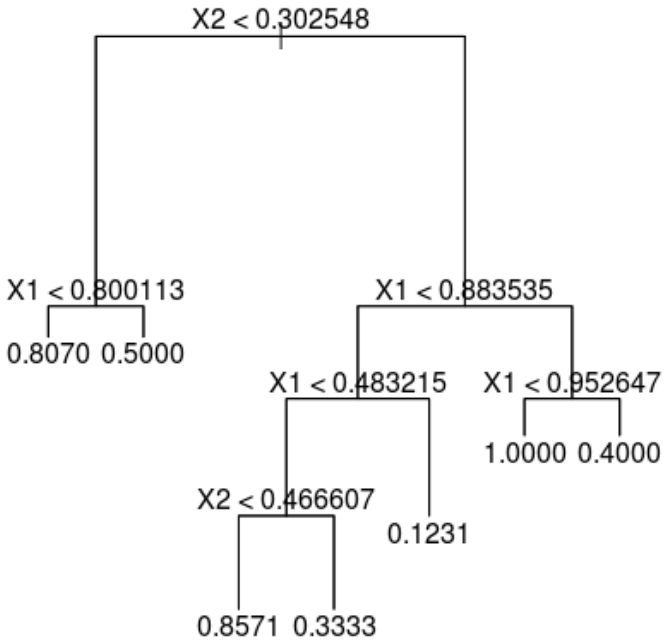
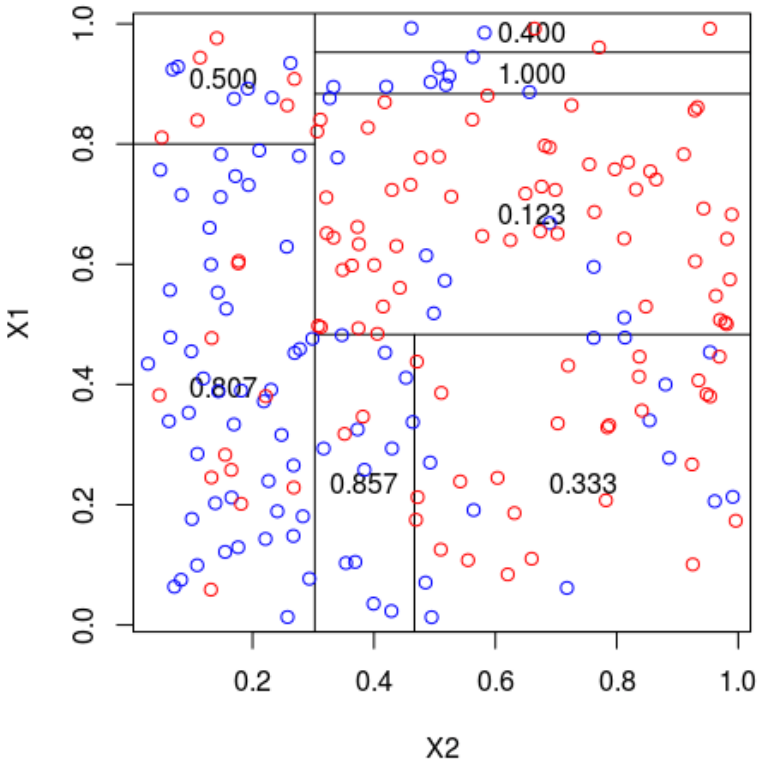
DECISION TREES

www Sources for figures & examples
https://scikit-learn.org/stable/
https://dimensionless.in/introduction-to-random-forest/
https://gluon.mxnet.io/index.html
https://skymind.ai/wiki/

Decision tree : deterministic data structure for modeling decision rules for a specific classification problem.

Construction : At each node, a single feature is selected to make separating decision. Splitting is stopped when leaf node has optimally less data points (wrt to a pre-defined criterion).





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Goal is to create a model that predicts the value of a target variable based on several input variables.

→ Each "interior" node of a tree corresponds to one of the input variables; there are edges to children for each of the possible values of that input variable. Each leaf represents a value of the target variable given the values of the input variables represented by the path from the root to the leaf.

→ A tree can be "learned" by splitting the source set into subsets based on an attribute value test. The "recursion" is completed when the subset at a node has all the same value of the target variable, or when splitting no longer adds value to the predictions (greedy algo).

→ As any multiway split may be summerized as a series of binary splits, the focus will be made on binary splits.

