台灣人工智慧學校

機器學習基礎與演算法

Chapter 6　決策樹系列 (Tree Based Model)

[講師投影片Chapter6]
[課程投影片]
[資料與程式碼]
[播放清單]

「版權聲明頁」

課程內容

6. 決策樹系列 (Decision tree)

-Decision tree
-Information gain
-Gain ratio
-Gini index
-Tree pruning
-Miscellaneous topics
[實作] 決策樹 (Decision Tree)

Code 放在Hub中的course內

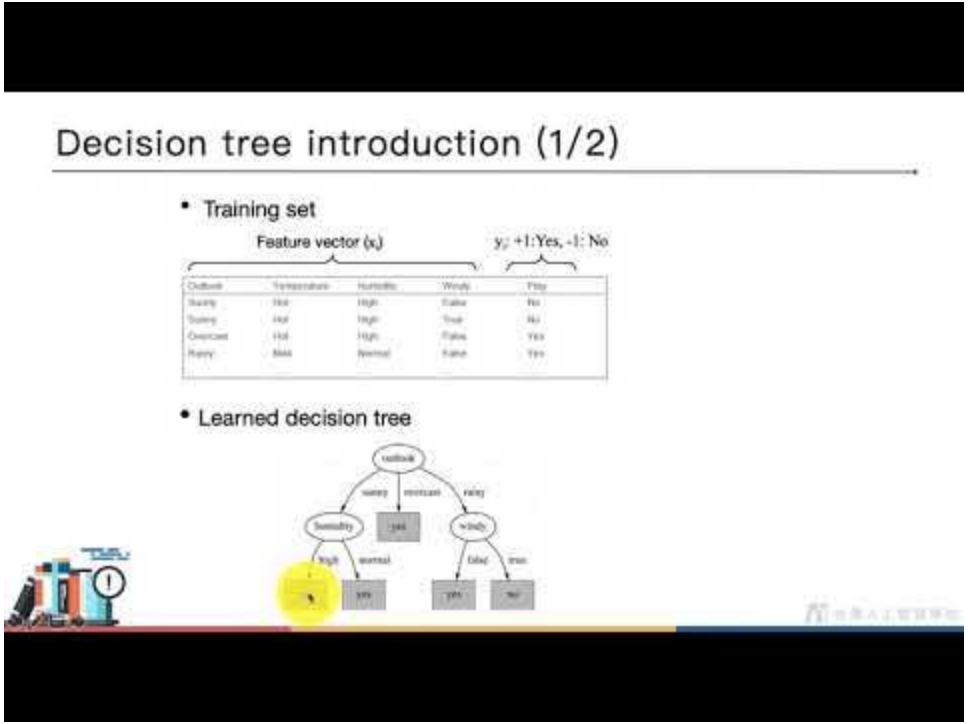
- 為維護課程資料，courses中的檔案皆為read-only，如需修改請cp至自身環境中
- 打開terminal，輸入

cp -r courses-tpe/Machine_Learning <存放至本機的名稱>

Chapter 6　決策樹 (Decision tree)

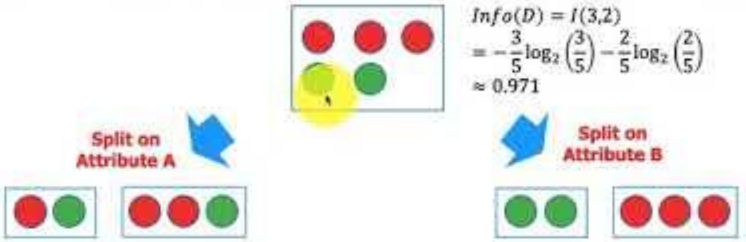
- 範例程式(example)的檔名會以**藍色字體**顯示且旁邊附上
- 練習(exercise)的檔案以**紅色字體**顯示且旁邊附上

06-1: Decision tree



06-2: Information gain

Information gain



$$Info(D) = I(3,2) = -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) \approx 0.971$$

