Artificial Intelligence

Decision trees,
for classification

Decision Tree (DT) ?

- **Supervised learning algorithm**
  - **For classification**
  - **And for regression**
- **It can be represented as a logical tree, with a root node, decision nodes, leaf nodes, connected by "decisions"**
- **A DT models decisions and their consequences**
- **For both tasks, scikit-learn uses the "CART" algorithm,**
  - **CART = "ClAssification and Regression Trees"**
    - **The one supported in scikit-learn**
  - **It produces "binary trees"**
    - **Each node has exactly 2 children**
  - **Classification with**
    - **Gini-index**
    - **Entropy**
  - **Regression with**
    - **MSE (Mean Squared Error)**

Decision Tree (DT) - Concept

- **Each node should represent a binary split of the samples being classified**
  - **By what criterion/attribute/feature?**
    - **The one that "best" separates the data into [2 different] classes**
    - **Gini-index is a metric to find that criterion**
      - **Also known as "Gini impurity"**
      - **Spoiler: pick the feature with the lowest Gini-index**
- **Start by considering the entire labelled dataset**
  - **Compute the "best" split criterion**
  - **When applied, that criterion splits the tree in 2 different branches**
    - **Conducting to 2 different sub-trees**
      - **representing sub-sets of the original dataset**
- **Repeat for each sub-set**
  - **So, it is a recursive approach**
 - **Until a stop condition is matched**

Decision Tree (DT) - When to stop?

- **The CART hyper-parameters (Leo Breiman, 1984)**
  - **max_depth**
  - **min_samples_split**
  - **min_samples_leaf**
- **Limit by metric**
  - **Gini of 0 (zero) means "no impurity"**
    - **All data belongs to a single class**
- **Limit the tree's depth**
  - **Control the recursive exploration**
- **Limit by number of samples in [leaf] nodes**
- **Take a look at some trees, as plotted by:**
  - **1_dt_classification_iris.py**
  - **1_dt_classification_wine.py**
  - **1_dt_regression_boston.py # fail - ethics**
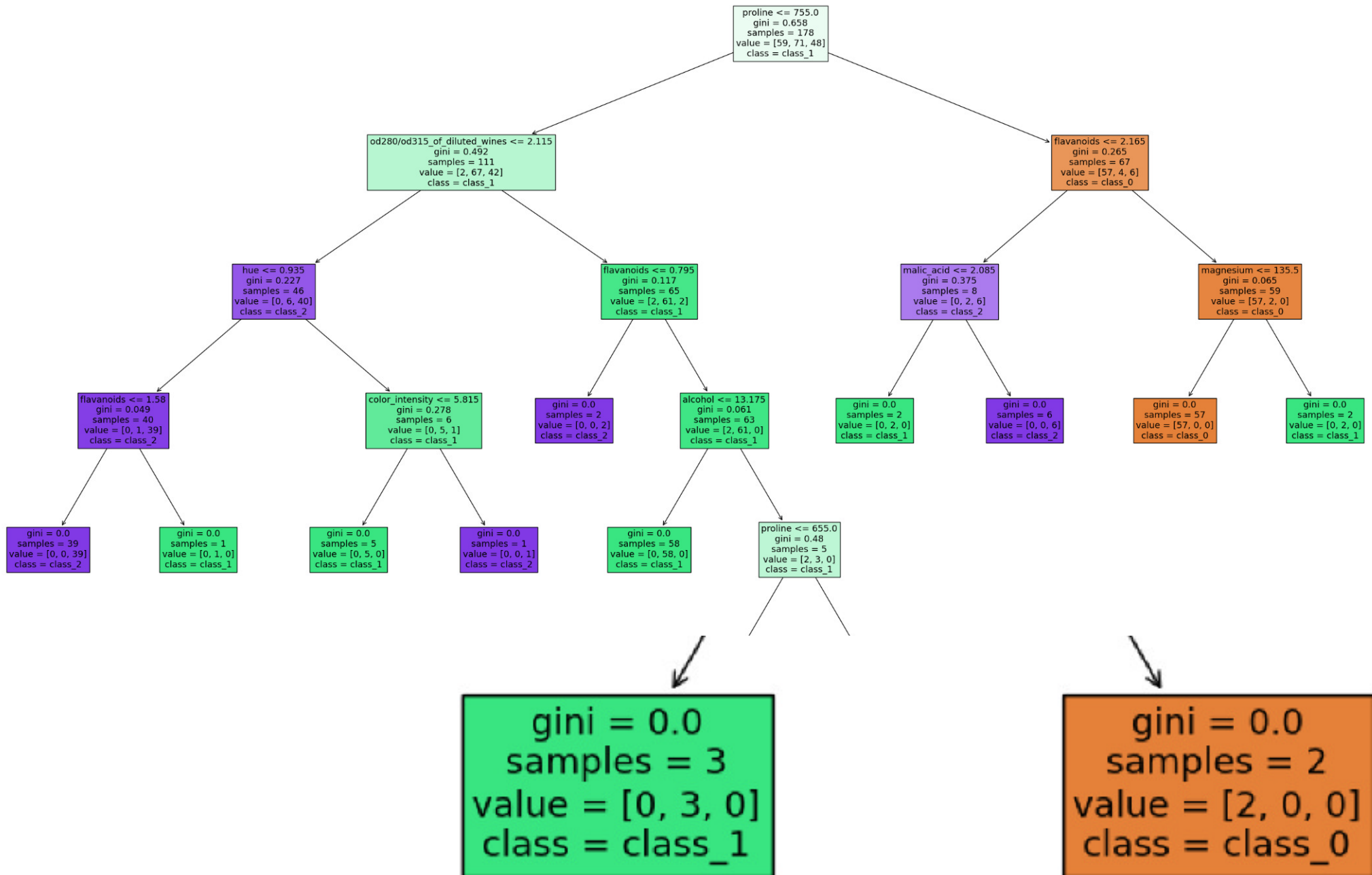 - **1_dt_regression_california.py**

