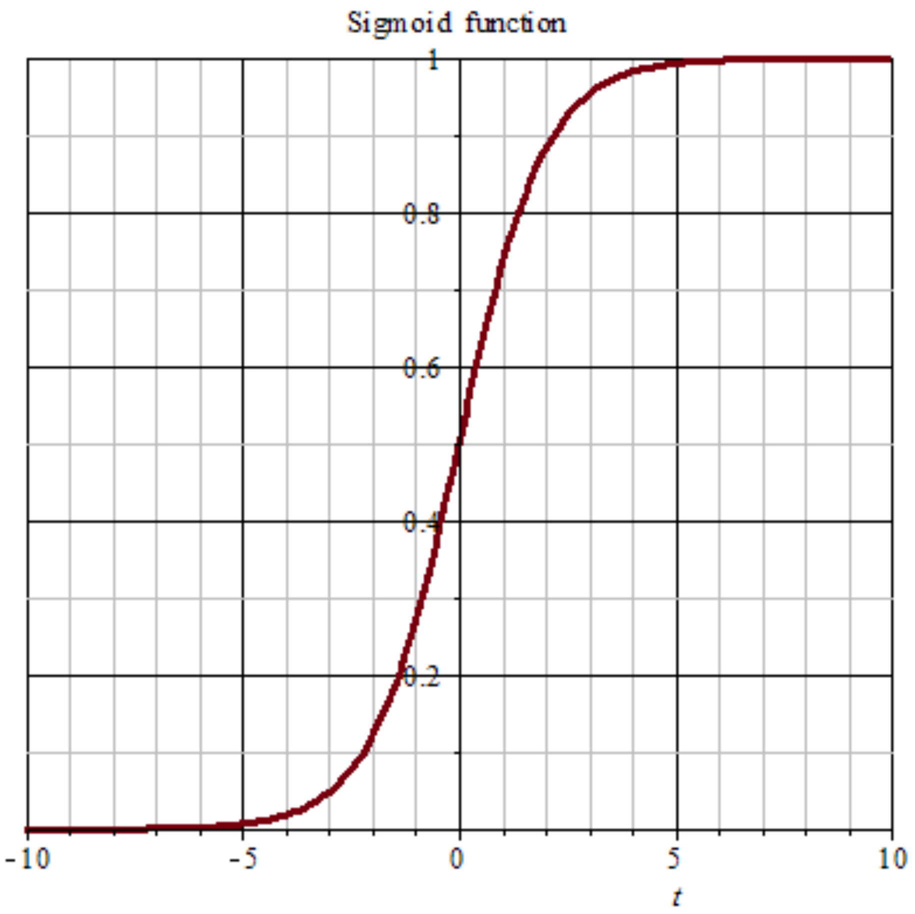


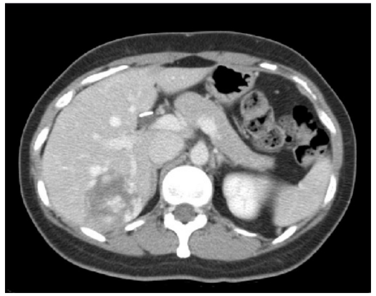
Figure source: https://zh.wikipedia.org/zh-tw/S型函數

Multi-class vs. Multi-label Classification

	標註 (label)	label_id
	貓	0
	狗	1
	馬	2

Multi-class Classification

一次只會有一個類別



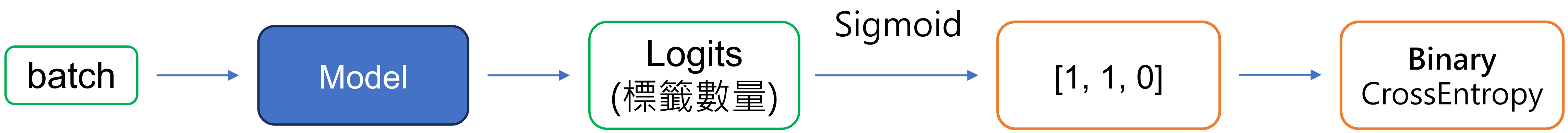
標註 (label)		
囊腫	✅	
血管瘤		[1, 0, 1]
脂肪瘤	✅	

Multi-label Classification

一次可以有多個類別

[注意事項] Multi-label Classification

- Multi-label Classification 實作上與二元分類任務類似：
  - Loss 同樣採用 BinaryCrossEntropy
    - 相當於是做很多次 (次數等於標籤數量) 的二元分類任務
  - 模型輸出需經過 Sigmoid function