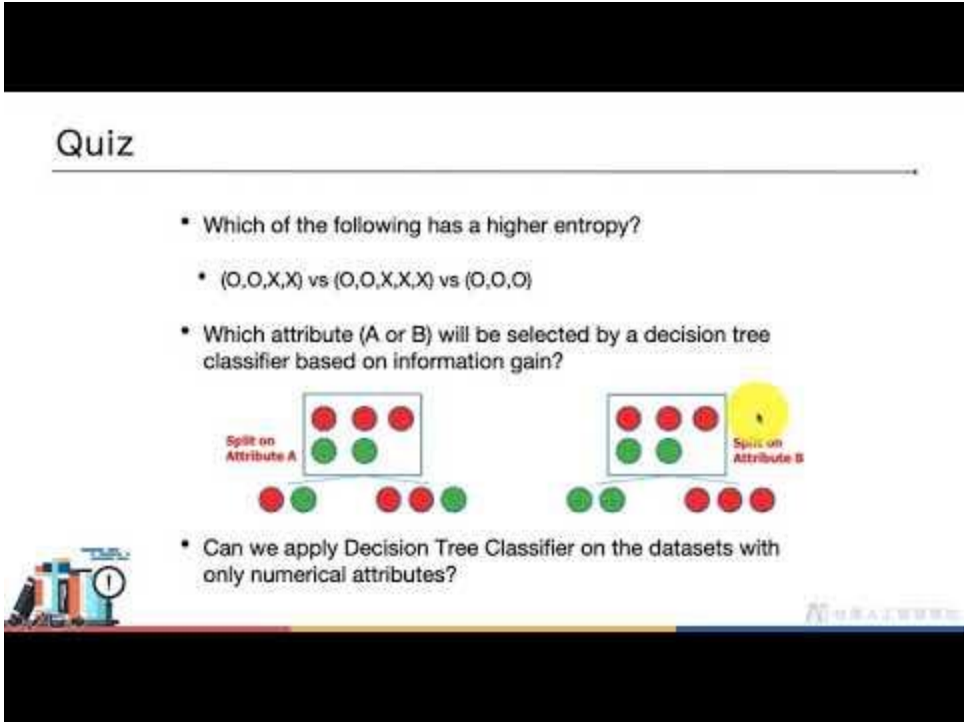
$$Info_A(D) = \frac{2}{5}Info(1,1) + \frac{3}{5}Info(2,1) = 0.918$$

$$Gain(A) = Info(D) - Info_A(D) = 0.971 - 0.918 = 0.053$$

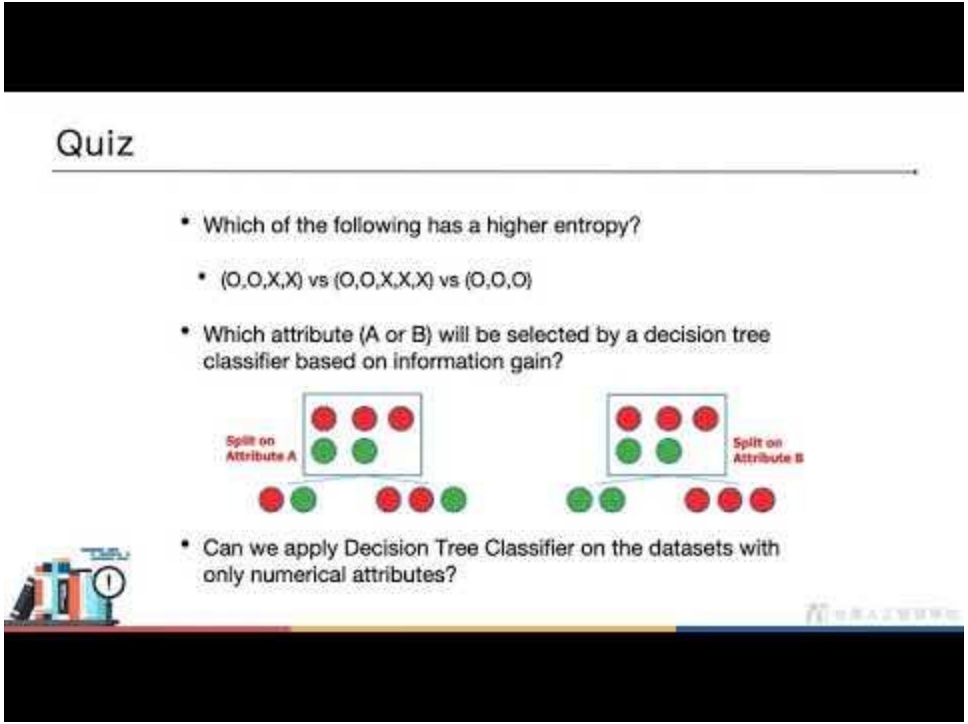
$$Info_B(D) = \frac{2}{5}Info(0,2) + \frac{3}{5}Info(3,0) = 0$$

$$Gain(B) = Info(D) - Info_B(D) = 0.917 - 0 = 0.917$$

06-3: Quiz


Quiz
Which of the following has a higher entropy?
(O,O,X,X) vs (O,O,X,X,X) vs (O,O,O)
Which attribute (A or B) will be selected by a decision tree classifier based on information gain?
Split on Attribute A
Can we apply Decision Tree Classifier on the datasets with only numerical attributes?

