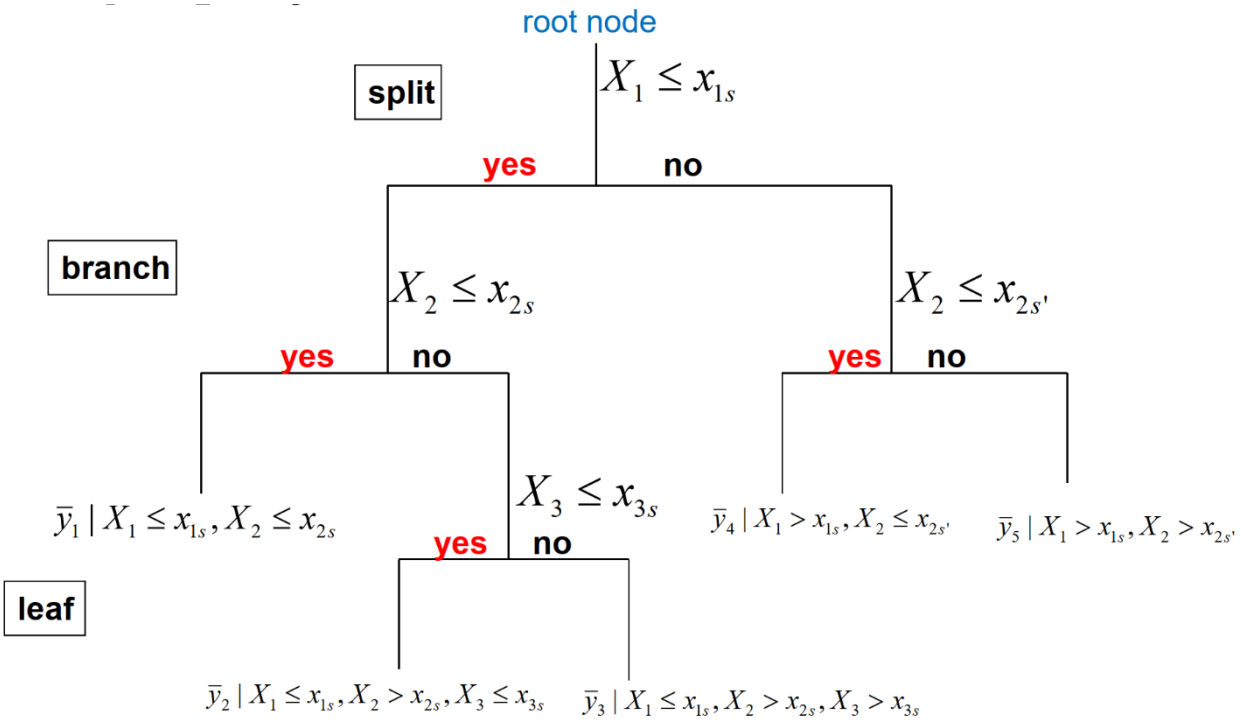
Classification and Regression Trees (CART)

stratify and segment the predictor space
use classification trees when the response variable is categorical
use regression trees when the response variable is continuous

Regression Tree



all the information is contained in the root node
divide the predictor space into k distinct and nonoverlapping regions, $R_1, R_2, \ldots R_k$, to minimize RSS
fitted value in a region R_i is the mean of the response values in this region $\hat{y}_i = \sum_{y \in R_i} \frac{y}{n_i}$

<u>Recursive Binary Splitting</u>
top-down greedy approach starts from the top of the tree and takes the best solution at each node
for each variable X_i, Y has variability