Multi-class vs. Multi-label Classification

- Multi-label (多標籤任務)：

batch → Model → Logits (標籤數量) $\xrightarrow{\text{Sigmoid}}$ [1, 1, 0] → **Binary** CrossEntropy

- Multi-class (多類別任務)：

batch → Model → Logits (標籤數量) $\xrightarrow{\text{Softmax}}$ [0.7, 0.1, 0.2] → CrossEntropy

深度學習
Deep Learning

PyTorch Modeling

Instructor: 林英嘉 (Ying-Jia Lin)
2025/10/01

Course GitHub

Slido # DL1001

PyTorch Tutorial

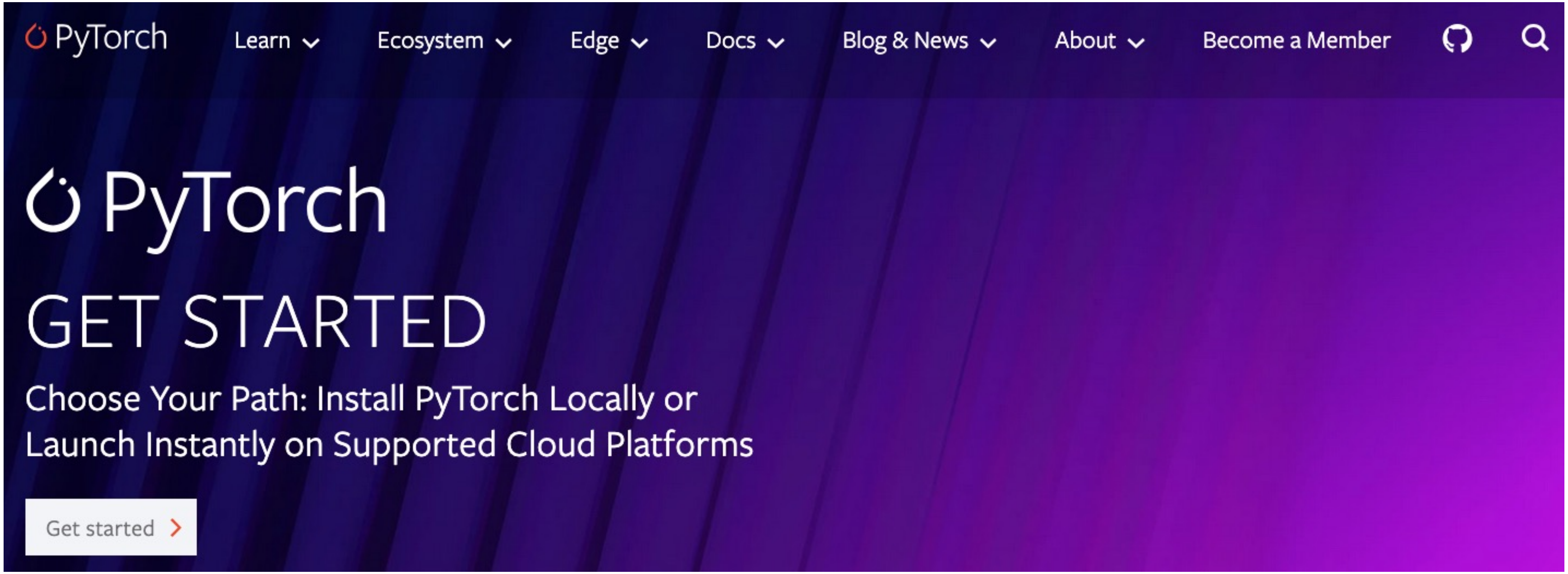
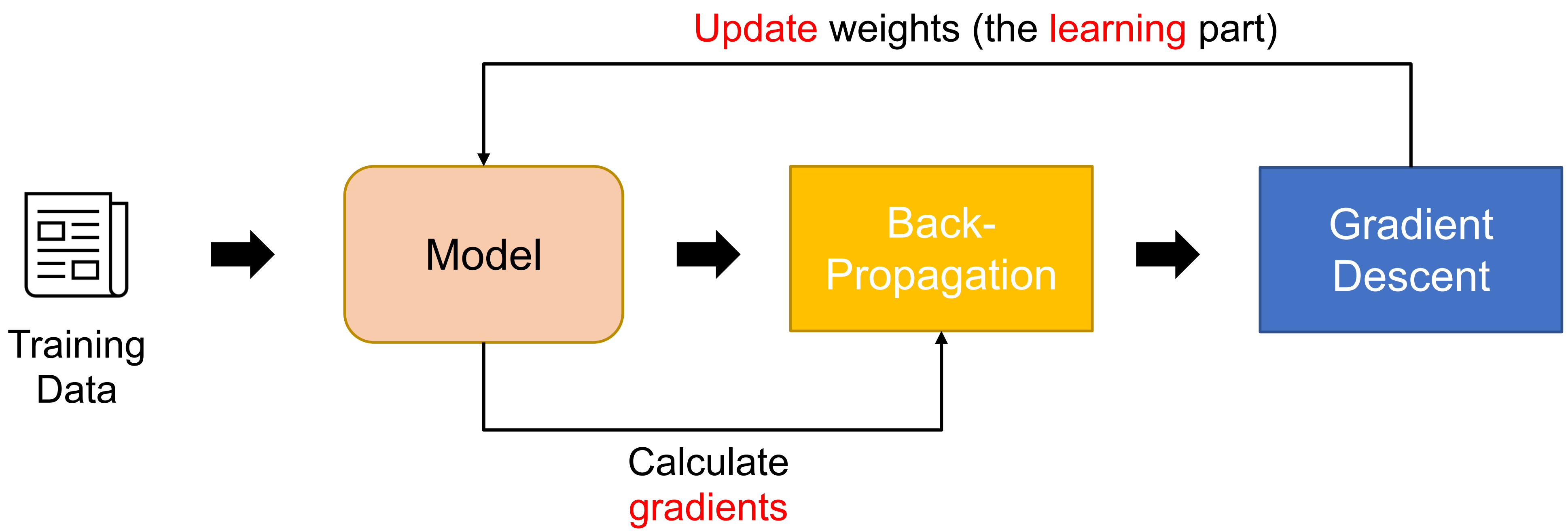


