TREE BASED METHODS

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INTRODUCTION TO DECISION TREES

MOTIVATION

- In many real-world applications, decisions need to be made based on complex, multi-dimensional data.
- One goal of statistical analysis is to provide insights and guidance to support these decisions.
- Decision trees provide a way to organize and summarize information in a way that is easy to understand and use in decision-making.

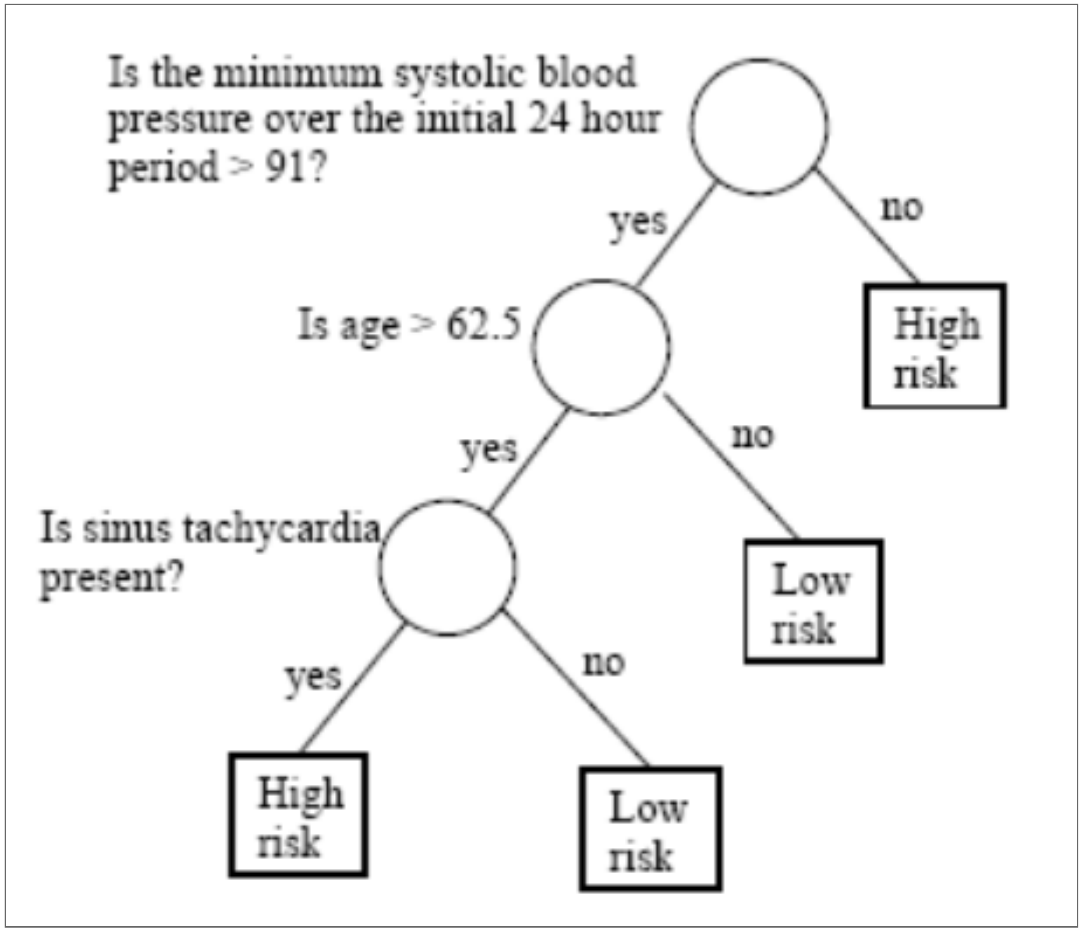
EXAMPLES (1)

- A bank need to have a way to decide if/when a customer can be granted a loan.
- A doctor may need to decide if an oncological patient has to undergo a surgery or a less aggressive treatment.
- A company may need to decide about investing in new technologies or stay with the traditional ones.

In all those cases a decision tree may provide a structured approach to decision-making that is based on data and can be easily explained and justified.

EXAMPLES (2)

- Similarly as would do a doctor, patients are classified into one of two classes: *high risk* versus *low risk* based on: systolic blood pressure, age and tachycardia.



SO, WHAT IS A DECISION TREE?

