APL 405: Machine Learning for Mechanics

Lecture 4: Decision Trees

by

Rajdip Nayek

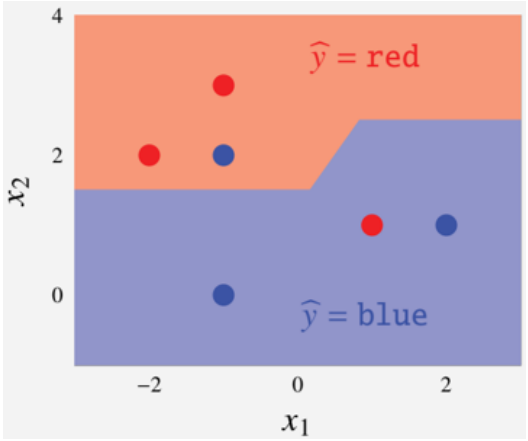
Assistant Professor,
Applied Mechanics Department,
IIT Delhi

Instructor email: rajdipn@am.iitd.ac.in

Supervised Learning: Recap of kNN

- In both regression and classification settings, we seek a function $f(\mathbf{x}^*)$ that maps the test input $\mathbf{x}^*$ to a prediction

- The k-NN method results in a prediction $\hat{y}(\mathbf{x}^*)$ that is a piecewise constant function of the input $\mathbf{x}^*$
  - The method partitions the input space into disjoint regions
  - Each region is associated with a certain constant prediction
  - These regions are describted by the k-neighbourhood of each possible test input

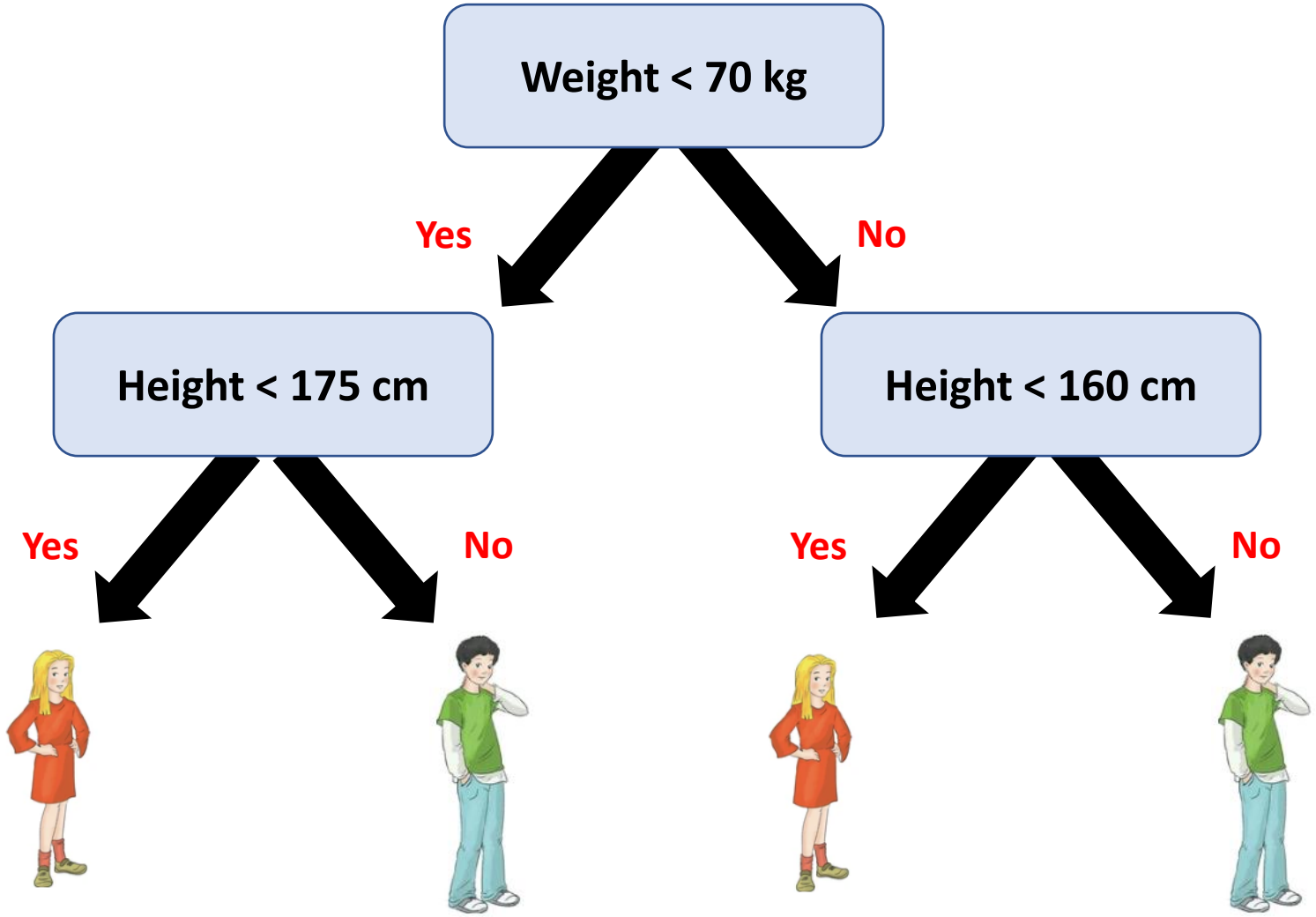


- Another way is to come up with a **set of rules** that defines the regions explicitly: **Decision Trees**
  - Also known as Classification and Regression Trees (CART)

Idea of decision trees (CART)