06-4: Answer


Quiz
Which of the following has a higher entropy?
(O,O,X,X) vs (O,O,X,X,X) vs (O,O,O)
Which attribute (A or B) will be selected by a decision tree classifier based on information gain?
Split on Attribute A
Split on Attribute B
Can we apply Decision Tree Classifier on the datasets with only numerical attributes?

06-5: Gain ratio

Attribute Selection: Gain ratio

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

income=high: 4
income=medium: 6
income=low: 4

- $SplitInfo_{income}(D) = -\frac{4}{14}\log_2\frac{4}{14} - \frac{6}{14}\log_2\frac{6}{14} - \frac{4}{14}\log_2\frac{4}{14} \approx 0.926$
- $GainRatio(income) = Gain(income)/SplitInfo_A(D) = \frac{0.029}{0.926} \approx 0.031$

06-6: Quiz

Quiz

- Given students' ID, height, weight, and gender as the training data, you are asked to build a decision tree classifier to predict a student's gender based on her/his ID, height, and weight
  - Which attribute (ID, height, or weight) is likely to be selected first if you use information gain as the attribute selection method?

06-7: Answer

Quiz

- Given students' ID, height, weight, and gender as the training data, you are asked to build a decision tree classifier to predict a student's gender based on her/his ID, height, and weight
  - Which attribute (ID, height, or weight) is likely to be selected first if you use information gain as the attribute selection method?

06-8: Gini index

Example of Gini index

age	income	student	credit_rating	buys_computer
youth	high	no	fair	no
youth	high	no	excellent	no
middle_aged	high	no	fair	yes
senior	medium	no	fair	yes
senior	low	yes	fair	yes
senior	low	yes	excellent	no
middle_aged	low	yes	excellent	yes
youth	medium	no	fair	no
youth	low	yes	fair	yes
senior	medium	yes	fair	yes
youth	medium	yes	excellent	yes
middle_aged	medium	no	excellent	yes
middle_aged	high	yes	fair	yes
senior	medium	no	excellent	no

When income = "high"
➔ 2 "yes" and 2 "no"

When income = "medium"
➔ 4 "yes" and 2 "no"

When income = "low"
➔ 3 "yes" and 1 "no"

- $Gini_{income}(D) = \frac{4}{14}\left(1-\left(\frac{2}{4}\right)^2-\left(\frac{2}{4}\right)^2\right)+\frac{6}{14}\left(1-\left(\frac{4}{6}\right)^2-\left(\frac{2}{6}\right)^2\right)+\frac{4}{14}\left(1-\left(\frac{3}{4}\right)^2-\left(\frac{1}{4}\right)^2\right)=0.325$
- $Gain(income) = Gini(D) - Gini_{income}(D) = 0.134$

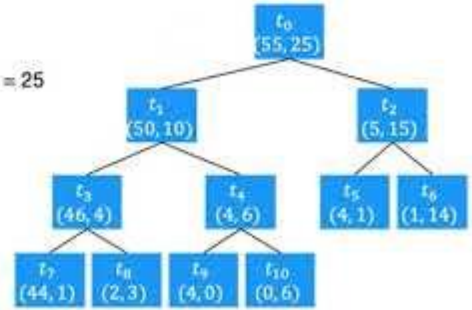
06-9: Tree pruning

Example of post-pruning

$$\alpha(t_i) = \frac{\#\text{ error after cut} - \#\text{ error before cut}}{\#\text{ leaves been cut} - 1}$$

$\alpha(t_0) = ?$

- If we cut the tree and leave only t_0, # errors = 25
- If we don't cut the tree, # errors = 1+2+0+0+1+1=5
- If we cut the tree, 6 leaves are cut
- $\alpha(t_0) = \frac{25-5}{6-1} = 4$