→ Splits are obtained by choosing a test at each step that "best" splits the set of items : What does mean Choosing the "best" split $S = S_r \cup S_l$ such that $S_r \cup S_l = \emptyset$ for e test property T ? An obvious heuristic is to choose the the query that decreases the impurity a much as possible.

Choice of a metrics Gini Impurity

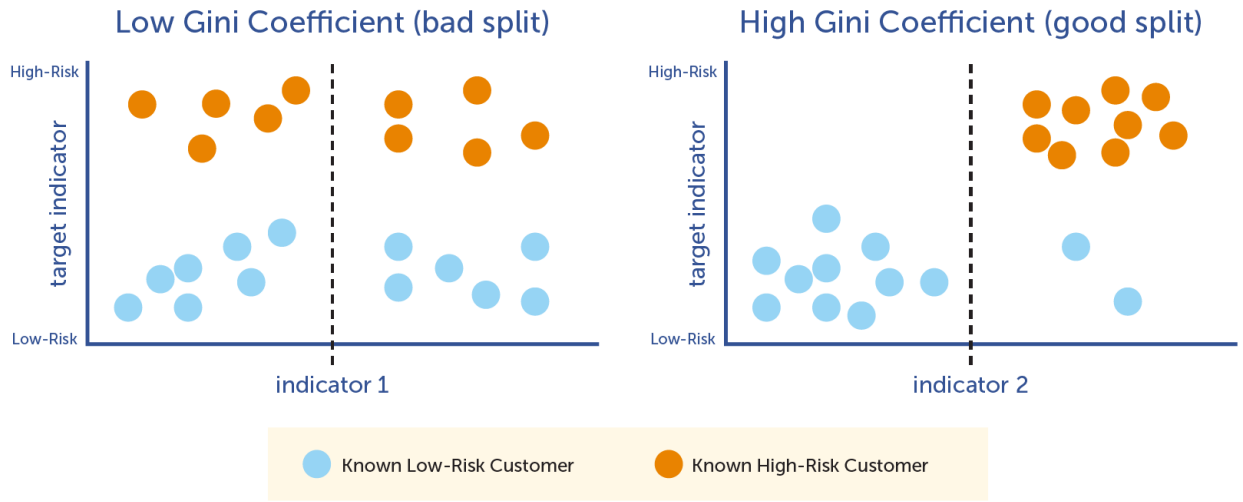
Gini Impurity of a set **S** of cardinal N measures the probability that a randomly chosen element of the set would be incorrectly labeled if randomly labeled according to the label distibution in **S**.

$$GI(S) = \sum_{k=1}^{K} P(y=k).P(y \neq k) = \sum_{k=1}^{K} P(y=k)[1-P(y \neq k)] = 1-\sum_{k=1}^{K} P^2(y=k)$$

then

$$\Delta GI(S) = GI(S) - P(S_l)GI(S_l) - (1 - P(S_l))GI(S_r)$$

where $P(S_l) = \frac{N_l}{N}$ and $N_l + N_r = N$



Choice of a metrics Entropy (Information) Impurity

$$H(S) = -\sum_{k=1}^{K} P(y=k) \log_2 P(y=k)$$

the the information gain (IG) associated to the split (or partition) (S_l, S_r) is

$$IG(S) = H(S) - H(S|(S_l, S_r)) = H(S) - P(S_l)H(S_l) - P(S_r)H(S_r)$$

where $H(S_l)$ (resp $H(S_r)$) are evaluated by using the empirical probabilities of the classes estimated from the subset S_l (resp S_r) :