$$RSS = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

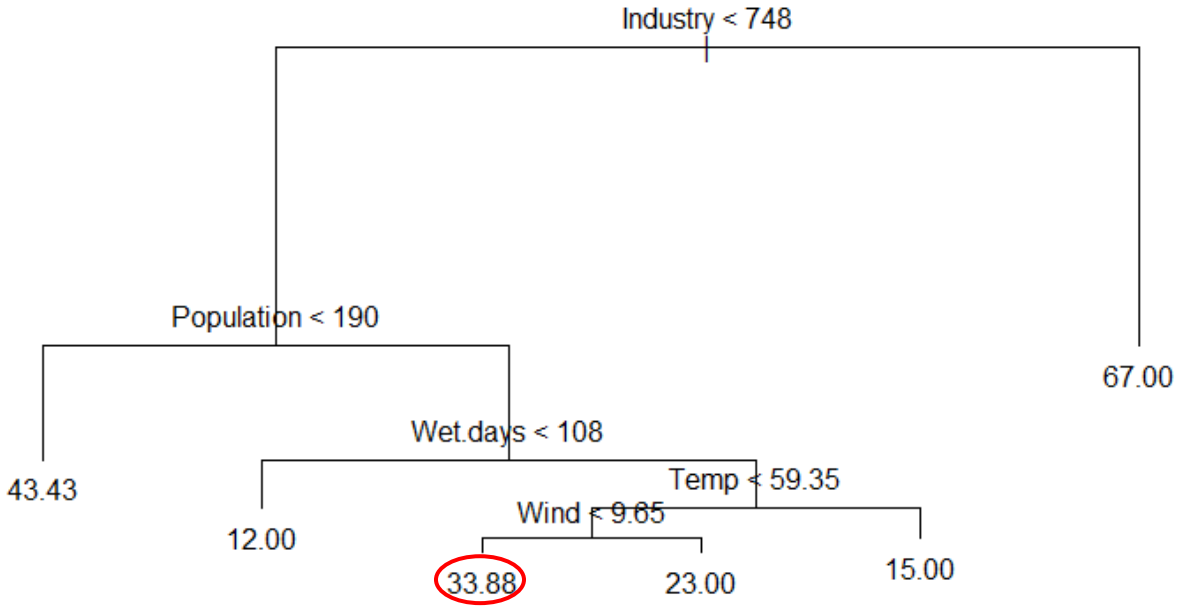
after splitting data by $X_i < s$

$$new\ RSS = \sum_{y \in R_1 = X_i < s}^{n} (y - \bar{y}_1)^2 + \sum_{y \in R_2 = X_i < s}^{n} (y - \bar{y}_2)^2$$

split each X_i to minimize the new RSS
repeat in each region recursively

$$residual\ mean\ deviance = \sum_{R_i\ in\ T_0} \sum_{y \in R_i} \frac{(y - \bar{y}_i)^2}{n - |T_0|}$$

T_0 = initial tree
$|T_0|$ = number of leaves/terminal nodes in initial tree
$\bar{y}_i$ = mean of the training observations in region R_i



length of branch is inversely related to its variance
to make a prediction for a given observation, use the mean or the mode of the training observations in the region it belongs to
e.g. the average pollution level of a city with less than 748 industry, population of less than 190,000, fewer than 108 wet days, average temperature of less than 59.35°, and wind of less than 9.65 is predicted to be 33.88

Pruning

recursive binary splitting usually overfits the data and creates too many splits, creating an overly complicated model that's hard to interpret
a smaller tree with fewer splits can lead to better interpretation at the cost of higher residual deviance
build a large tree and fold the terminal branches back

Maximum Number of Leaves
specify total number of terminal nodes
compare mean deviance of new tree to mean deviance of original tree T_0

Cost-Complexity

$$penalized\ RSS\ (pRSS) = \sum_{R_i\ in\ T} \sum_{y \in R_k} (y - \bar{y}_i)^2 + \alpha|T|$$

α = penalty given to additional leaves

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$|T|$ = number of leaves/terminal nodes in subtree

