

Decision Trees: CART

Machine Learning

Classification and Regression

- Decision Trees can be used for both

X1	X2	Y
0.268	0.266	Bad
0.219	0.372	Bad
0.517	0.573	Bad
0.269	0.908	Good
0.181	0.202	Bad
0.519	0.898	Good
0.563	0.945	Bad
0.129	0.661	Bad

- Classification

- Spam / not Spam
- Admit to ICU /not
- Lend money / deny
- Intrusion detections

X1	X2	Y
0.268	0.266	64.41
0.219	0.372	28.08
0.517	0.573	95.76
0.269	0.908	15.84
0.181	0.202	41.83
0.519	0.898	25.20
0.563	0.945	9.44
0.129	0.661	82.77

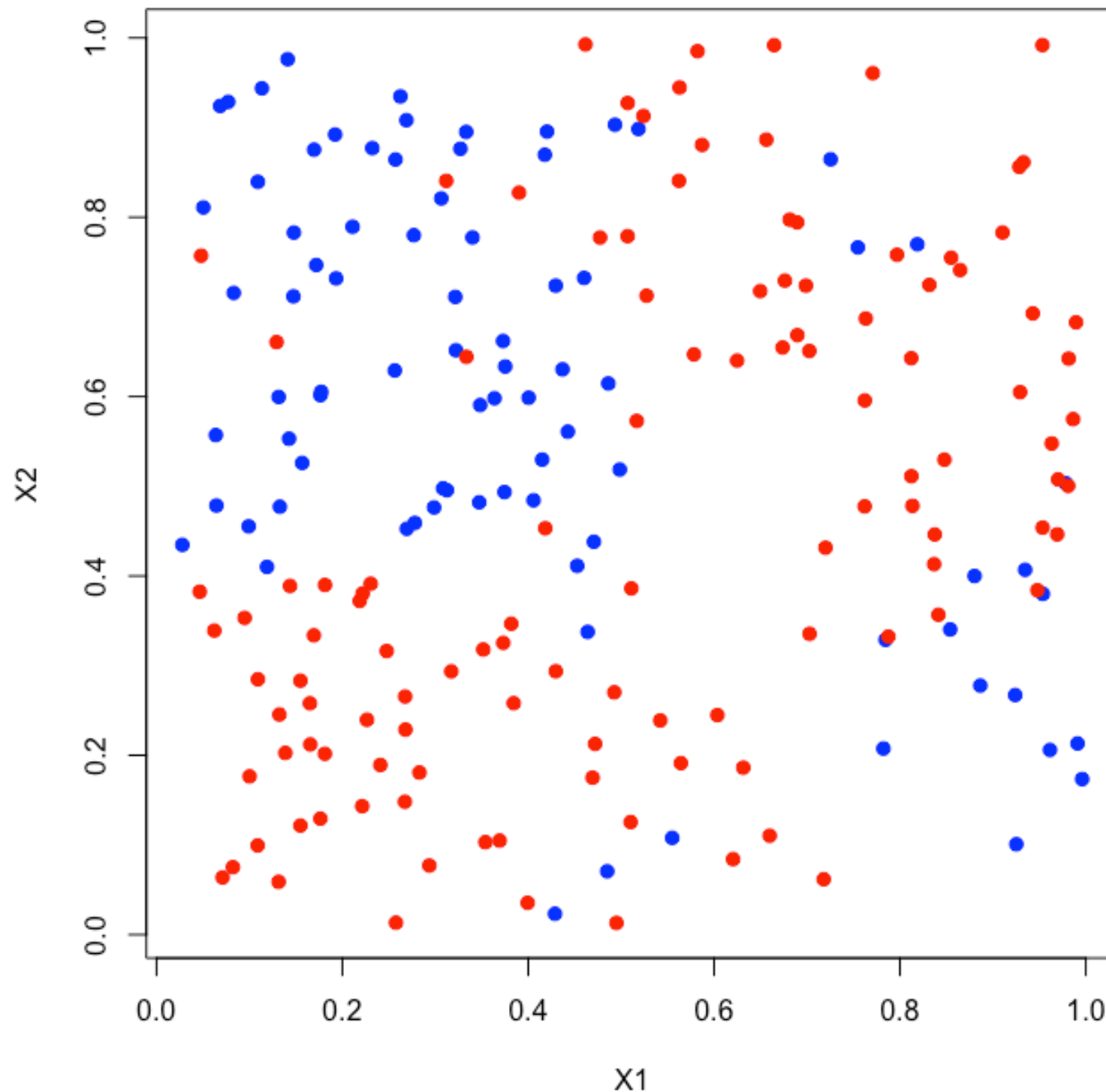
- Regression

- Predict stock returns
- Pricing a house or a car
- Weather predictions (temp, rain fall etc)
- Economic growth predictions
- Predicting sports scores