06-10: Miscellaneous topics

DT is constructed in a "greedy" manner

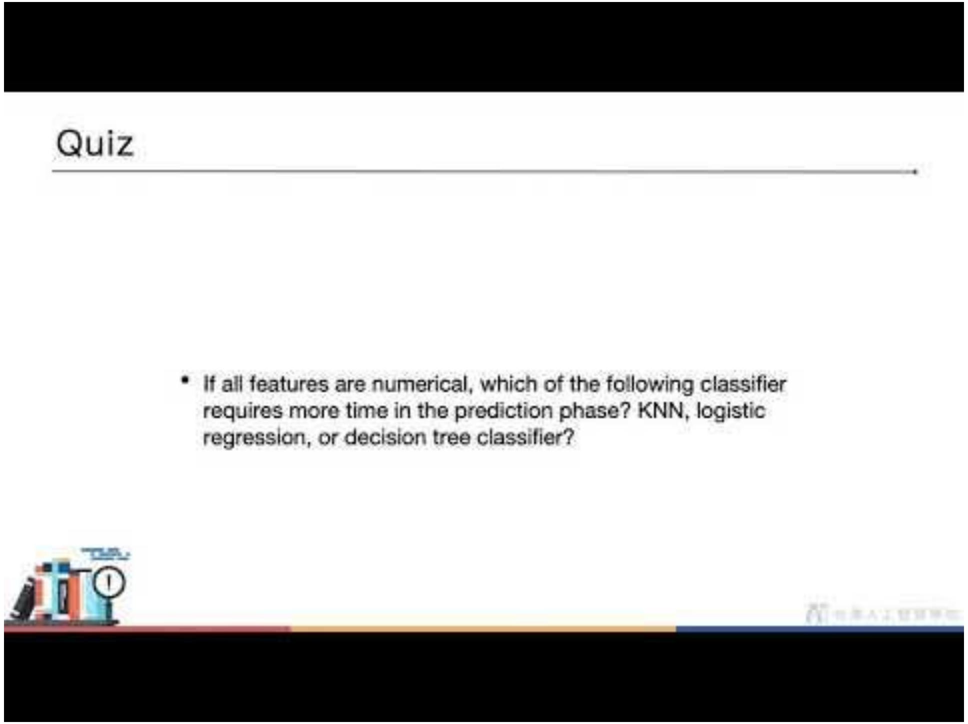
- Greedy: pick a feature to split the data best on the ***current*** information
  - This may lead to a local optimal

06-11: Quiz

Quiz

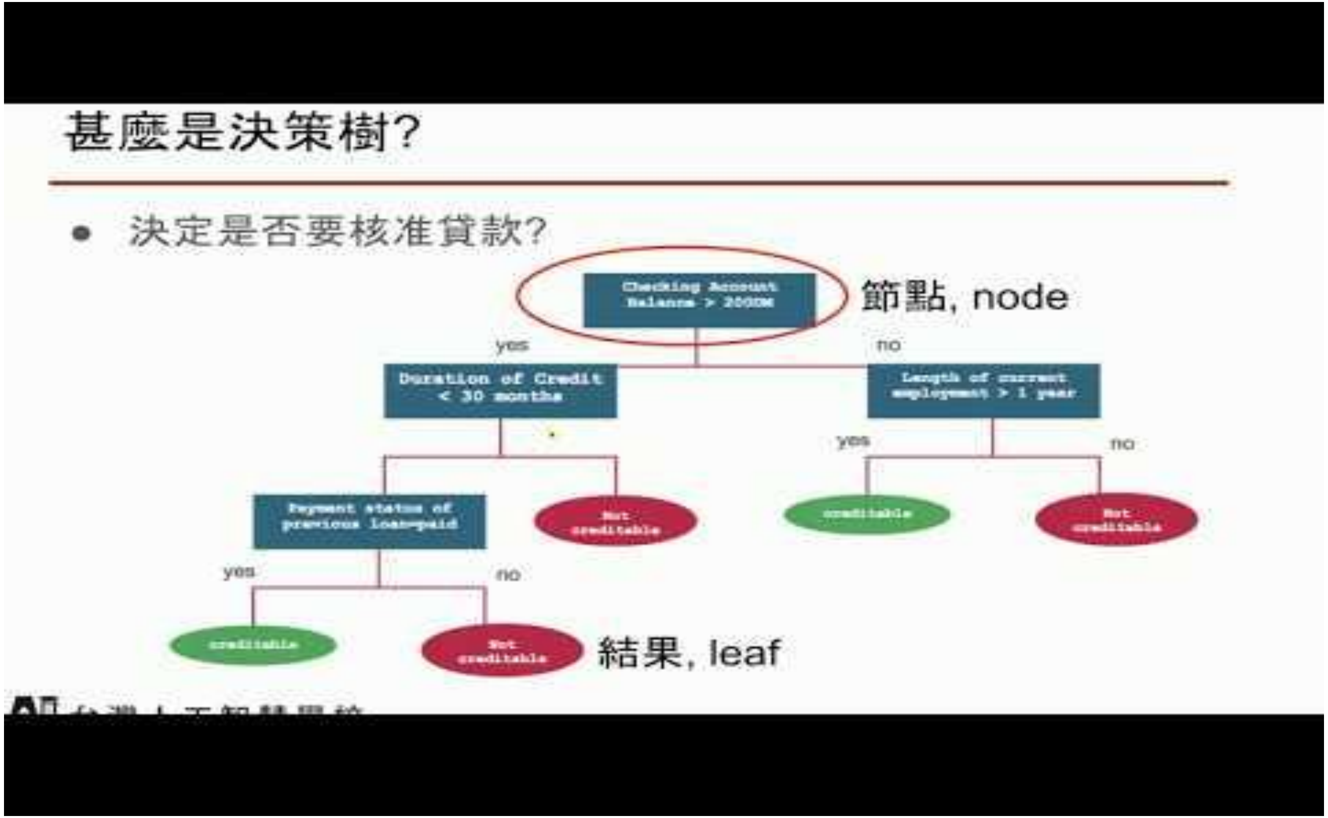
- If all features are numerical, which of the following classifier requires more time in the prediction phase? KNN, logistic regression, or decision tree classifier?

