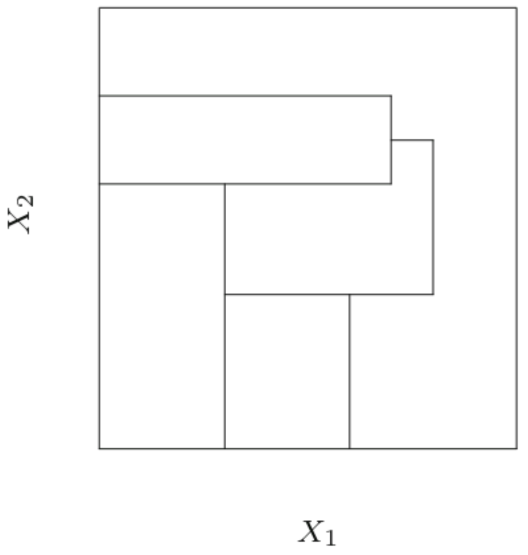
Decision Trees

Decision tress can be applied to both **regression** and **classification** problems, which makes it very flexible and interpretable.

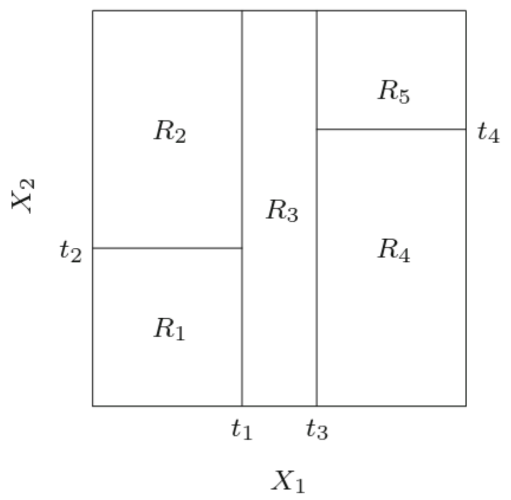
CART

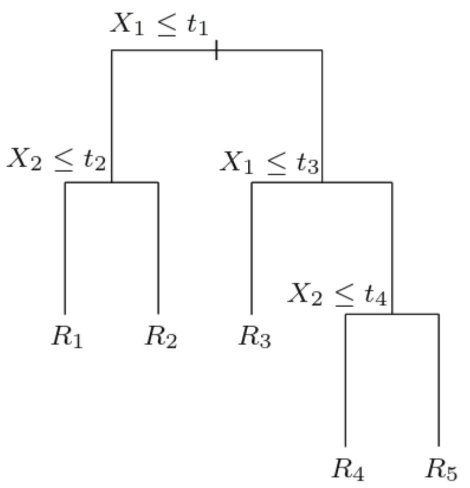
Stands for **Classification and Regression Trees** which is an (algorithm/method) for tree based methods.

Considering a response Y and predictor X_1, X_2



By restricting it to **recursive binary partitions** by splitting the region into two and model the response by the mean of Y





Regression Trees

To construct a **regression tress**, the algorithm needs to automatically decide on splitting variables(feature) and splitting point s also what **shape** the tree should have.

$$y = \sum_{m=1}^{M} c_m I(x \in R_m)$$

- This models the response as a constant c_m in each region R_m.
  Using the Residual Sum of Squares :

  $$\sum_{i=1}(y_i - \sum^{M} c_m I(x \in R_m))^2$$

  For one **Region** we get :

  $$\mathcal{L}(c) = \sum^{n}(y_i - c)^2$$

  Deriving w.r.t. c :

  $$\frac{d\,\mathcal{L}}{d\,c} = \sum^{n} 2(c - y_i)$$

  Setting it to zero results in:

  $$\hat{c} = \frac{1}{N_m}\sum_{i=1}^{n} y_i \equiv \hat{c}_m = \text{ave}(y_i | x_i \in R_m)$$

  Note:
- $\sum_{i \in R_m} c = N_m.c$
- The constant $\hat{c}$ represent the mean of $\bar{y}$ on that region m
- $\text{avg}(y_i | x_i \in R_m)$ means the average of y_i given that x_i is in the region m