- A decision tree is a graphical representation of a series of decisions and their potential outcomes.
- It is obtained by recursively *stratifying* or *segmenting* the *feature space* into a number of simple regions.
- Each region (decision) corresponds to a *node* in the tree, and each potential outcome corresponds to a *branch*.
- The tree structure can be used to guide decision-making based on data.

WHAT DO WE NEED TO LEARN?

- We need **context** and also, we need to learn how to **build**, **evaluate** and **optimize** trees.
- **Context**
  - When is it appropriate to rely on decision trees?
  - When would other approaches be preferable?
  - What type of decision trees can be used?
- **Build the tree**
  - How do we build a decision tree?
  - What are the algorithms available?
  - How do we optimize the tree?
  - How do we evaluate it?

MORE ABOUT CONTEXT

- Decision trees are non parametric data guided predictors well suited for a variety of situations such as:
  - Non-linear relationships.
  - High-dimensional data.
  - Interaction effects.
  - Non-parametric data.
  - Mixed data types.
- Complex problems, that require expert knowledge are not well suited for decision trees.

TYPES OF DECISION TREES

- The two main types of trees are Classification and Regression Trees (CART).
  - **Classification Trees** are built when the response variable is categorical.
    - They aim to *classify a new observation* based on the values of the predictor variables.
  - **Regression Trees** are used when the response variable is numerical.
    - They aim to *predict the value* of a continuous response variable based on the values of the predictor variables.
- Both types of decision trees follow the same basic principles for constructing the tree, but the splitting criteria and the method for predicting the response variable differ.

BUILDING THE TREES

- Building the tree requires deciding:
  - how to partition (“split”) the space,
  - Which *impurity* measures to use,
  - When to stop splitting
- Evaluation is similar to other classifiers.
- Optimization involves deciding:
  - How to *prune* the tree,
  - Which features are most important.

TREE BUILDING WITH R

- There are mutliple packages for working with trees in R.
- We will mostly use `rpart` and `caret`.
- Check the document “CART_Examples.qmd” for a series of examples on how to build, validate and optimize trees with R.