Figure source: https://pytorch.org/

[Recap] 深度學習模型訓練流程



Steps for building your first PyTorch program

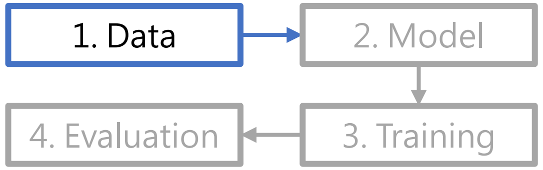
Step 1 (Data):
- Prepare the dataset
- Overwrite PyTorch Dataset
- Define DataLoader

Step 2 (Model):
- Construct the model
- Define the loss function
- Define the optimizer

Step 3 (Training):
Write the training process

Step 4 (Evaluation):
Write the evaluation process

Step 1: Prepare the dataset



- From torchvision (image data) or torchtext (text data)
  - You may skip Step 1-2.
- User-defined dataset
  - Download from the Internet
  - Your own dataset

What is a dataset?

1. Data → 2. Model → 3. Training → 4. Evaluation

dataset

PassengerId	Survived	Pclass	Name	Sex
1 891	0 1	1 3	891 unique values	male 65% female 35%
1	0	3	Braund, Mr. Owen Harris	male
2	1	1	Cumings, Mrs. John Bradley (Florence Briggs Thayer)	female
3	1	3	Heikkinen, Miss. Laina	female
4	1	1	Futrelle, Mrs. Jacques Heath (Lily May Peel)	female
5	0	3	Allen, Mr. William Henry	male
6	0	3	Moran, Mr. James	male
7	0	1	McCarthy, Mr. Timothy J	male

data / instance /example

https://www.kaggle.com/competitions/titanic/data?select=train.csv

Step 1-2: 建立 PyTorch Dataset

- 為了符合我們載入資料的需求
  - 例如：適合我們資料的前處理過程
- 簡潔且容易維護的資料存取介面：

```
img, label = dataset[0] # `dataset` 是透過 PyTorch Dataset 所建立的
```

index

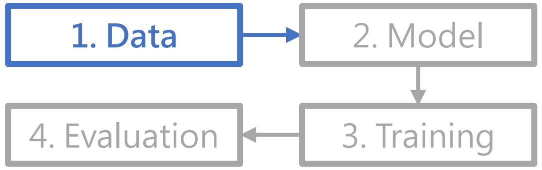
Step 1-2: 建立 PyTorch Dataset

- 我們需要繼承 torch.utils.data.Dataset，並改寫三個項目 (__init__, __getitem__, __len__)：

```
import torch

class CustomDataset(torch.utils.data.Dataset):
    def __init__(self, parameter_1, parameter_2, ...):
        # Prepare some things
        # that you are going to use in `__getitem__` and `__len__`

    def __getitem__(self, index):
        # do_something
        return data, label

    def __len__(self):
        return len(data_variable)
```

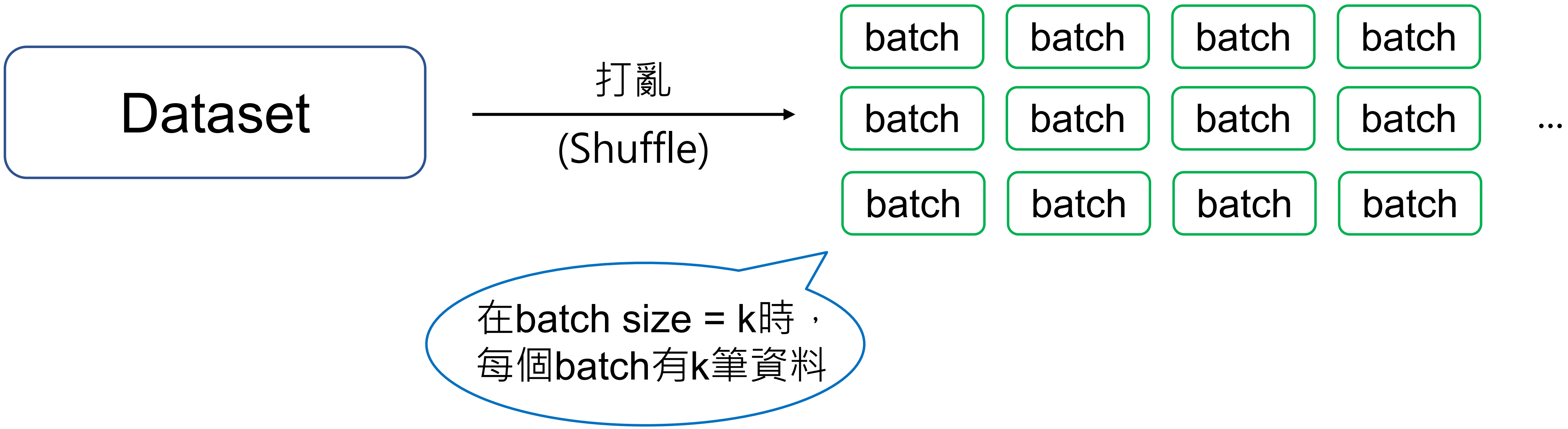
- __init__ ：初始化 class 中的變數
- __getitem__ ：讓 PyTorch Dataset 可以透過 index 來取得任一筆資料
- __len__ ：取得資料集的總數