06-12: Answer



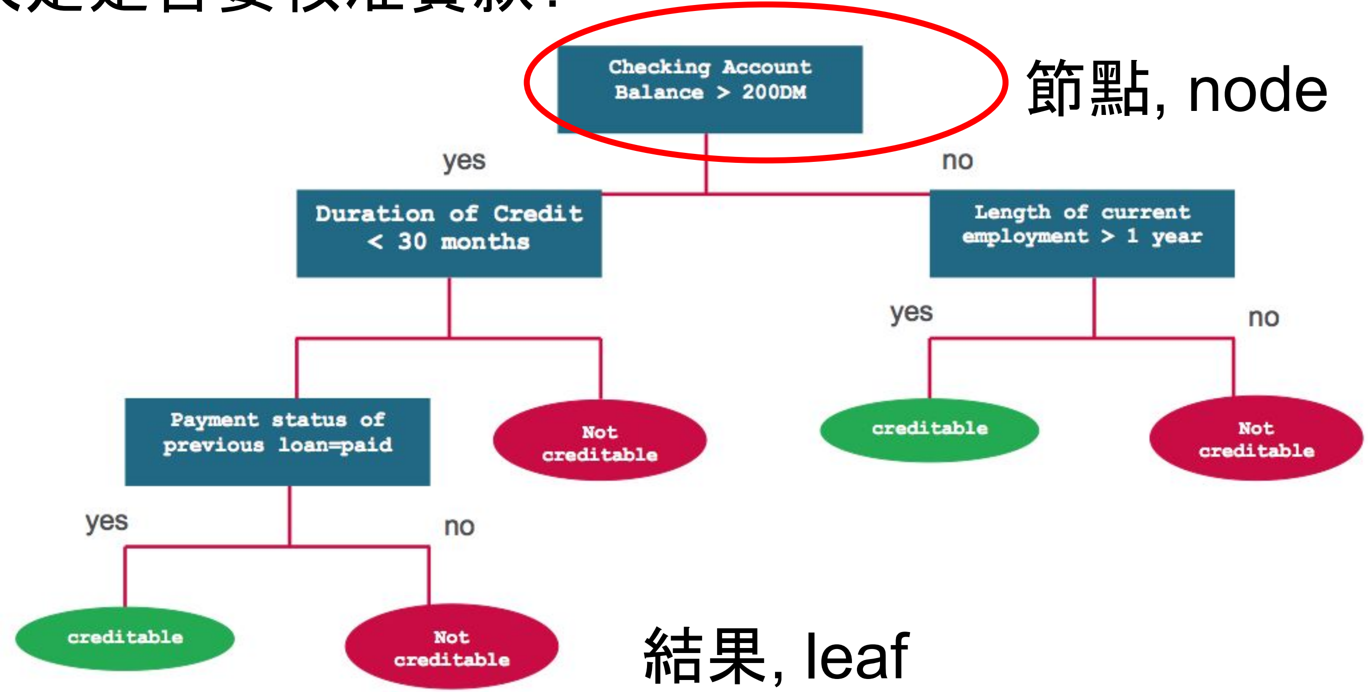
Quiz
If all features are numerical, which of the following classifier requires more time in the prediction phase? KNN, logistic regression, or decision tree classifier?

[實作課程] 決策樹 (Decision Tree)



甚麼是決策樹?

- 決定是否要核准貸款?



節點, node

結果, leaf

如何做決策?