Decision Trees

- The general idea is that we will segment the space into a number of simple regions.
- The segmentation can be illustrated as a tree
- The end nodes can have a category (classification) or a continuous number (regression)
- These methods, while quite simple are very powerful.

Visualizing Classification as a Tree



Metrics

- Algorithms for constructing decision trees usually work top-down, by choosing a variable at each step that best splits the set of items.
- Different algorithms use different metrics for measuring “best”
- These metrics measure how similar a region or a node is. They are said to measure the impurity of a region.
- Larger these impurity metrics the larger the “dissimilarity” of a nodes/regions data.
- Examples: Gini impurity, Entropy, Variance

Algorithms for building Decision Trees

- Popular ones include
 - CART (Classification And Regression Tree)
 - CHAID (CHi-squared Automatic Interaction Detector)
 - C4.5
- We will focus on CART, that uses the Gini impurity as its impurity measure.

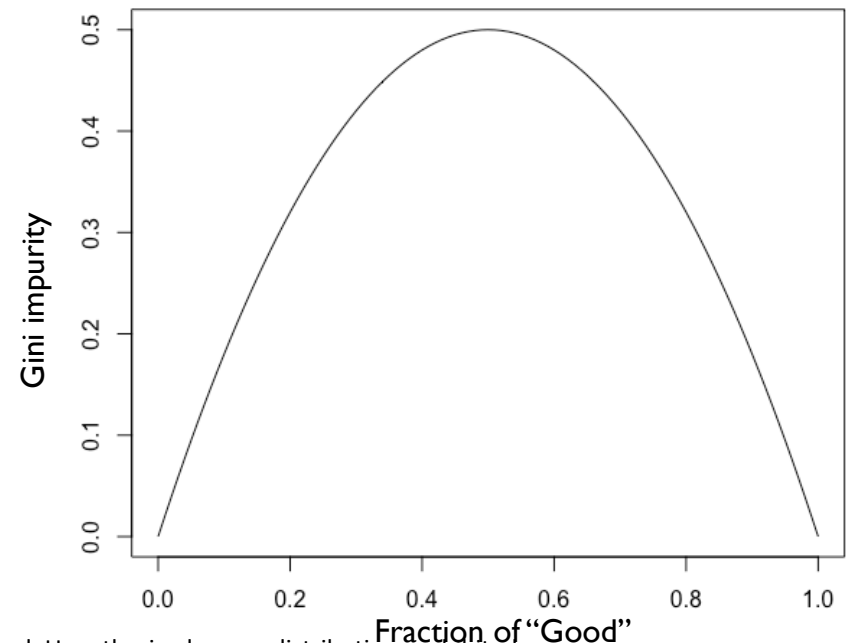
CART: An Example

Cust_ID	Gender	Occupati on	Age	Target
1	M	Sal	22	1
2	M	Sal	22	0
3	M	Self-Emp	23	1
4	M	Self-Emp	23	0
5	M	Self-Emp	24	1
6	M	Self-Emp	24	0
7	F	Sal	25	1
8	F	Sal	25	0
9	F	Sal	26	0
10	F	Self-Emp	26	0

Gini impurity

- Used by the CART
- Is a measure of how often a randomly chosen element from the set would be incorrectly labeled if it was randomly labeled according to the distribution of labels in the subset.
- Can be computed by summing the probability of an item with label i being chosen (p_i), times the probability of a mistake ($1 - p_i$) in categorizing that item.
- Simplifying gives, the Gini impurity of a set:

$$1 - \sum_{i=1}^J p_i^2$$

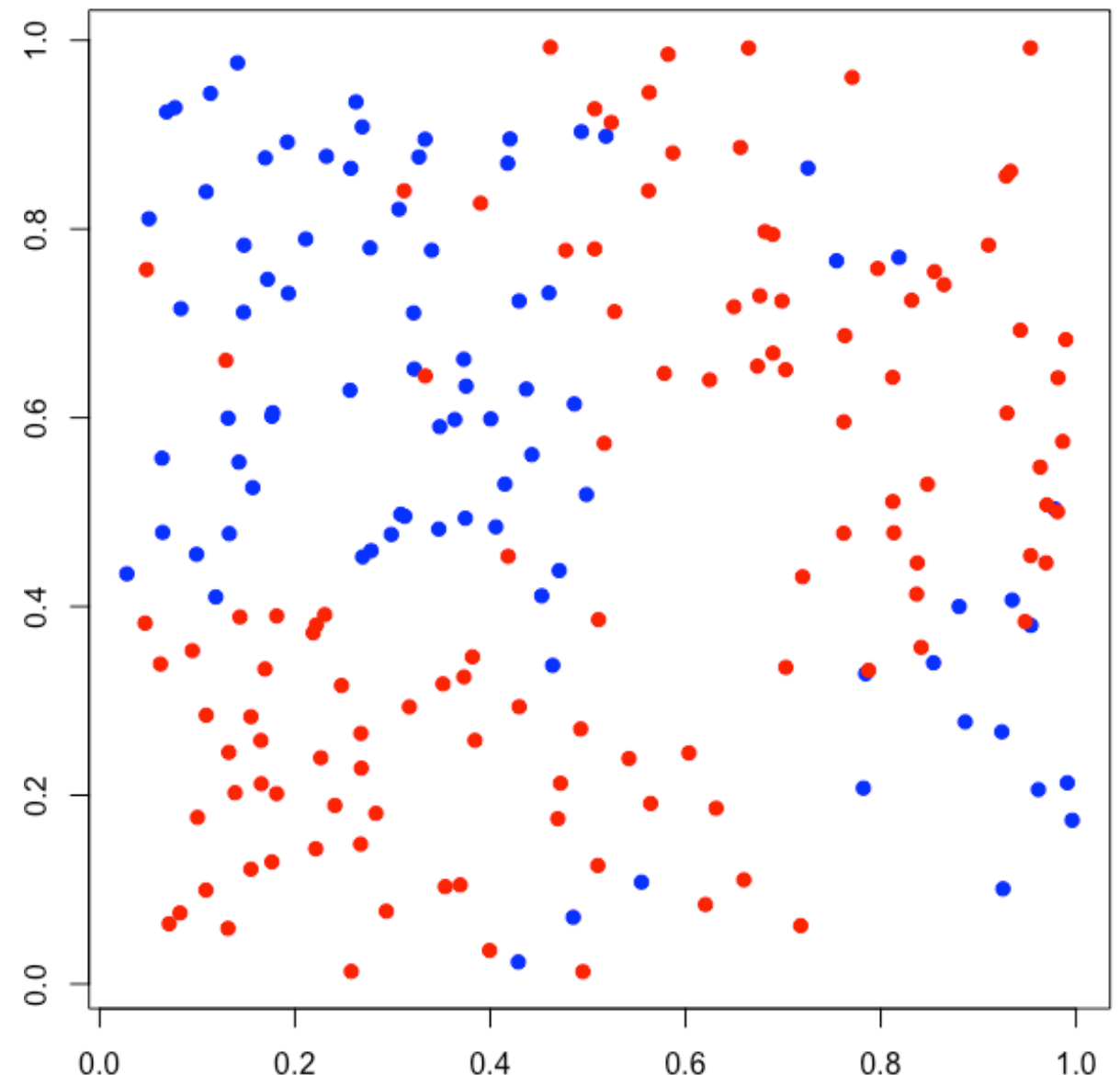


Splitting using Gini impurity

- When splitting, the Gini impurity of the two resulting nodes are combined using a weighted average.
- With weights being the fraction of data on each node.
- The CART algorithm simply chooses the right “split” by finding the split that maximizes the “decrease in Gini impurity” - also called the Gini Gain.