Step 1-2: 建立 PyTorch Dataset




```
import torch

class HandWrite(torch.utils.data.Dataset):
    def __init__(self, files: list, word_to_id: dict, transform=None):
        self.files = files # 全部的資料
        self.transform = transform # 影像資料前處理的流程

    def __getitem__(self, index):
        fname = self.files[index]
        image = Image.open(fname)
        if self.transform is not None:
        image = self.transform(image)

        label = fname.split('/')[-1].split('_')[0]
        return image, torch.tensor(word_to_id[label])

    def __len__(self):
        return len(self.files)
```

Step 1-3: 建立 DataLoader




```
# We should split the dataset into train / validation / test sets first.
train_loader = torch.utils.data.DataLoader(trainset, batch_size=TRAIN_BS, shuffle=True)
val_loader = torch.utils.data.DataLoader(valset, batch_size=VAL_BS, shuffle=False)
test_loader = torch.utils.data.DataLoader(testset, batch_size=TEST_BS, shuffle=False)
```

Advantages of batching

- Training:
  - mini-batch gradient descent 有機會避免模型陷入局部最小值
- Inference (validation or test):
  - 省記憶體
  - 不需要累積梯度，所以 inference 時期的 batch size (bs) 通常可以比 training 時期的 bs 還大

Step 2-1: Construct the model

1. Data → **2. Model** → 3. Training → 4. Evaluation

- 我們需要：
  1. 繼承 torch.nn.Module，
  2. 初始化 torch.nn.Module 原本定義的內容
  3. 改寫兩個項目 (__init__, forward)

```
class MyModel(torch.nn.Module):
    def __init__(self):
        super().__init__() # 初始化 torch.nn.Module 原本定義的內容
        # Define our new variables
        # Define our model layers

    def forward(self, x):
        # Do something (forward pass)
        return output
```

https://pytorch.org/tutorials/beginner/basics/buildmodel_tutorial.html

為什麼需要 super().__init__()？

- 模型需要繼承 torch.nn.Module，並且透過 super().__init__() 初始化原本在 nn.Module 中被定義好的內容，如下圖所示：

```python
    def __init__(self):
        """
        Initializes internal Module state, shared by both nn.Module and ScriptModule.
        """
        torch._C._log_api_usage_once("python.nn_module")

        self.training = True
        self._parameters = OrderedDict()
        self._buffers = OrderedDict()
        self._non_persistent_buffers_set = set()
        self._backward_hooks = OrderedDict()
        self._forward_hooks = OrderedDict()
        self._forward_pre_hooks = OrderedDict()
        self._state_dict_hooks = OrderedDict()
        self._load_state_dict_pre_hooks = OrderedDict()
        self._modules = OrderedDict()
```

https://github.com/pytorch/pytorch/blob/266657182a4040937f6f27011d7ddf77716db83d/torch/nn/modules/module.py#L206-L221

ImageNet Competition

Complete name: ImageNet Large Scale Visual Recognition Challenge (ILSVRC)