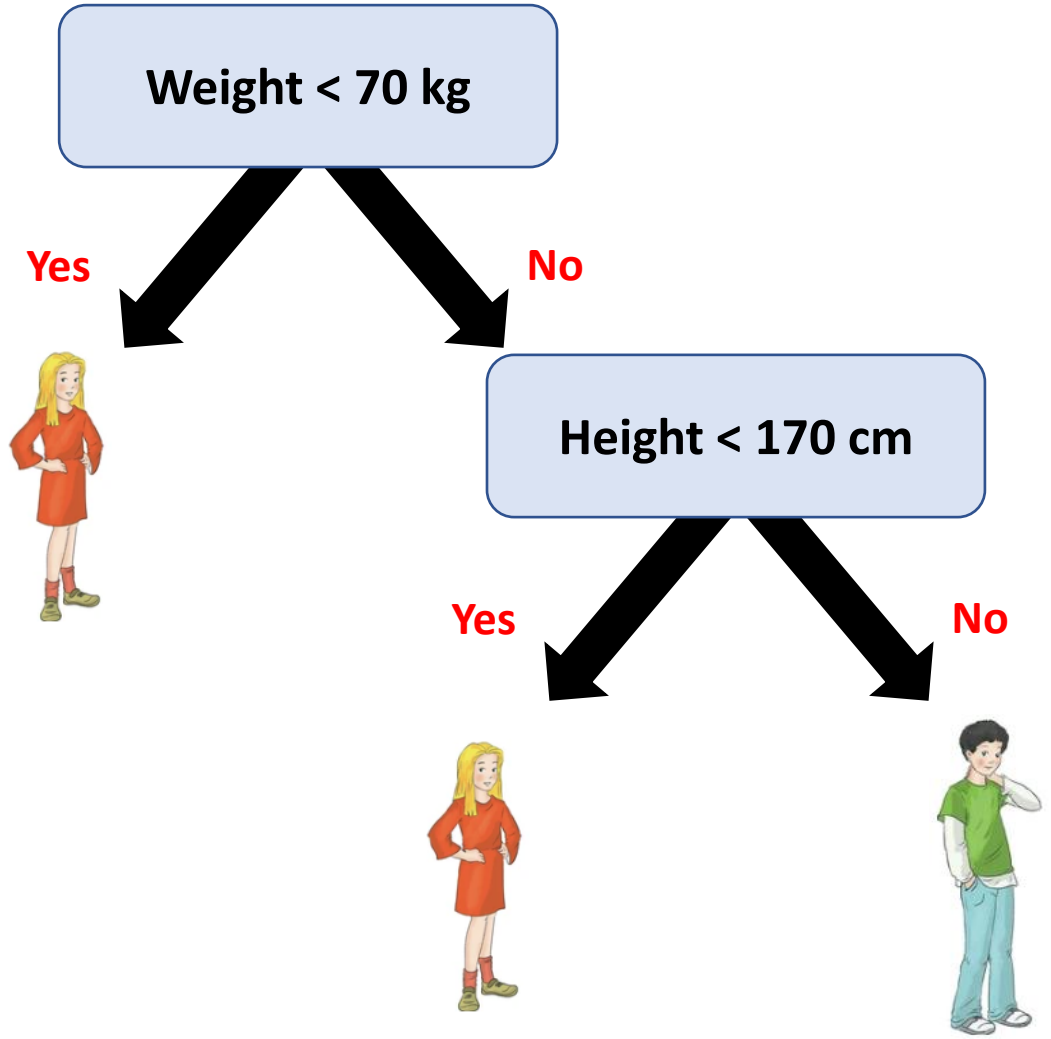
- **Scenario**: Decide Male or Female?
- Features measured: height and weight

Idea of decision trees (CART)



Split continuous features by checking whether that feature is greater than or less than some threshold

Idea of decision trees (CART)

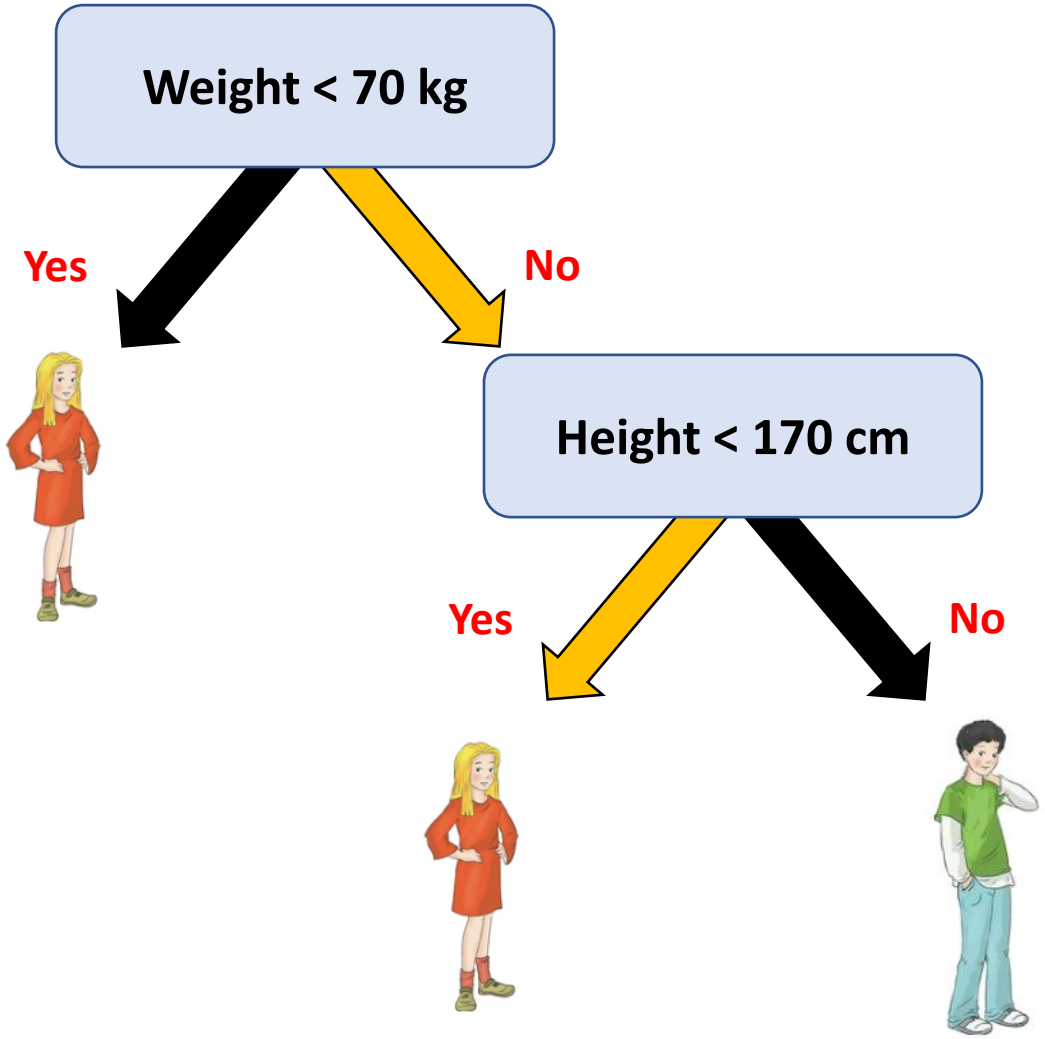


Split continuous features by checking whether that feature is greater than or less than some threshold

Idea of decision trees (CART)