DT for classification using the "Iris" DS

- **Each node: criterion ; gini ; samples in it ; samples distribution ; majority class**
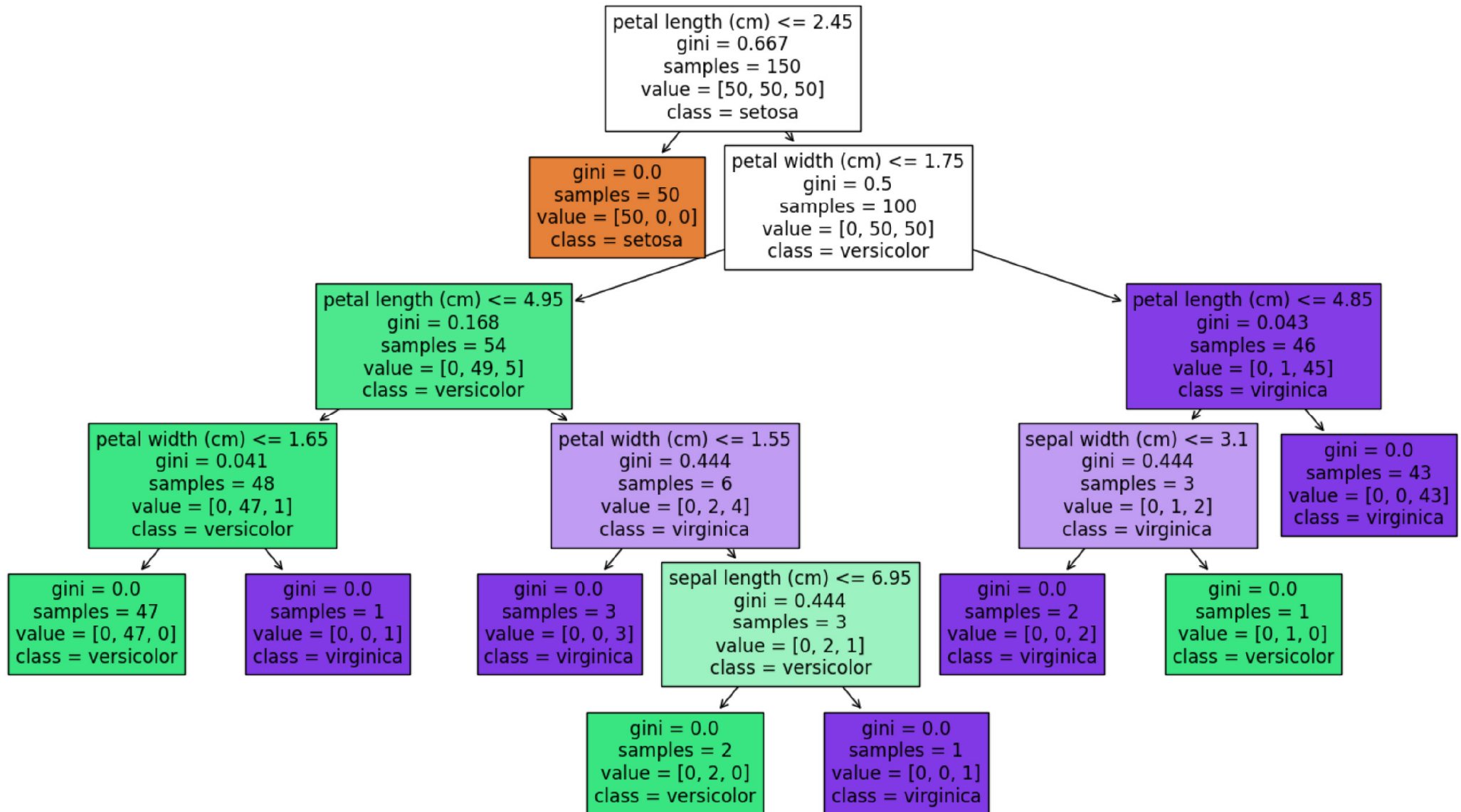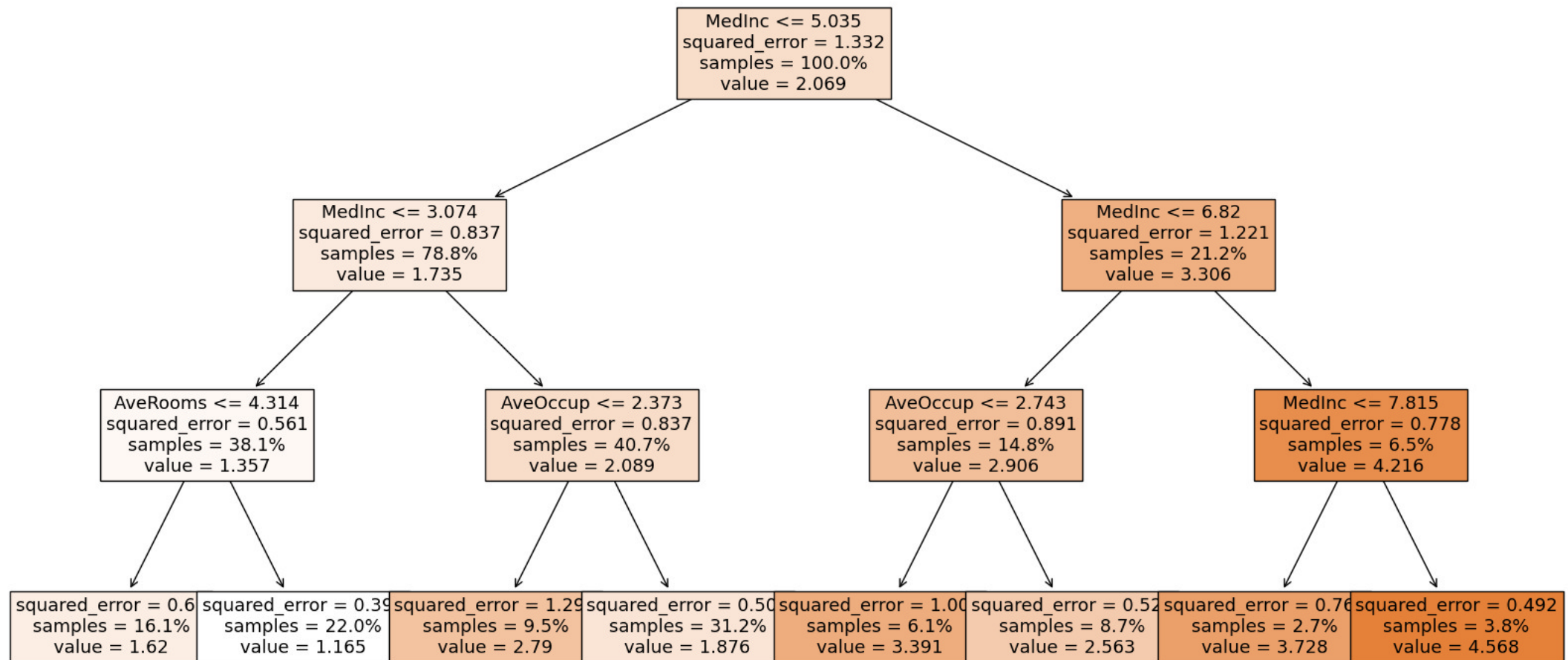
DT for classification using the "Wine" DS