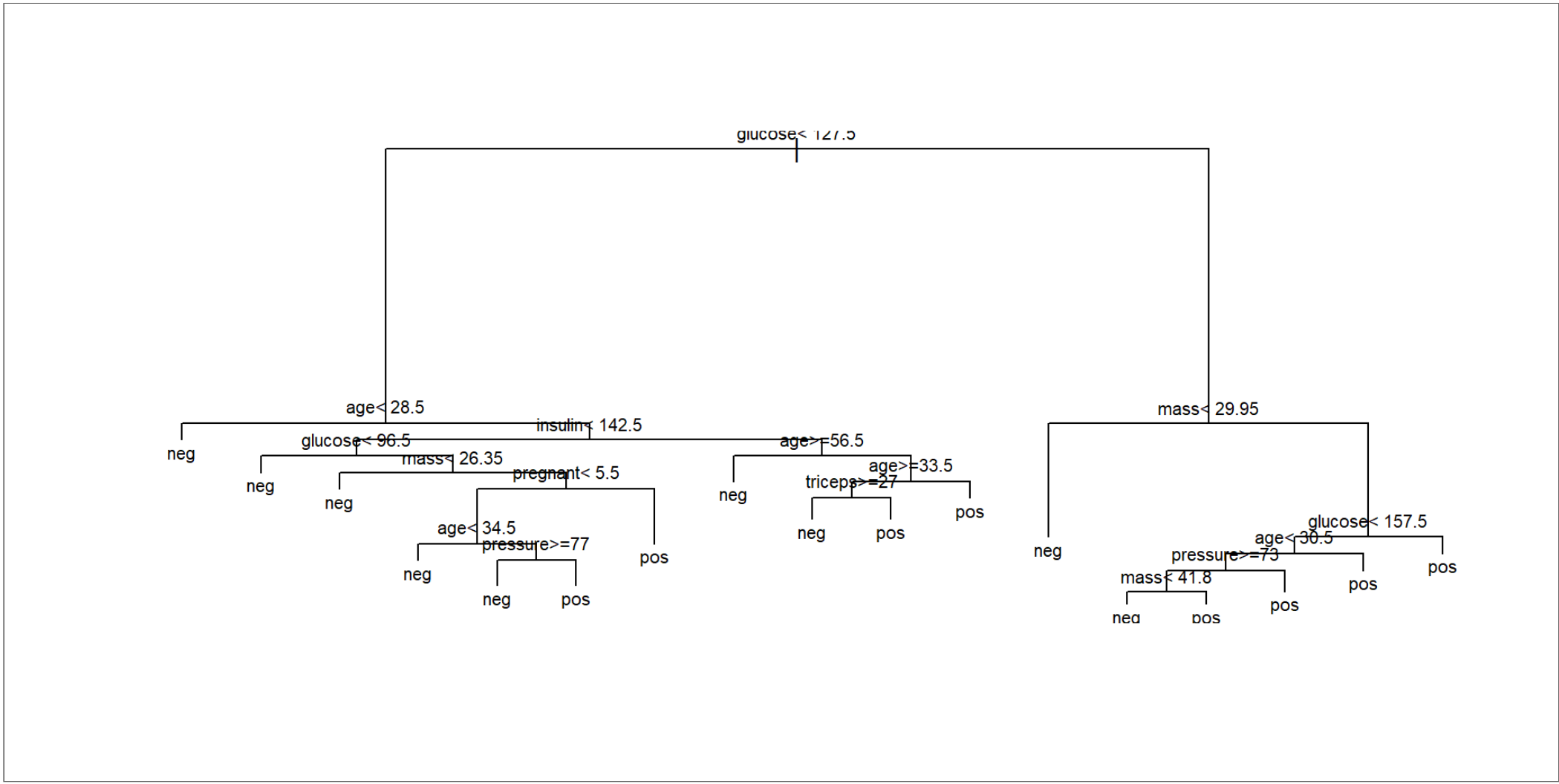
A "QUICK AND DIRTY" EXAMPLE IN R

- The Pima Indian Diabetes data set contains 768 individuals (female) and 9 clinical variables for predicting the probability of individuals in being diabete-positive or negative.

```
library(rpart)
data("PimaIndiansDiabetes2", package = "mlbench")
model1 <- rpart(diabetes ~., data = PimaIndiansDiabetes2)
```

```
plot(model1)
text(model1, digits = 3, cex=0.7)
```

A SIMPLE, UNPRUNNED TREE



HOW ACCURATE IS THE MODEL?

```
predicted.classes<- predict(model1, PimaIndiansDiabetes2, "class")
mean(predicted.classes == PimaIndiansDiabetes2$diabetes)
```

```
[1] 0.8294271
```

A better strategy is to use train dataset to build the model and a test dataset to check how it works.