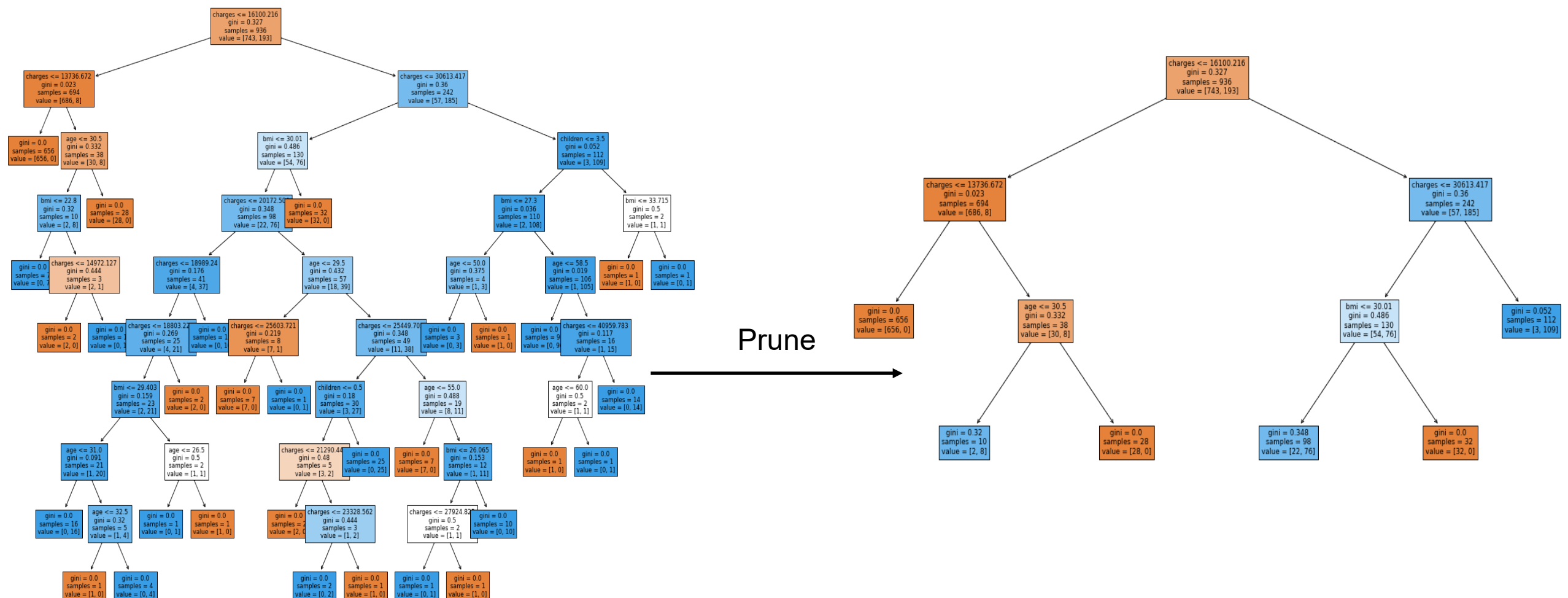
Decision trees are prone to 'overfitting'

- Decision Tree is a powerful algorithm that can adapt well and capture various patterns in the data
- If allowed to grow fully, they become over-complex & tend to fit even the noise
- Thus, a fully grown tree may not 'generalize' well on test or new unseen data



Pruning

- Ideally we would like a tree that does not over-fit the given data
- One popular and simple way to prune a decision tree is by limiting the depth of the tree to avoid over fitting.
- For example the tree on the right below is generated with a max depth of 2 while the tree on the left has no depth restriction (and hence overfits the data)



Pre-Pruning

- Stop growing the tree before it grows too big
- This can be achieved by bounding hyperparameters

Hyperparameters in Decision Trees

- **max_depth** - The maximum depth of the tree. If set to 'None', then nodes are expanded until all leaves are pure. Higher the value, more complex the tree
- **min_samples_split** - The minimum number of samples required to split a node. Doesn't split any node that is smaller than this number. Higher the values, less complex the tree
- **min_samples_leaf** - The minimum number of samples required at a leaf node. All leaf nodes have at least these many data points. Higher the value, less complex the tree

Hyperparameter Tuning using Grid Search

- Grid Search is a process of searching the best combination of hyperparameters from a predefined set of values
- A parameter grid (Hyperparameters and corresponding values) is provided as an input to the Grid-search function
- It tries all the combinations of the values passed and evaluates the model for each combination
- It returns the combination of hyperparameter values that works best as per the metric provided for model evaluation
- GridSearchCV() is an implementation of Grid Search with Cross Validation

