

# Decision Trees

DESU IA4Health

Info-GRAM

# Characteristics

- *Decision Trees* can perform both classification and regression tasks, and even multioutput tasks.
- Decision Trees are also the fundamental components of Random Forests.
- Non-parametrics models
- they don't require feature scaling or centering at all.
- Decision Trees are fairly intuitive and their decisions are easy to interpret. They are often called *white box models*. In contrast, as we will see, Random Forests or neural networks are generally considered *black box models*.

# Objectives

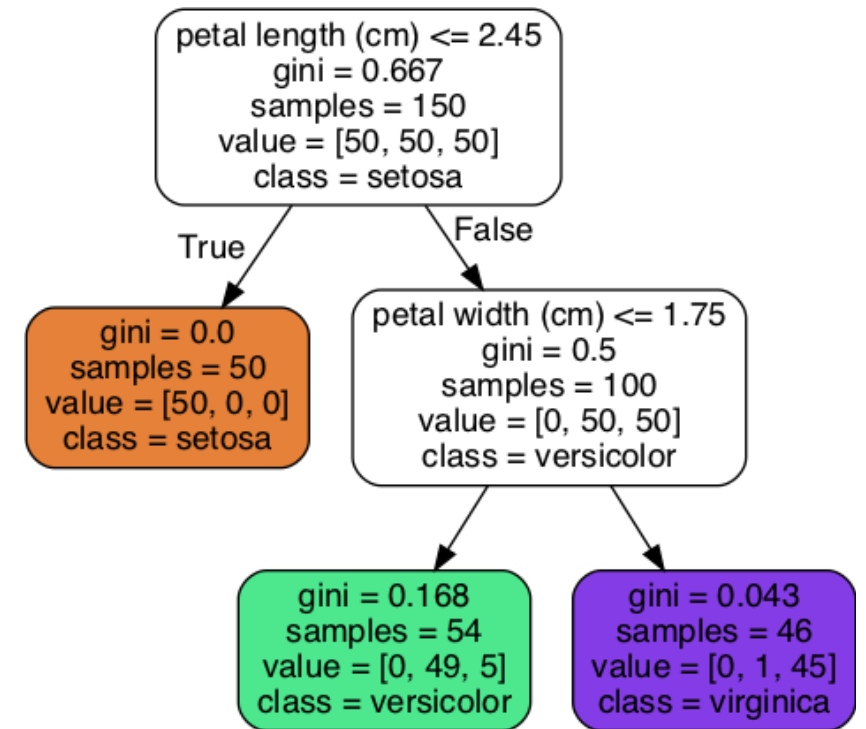
- Training
- Trees visualization
- Make predictions
- Regularization
- Trees for regression

# Tree representation

- **Samples** : counts how many training instances it applies to.
- **Value** : tells you how many training instances of each class this node applies
- **Gini** : measures its *impurity*.
  - a node is “pure” (gini=0) if all training instances it applies to belong to the same class.

$$G_i = 1 - \sum_{k=1}^n p_{i,k}^2$$

$p_{i,k}$  is the ratio of class  $k$  instances among the training instances in the  $i^{\text{th}}$  node.

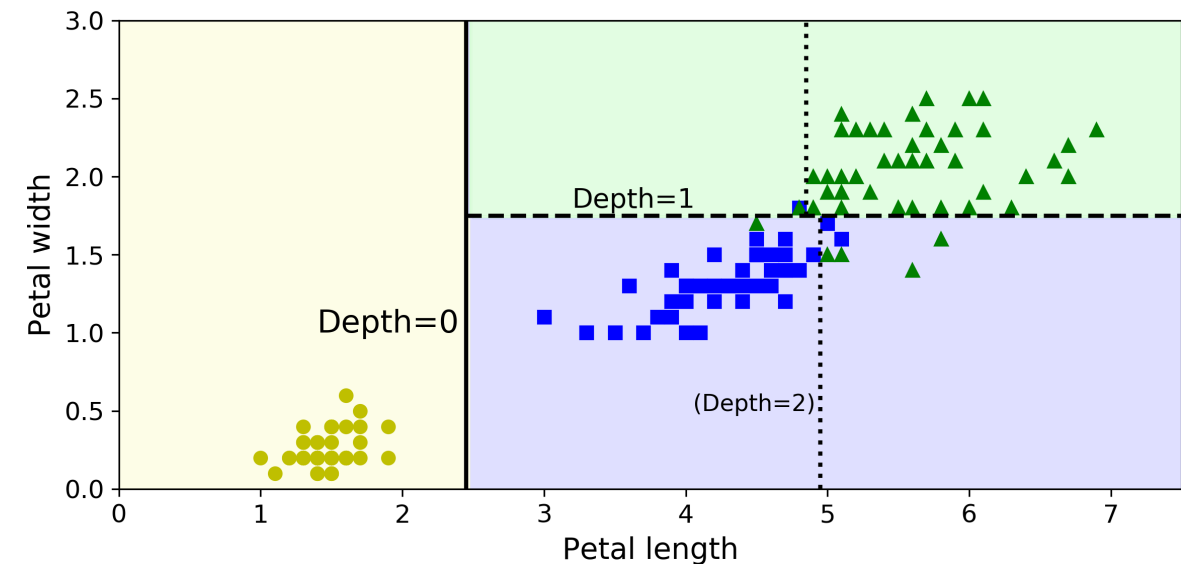


# Entropy

- The concept of entropy originated in thermodynamics as a measure of molecular disorder: entropy approaches zero when molecules are still and well ordered.
- Shannon's *information theory*, where it measures the average information content of a message: entropy is zero when all messages are identical.