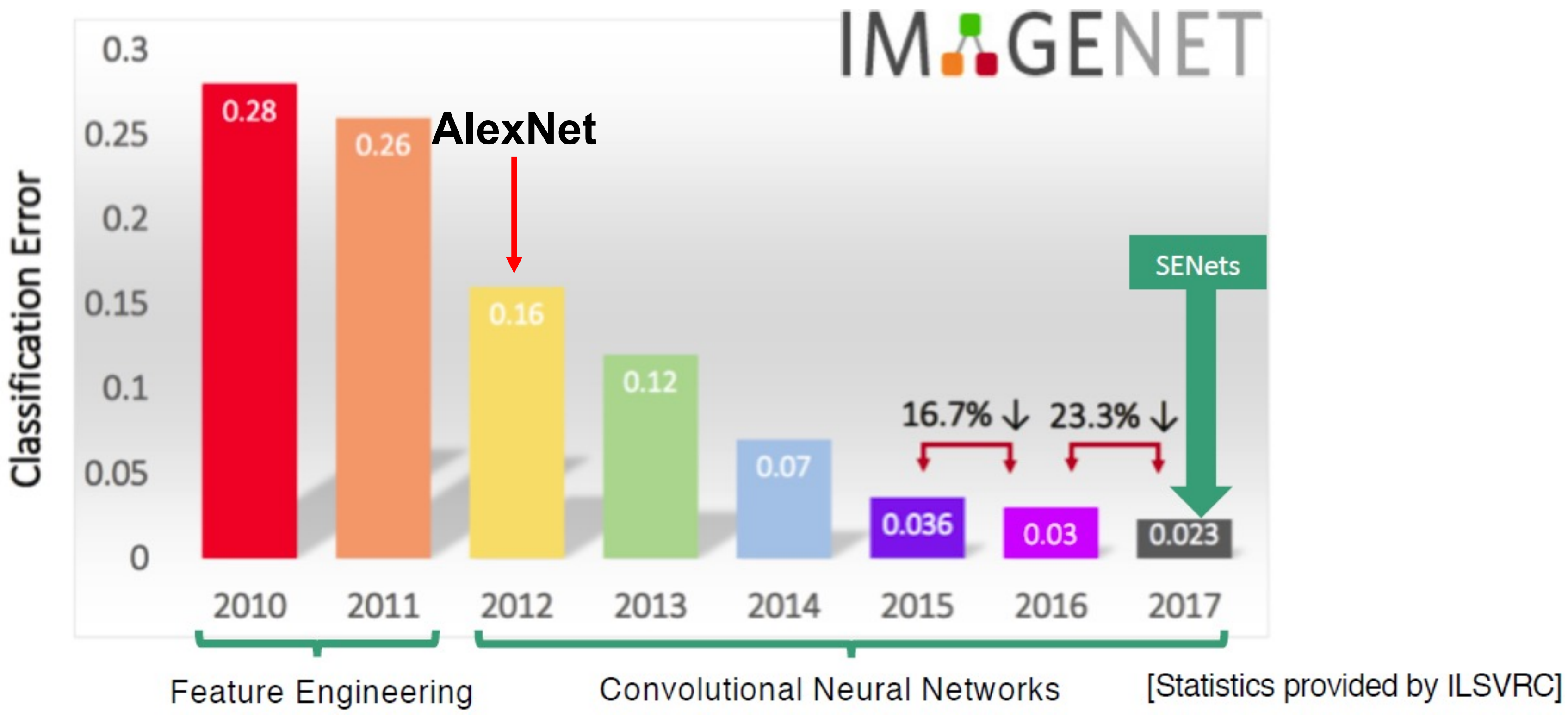
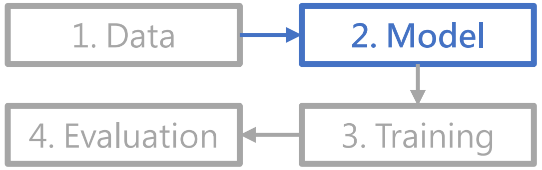


Figure source: https://www.kaggle.com/discussions/getting-started/149448

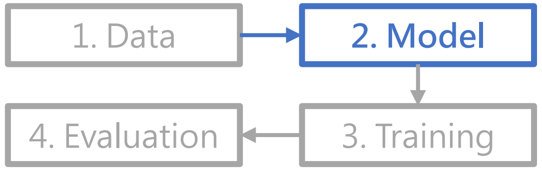
Step 2-2: Define the optimizer



Loss functions	Meaning
torch.optim.SGD	**Stochastic gradient descent** (with momentum)
torch.optim.RMSprop	**RMSProp** (Root Mean Square Propagation)
torch.optim.Adam	**Adam** (Adaptive Moment Estimation)
torch.optim.AdamW	**AdamW** (Adam with decoupled weight decay)

```
learning_rate = 1e-3 # 代表 0.001
optimizer = optim.Adam(model.parameters(), lr=learning_rate)
```