Test input

- Weight = 70 kg
- Height = 168 cm

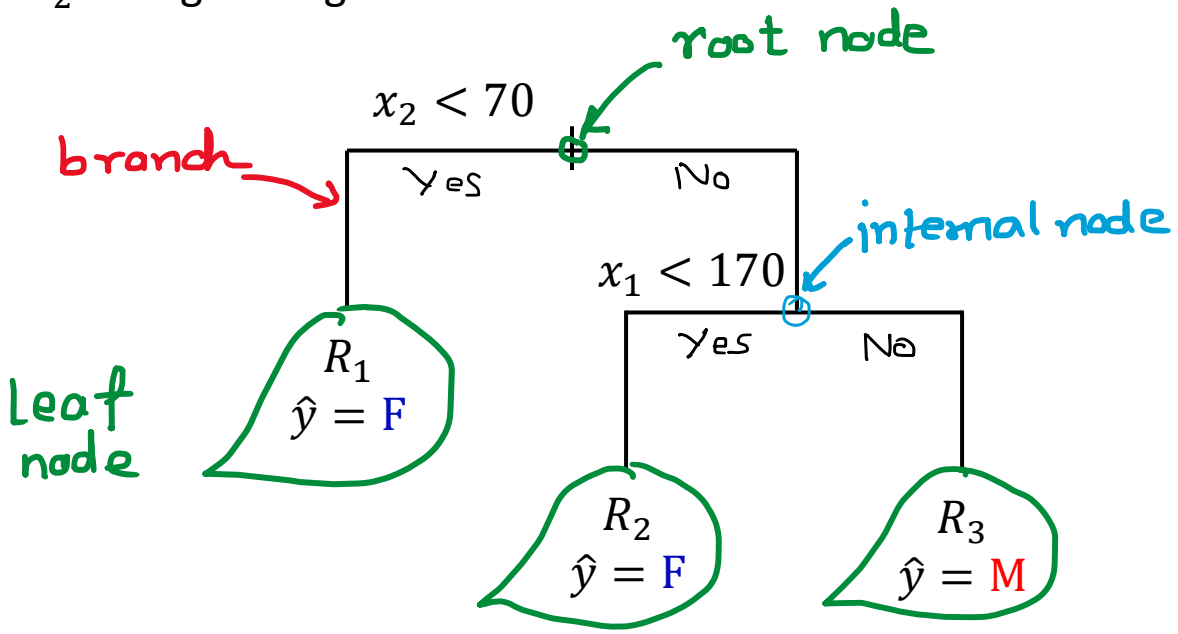


Make predictions by splitting on features according to a tree structure

Structure of a Decision Tree

Structure of a Decision Tree

- Consider the classification example with two numerical inputs $\mathbf{x} = [x_1 \quad x_2]^T$ and a categorical output $y \in \{\mathrm{F}, \mathrm{M}\}$
  - x_1 - height in centimeters
  - x_2 - weight in kg



Structure of a **decision** tree

- Internal nodes check an input variable
- Left/Right branch is determined by value of input variable → $x_j < s_k$
- Leaf nodes are outputs (predictions)

The tree shown has two internal nodes (including the root) and three leaf nodes

The tree is referred to as ***binary tree*** since each internal node splits into exactly two branches

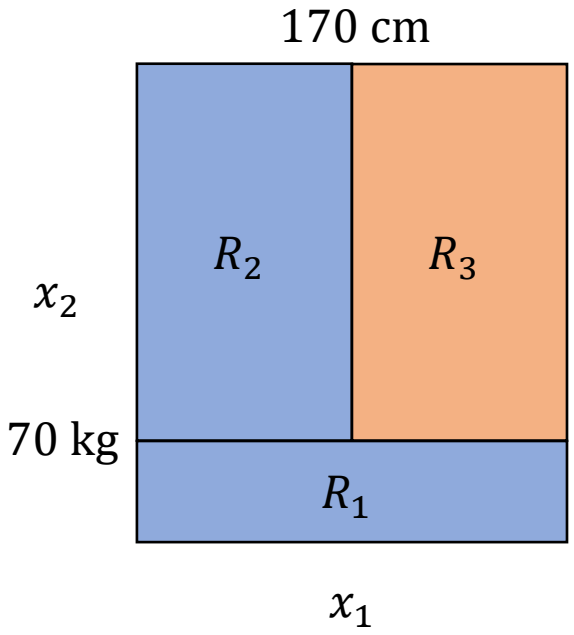
Set of Rules

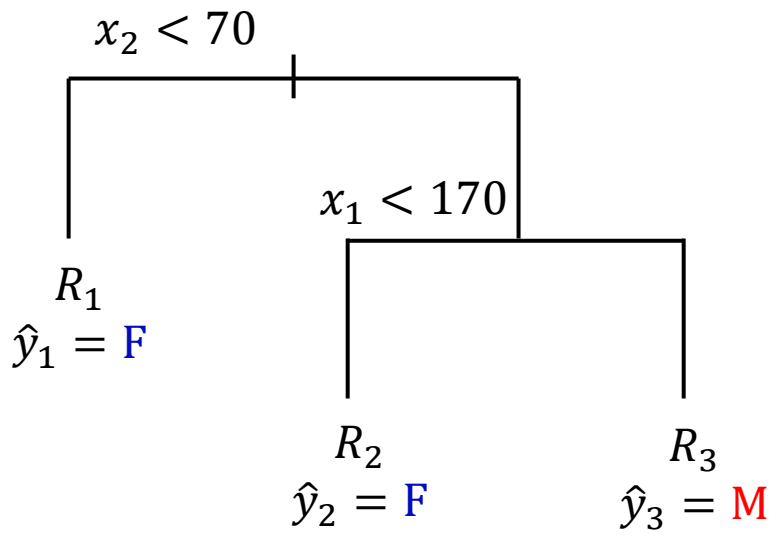
```
If Height < 170 cm Then Female
If Height >= 170 cm AND Weight < 70 kg Then Female
If Height <= 170 cm AND Weight >= 70 kg Then Male
```

Decision boundaries of a Decision Tree

- Consider a classification example with two numerical inputs $\mathbf{x} = [x_1 \quad x_2]^T$ and a categorical output $y \in \{\text{F}, \text{M}\}$

- Each path from root node to a leaf defines a region R_m of input space

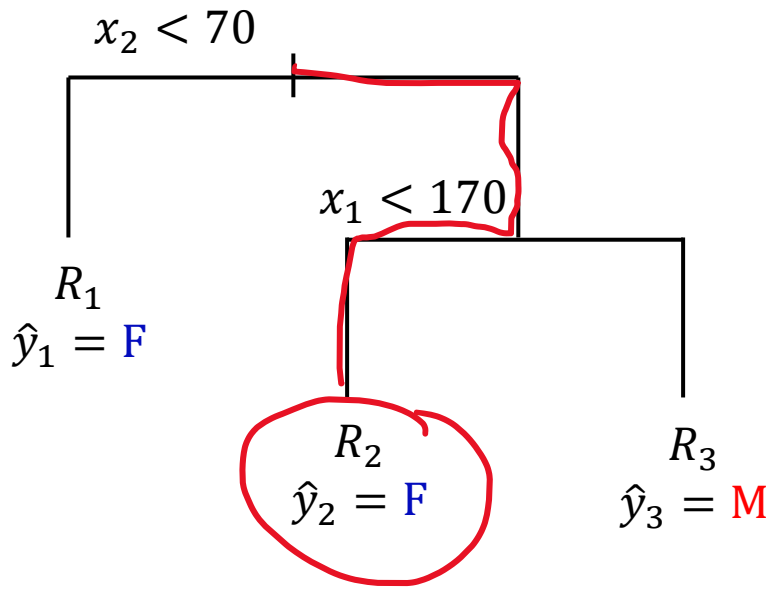




- The decision tree partitions the input space into axis-aligned 'boxes' or rectangles. So the **decision boundaries** are in the shape of **rectangles**

Make a prediction using a Classification tree

- Consider a test input $\mathbf{x}^* = [70 \quad 168]^T$
  - x_1 - height in centimeters
  - x_2 - weight in kg