To find the best binary partition in terms of minimum sum of squares is computationally infeasible. Hence **regression trees** use a greedy algorithm.
At a given node we consider all possible splits (j, s) by :

- Consider all features p of X given by X_j
  - For every possible threshold s
  - We evaluate the $R_1(j, s) = \{X | X_j \leq s\}$ and $R_2(j, s) = X | X_j > s$
- Repeat for each **feature** resulting in pairs $(j, s) \rightarrow (\text{feature,split point})$
  ex : $(age, 50), (age, 40), (height, 170), (height, 167)\ldots$

Then we seek the **splitting variable** j and **split point** s that (minimize/solves) this :

$$\min_{j,s}\left[\min_{c_1}\sum_{x_i \in R_1(j,s)}(y_i - c_1)^2 + \min_{c_2}\sum_{x_i \in R_2(j,s)}(y_i - c_2)^2\right]$$

The inner minimization is solved by:

$$\hat{c}_1 = \text{ave}(y_i | x_i \in R_1(j, s)) \text{ and } \hat{c}_2 = \text{ave}(y_i | x_i \in R_2(j, s))$$

The greedy algorithm Summary :

- Select splits which are pairs (j, s)
- Calculate the constant for the split c_1, c_2
- Evaluate the split by calculating the Residual Sum of Squares
- Choose the split (j, s) that yields the smallest RSS

The question now is how large should we grow the tree? , very large tree might overfit the data easily while small might not learn the data and the underline structure.

Classification Trees

A **classification tree** is very similar to regression tree, except that is used to predict **qualitative** response , for regression tree the predicted response for an observation is given by the mean response $\hat{c}$ of the training observations.

For a **classification tree** we predict each observation belongs to the **most common occurring class** of training observations in the region m.
To interpret the results of a classification tree we are often interested not only in class prediction on node/region, but also in the class **proportions** among the training observations.

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

- $I(y_i = k)$ is indication function returns 1 if the condition is met , 0 otherwise
  To perform the binary split so we grow the classification tree we use **Missclassification error**

  $$\text{Missclassificaion error} = \frac{1}{N_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$$

  With :

  $$k(m) = \arg\max_k (\hat{p}_{mk})$$

- Representing the majority class in node m

A simpler form of **Missclassification error**

$$E = 1 - \max_k (\hat{p}_{mk})$$

The problem with missclassification error is not **sufficiently sensitive for tree-growing**, for example :

- **Node** X has 400 **observation** from class A and 380 from class B

  $$E = 1 - \max(\hat{p}_A, \hat{p}_B)$$

  $$\hat{p}_A = \frac{400}{780} = 0.51$$
  $$\hat{p}_A = \frac{380}{780} = 0.49$$
  $$\text{Results in: } E = 1 - \max(0.51, 0.49)$$
  $$E = 1 - 0.51 = 0.49$$

- **Node** Y had 700 **observation** from class A and 80 from class B

  $$E = 1 - \max(0.89, 0.11)$$

  $$E = 1 - 0.89 = 0.11$$

  For missclassification both node X and node Y are the same and both have class A **majority**, not taking into **consideration** that node Y is more pure and that the probabilities in node X are closer and almost the same, that's what not **sufficiently sensitive** means.

In practice **Gini index** and **Cross-entropy** are more preferable :

Gini index

The $Gini\ index$ is defined by :

$$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$

Or the **Computationally efficient** form :

$$G = 1 - \sum_{k=1}^{K} (\hat{p}_{mk})^2$$

It's measure of total **variance** across the K classes, takes values between $[0, 1]$.