Cross Validation

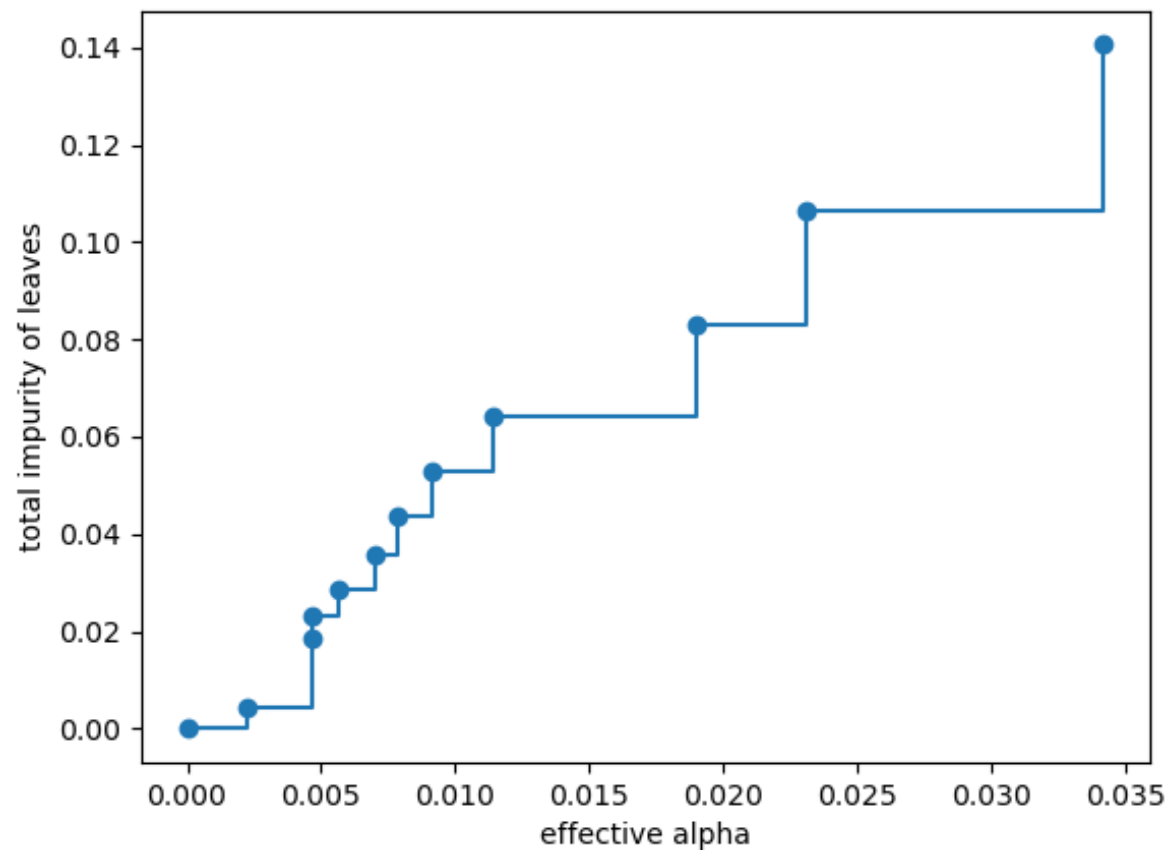
- Cross Validation is a common Machine Learning technique that splits the data into n non-overlapping groups, and runs n experiments:
 - In each experiment, $n-1$ groups are used to train a model and the model is tested on the left out group.
 - The results are summarized over the n experiments.
- It gives a mechanism that allows us to test a model repeatedly on data that was not used to build the model.
- For Decision Trees, a very common approach is simply to choose the tree with minimum cross validation error