$$H(S_l) = -\sum_{k=1}^{K} P(y=k|X \in S_l) \log_2 P(y=k|X \in S_l)$$

Choice of a metrics Misclassification Impurity

$$MI(N) = 1 - \max_k P(y = k)$$

and hence the gain in MI

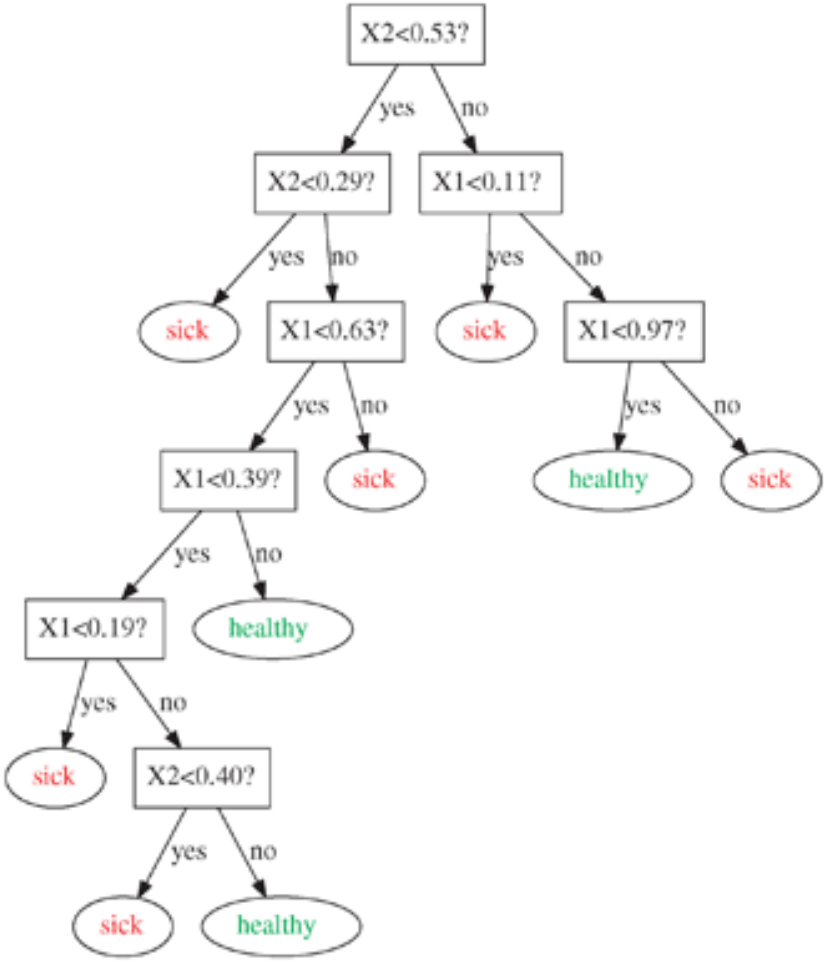
$$\begin{aligned} \Delta MI(N) &= MI(N) - P(S_l)MI(N_l) - P(S_r)MI(N_r) \\ &= MI(N) - 1 + P(S_l)\max_k P(y = k|X \in S_l) + P(S_r)\max_k P(y = k|X \in S_r) \end{aligned}$$

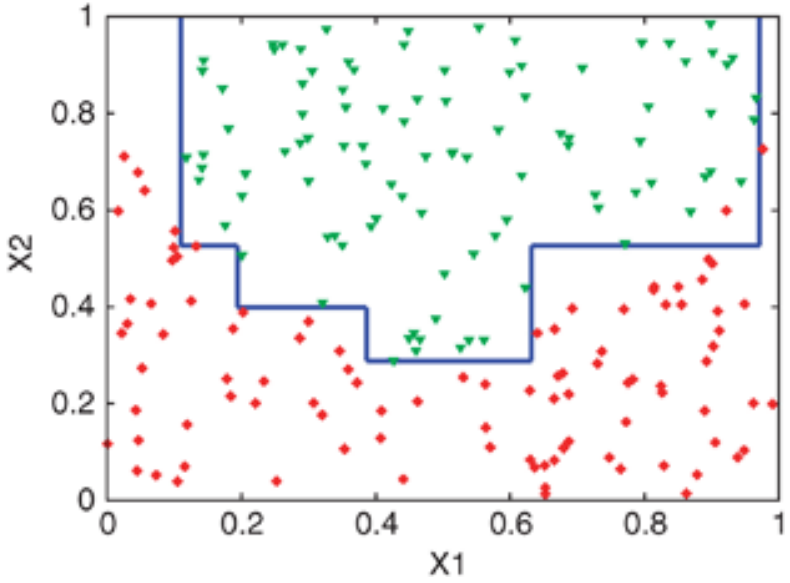
Splitting strategy

Designers usually choose to split wrt a single attribute. In general for non numerical attributes, an exhaustive search over all possibilities is performed. For real values attribute, gradient method for identifying a separating hyperplane may be used; However, simple threshold on a single attribute is often preferred.