- Gini index of 1 represent impure region/dataset
- While Gini index of 0 represent pure dataset

Calculating the **Gini index** for each feature, help us decide on which feature to pick as the root node

- Fast computation than both $entropy$ and $missclassification\ error$
- Create splits quickly
- Efficient for large high-dimensional datasets

Cross-entropy/deviance

The $Cross-entropy$ is defined by :

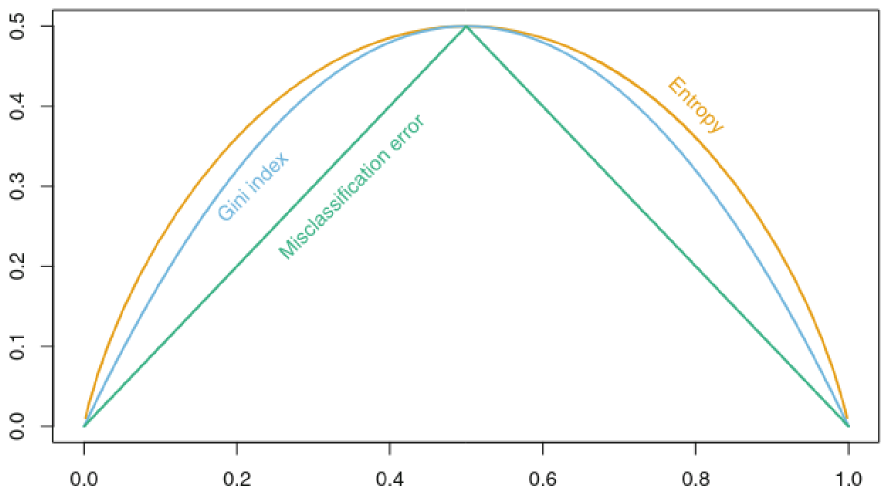
$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Entropy measures uncertainty in a node's class distribution, derived from **information gain** lower entropy indicates that the node m is pure.

- Sensitive to probability changes
- Produce more balanced nodes partitions
- Suited for more balanced datasets

Use Cases

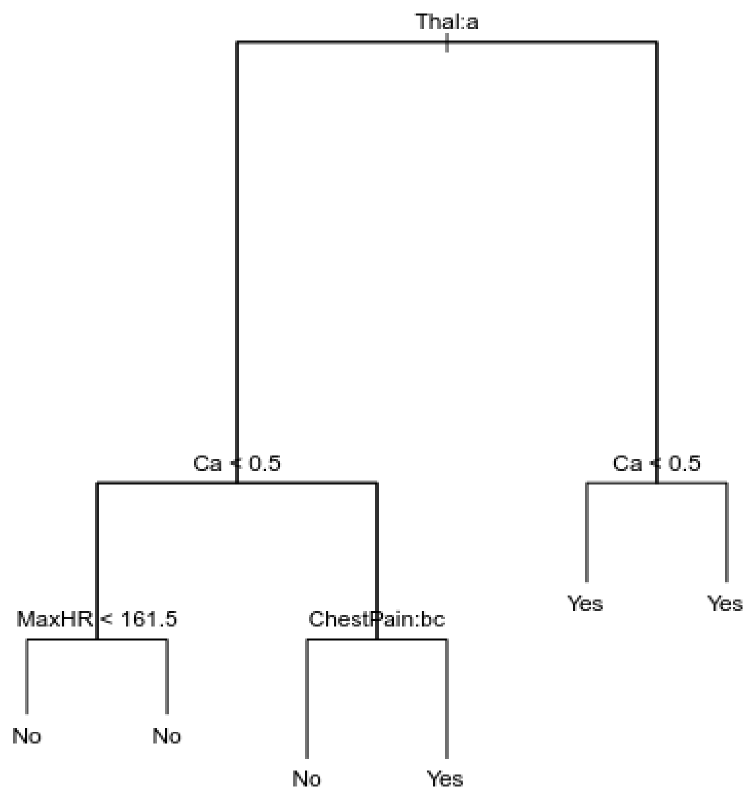
Split Evaluation :
Both of **entropy** and **gini index** are numerically similar, they are used to evaluate the quality of a particular split since they are sensitive to **node purity** more than **missclassification error**.



Why node purity important ?

an important aspect in **Decision Tress** is that the leaves should represent regions with strong **confident predictions**, and that is determined by **node purity**.