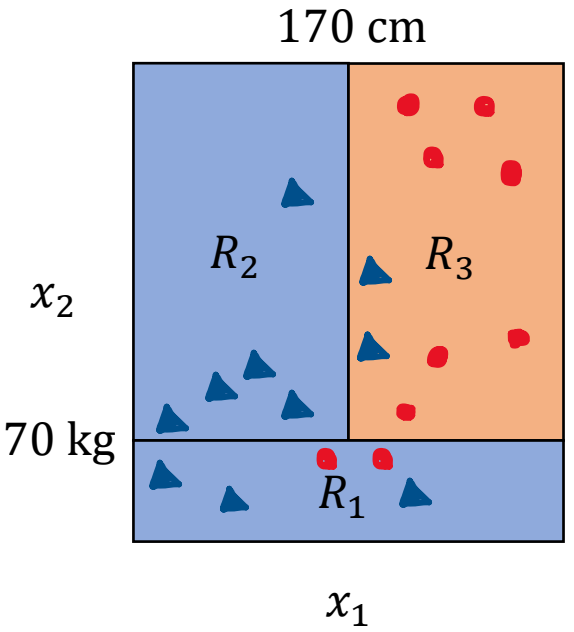
Set of Rules

```
If Height < 170 cm Then Female
If Height >= 170 cm AND Weight < 70 kg Then Female
If Height <= 170 cm AND Weight >= 70 kg Then Male
```

Structure of Decision Trees

- The same partitioning can be done for a general input vector $\mathbf{x} = [x_1 \quad x_2 \quad \cdots \quad x_p]^T$, however, the partitioned space is difficult to illustrate

- For a p-dimensional input space, the decision boundaries would be represented by hyper-rectangles (boxes in higher dimensions)



- Let $\{(\mathbf{x}^{(m_1)}, y^{(m_1)}), (\mathbf{x}^{(m_2)}, y^{(m_2)}), \cdots, (\mathbf{x}^{(m_k)}, y^{(m_k)})\}$ be the training examples that fall into R_m
  - $m = 3, k = 9$ for the top-right reddish box

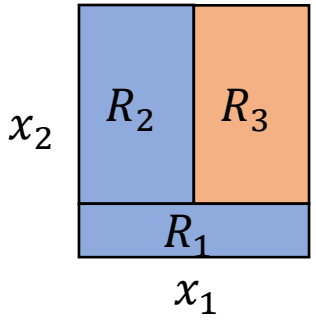
- Regression tree
  - Numerical output
  - Leaf value $\hat{y}_m$ typically set to the mean value in $\{(\mathbf{x}^{(m_1)}, y^{(m_1)}), \cdots, (\mathbf{x}^{(m_k)}, y^{(m_k)})\}$

- Classification tree
  - Catergorical output
  - Leaf value $\hat{y}_m$ typically set to the most common value (mode) in $\{(\mathbf{x}^{(m_1)}, y^{(m_1)}), \cdots, (\mathbf{x}^{(m_k)}, y^{(m_k)})\}$

Learning Decision Trees

- We saw how a decision tree can be used to make a prediction. Now, how a tree can be learned from training data?

- Learning a decision tree involves deciding the shape of the tree
  - Finding the number of regions (boxes), say L regions, $R_1, R_2, \cdots, R_L$, and
  - Finding the partitions of the boxes



- We should select the number of regions and partitions such that the tree fits the training data well
  - the output predictions from the tree should match the output values in the training data

- However, finding the tree (a collection of splitting rules) that optimally partitions the input space to fit the training data is computationally infeasible due to combinatorial explosion in the number of ways you can partition the input space

- Searching through all possible binary trees is not possible in practice unless the tree size is very small

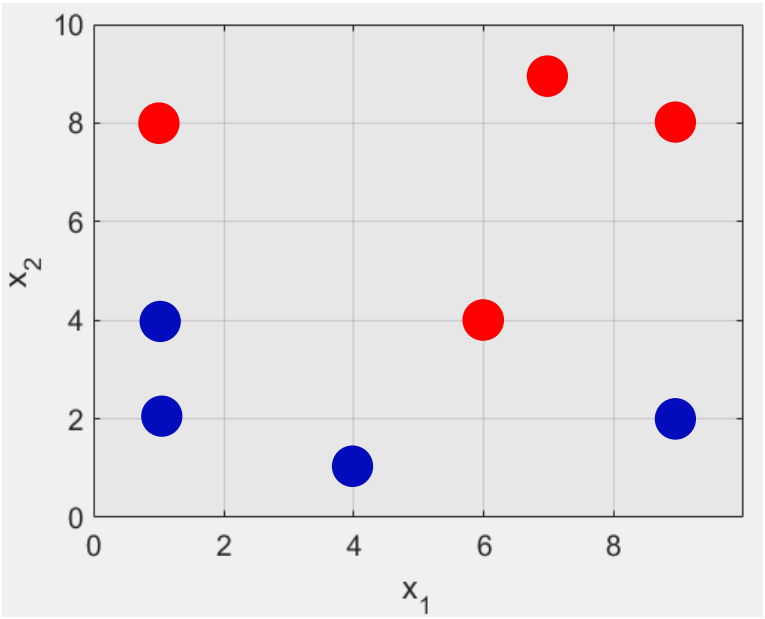
- To handle this situation, a heuristic algorithm known as **recursive binary splitting** is used for learning decision trees.

Learning Classification Trees using Recursive Binary Splitting

Start with the first split at the root and then build the tree from top to bottom

- When determining the splitting rule at the root node, the objective is to obtain a model that best explains the training data after a single split, without taking into consideration that additional splits may be added afterwards

i	x_1	x_2	y
1	9	2	**Blue**
2	4	1	**Blue**
3	1	2	**Blue**
4	1	4	**Blue**
5	1	8	**Red**
6	6	4	**Red**
7	7	9	**Red**
8	9	8	**Red**



Learning Classification Trees using Recursive Binary Splitting

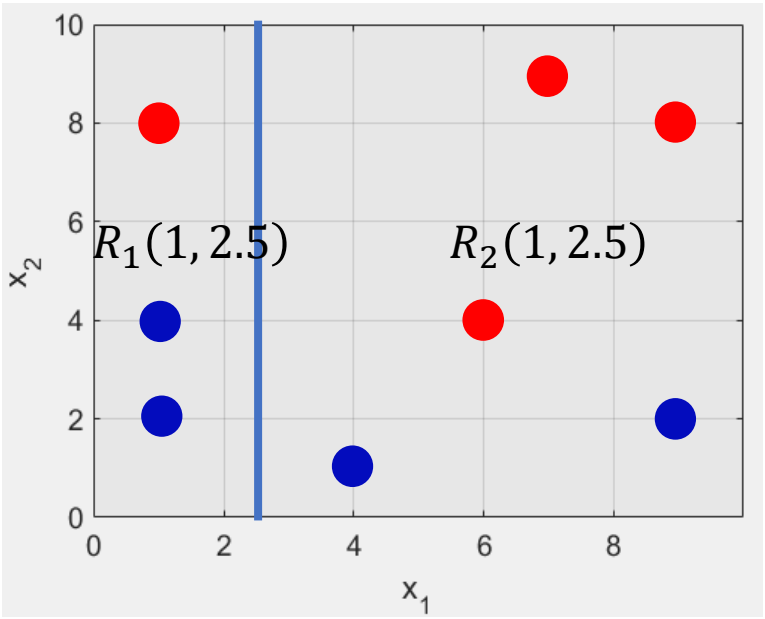
Start with the first split at the root and then build the tree from top to bottom