Step 2-2: Define the loss function



Loss functions	Usage
torch.nn.CrossEntropyLoss	Classification
torch.nn.MSELoss	Regression
torch.nn.BCELoss	Binary classification

```
# example
loss_function = torch.nn.CrossEntropyLoss()
```

[PyTorch小細節]
BCEWithLogitsLoss 已經包含了 Sigmoid
CrossEntropyLoss 已經包含了 Softmax

Step 2-2: 訓練過程中的模型輸出

- 迴歸任務：

batch → Model → Logits (模型原始輸出) → MSE

- 二分類任務：

batch → Model → Logits (模型原始輸出) → 1 或 0 $\xrightarrow{\text{Sigmoid}}$ **Binary** CrossEntropy

- 多分類任務：

batch → Model → Logits (模型原始輸出) → N classes $\xrightarrow{\text{Softmax}}$ CrossEntropy

Step 3: 訓練模型

1. Data → 2. Model → 3. Training → 4. Evaluation

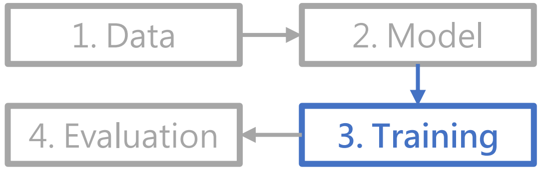
重複直到訓練完成或到達指定條件

清空 optimizer (過去累積)的梯度	`optimizer.zero_grad()`
模型前向傳播得到輸出	`output = model(inputs)`
模型反向傳播計算梯度	`loss = loss_function(output, target)` `loss.backward()`
optimizer 更新模型參數	`optimizer.step()`

Step 3: 訓練模型


```
for batch in train_loader:
    # 把資料移動到 GPU
    images, labels = batch[0].to(device), batch[1].to(device)

    optimizer.zero_grad()

    # 1. 前向傳播
    outputs = model(images) # 形狀是 (batch_size, num_classes)
    loss = loss_fn(outputs, labels)

    # 2. 反向傳播 (計算梯度)
    loss.backward()

    # 3. 更新模型權重
    optimizer.step()
```

Step 3: 訓練模型



外層通常會有epoch (模型經過一次完整訓練集的更新稱為1個epoch)

```
for epoch in range(epochs):
    for batch in train_loader:
        # 把資料移動到 GPU
        images, labels = batch[0].to(device), batch[1].to(device)

        optimizer.zero_grad()

        # 1. 前向傳播
        outputs = model(inputs) # 形狀是 (batch_size, num_classes)
        loss = loss_fn(outputs, labels)

        # 2. 反向傳播 (計算梯度)
        loss.backward()

        # 3. 更新模型權重
        optimizer.step()
```

Step 4: 模型評估

1. Data → 2. Model → 3. Training → **4. Evaluation**

```
with torch.no_grad():  ← 在這底下縮排屬於不計算梯度的環境
    for batch in test_loader:
        images, labels = batch[0].to(device), batch[1].to(device)

        outputs = model(inputs) # 形狀是 (batch_size, num_classes)
        loss = loss_fn(outputs, labels) # 純粹紀錄數值用，沒有要更新模型
        total_loss += loss.item()
```

Step 4: 模型評估

1. Data → 2. Model → 3. Training → 4. Evaluation

```python
with torch.no_grad():
    for batch in progress_bar:
        images, labels = batch[0].to(device), batch[1].to(device)
        outputs = model(images) # `outputs` 的形狀是 (batch_size, 10)
        loss = loss_fn(outputs, labels)
        total_loss += loss.item()

        prediction = outputs.argmax(dim=1) # 找出數值最大的類別作爲模型預測

        # 我們希望 `predictions` 的長相是 [1, 2, 0, 4, 5, 7, ...]
        # 如果用 append 的話可能會變成 [[1, 2, 0], [4, 5, 7], ...]
        prediction_list.extend(prediction.tolist())
        label_list.extend(labels.tolist())

avg_loss = total_loss / len(data_loader)
accuracy = accuracy_score(label_list, prediction_list)
```

```python
from sklearn.metrics import accuracy_score
```

Thank you!

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