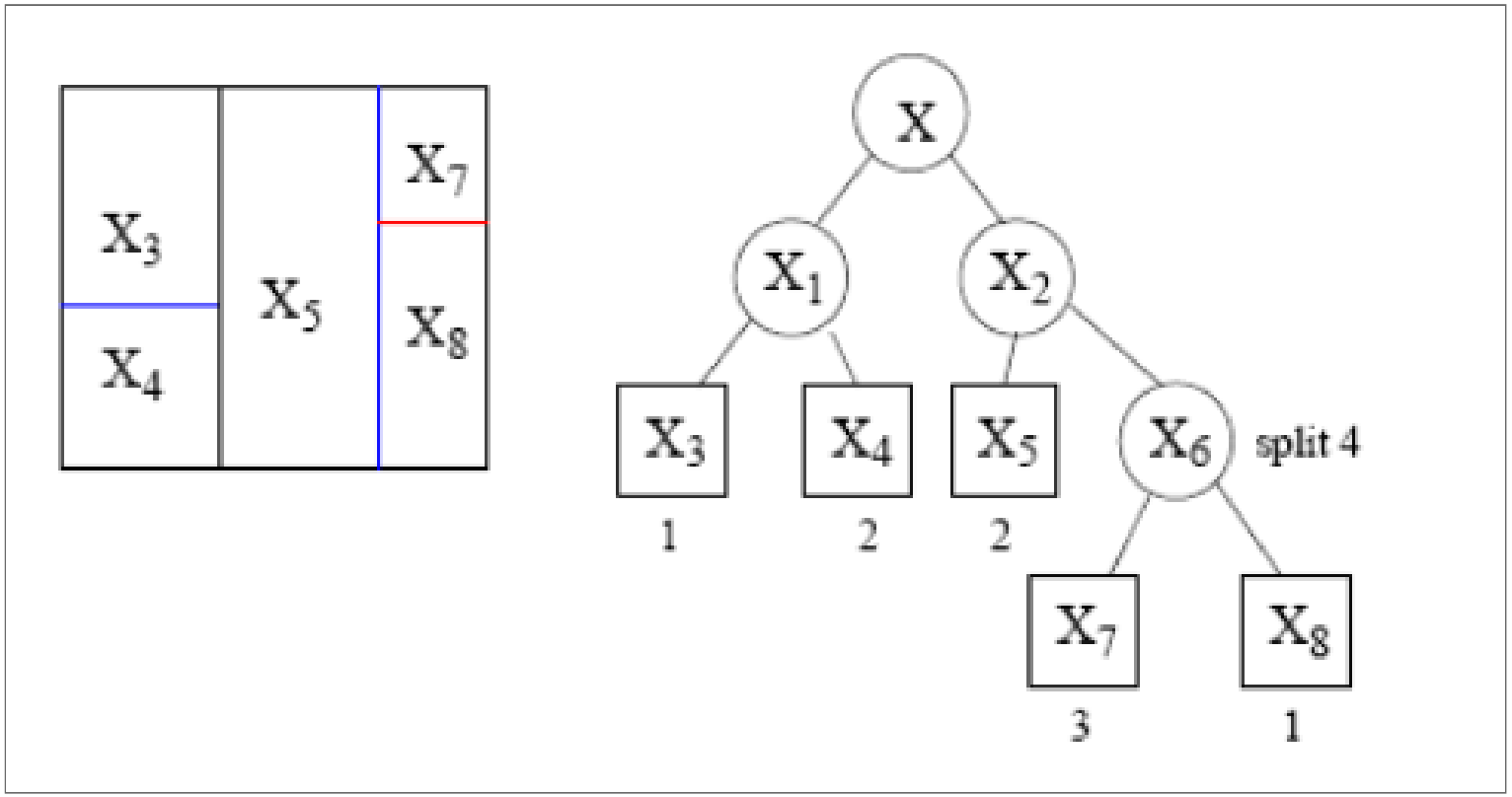
```
set.seed(123)
ssize <- nrow(PimaIndiansDiabetes2)
propTrain <- 0.8
training.indices <-sample(1:ssize, floor(ssize*propTrain))
train.data  <- PimaIndiansDiabetes2[training.indices, ]
test.data <- PimaIndiansDiabetes2[-training.indices, ]
```

Now we build the model on the train data and check its accuracy on the test data.

```
model2 <- rpart(diabetes ~., data = train.data)
predicted.classes.test<- predict(model2, test.data, "class")
mean(predicted.classes.test == test.data$diabetes)
```

```
[1] 0.7272727
```

CONSTRUCTING THE TREE



NOTATION AND BASIC CONCEPTS

- $\mathbb{X}$: Space of variables, or *feature space*
  - Usually $\mathbb{X} \subseteq \mathbb{R}^p$
  - But it can contain numerical/categorical variables.
- $X \in \mathbb{X}$: Input vector: $X_1, X_2, \ldots, X_p$.
- Tree-structured classifiers are constructed by repeated splits of the space X into smaller and smaller subsets, beginning with X itself.
  - That is by *recursive splitting*

ADDITIONAL NOTATION

- A node is denoted by t. We will also denote the left child node by t_L and the right one by t_R.
- Denote the collection of all the nodes in the tree by T and the collection of all the leaf nodes by $\tilde{T}$
- A split will be denoted by s. The set of splits is denoted by S.
- **Nice definition of basic terminology:**

TREES PARTITION THE SPACE

- Keep in mind: *the tree represents the recursive splitting of the space*.
  - Every node of interest corresponds to one region in the original space.
  - Two child nodes will occupy two different regions and
  - Put together, we get the same region as that of the parent node.
- In the end, every leaf node is assigned with a class and a test point is assigned with the class of the leaf node it lands in.
- **Animation**

THE TREE REPRESENTS THE SPLITTING

CONSTRUCTION OF A TREE

The construction of a tree involves the following three general elements:

1. The selection of the splits, i.e., how do we decide which node (region) to split and how to split it?
   - How to select from the pool of candidate splits?
   - What are appropriate *goodness of split* criteria?
2. If we know how to make splits (‘grow’ the tree), how do we decide when to declare a node terminal and *stop splitting*?
3. We have to assign each terminal node to a class. How do we assign these class labels?