Post-Pruning: Cost-complexity pruning

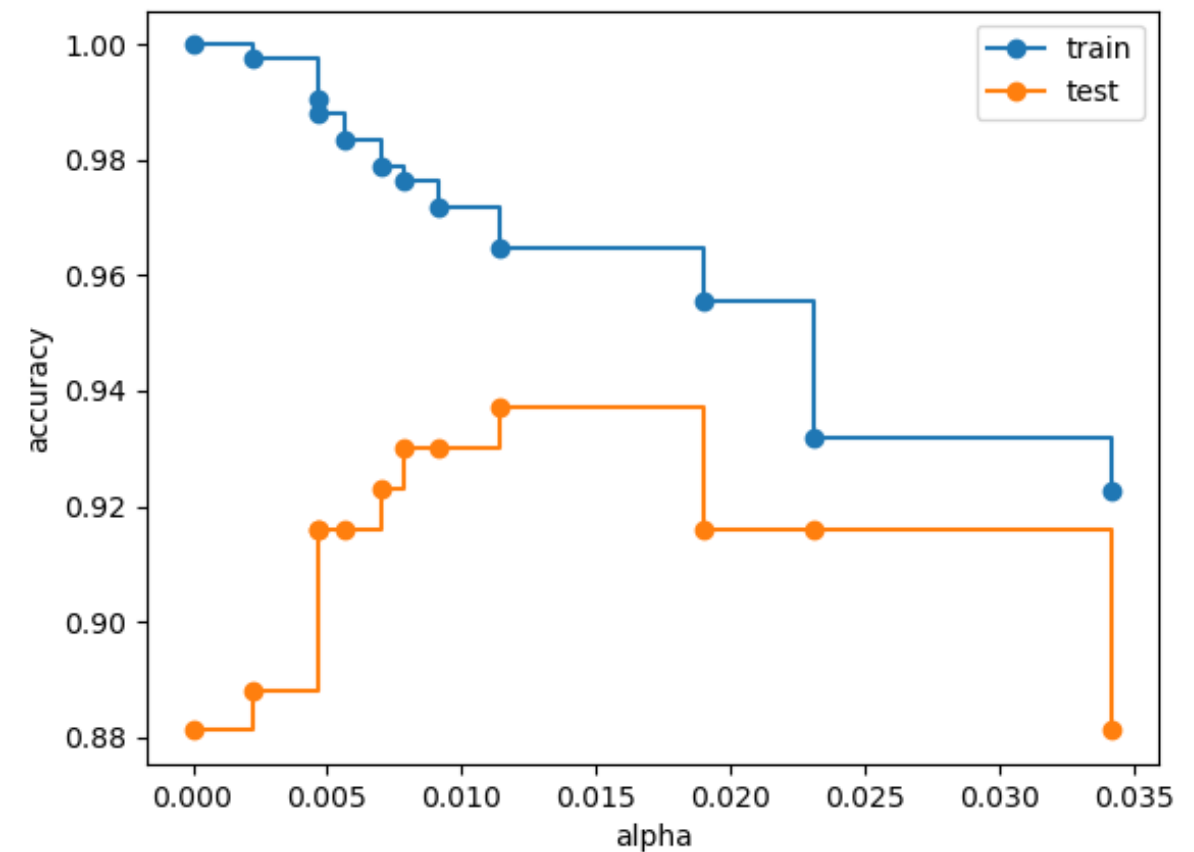
α

- Starting from the Full tree, create a sequence of trees that are sequentially smaller (pruned)
- At each step the algorithm
 - try removing each possible subtree
 - find the 'relative error decrease per node' for that subtree - Complexity parameter,
 - And remove the subtree with the minimum
- With the list of subtrees, one usually reverts back to using cross-validation errors to find the best final pruned tree