- **Notice the gini = 0 on leaf nodes**

DT for classification using the "Iris" DS

- **Each node: criterion ; gini ; samples in it ; samples distribution ; majority class**

$$G = 1 - \sum_{i=1}^{c} (p_i)^2$$

Computing the Gini-index

- **Gini-index or Gini impurity (or just G in this doc)**

- **Computed <mark>per feature</mark> and <mark>in parts</mark>**
  - **G = 1 - sum(proportion of class i "in the node"**2)**
  - **One part per feature value**
  - **For example, if the possible values for a feature F are**
    - **Yes or No, then compute**
    - **G(Yes)**
    - **G(No)**
    - **G = weight(Yes) * G(Yes) + weight(No) * G(No)**
      - **Weight(Yes) = number of samples with F=Yes / total number of samples**
      - **Weight(No) = number of samples with F=No / total number of samples**

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

Computing gini algorithm by example 1/5

- **Consider the supervised dataset above**
  - **The labels/targets column is named "preferred"**
- **Start with any feature,**
  - **for example with features F = "Account age > 1"**
- **Step #1 - build as many sets as the diff values for F**
  - **Each set will contain the samples with different values**
- **2 sets, in this case, one set for "No", other for "Yes"**
- **set_no = [3, 7, 8] ; set_yes = [1, 2, 4, 5, 6]**

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

- **set_no** = [3, 7, 8] ; **set_yes** = [1, 2, 4, 5, 6]
- **Step #2 - build *aux* groups representing the dataset's different values, according to the supervised label**
  - group_no = [1, 2, 3, 5, 8] ; group_yes = [4, 6, 7]
- **Next, find the intersections between the sets formed in step #1 and the labels' groups**
  - set_no.intercept[group_no] = [3, 8]
  - set_no.intercept[group_yes] = [7]
  - *set*_yes.intercept[group_no] = [1, 2, 5]
  - *set*_yes.intercept[group_yes] = [4, 6]

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

- **Remember**
  - set_no = [3, 7, 8] ; set_yes = [1, 2, 4, 5, 6]
  - set_no.intercept[group_no] = [3, 8] ; set_no.intercept[group_yes] = [7]
  - set_yes.intercept[group_no] = [1, 2, 5] ; set_yes.intercept[group_yes] = [4, 6]

Step #3 – Compute the proportions, per set

- set_no has **3** elements
- **2** of set_no are in the intercept with group_no
- **1** of set_no is in the intercept with group_yes
- Pno1 = 2/3 ; Pno2 = 1/3
- set_yes has **5** elements
- **3** of set_yes are in the intercept with group_no
- **2** of set_yes are in the intercept with group_yes
- Pyes1 = 3/5 ; Pyes2 = 2/5

Computing gini algorithm by example 3/5

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Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

Computing gini algorithm by example 4/5

- **Remember**
  - set_no = [3, 7, 8] ; set_yes = [1, 2, 4, 5, 6]
  - set_no.intercept[group_no] = [3, 8] ; set_no.intercept[group_yes] = [7]
  - set_yes.intercept[group_no] = [1, 2, 5] ; set_yes.intercept[group_yes] = [4, 6]
  - Pno1 = 2/3 ; Pno2 = 1/3 ; Pyes1 = 3/5 ; Pyes2 = 2/5

- # Step #4 – Compute the partials
  - G(No) = 1 - (2/3**2 + 1/3**2) = 0.44
  - G(Yes) = 1 – (3/5**2 + 2/5**2) = 0.48

- # Next, compute the weights for the partials
  - set_no has 3 elements ; set_yes has 5 elements
  - The dataset has 8 elements
  - W(No) = 3/8
  - W(Yes) = 5/8

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

Computing gini algorithm by example 5/5

- **Remember**
  - set_no = [3, 7, 8] ; set_yes = [1, 2, 4, 5, 6]
  - set_no.intercept[group_no] = [3, 8] ; set_no.intercept[group_yes] = [7]
  - set_yes.intercept[group_no] = [1, 2, 5] ; set_yes.intercept[group_yes] = [4, 6]
  - Pno1 = 2/3 ; Pno2 = 1/3 ; Pyes1 = 3/5 ; Pyes2 = 2/5
  - G(No) = 0.44 ; G(Yes) = 0.48 ; W(No) = 3/8 ; W(Yes) = 5/8

- **Step #5 – Compute the Gini-index for the feature**
  - G = W(No)*G(No) + W(Yes)*G(Yes)
  - G = 3/8 * 0.44 + 5/8 * 0.48 = 0.465 ~ 0.47