- When determining the splitting rule at the root node, the objective is to obtain a model that best explains the training data after a single split, without taking into consideration that additional splits may be afterwards
  - Select one of the p input variables $x_1, \cdots x_j, \cdots, x_p$ and a corresponding cutpoint s which divide the input space into two half-spaces

$$R_1(j,s) = \{\mathbf{x} \mid x_j < s\} \text{ and } R_2(j,s) = \{\mathbf{x} \mid x_j \geq s\}$$

i	x_1	x_2	y
1	9	2	Blue
2	4	1	Blue
3	1	2	Blue
4	1	4	Blue
5	1	8	Red
6	6	4	Red
7	7	9	Red
8	9	8	Red

Split at say $x_1 = 2.5$



Learning Classification Trees using Recursive Binary Splitting

Start with the first split at the root and then build the tree from top to bottom

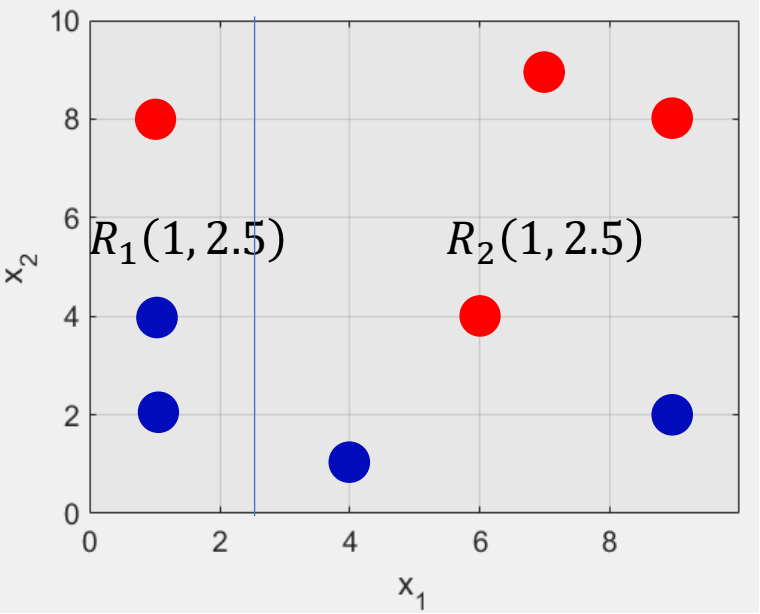
- When determining the splitting rule at the root node, the objective is to obtain a model that best explains the training data after a single split, without taking into consideration that additional splits may be added afterwards
  - Select one of the p input variables $x_1, \cdots x_j, \cdots, x_p$ and a corresponding cutpoint s which divide the input space into two half-spaces

$$R_1(j,s) = \{\mathbf{x} \mid x_j < s\} \quad \text{and} \quad R_2(j,s) = \{\mathbf{x} \mid x_j \geq s\}$$

  - The predictions associated with the two regions will be

$$\hat{y}_1(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_1(j,s)\} \quad \text{and} \quad \hat{y}_2(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_2(j,s)\}$$

Blue **Red**

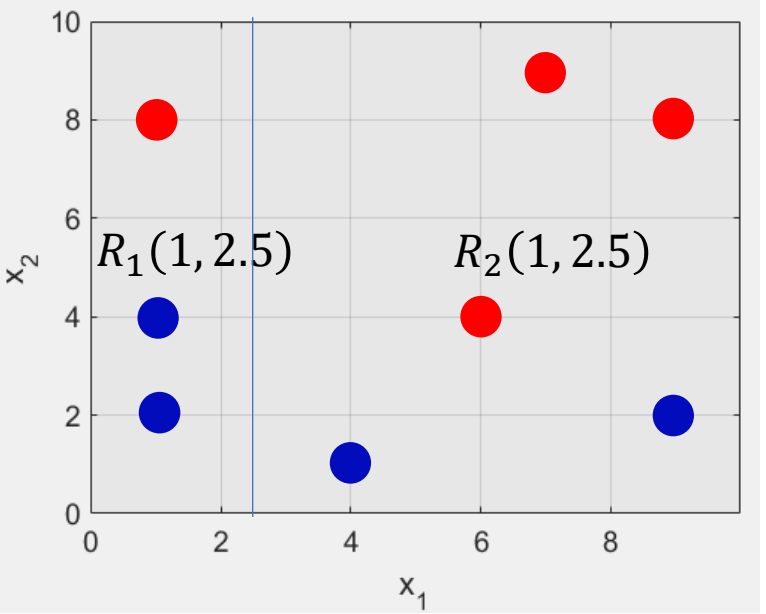


Learning Classification Trees using Recursive Binary Splitting

Start with the first split at the root and then build the tree from top to bottom

- When determining the splitting rule at the root node, the objective is to obtain a mod data after a single split, without taking into consideration that additional splits may ac
  - Select one of the p input variables $x_1, \cdots, x_p$ and a corresponding cutpoint s w half-spaces

$$R_1(j,s) = \{\mathbf{x} \mid x_j < s\} \quad \text{and} \quad R_2(j,s) = \{\mathbf{x} \mid x_j \geq s$$



  - The predictions associated with the two regions will be

$$\hat{y}_1(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_1(j,s)\} \quad \text{and} \quad \hat{y}_2(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_2(j,s)\}$$

- Compute prediction *loss* for all training data points $\left(\mathbf{x}^{(i)}, y^{(i)}\right)_{i=1}^{N}$ at the node to determine goodness-of-fit

$$\text{Loss} = n_1 Q_{\ell,L}(j,s) + n_2 Q_{\ell,R}(j,s)$$

where, n_1, n_2 are the number of data points in left and right nodes of current split and $Q_{\ell,L}, Q_{\ell,R}$ are the associated prediction errors of the left (L) branch and right (R) branch for the ℓth region

Loss → When learning a model, we use a **scalar number** to assess whether we are on track; **low is good**, high is bad

Prediction errors for classification trees

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_\ell(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

Indicator function

- **Misclassification rate:** proportion of data points in region R_ℓ which do not belong to the most common class

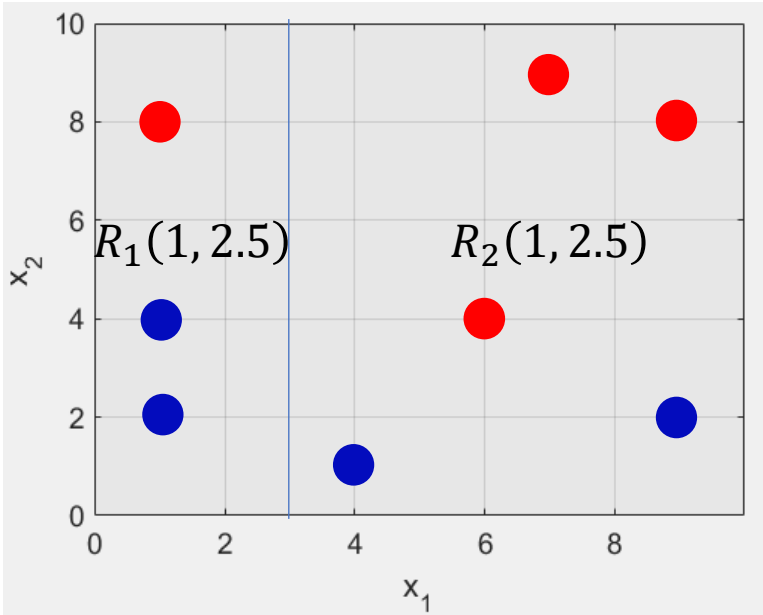
$$Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$$