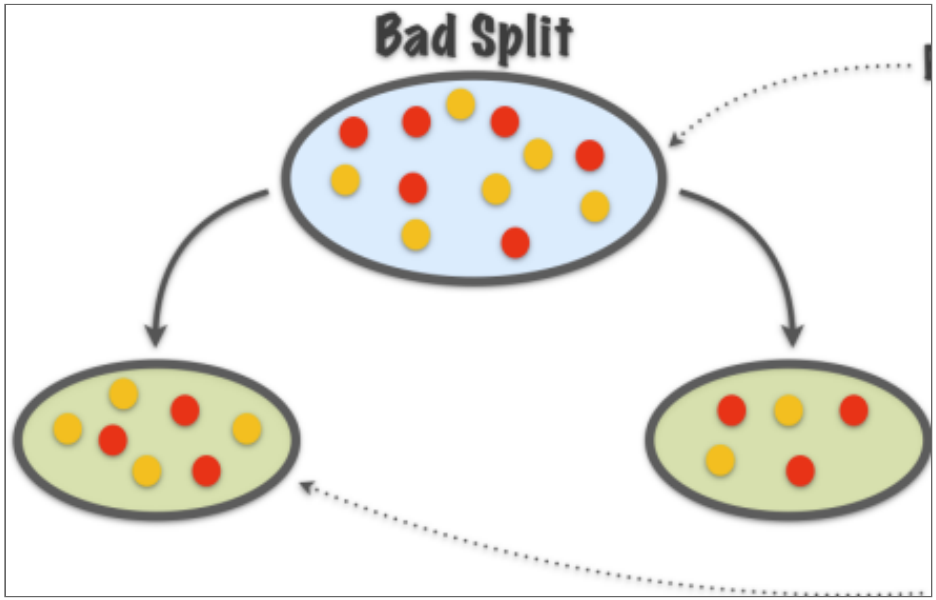
WHICH QUESTIONS TO SPLIT THE TREE

- To build a Tree, questions have to be generated that induce splits based on the value of a single variable.
- Ordered variable X_j:
  - $\text{Is } X_j \leq c$? for all possible thresholds c.
  - Restricts the split line to be parallel to the coordinates.
- Categorical variables, $X_j \in \{1, 2, \ldots, M\}$:
  - $\text{Is } X_j \in A$? where A is any subset of $\{1, 2, \ldots, M\}$.
- The pool of candidate splits for all p variables is formed by combining all the generated questions.

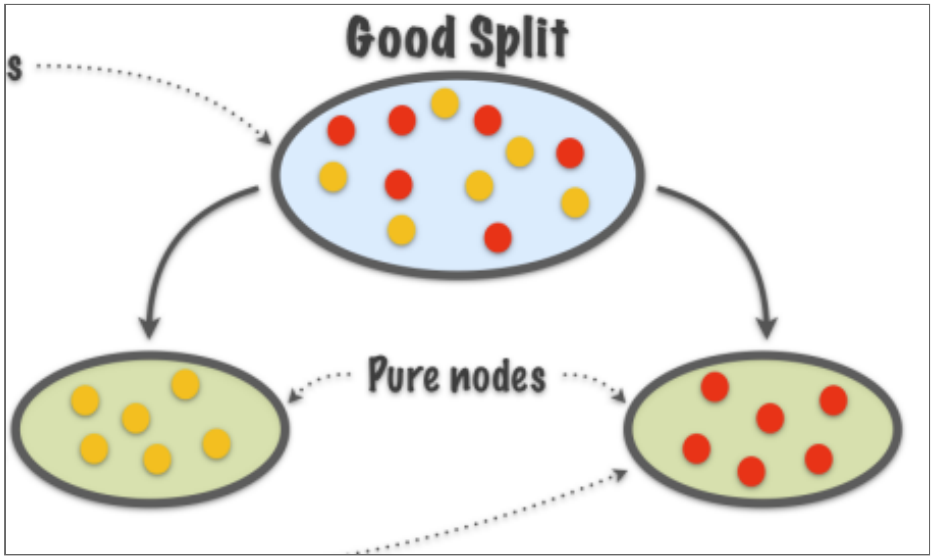
DETERMINING GOODNESS OF SPLIT

- The way we choose the split, is *to measure every split by a 'goodness of split' measure*, which depends on:
  - the split question as well as
  - the node to split.
- The 'goodness of split' in turn is measured by an *impurity function*.
- Intuitively, when we split the points we want the region corresponding to each leaf node to be "pure", that is, most points in this region come from the same class, that is, one class dominates.