- **Interpretation?**
  - Do this for ALL features
  - The lowest G value represents the feature to be used for splitting the dataset in the decision tree

Using the Gini-index

$$G = 1 - \sum_{i=1}^{c} (p_i)^2$$

- **Exercise: compute the Gini-index for the dataset, for the other features "Violations > 0" and "Balance > 50.000"**

- **Help:**

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

Feature	F-V	P1	P2	P1**2	P**2	sum	G	
Account Age > 1	No	2/3	1/3	4/9	1/9	0.56	0.44	GNo
Account Age > 1	Yes	3/5	2/5	1/3	1/6	0.52	0.48	GYes
Violations > 0	No	1/2	1/2	1/4	1/4	0.50	0.50	GNo
Violations > 0	Yes	1	0	1	0	1.00	0.00	GYes
Balance > 50.000	No	1	0	1	0	1.00	0.00	GNo
Balance > 50.000	Yes	4/7	3/7	1/3	1/5	0.51	0.49	GYes

Using the Gini-index

$$G = 1 - \sum_{i=1}^{c} (p_i)^2$$

- **G(Violations>0) = 6/8 * 0.5 + 2/8 * 0 = 0.375**
- **G(Balance > 50.000) = 1/8*0 + 7/8 * 0.49 = 0.42875**
- **Help:**

Account age > 1	Violations > 0	Balance > $50,000	Preferred
Yes	No	Yes	No
Yes	Yes	Yes	No
No	No	Yes	No
Yes	No	Yes	Yes
Yes	No	No	No
Yes	No	Yes	Yes
No	No	Yes	Yes
No	Yes	Yes	No

Feature	F-V	P1	P2	P1**2	P**2	sum	G	
Account Age > 1	No	2/3	1/3	4/9	1/9	0.56	0.44	GNo
Account Age > 1	Yes	3/5	2/5	1/3	1/6	0.52	0.48	GYes
Violations > 0	No	1/2	1/2	1/4	1/4	0.50	0.50	GNo
Violations > 0	Yes	1	0	1	0	1.00	0.00	GYes
Balance > 50.000	No	1	0	1	0	1.00	0.00	GNo
Balance > 50.000	Yes	4/7	3/7	1/3	1/5	0.51	0.49	GYes

$$G = 1 - \sum_{i=1}^{c} (p_i)^2$$

Using the Gini-index

- **G(Account Age>1) = 0.465 ~ 0.47**
- **G(Violations>0) = 0.375 ~ 0.38 lowest impurity**
- **G(Balance > 50.000) = 0.42875 ~ 0.43**
- **Continue, recursively**
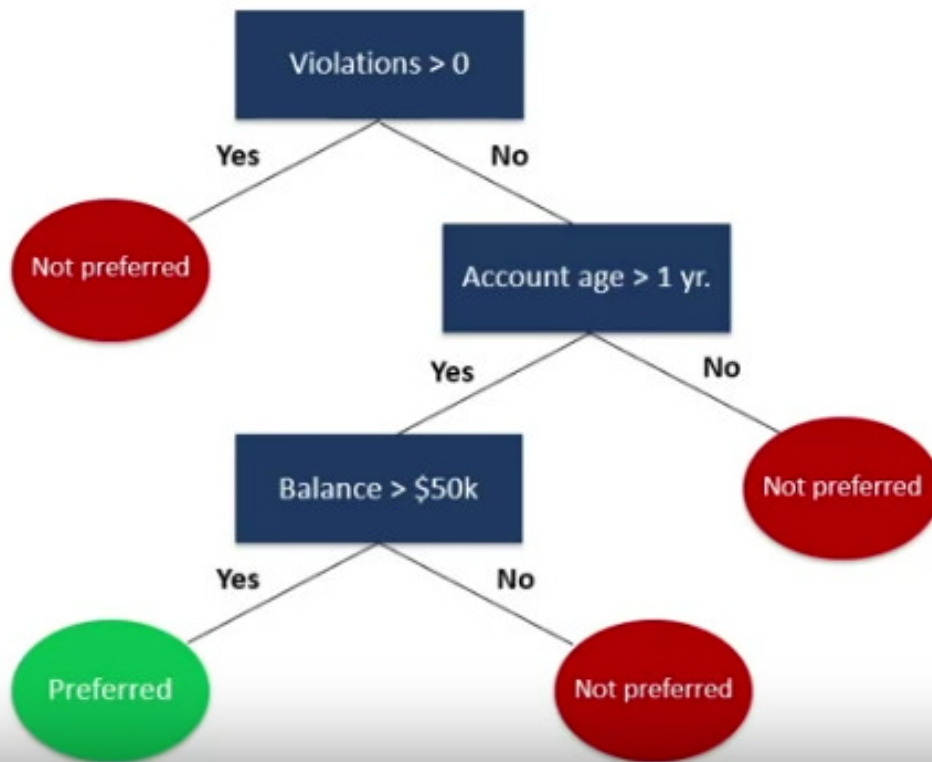
$$G = 1 - \sum_{i=1}^{c} (p_i)^2$$