- **Gini index**

$$Q_\ell = \sum_{m=1}^{M} \hat{\pi}_{\ell,m} \left(1 - \hat{\pi}_{\ell,m}\right)$$

- **Entropy criteria** (commonly used)

$$Q_\ell = -\sum_{m=1}^{M} \hat{\pi}_{\ell,m} \ln \hat{\pi}_{\ell,m}$$

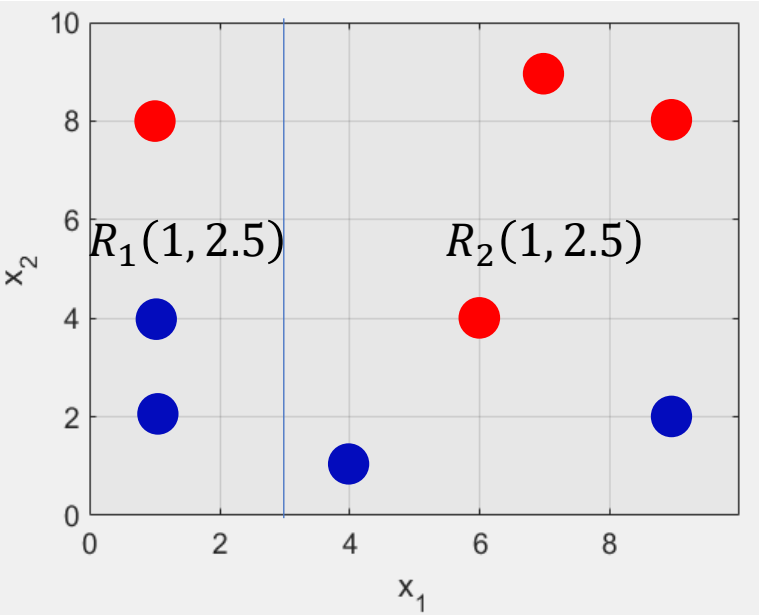


Calculating the loss for 1st split

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region of that belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

- Let's use **Misclassification rate:** $Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$



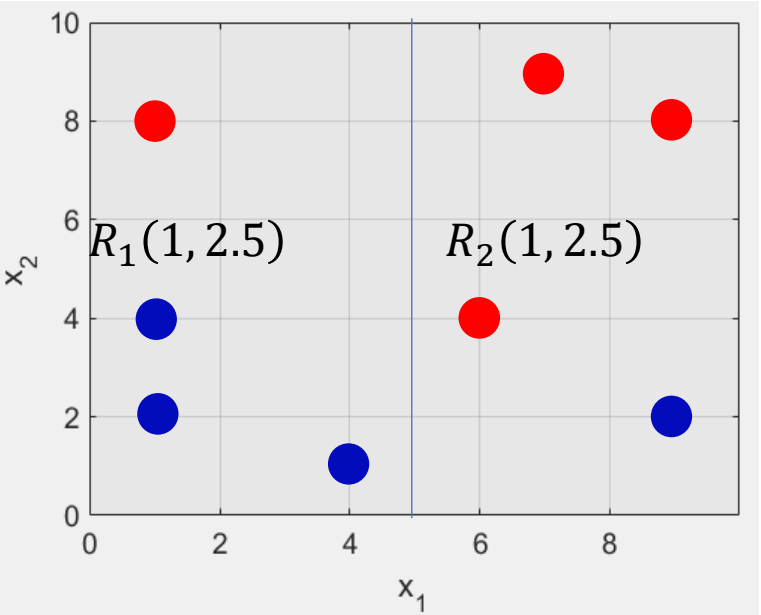
Splits (R_1)	n_1	$\hat{\pi}_{1,B}$	$\hat{\pi}_{1,R}$	Q_1	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	1/3	5	2/5	3/5	2/5	3

Calculating the loss for 1st split

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region of that belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

- Let's use **Misclassification rate:** $Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$



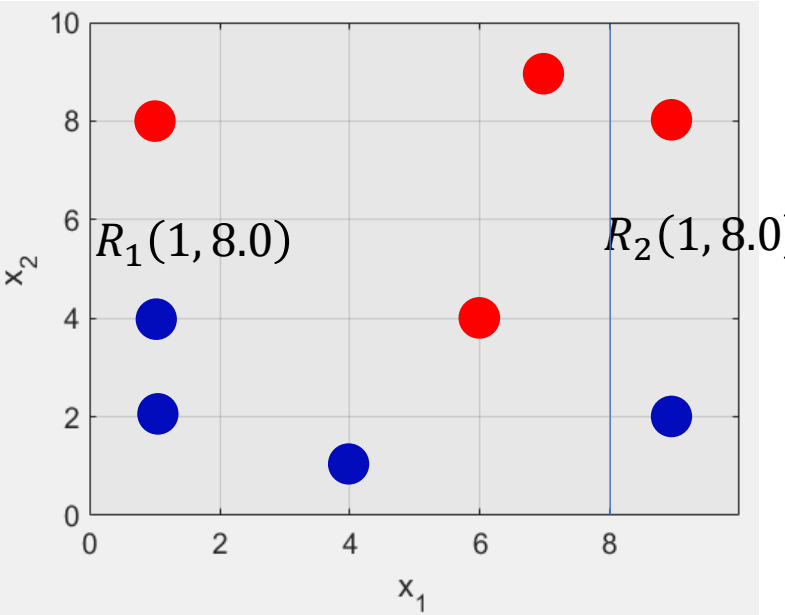
Splits (R_1)	n_1	$\hat{\pi}_{1,B}$	$\hat{\pi}_{1,R}$	Q_1	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	1/3	5	2/5	3/5	2/5	3
$x_1 < 5.0$	4	3/4	1/4	1/4	4	1/4	3/4	1/4	2

Calculating the loss for 1st split

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region of that belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

- Let's use **Misclassification rate:** $Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$



Splits (R_1)	n_1	$\hat{\pi}_{1,B}$	$\hat{\pi}_{1,R}$	Q_1	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	1/3	5	2/5	3/5	2/5	3
$x_1 < 5.0$	4	3/4	1/4	1/4	4	1/4	3/4	1/4	2
$x_1 < 8.0$	6	3/6	3/6	3/6	2	1/2	1/2	1/2	4