GOOD SPLITS VS BAD SPLITS



Purity not increased



Purity increased

IMPURITY FUNCTIONS

Impurity functions measure the extent of purity for a region containing data points from possibly different classes.
Definition: An impurity function is a function Φ defined on the set of all K-tuples of numbers $(p_1, \cdots, p_K)$ satisfying
$p_j \geq 0, \quad j = 1, \cdots, K, \Sigma_j p_j = 1$ with the properties:

1. Φ achieves maximum only for the uniform distribution, that is all the p_j are equal.
2. Φ achieves minimum only at the points $(1, 0, \ldots, 0)$,$(0, 1, 0, \ldots, 0)$, $\ldots, (0, 0, \ldots, 0, 1)$, i.e., when the probability of being in a certain class is 1 and 0 for all the other classes.
3. Φ is a symmetric function of $p_1, \cdots, p_K$, i.e., if we permute p_j, Φ remains constant.

SOME IMPURITY FUNCTIONS

Commonly used impurity functions:

1. **Entropy function**: $\sum_{j=1}^{K} p_j \log \frac{1}{p_j} = -\sum_{j=1}^{K} p_j \log p_j$.

   If $p_j = 0$, use the limit $\lim p_j \to \log p_j = 0$.
2. **Misclassification rate**: $1 - \max_j p_j$.
3. **Gini index**: $\sum_{j=1}^{K} p_j (1 - p_j) = 1 - \sum_{j=1}^{K} p_j^2$.

ENTROPY GUIDED SPLITTING

- Entropy gives low values for purer nodes
  - We may choose the split that minimises entropy.
- This set up can be abused by certain splits
  - E.g Large child node with almost plus a second tiny child node pure
- This split
  - doesn’t really improve the overall performance while
  - It also adds unnecessary depth and complexity to the tree, especially if this happens repeatedly in the same tree.

INFORMATION GAIN

- An information theoretic approach that compares:
  - the entropy of the parent node before the split to
  - that of a weighted sum of the child nodes after the split where the weights are proportional to the number of observations in each node.
- Given a split {F} and a set of observations {X}, information gain is defined as:

$$IG(X,F) = \ (\text{original entropy}) - (\ \text{entropy after the split})$$

$$IG(X,F) = H(X) - \sum_{i=1}^{n} \frac{|x_i|}{X} H\left(x_i\right)$$

INFORMATION GAIN ACCOUNTS FOR NODE SIZES

$$IG(X, F) = H(X) - \sum_{i=1}^{n} \frac{|x_i|}{X} H\left(x_i\right)$$

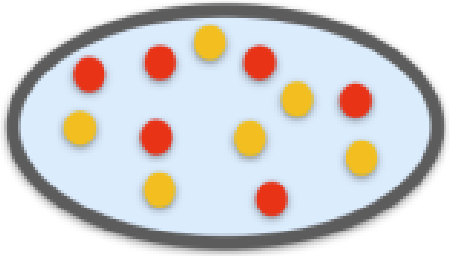
- Since information gain subtracts the entropy of the child nodes our choice of split will be the one that maximises the information gain.-
- This effectively penalizes small, pure nodes based on their size just as we needed.

EXAMPLE

Consider the problem of designing an algorithm to automatically differentiate between apples and pears (class labels) given only their width and height measurements (features).