- 該怎麼知道要用哪個 feature? 要用多少的值來做出我們的決策呢?
- 透過從訓練資料找出規則，讓每一個決策能夠使**訊息增益** (Information gain) 最大化
- 如何衡量訊息增益?
    - 吉尼不純度, Gini impurity
    - 熵, Entropy

吉尼不純度 (Gini impurity)

- 數字越大，代表序列中的資料越混亂

$$Gini = 1 - \sum_j p_j^2$$

	Parent
C0	6
C1	6
Gini = 0.5	

Gini :
$1 - (6/12)^2 - (6/12)^2$
= 0.5

熵 (Entropy)

$$Entropy = -\sum_j p_j \log_2 p_j$$

- 如果序列中所有 sample 都是同一個類別

$$entropy = -1 \log_2 1 = 0$$

- 若序列中各有一半的 sample 分屬不同的類別

$$entropy = -0.5 \log_2 0.5 - 0.5 \log_2 0.5 = 1$$

Gini vs. Entropy

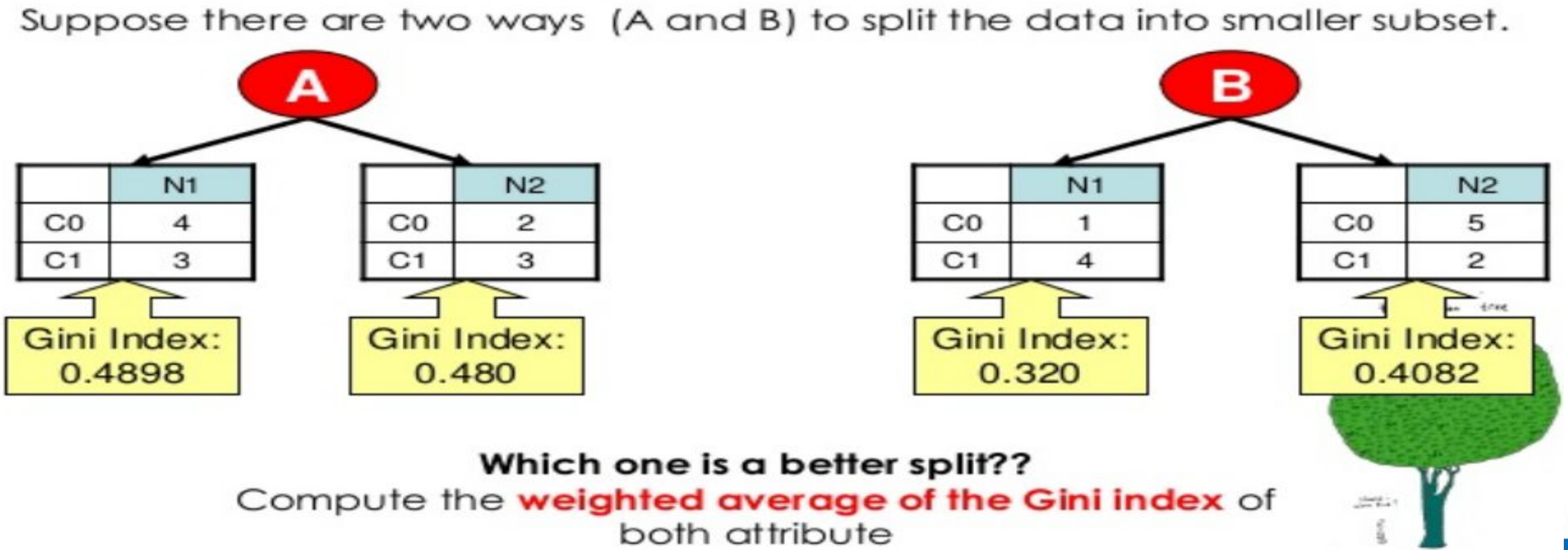
- 都是在衡量一個序列中的混亂程度，越高越混亂
- 數值皆為 0 ~ 1 之間。0 代表序列都是同樣的值
- Scikit-learn 預設使用 Gini

$$Gini = 1 - \sum_j p_j^2$$

$$Entropy = -\sum_j p_j \log_2 p_j$$

Information Gain 訊息增益

- 決策樹中，試著用 feature 將資料做切分，選取的 feature 必須能最大化訊息增益。而訊息增益則是由 Gini 或 Entropy 衡量，我們希望切分後的資料越純越好 (Gini=0)