Total Impurity vs effective alpha for training set



Accuracy vs alpha for training and testing sets



Few Additional Thoughts

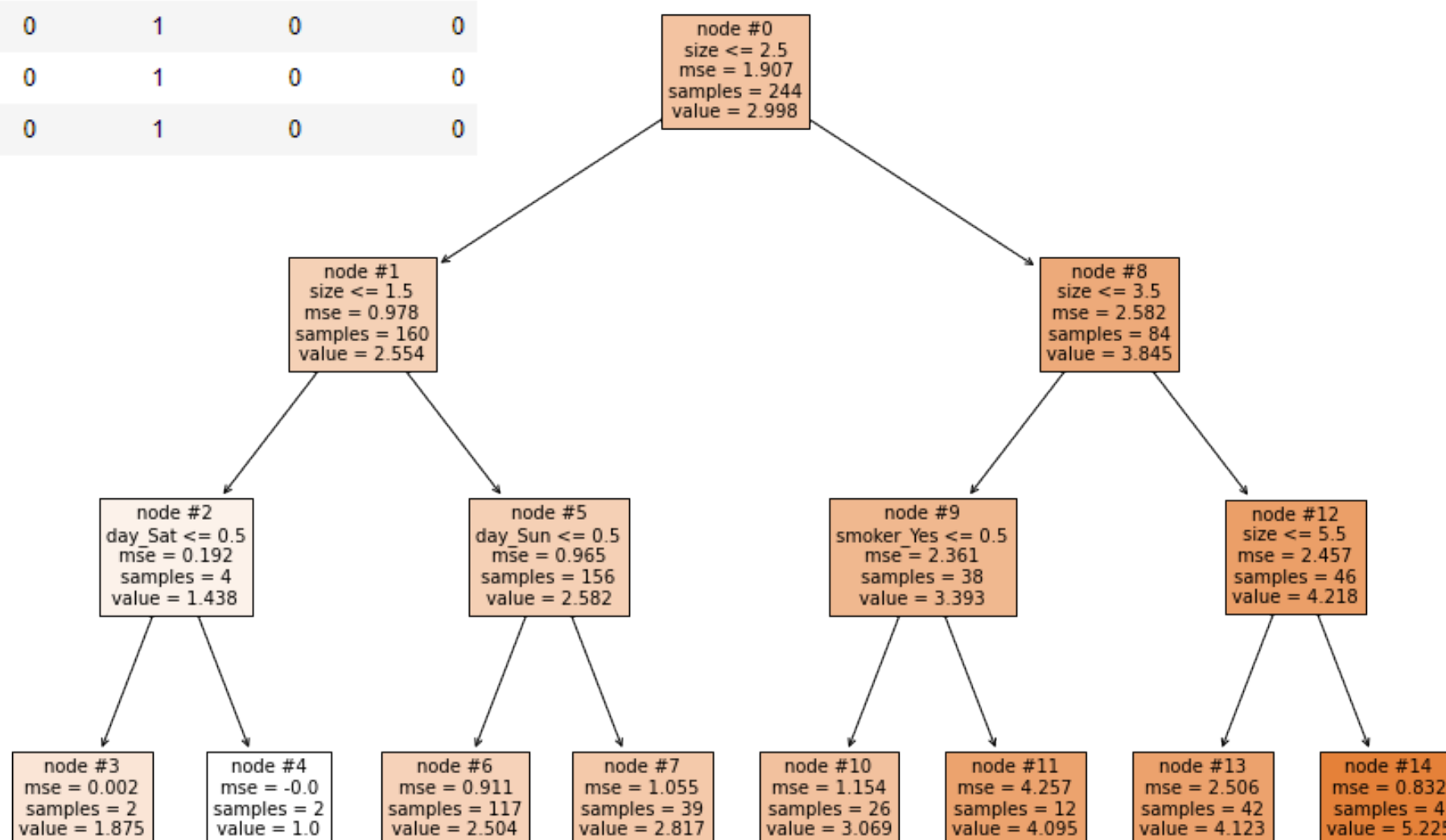
- Other impurity measures
- Regression Trees
- Pros and Cons

Impurity Measures in Decision Trees

	GINI INDEX	ENTROPY	INFORMATION GAIN	VARIANCE
When to use	Classification	Classification	Classification	Regression
Formula	$1 - \sum p_i^2$	$-\sum p_i \log(p_i)$	$E(Y) - E(Y X)$	$\Sigma(x - \bar{x})^2 / N$
Range	0 to 0.5 0 = most pure 0.5 = most impure	0 to 1 0 = most pure 1 = most impure	0 to 1 0 = less gain 1 = more gain	≥ 0
Characteristics	Easy to compute Non-additive	Computationally intensive Additive	Computationally intensive	The most common measure of spread

Regression Trees

	tip	size	sex_Male	smoker_Yes	day_Sat	day_Sun	day_Thur	time_Lunch
0	1.01	2	0	0	0	1	0	0
1	1.66	3	1	0	0	1	0	0
2	3.50	3	1	0	0	1	0	0
3	3.31	2	1	0	0	1	0	0
4	3.61	4	0	0	0	1	0	0
5	4.71	4	1	0	0	1	0	0
6	2.00	2	1	0	0	1	0	0



Pros and Cons of Decision Trees

Pros -

- Easy to understand and interpret
- Useful in data exploration as it gives the splitting based on the significance of variables
- Not influenced by the outlier/Null values and hence requires less data cleaning. Requires less time and effort during data pre-processing than other algorithms.
- Can handle both continuous and categorical variables
- Does not require any underlying assumptions in data. Works with both linearly and nonlinearly related variables.

Pros and Cons of Decision Trees

Cons-

- A small change in the data-set can result in large change in the structure of the decision tree causing instability in the model.
- Large trees can be difficult to interpret.
- Tends to overfit.