Width	Height	Fruit
7.1	7.3	Apple
7.9	7.5	Apple
7.4	7.0	Apple
8.2	7.3	Apple
7.6	6.9	Apple
7.8	8.0	Apple
7.0	7.5	Pear
7.1	7.9	Pear
6.8	8.0	Pear
6.6	7.7	Pear
7.3	8.2	Pear
7.2	7.9	Pear

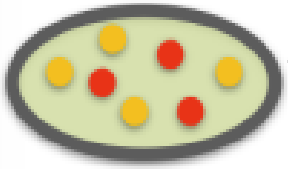
EXAMPLE. ENTROPY CALCULATION



$$H(X) = \sum_{i=1}^{n} P(x_i) log_2 P(x_i)$$

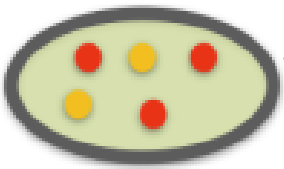
$$= -\frac{6}{12} \cdot log_2(\frac{6}{12}) - \frac{6}{12} \cdot log_2(\frac{6}{12})$$

$$= \frac{1}{2} + \frac{1}{2} = 1$$



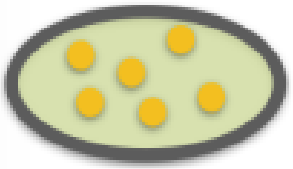
$$H(X) = -\overbrace{\frac{4}{7} \cdot log_2(\frac{4}{7})}^{\text{yellow}} - \overbrace{\frac{3}{7} \cdot log_2(\frac{3}{7})}^{\text{red}}$$

$$= 0.4613 + 0.5239 = 0.9852$$

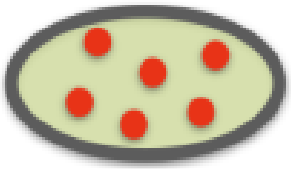


$$H(X) = -\overbrace{\frac{3}{5} \cdot log_2(\frac{3}{5})}^{\text{red}} - \overbrace{\frac{2}{5} \cdot log_2(\frac{2}{5})}^{\text{yellow}}$$