- The higher the purity $\rightarrow$ the node gives you confident predictions
- The lower the purity $\rightarrow$ the node is uncertain even tho it gives the same results
  for example :



- The right hand node `Ca<0.5` both of it's leaves are yes , which seems useless why not prune them
- The **right hand leaf** is more certain and confident on it's prediction than the **left hand leaf** which is less certain and *probably yes*
- Splitting `Ca<0.5` does not reduce the **missclassification error** but improves **gini index** and **entropy** which are more sensitive to node purity

More explanation :
Say we have a node/region with :

- $Yes \rightarrow 80\%$
- $No \rightarrow 20\%$
  After the split :
- $Right\ Leaf \rightarrow Yes\ 90\%$, $No\ 10\% \implies$ very pure , results in a Yes
- $Left\ Leaf \rightarrow Yes\ 55\%$, $No\ 45\% \implies$ still mixed and uncertain but still results in a Yes
  For **missclassification** both leaves are the same, but for **gini index/entropy** the right leaf is more certain and can be trusted.

Tree Pruning

Tree Pruning algorithms reduce the size of decision trees to avoid overfitting and complexity, there is two types of **pruning**

Pre-Pruning (Early Stopping)

Stop growing the tree before it perfectly classifies the training data(fully developed) by setting some conditions such as :

- maximum depth
- minimum threshold(number of samples in a node)
- information gain or gini impurity threshold
- maximum leaf nodes
- maximum features to be considered at each split

These conditions lead to faster training and less memory usage but often leads to underfitting the data where the DT is unable to capture the patterns in the data

Post-Pruning

This approach allow the tree to grow to it's maximum depth, often leading to overfitting, the pruning process here the sub-trees
are removed if they don't improve performance on a validation set

The size of tree is a **tuning parameter** which correspond to the model complexity, the **greedy** strategy is to grow a large tree T_0 and then stop growing after the minimum **node size** is reached(4 observations per region).

The large tree T_0 is pruned using $\text{cost-complexity prunning}$:

- The number of Observations in a region m is denoted :

$$N_m = \#\{x_i \in R_m\},$$

- The constant for region m is denoted :

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i$$

- The **MSE** for region m is denoted(**impurity measure**) :

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

  The **Cost complexity criterion** :

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$$

  With :

- $|T|$ the number of terminal nodes(leafs)
- α penalty parameter

The idea is to find for each α a subtree $T_\alpha \subseteq T_0$ that minimize $C_\alpha(T)$,$\alpha \geq 0$ results in a tradeoff between the tree size and it's **goodness of fit**.

- Large values results in smaller trees T_α
- $\alpha = 0$ results in T_0

Weakest Link Pruning

To find T_α that minimize $C_\alpha(T)$ we use **weakest link pruning**:

First the starting point for the pruning is not T_0 , but rather $T_1 = T(0)$ which is the smallest subtree of T_0 that satisfy:

$$R(T_1) = R(T_0)$$

With $R(T) = \sum^{|T|} N_m Q_m(T)$

To Obtain T_1 First, we look at T_0 the biggest tree and for any **two terminal nodes(leafs)** from the same parent node, if we sum the error rate and it's the same as their parent node, we prune off these two terminal nodes :

$$R(t) = T(t_L) + R(t_R)$$

- Parent node t
- Two terminal nodes t_L and t_R

This process is applied recursively. which results in a pruned T_0 while having the same error rate.

```
T_0:          T₁ (after pruning):
    A              A
   / \            / \
  B   C          B   C
 / \
D   E
```

- Since $R(B) = R(D) + R(E)$

- Making a prediction using the region B or in D and E will results in the same error rate
- The **child nodes** doesn't provide any improvements over their **parents**

The **weakest link** method not only find the next α which results in different optimal subtree, but find that optimal subtree.

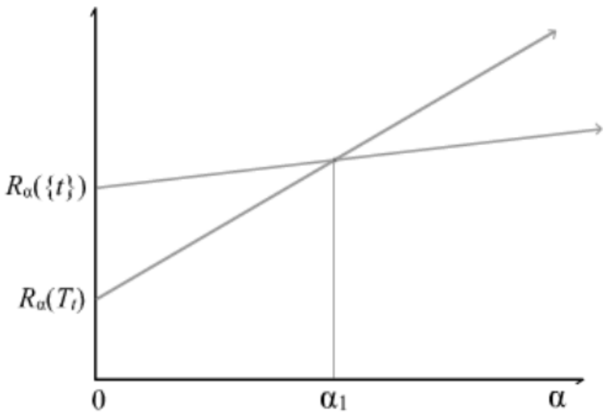
Let $t \in T_1$ is any node $\rightarrow R_\alpha(t) = R(t) + \alpha$.
and T_t any branch $\rightarrow R_\alpha(T_t) = R(T_t) + \alpha|T_t|$.
For more details on these formulas check Weakest link lagrangian derivation