Using the Gini-index

- **But scikit-learn's tree shows gini = 0.469, why?**
- **Because it is the value computed before any split, considering only the labels**
- **G = 1 - (5/8 No ** 2 + 3/8 Yes ** 2) = 0.46875 ~ 0.469**

```
Violations > 0 <= 0.5
gini = 0.469
samples = 8
value = [5, 3]
class = No
```

```
Balance > $50.000 <= 0.5
gini = 0.5
samples = 6
value = [3, 3]
class = No
```

```
gini = 0.0
samples = 2
value = [2, 0]
class = No
```

```
gini = 0.0
samples = 1
value = [1, 0]
class = No
```

```
Account age > 1 <= 0.5
gini = 0.48
samples = 5
value = [2, 3]
class = Yes
```

```
gini = 0.5
samples = 2
value = [1, 1]
class = No
```

```
gini = 0.444
samples = 3
value = [1, 2]
class = Yes
```

References

- https://scikit-learn.org/stable/modules/tree.html
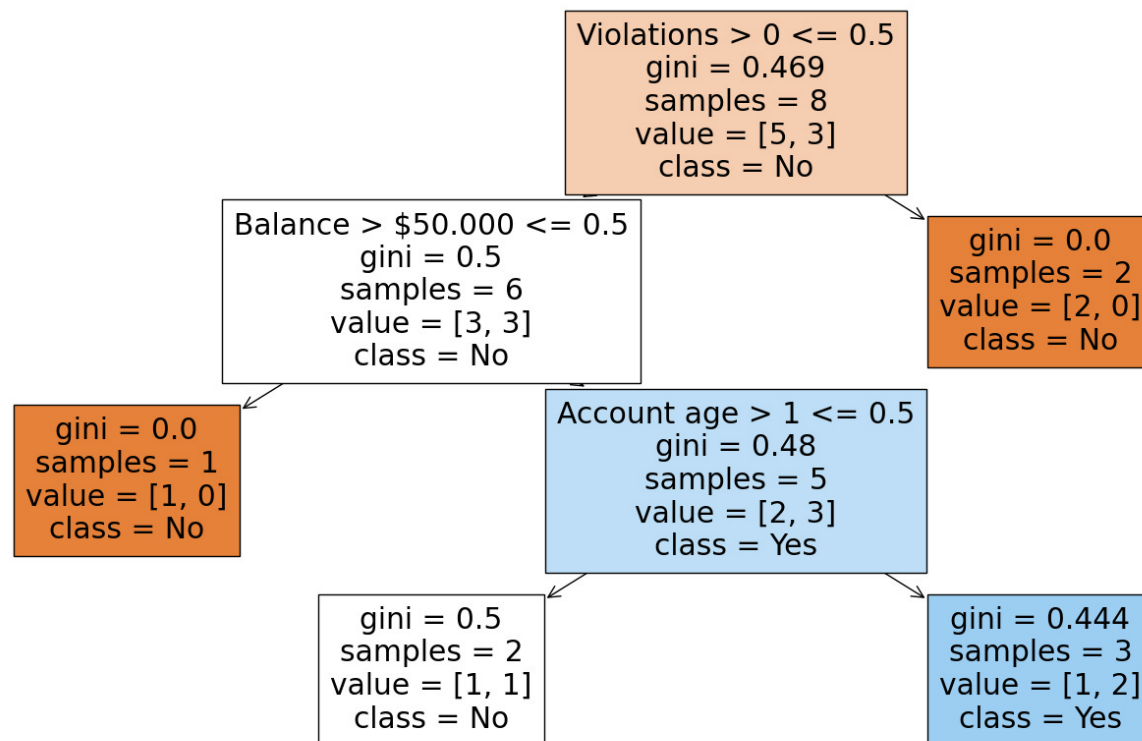
- https://github.com/amsm/am_decision_trees