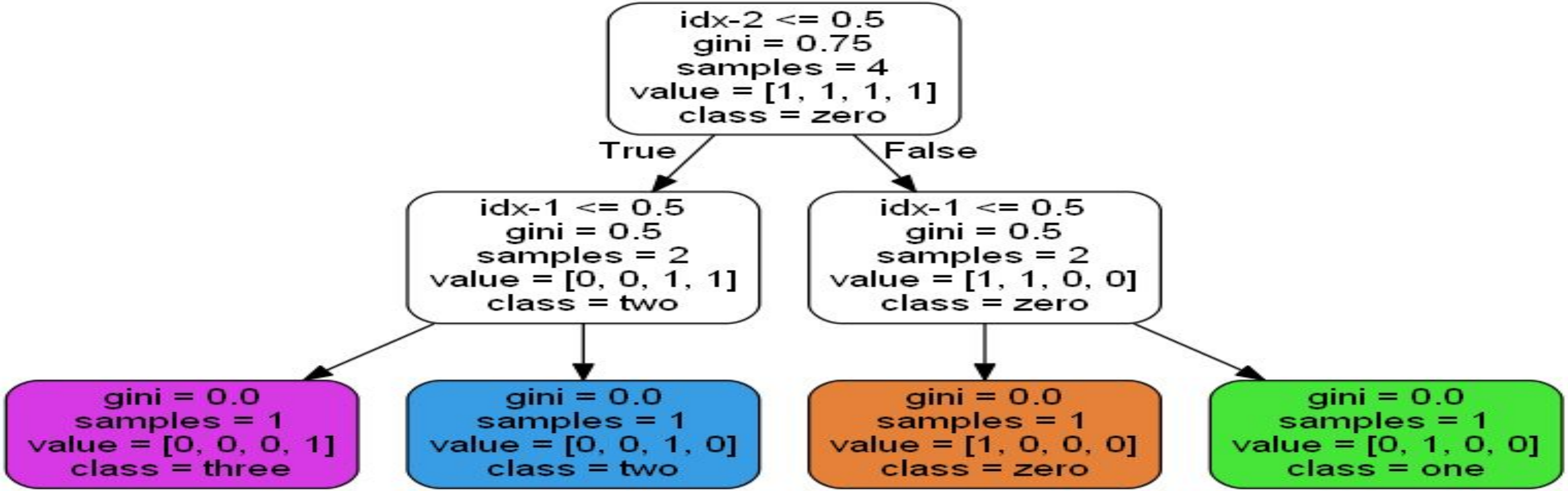


決策樹建立 (1/2)

- 不斷尋找 feature 進行決策，試著將資料切分為同一個類別 (minimize Gini)
  - 這樣會造成甚麼後果?

決策樹建立 (2/2)

- 當我們拿一批訓練資料給決策樹進行分類時，若沒有給定任何條件，決策樹會不斷進行分枝，直到所有 leaf 的資料都屬於同一個類別為止



決策樹 in Scikit-learn

- 兩行 code 建立決策樹

```python
from sklearn.tree import DecisionTreeRegressor

from sklearn.tree import DecisionTreeClassifier

clf = DecisionTreeClassifier()
```

決策樹模型中的參數

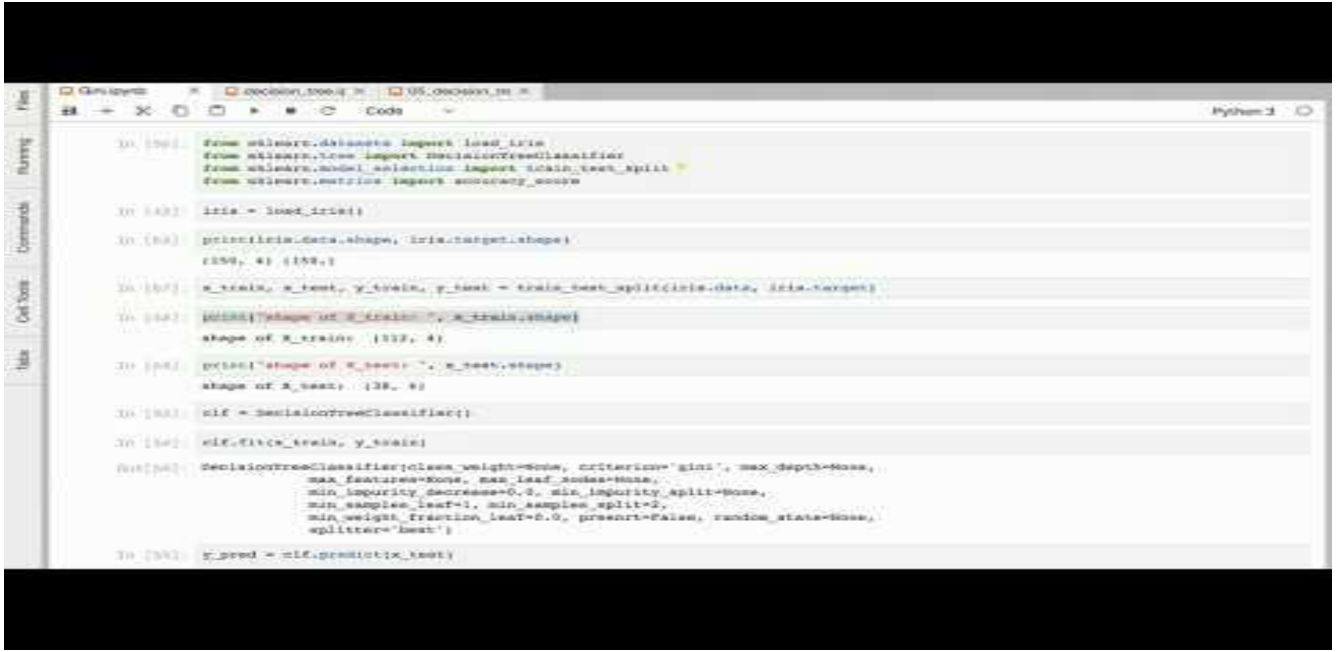
```
from sklearn.tree import DecisionTreeClassifier

clf = DecisionTreeClassifier(
        criterion = ‘gini’,
        max_depth = None,
        min_samples_split = 2,
        min_samples_leaf = 1,
)
```