# Decision Boundaries

- The thick vertical line represents the decision boundary of the root node (depth 0): petal length = 2.45 cm. Since the left area is pure (only Iris-Setosa), it cannot be split any further.
- The right area is impure, so the depth-1 right node splits it at petal width = 1.75 cm (represented by the dashed line). Since `max_depth` was set to 2, the Decision Tree stops right there.
- if `max_depth` would have been 3, then the two depth-2 nodes would each add another decision boundary (represented by the dotted lines).



# Estimating Class Probabilities

- A Decision Tree can also estimate the probability that an instance belongs to a particular class  $k$ : first it traverses the tree to find the leaf node for this instance, and then it returns the ratio of training instances of class  $k$  in this node

# CART Training Algorithm

- The algorithm first splits the training set in two subsets using a single feature  $k$  and a threshold  $t_k$  (e.g., "petal length  $\leq 2.45$  cm").
  - It searches for the pair  $(k, t_k)$  that produces the purest subsets (weighted by their size).
- The cost function that the algorithm tries to minimize

$$J(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}}$$

where  $\begin{cases} G_{\text{left/right}} & \text{measures the impurity of the left/right subset,} \\ m_{\text{left/right}} & \text{is the number of instances in the left/right subset.} \end{cases}$

- Once it has successfully split the training set in two, it splits the subsets, recursively. It stops recursing once it reaches the maximum depth (defined by the max\_depth hyperparameter),



# Regularization Hyperparameters

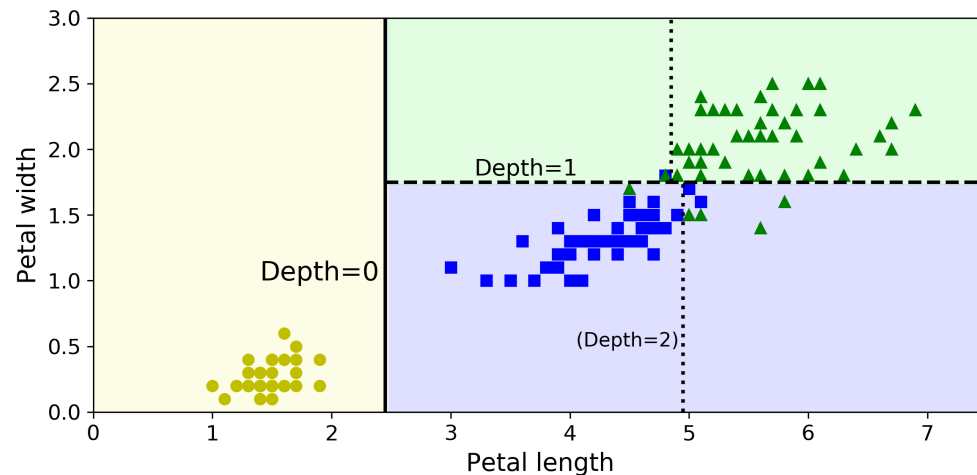
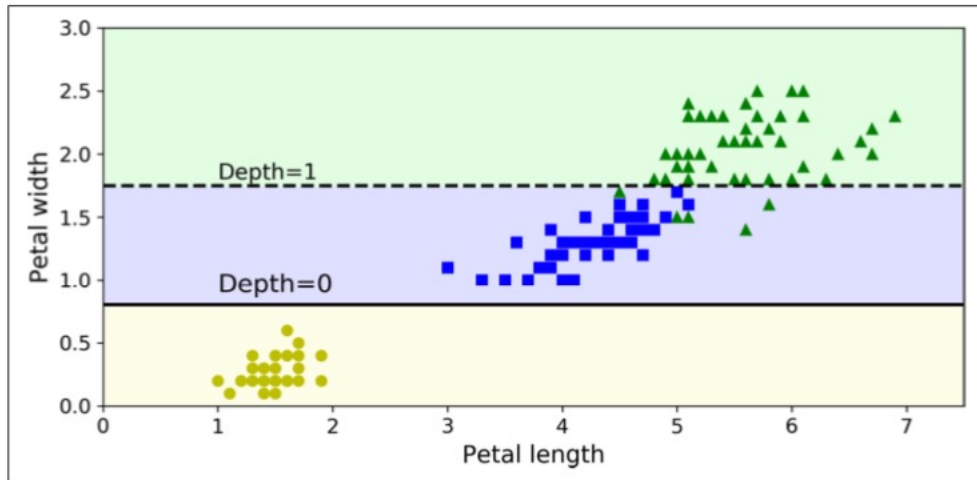
- ***max\_depth***
- ***max\_leaf\_nodes*** (maximum number of leaf nodes),
- ***max\_features*** (maximum number of features that are evaluated for splitting at each node).
- ***min\_samples\_split*** (the minimum number of samples a node must have before it can be split),
- ***min\_samples\_leaf*** (the minimum number of samples a leaf node must have),
- ***min\_weight\_fraction\_leaf*** (same as `min_samples_leaf` but expressed as a fraction of the total number of weighted instances)

## To regularize the model :

- Increase `min_*` hyperparameters
- Reduce `max_*` hyperparameters

# Inestability

- Decision Trees are very sensitive to small variations in the training data.
- For example, if you just remove the widest Iris-Versicolor from the iris training set (the one with petals 4.8 cm long and 1.8 cm wide) and train a new Decision Tree, you may get the model represented in the left very different from the previous Decision Tree in the right



## Solution :

- Ensemble classifiers