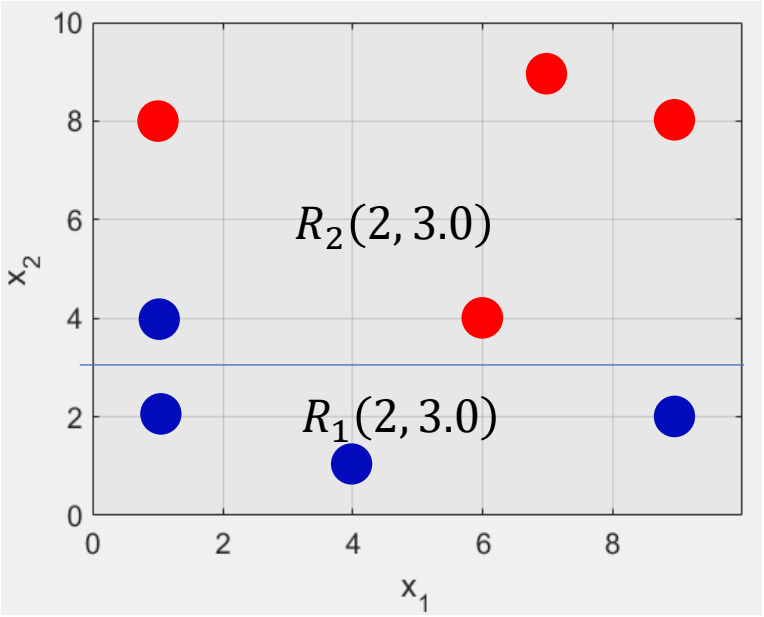
Calculating the loss for 1st split

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region of that belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

- Let's use **Misclassification rate:** $Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$

- To find the optimal split, we select the values for j and s that minimise the loss



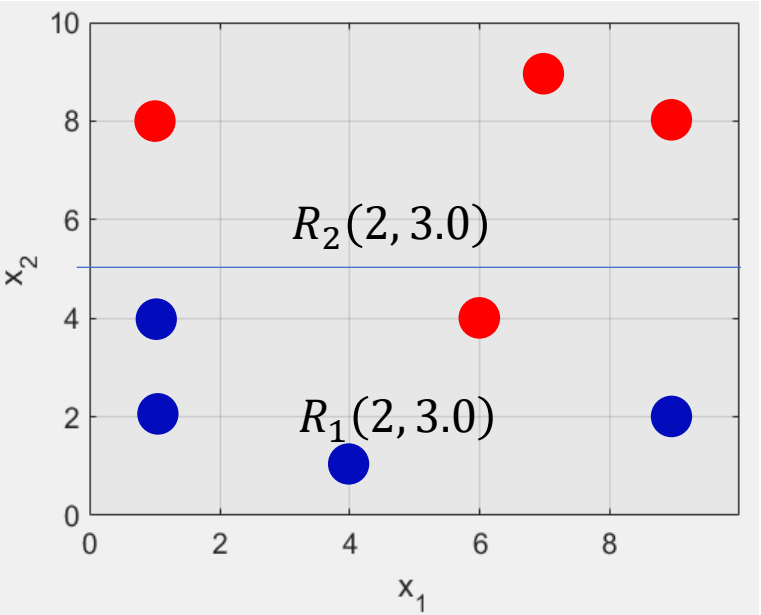
Splits (R_1)	n_1	$\hat{\pi}_{1,B}$	$\hat{\pi}_{1,R}$	Q_1	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	1/3	5	2/5	3/5	2/5	3
$x_1 < 5.0$	4	3/4	1/4	1/4	4	1/4	3/4	1/4	2
$x_1 < 8.0$	6	3/6	3/6	3/6	2	1/2	1/2	1/2	4
$x_2 < 3.0$	3	3/3	0/3	0/3	5	1/5	4/5	1/5	1

Calculating the loss for 1st split

- Define $\hat{\pi}_{\ell,m}$ as the proportion of training observations in the ℓth region of that belong to the mth class

$$\hat{\pi}_{\ell,m} = \frac{1}{n_\ell} \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \mathbf{I}\left(y^{(i)} = m\right)$$

- Let's use **Misclassification rate:** $Q_\ell = 1 - \max_m \hat{\pi}_{\ell,m}$



Splits (R_1)	n_1	$\hat{\pi}_{1,B}$	$\hat{\pi}_{1,R}$	Q_1	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	$n_1Q_1 + n_2Q_2$
$x_1 < 2.5$	3	2/3	1/3	1/3	5	2/5	3/5	2/5	3
$x_1 < 5.0$	4	3/4	1/4	1/4	4	1/4	3/4	1/4	2
$x_1 < 8.0$	6	3/6	3/6	3/6	2	1/2	1/2	1/2	4
$x_2 < 3.0$	3	3/3	0/3	0/3	5	1/5	4/5	1/5	**1**
$x_2 < 5.0$	5	4/5	1/5	1/5	3	0/3	3/3	0/3	**1**

Learning Classification Trees using Recursive Binary Splitting

Start with the first split at the root and then build the tree from top to bottom

- When determining the splitting rule at the root node, the objective is to obtain a model that best explains the training data after a single split, without taking into consideration that additional splits may be added before arriving at the final model
  - Select one of the p input variables $x_1, \cdots, x_p$ and a corresponding cutpoint s which divide the input space into two half-spaces

$$R_1(j,s) = \{\mathbf{x} \mid x_j < s\} \quad \text{and} \quad R_2(j,s) = \{\mathbf{x} \mid x_j \geq s\}$$

  - The predictions associated with the two regions will be

$$\hat{y}_1(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_1(j,s)\} \quad \text{and} \quad \hat{y}_2(j,s) = \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_2(j,s)\}$$

  - Compute *loss* (squared error) for all training data points $\left(\mathbf{x}^{(i)}, y^{(i)}\right)_{i=1}^{N}$ at the node to determine goodness-of-fit

$$n_1 Q_1 + n_2 Q_2$$

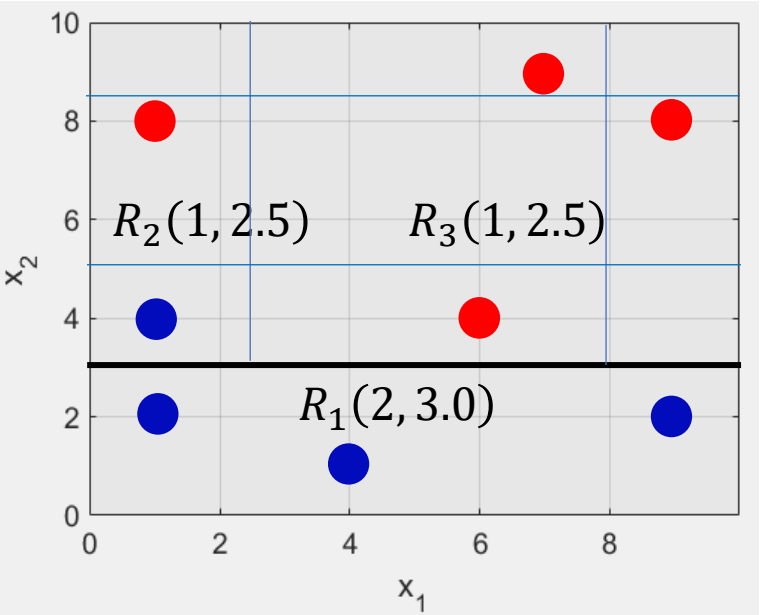
  where, n_1, n_2 are # of data points in left and right nodes of current split and Q_1, Q_2 are associated prediction errors