Feature Importance

- 決策樹的另一優點是，我們可以從構建樹的過程中，透過 feature 被用來切分的次數，來得知哪些 features 是相對有用的
- 所有 feature importance 的總和會是 1
- 實務上，我們經常會用 feature importance 來排序 feature 的重要性以及選取要使用的 feature

```
# feature importance
clf.feature_importances_
```

決策樹實戰

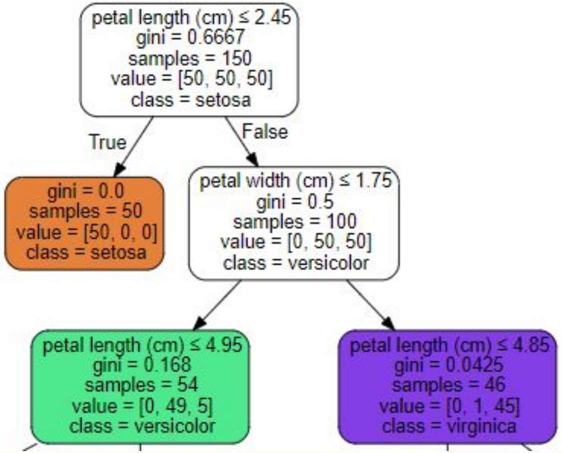


*影片中 code 有誤: **accuracy_score(y_test, y_pred)**

決策樹視覺化

● 生成好的樹，可以用額外的套件 graphviz，自動從 code 繪製成圖形，讓我們了解決策樹究竟學到了甚麼決策

```
>>> dot_data = tree.export_graphviz(clf, out_file=None,
                         feature_names=iris.feature_names,
                         class_names=iris.target_names,
                         filled=True, rounded=True,
                         special_characters=True)
>>> graph = graphviz.Source(dot_data)
>>> graph
```



決策樹小結

決策樹 summary

- 掃過所有 feature 與對應的值將資料做切分
- 希望資料盡可能分開, 透過切分後的資料純度 (Gini or Entropy) 來衡量
- 如果不對決策樹進行任何限制 (樹的深度、葉子至少要有多少樣本), 容易造成 Overfitting
- 透過 feature importance 來排序重要性

決策樹 Summary

- 掃過所有 feature 與對應的值將資料做切分
- 希望資料盡可能分開，透過切分後的資料純度 (Gini or Entropy) 來衡量
- 如果不對決策樹進行任何限制 (樹的深度、葉子至少要有多少樣本)，容易造成 Overfitting
- 透過 feature importance 來排序重要性

決策樹進化! Ensemble

- 決策樹有著非常容易被理解的優點，但是通常預測結果不會那麼準確
- 之後的學者想出方法，把樹結合起來 (ensemble) 做改進
  - **Bagging (Bootstrap aggregating)**: Fit many large trees to bootstrap-resampled versions of the training data, and classify by majority vote.
  - **Boosting**: Fit many large or small trees to reweighted versions of the training data. Classify by weighted majority vote.

練習 decision_tree_example.ipynb

- 請使用 Iris Dataset，建立決策樹模型，試著更改 Decision Tree 中的 **criterion, max_depth, min_samples_split** 等參數，並評估不同的參數是否會影響以下結果
  - training error / loss
  - testing error / loss
  - training speed (可用 %%timeit 計算 cell 執行的速度)

Write a Decision Tree from Scratch (optional, but 推薦)

補充閱讀

- 如果前面助教講的影片你都聽不懂，肯定是因為助教講的不夠清楚，只好幫各位找一些寫的不錯的文章，給大家參考
    - 決策樹 (Decision Tree) - 中文
    - how decision tree works - 英文

思考問題

- 在分類問題中，若沒有任何限制，決策樹有辦法把訓練資料的 loss 完全降成 0 嗎？
- 決策樹做分類問題時，資料的不純度比較容易計算 (是否屬於同一個類別)。那如果變成回歸問題，這時切分後的資料不純度該如何計算？樹建置完成後，又該如何進行預測呢？