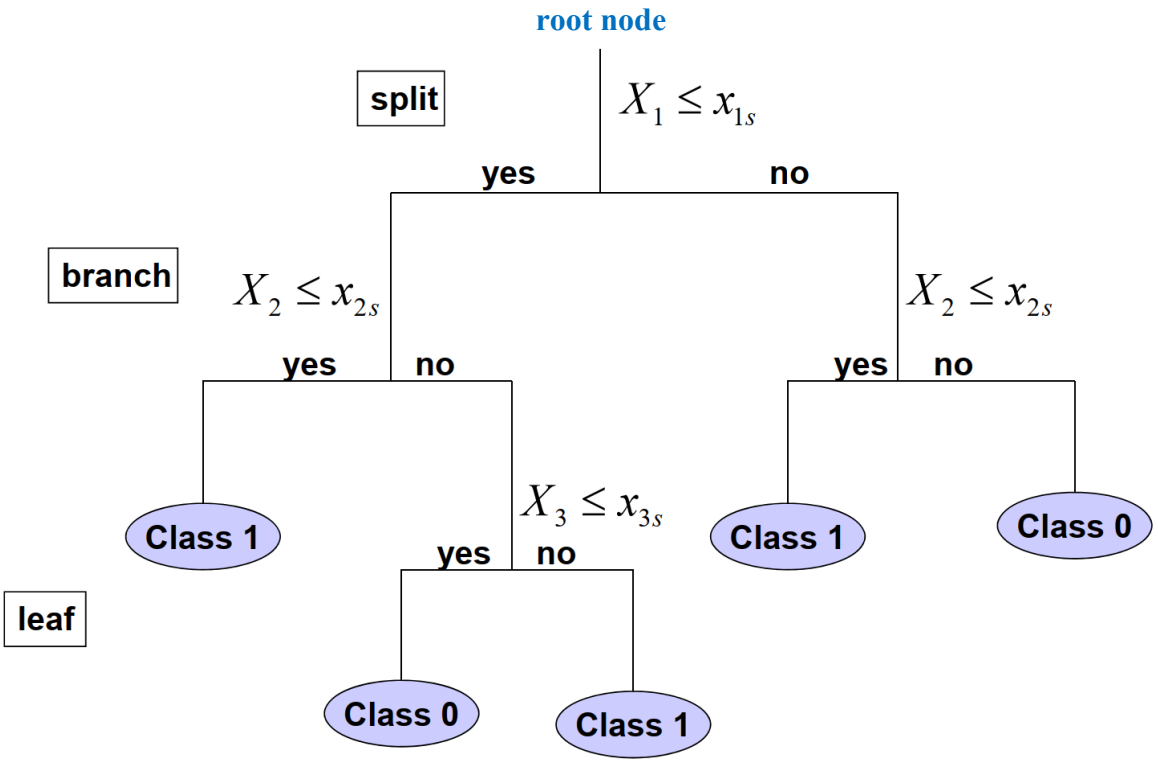
for each α, choose the subtree T nested in T_0 that minimizes $pRSS$
α controls a trade-off between the subtree's complexity and its fit to the training data
when $\alpha = 0$, $T = T_0$ because $pRSS$ measures training error
the higher α is, the higher the penalty for having many terminal nodes so $pRSS$ is minimized for smaller subtrees
as α increases from 0, branches get pruned from the tree in a nested and predictable fashion

K-fold Cross-Validation
divide the number of training observations into k folds
$\frac{k-1}{k}$ are training observations, $\frac{1}{k}$ are testing observations
for each fold 1) use recursive binary splitting to grow a large tree on the training data, stopping when each terminal node has fewer than a minimum number of observations
2) apply cost complexity pruning to the large tree to obtain a sequence of best subtrees as a function of α for each fold
calculate the mean squared prediction error on the data in the last k^{th} fold as a function of α
average the results for each value of α
choose α and corresponding subtree with the least number of terminal nodes that minimize $pRSS$

Tree vs. Linear Models

linear regression is appropriate if there is a linear relationship between covariates and response variable
CART works well for highly non-linear problems
regression trees are multiple linear models with dummy variables representing the branches

Classification Tree



class labels for different samples
label at each terminal node is the modal value, value with the largest probability
use binary splits to minimize deviance/misclassification error and maximize information gain

$$deviance = -2 \sum_{m} n_{mk} \, log(p_{mk})$$

n_{mk} = number of observations in the m[th] terminal node that belongs to class k