Consequences :

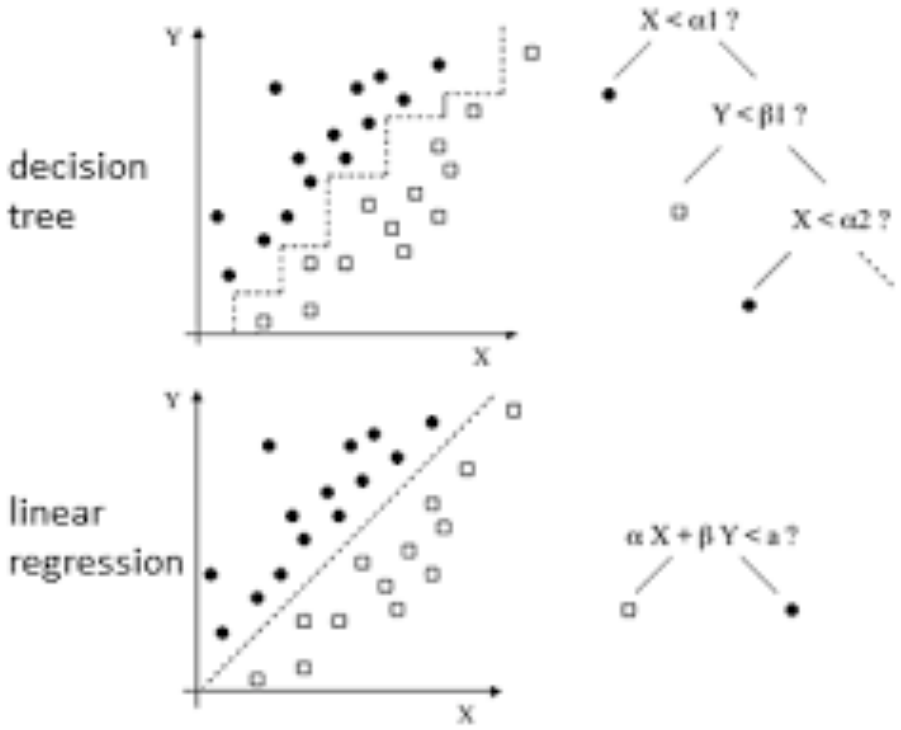
Each split leads to a straight line classifying the dataset into two parts.
Thus, the final decision boundary will consist of straight lines (or boxes).





Consequences :

In comparison to regression, a decision tree can fit a stair case boundary to classify data.