When $\alpha = 0$:

$$R_0(T_t) < R_0(t)$$

- That is the **penalty error rate** of the node is bigger than it's branch

Increasing α leads to a faster increase in $R_\alpha(T_t)$ since it's $\alpha|T_t|$ at a certain α_1 we will have $R_{\alpha_1}(T_t) = R_{\alpha_1}(t)$.



Solving the inequality $R_\alpha(T_t) < R_\alpha(t)$:

$$\alpha < \frac{R(t) - R(T_t)}{|\tilde{T}_t| - 1}$$

- The numerator is the increase in **error rate** if we prune
- The denominator is the number of leaves removed

$$g_1(t) \begin{cases} \frac{R(t)-R(T_t)}{|\tilde{T}_t|-1}, & t \notin \tilde{T}_1 \\ +\infty, & t \in \tilde{T}_1 \end{cases}$$

With $\tilde{T}$ is set of **terminal nodes**

- If $t \in \tilde{T}_1$ means t is a **leaf/terminal node**, that's why we set it to $+\infty$ to exclude it
  The **weakest link** t^* in T_1 achieves the minimum of $g_1(t)$

  $$g_1(t^*) = \min_{t \in T_1} g_1(t)$$

  put $\alpha_2 = g_1(t^*)$, to get the optimal subtree corresponding to α_2 and removing the branch growing out of t^* since it increase the error rate the least if removed , keep in mind there can be several nodes that reach or achieve the minimum of $g_1(t)$

Steps Summary :

- For T_1 Tree compute for every internal node $t \in T$, $g(t)$ interpreted as the increase in the error rate if that node t is pruned
- Find $t^* = \min g_1(t)$, Let $\alpha^* = g(t^*)$ so that the next subtree is smaller
- Prune by replacing the subtree T_{t^*} by a single leaf t^* resulting in a new tree T_k
- Save the pair(α_k, T_k), and set T_k as the main tree and repeat it
  Resulting in guaranteed nested sub trees :

  $$T_1 \supset T_2 \supset \cdots \supset T_k$$

  With :

$$\alpha_1 < \alpha_2 < \cdots < \alpha_{k+1}$$

Intuition :

The weakest link pruning **iteratively** removes internal nodes(non-terminal) whose pruning causes the **smallest increase in error rate**. Simply :

- Remove the nodes to reduce complexity but only the one that effort the error rate the least $\min_{t \in T_1} g_i(t)$
- α is the threshold computed to decide on the optimal prune using $g(t)$
- Running **weakest link** to completion will results in the **root** node only, that's why the results is guaranteed **nested sub trees**
- **Weakest link** pruning main goal is the reduce complexity

Why Decision Trees Fails

First let's talk about the Bias-Variance Trade-Off in DT:

High Bias (Shallow Trees) :

Decision tress with low depth will results in a **high bias** model where it fails to capture the underline data patterns by being overly generalized that missed the relationships between features and response.
Bias Source: The inability of the model to approximate the true function due to its oversimplified structure.

High Variance

Allowing Decision trees to fully grow until it fit perfectly the training data will results in a **overfit** model where it's so sensitive to changes and fails to generalize for new unseen data.
Variance Source: The model’s ability to capture idiosyncrasies in the training data that do not generalize to new data.

Balancing The Trade-off

The goal is to find a sweet spot between variance and bias , we talked about pre-pruning, post-pruning methods which they reduce the complexity and try to find a balance but in practice the best way to balance the trade off is **Ensembling** methods such :

- Bagging
- Boosting

For more details and considerations when using **Decision Trees** Read :

- Other Considerations on Decision Trees
- Trees Versus Linear Models
  For more advance **Decision Trees** see:
- Random Forests
- Boosting
- Bayesian Additive Regression Tress