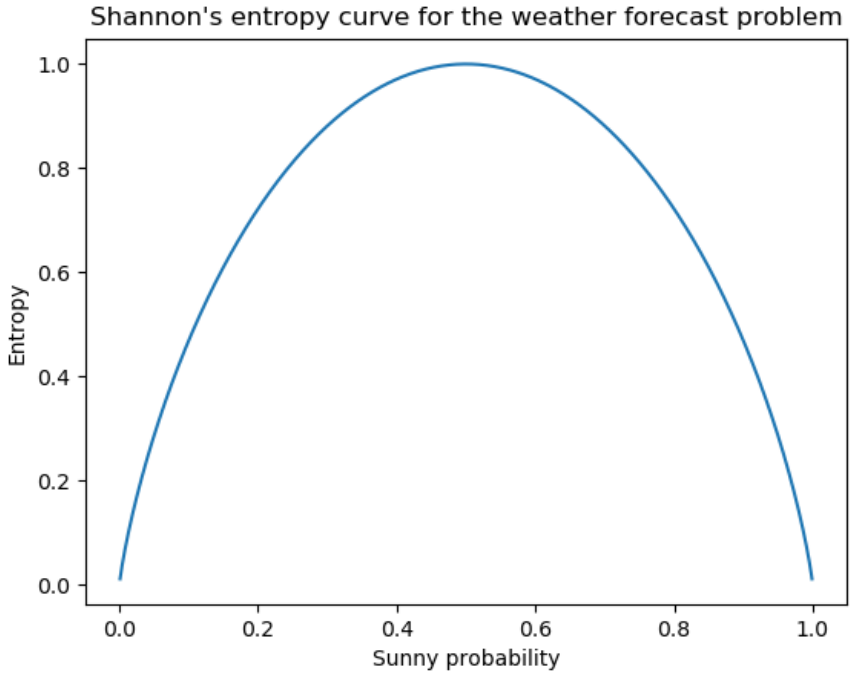
Misclassification Error

Shannon Entropy

measures the lack of information contained in a binary variable

the closer p is to 0 or 1, the smaller the entropy is and the less random the data is

entropy is largest at $p = 0.5$, where using classification tree would be no better than randomly guessing



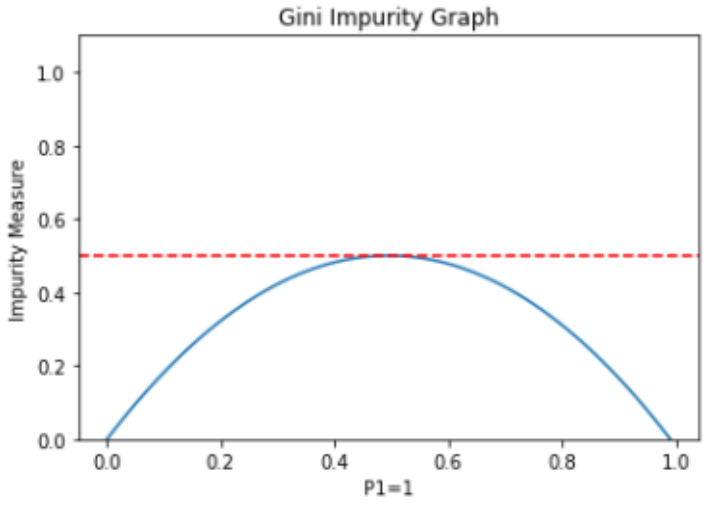
Gini's Impurity Index

probability of an incorrect classification of a new instance

the closer p is to 0 or 1, the purer the data is and the lower the likelihood of misclassification

maximum impurity of 0.5 at $p = 0.5$, where using classification tree would be no better than randomly guessing

Gini's impurity index is used for growing a tree and misclassification error is used for pruning a tree



Advantages and Disadvantages of Trees

trees are easy to explain than linear regression
decision trees closely mirror human decision making than regression analysis
trees can be displayed graphically and are easily interpreted by non-experts
trees can easily handle qualitative predictors without the need to create dummy variables
trees don't always make precise predictions, so need to aggregate many decision trees using methods like bagging and random forests

Ensemble Methods

bagging and random forests aim to reduce the complexity of models that overfit the training data
bagging and random forests improve prediction at the cost of interpretability
boosting tries to increase the complexity of models that suffer from high bias and underfit the training data

Bagging
generate many subsets of the data by taking bootstrap samples of the data
for each subset, generate a tree without pruning
average the predictions from all the trees to get final prediction

Random Forest
generate many subsets of the data by taking bootstrap samples of the data
for each subset, randomly select a set of covariates to build the tree
cannot make a generalization for all the trees

Boosting
build one tree then train the next tree based on the RSS of T_0
grow a family of trees sequentially