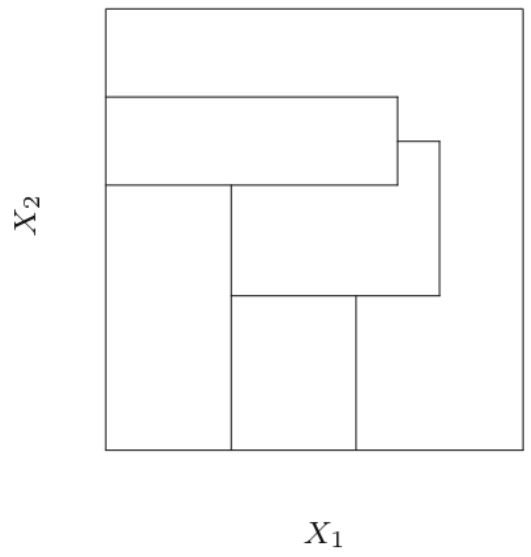
Decision Trees

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

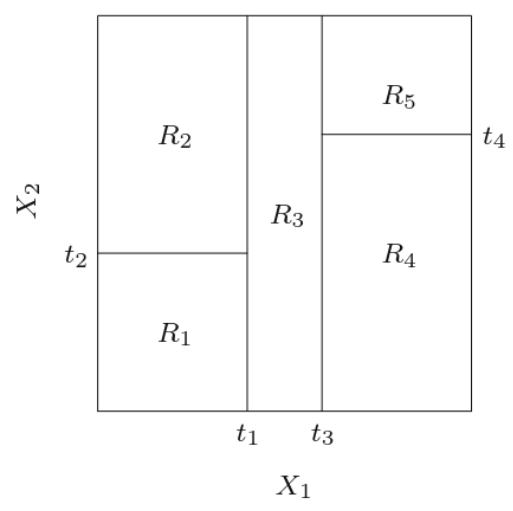
CART

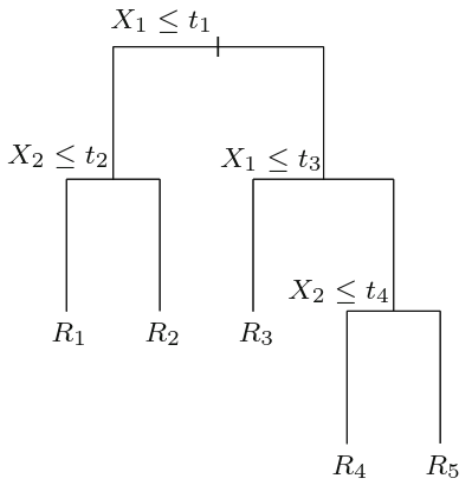
Stands for **Classification and Regression Trees** which is an (algorithm/method) for tree based methods.

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 : $(age, 50), (age, 40), (height, 170), (height, 167) \dots$

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.

Tree Pruning

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 :

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

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.

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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.

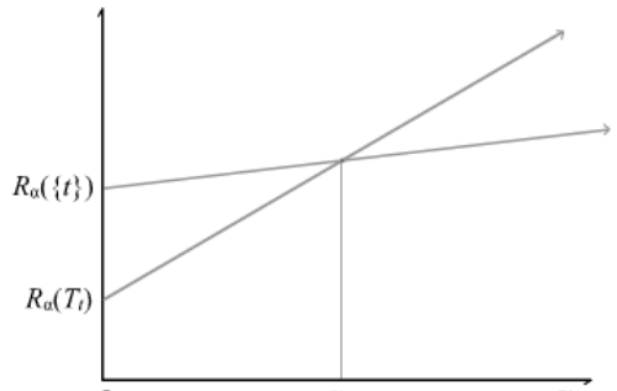
Let $t \in T_1$ is any node $\rightarrow R_\alpha(t) = R(t) + \alpha$.
and T_t any branch $\rightarrow R_\alpha(T_t) = R(T_t) + \alpha|T_t|$.
For more details on these formulas check Weakest link lagrangian derivation

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