$$= 0.4422 + 0.5288 = 0.9710$$

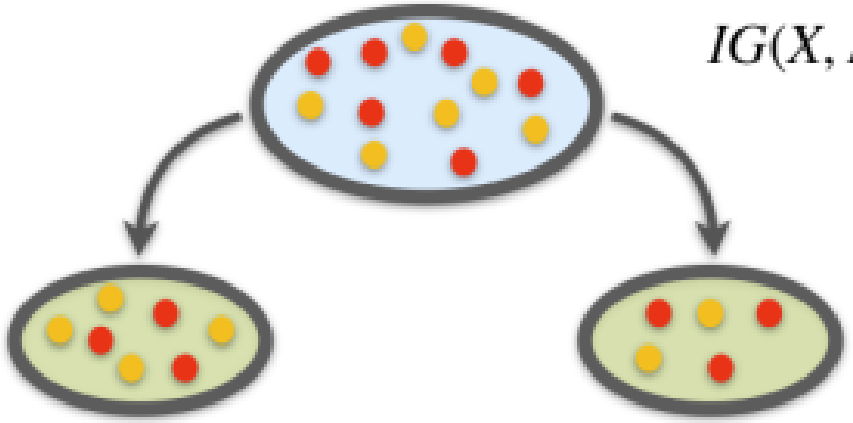


$$H(X) = -\frac{6}{6} \cdot log_2(\frac{6}{6}) = 0$$



$$H(X) = -\frac{6}{6} \cdot log_2(\frac{6}{6}) = 0$$

EXAMPLE. INFORMATION GAIN

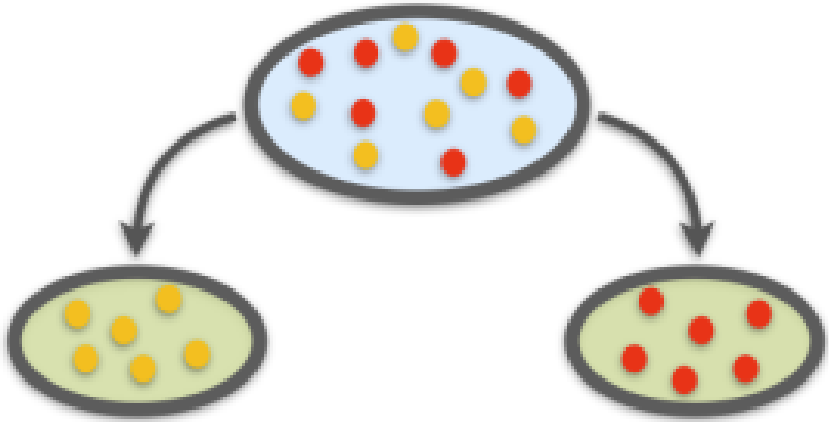


$$IG(X, F) = (original\ entropy) - (entropy\ after\ split)$$

$$= H(X) - \sum_{i=1}^{n} \frac{|x_i|}{X} H(x_i)$$

$$= 1 - \frac{7}{12} \cdot (0.9852) - \frac{5}{12} \cdot (0.9710) = 0.0213$$

$$IG(X, F) = 1 - \frac{6}{12} \cdot (0) - \frac{6}{12} \cdot (0) = 1$$



WHEN TO STOP GROWING

- Maximizing information gain is one possible criteria to choose among splits.
- In order to avoid excessive complexity it is usually decided to stop splitting when “information gain does not compensate for increase in complexity”.
- In practice stop splitting if:
  $\max_{s \in S} \Delta I(s, t) < \beta$
  where ΔI represents the information gain associated with an optima split s and a node t, and β is a pre-determined threshold.

CLASS ASSIGNMENT RULES (1)

- The decision tree classifies new data points as follows.
  - We let a data point pass down the tree and see which leaf node it lands in.
  - The class of the leaf node is assigned to the new data point. Basically, all the points that land in the same leaf node will be given the same class. This is similar to k-means or any prototype method.

CLASS ASSIGNMENT RULES (2)

- A class assignment rule assigns a class $j = 1, \cdots, K$ to every terminal (leaf) node $t \in \tilde{T}$.
- The class is assigned to node t. $\tilde{T}$ is denoted by $\kappa(t)$, e.g., if $\kappa(t) = 2$, all the points in node t would be assigned to class 2.

  If we use 0-1 loss, the class assignment rule is very similar to k-means (where we pick the majority class or the class with the maximum posterior probability):
  $\kappa(t) = \arg\max_j p(j \mid t)$

ESTIMATING THE ERROR RATE (1)

- Let's assume we have built a tree and have the classes assigned for the leaf nodes.
- We want to estimate the classification error rate for this tree.
- We need to introduce the resubstitution estimate $r(t)$ for the probability of misclassification, given that a case falls into node t. This is:

$$r(t) = 1 - \max_j p(j \mid t) = 1 - p(\kappa(t) \mid t)$$

ESTIMATING THE ERROR RATE (2)

- Denote $R(t) = r(t)p(t)$. The resubstitution estimation for the overall misclassification rate $R(T)$ of the tree classifier T is:

$$R(T) = \sum_{t \in \tilde{T}} R(t)$$

OPTIMIZING THE TREE

- Trees obtained by looking for optimal splits tend to overfit: good for the data in the tree, but generalize badly and tend to fail more in predictions.
- In order to reduce complexity and overfitting while keeping the tree as good as possible tree pruning may be applied.
- Essentially pruning works by removing branches that are unlikely to improve the accuracy of the model on new data.

PRUNING METHODS

- There are different pruning methods, but the most common one is the *cost-complexity* pruning algorithm, also known as the weakest link pruning.
- The algorithm works by adding a penalty term to the impurity function, which measures the quality of a split.
- The penalty term depends on a parameter called alpha, which controls the trade-off between tree complexity and accuracy.

COST COMPLEXITY PRUNING

- Start by building a large tree that overfits the data.
- Then, use cross-validation to estimate the optimal value of alpha that minimizes the generalization error.
- Finally, prune the tree by removing the branches that have a smaller improvement in impurity than the penalty term multiplied by alpha.
- Iterate the process continues until no more branches can be pruned, or until a minimum tree size is reached.

REGRESSION TREES

- When the response variable is numeric decision trees are *regression trees*.
- Some differences with classification trees are:
  - The splitting criteria used in regression trees are typically based on mean squared error or mean absolute error.
  - The leaf node prediction in regression trees is typically the mean or median of the target variable in that region
  - The evaluation metrics used to assess the performance of regression trees are typically based on measures of the difference between the predicted and actual values (such as mean squared error or R-squared)

REFERENCES AND RESOURCES

REFERENCES

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- Hastie, T., Tibshirani, R., & Friedman, J. (2009). The elements of statistical learning: Data mining, inference, and prediction. Springer.
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RESOURCES

- **Applied Data Mining and Statistical Learning (Penn Statte-University)**
- **R for statistical learning**
- **CART Model: Decision Tree Essentials**
- **Introduction to Artificial Neural Networks**