  - To find the optimal split, we select the values for j and s that minimise the loss

- When we have decided on the first split of the input space (corresponding to the root node of the tree), this split is kept fixed, and we continue in a similar way for the two resulting half-spaces (corresponding to the two branches of the tree)

Calculating the loss for 2nd split

- There is no point splitting region R_1 further since it only contains data points from the same class (**Blue**)
- We therefore split the upper region into two new regions, R_2 and R_3
- We split in the same manner as before



Splits (R_2)	n_2	$\hat{\pi}_{2,B}$	$\hat{\pi}_{2,R}$	Q_2	n_3	$\hat{\pi}_{3,B}$	$\hat{\pi}_{3,R}$	Q_3	$n_2Q_2 + n_3Q_3$
$x_1 < 2.5$	2	1/2	1/2	1/2	3	0/3	3/3	0/3	1
$x_1 < 8.0$	4	1/4	3/4	1/4	1	0/1	1/1	0/1	1
$x_2 < 5.0$	2	1/2	1/2	1/2	3	0/3	3/3	0/3	1
$x_2 < 8.5$	4	1/4	3/4	1/4	1	0/1	1/1	0/1	1

Learning Regression Trees using Recursive Binary Splitting

Start with the first split at the root and then build the tree from top to bottom

- When determining the splitting rule at the root node, the objective is to obtain a model that best explains the training data after a single split, without taking into consideration that additional splits may be added before arriving at the final model
  - Select one of the p input variables $x_1, \cdots, x_p$ and a corresponding cutpoint s which divide the input space into two half-spaces

$$R_1(j,s) = \{\mathbf{x} \mid x_j < s\} \quad \text{and} \quad R_2(j,s) = \{\mathbf{x} \mid x_j \geq s\}$$

  - The predictions associated with the two regions will be

$$\hat{y}_1(j,s) = \text{Mean}\{y^{(i)} : \mathbf{x}^{(i)} \in R_1(j,s)\} \quad \text{and} \quad \hat{y}_2(j,s) = \text{Mean}\{y^{(i)} : \mathbf{x}^{(i)} \in R_2(j,s)\}$$

  - Compute *loss* (squared error) for all training data points $\left(\mathbf{x}^{(i)}, y^{(i)}\right)_{i=1}^{N}$ at the node to determine goodness-of-fit

$$n_1 Q_1 + n_2 Q_2 = \sum_{i:\mathbf{x}^{(i)} \in R_1(j,s)} \left(y^{(i)} - \hat{y}_1(j,s)\right)^2 + \sum_{i:\mathbf{x}^{(i)} \in R_2(j,s)} \left(y^{(i)} - \hat{y}_2(j,s)\right)^2$$

    where, n_1, n_2 are # of data points in left and right nodes of current split and Q_1, Q_2 are associated prediction errors
    - To find the optimal split, we select the values for j and s that minimise the loss
- When we have decided on the first split of the input space (corresponding to the root node of the tree), this split is kept fixed, and we continue in a similar way for the two resulting half-spaces (corresponding to the two branches of the tree)

Algorithm for CART using Recursive Binary Splitting

Data: $\{(\mathbf{x}^{(1)}, y^{(1)}), (\mathbf{x}^{(2)}, y^{(2)}), \ldots, (\mathbf{x}^{(N)}, y^{(N)})\}$
Output: Decision tree with regions $R_1, R_2, \ldots, R_L$ and corresponding predictions $\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_L$

1. Let R denote the entire input space
2. Compute the regions $(R_1, \cdots, R_L) = \textbf{split}(R, \mathcal{T})$
3. Compute the predictions $\hat{y}_\ell$ for $\ell = 1,2, \ldots, L$ as

$$\hat{y}_\ell = \begin{cases} \text{Mean}\{y^{(i)} : \mathbf{x}^{(i)} \in R_\ell\} & \textbf{(Regression)} \\ \text{Mode}\{y^{(i)} : \mathbf{x}^{(i)} \in R_\ell\} & \textbf{(Classification)} \end{cases}$$

function **split**$(R_\ell, \mathcal{T}_\ell)$

if *stopping criterion fulfilled*

return R_ℓ

else

Go through all possible splits $x_j < s$ for all input variables

Pick pair (j, s) that minimizes the chosen loss

Split the region R_ℓ into two half-spaces R_ℓ and $R_{\ell+1}$

Split the data $\mathcal{T}_\ell$ into two parts, $\mathcal{T}_\ell$ and $\mathcal{T}_{\ell+1}$, respectively

return (R_ℓ, T_ℓ) and $(R_{\ell+1}, T_{\ell+1})$

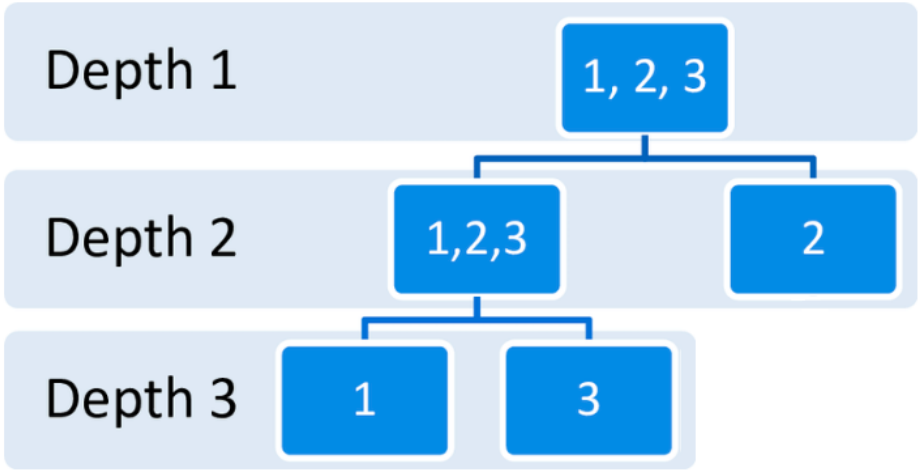
Test Data: $\mathbf{x}^*$
Output: $\hat{y}(\mathbf{x}^*)$

1. Find the region R_ℓ in which $\mathbf{x}^*$ belongs to
2. Return the prediction $\hat{y}(\mathbf{x}^*) = \hat{y}_\ell$

Example of *stopping criterion*
No further splits if there are less than a certain number of training data points in the corresponding region

How deep should be a decision tree?

- The depth of a decision tree (the maximum distance between the root node and any leaf node) has a big impact on the final predictions



- The tree depth impacts the predictions in a somewhat similar way to the hyperparameter k in k-NN

- **Not too shallow (or small)**: Need to handle important but possibly subtle distinctions in data
- **Not too deep (or big):** Avoid over-fitting training examples
- **Optimal tree depth (or size)**: Is a trade-off between flexibility and rigidity of the final model
- Typically, we desire small trees with informative nodes near the root

kNN vs Decision Trees

- **Advantages of Decision trees over kNNs**
  - Simple to deal with poorly scaled data
  - Fast at test time (no need to calculate distances like in kNN)
  - More interpretable

- **Advantages of kNNs over Decision trees**
  - Fewer hyperparameters (need to decide on just the value of k)
  - Can incorporate interesting distance measures