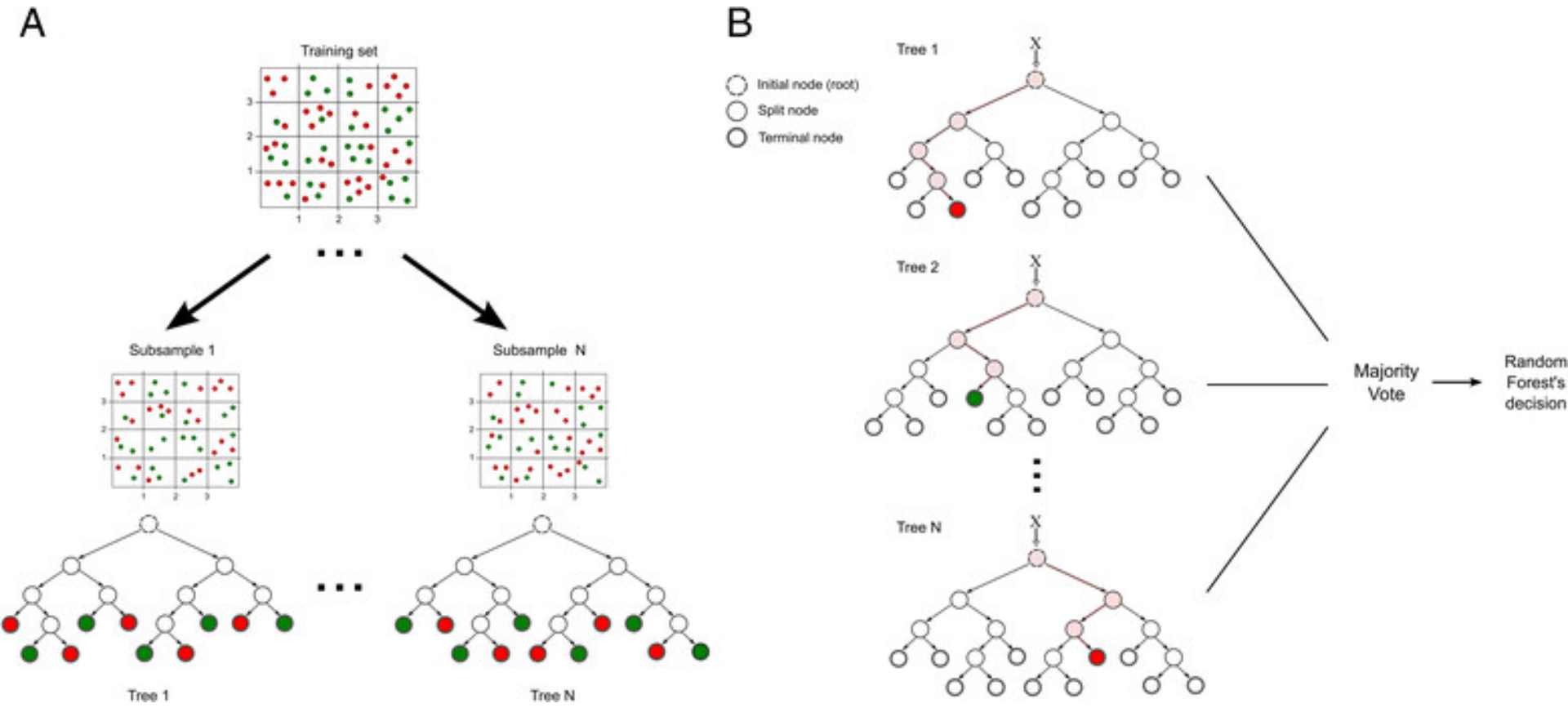
Random forests

Random Forest consists in generating multiple small decision trees from random subsets of the data (hence the name "Random Forest").

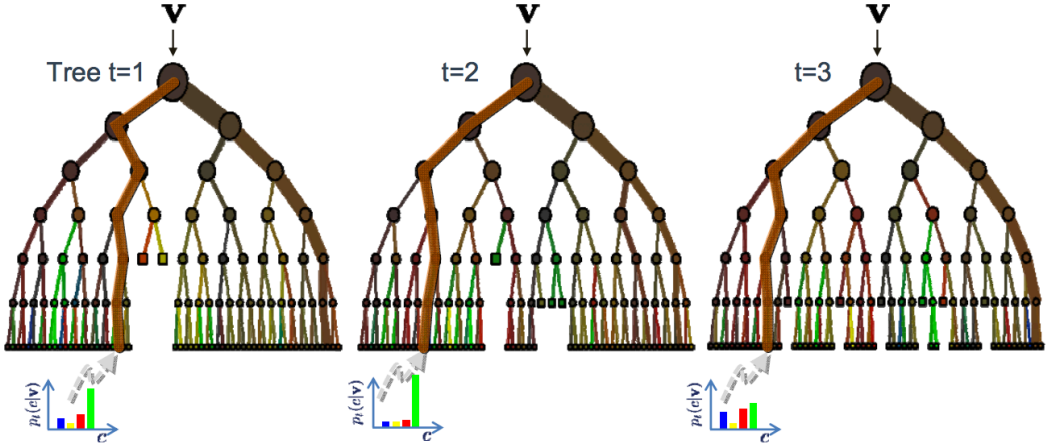
→ Each of the decision tree gives a biased classifier (as it only considers a subset of the data).
→ Each decision tree capture different trends in the data. This ensemble of trees is like a team of experts each with a little knowledge over the overall subject but thourough in their area of expertise. →

- In case of classification the majority vote is considered to classify a class.
- In case of Regression, we can use the avg. of all trees as our prediction.
- In addition to this, we can also weight some more decisive trees high relative to others by testing on the validation data.

Random forest, illustrations :



Recap :



Pros:

- One of the most accurate decision model
- Works well on large datasets.
- Can be used to extract variable importance.
- Do not require feature engineering (scaling and normalization)
- Probabilities and set the threshold for classification.
- Capable of generating complex decision boundaries

Cons:

- Overfitting in case of noisy data.
- Unlike decision trees, results may be quite difficult to interpret.
- Hyperparamters needs good tuning for high accuracy :
  - Ntree : Nb of trees to grow in the forest
  - N_features : Nb of variables randomly sampled as candidates for each split for a given tree
  - Replacement : Sampling done with or without replacement