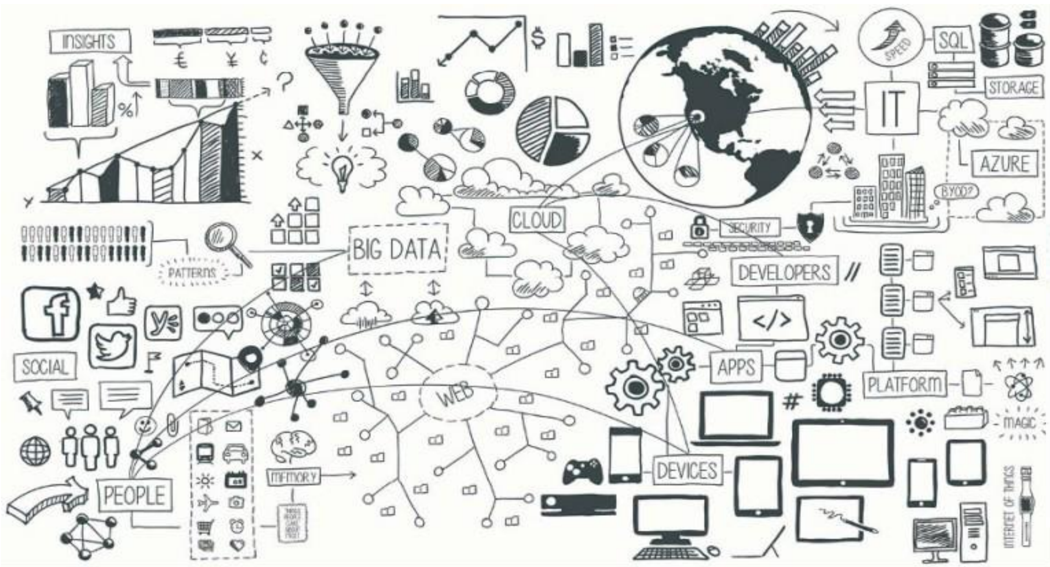
Data Mining (Minería de Datos)

Classification Trees



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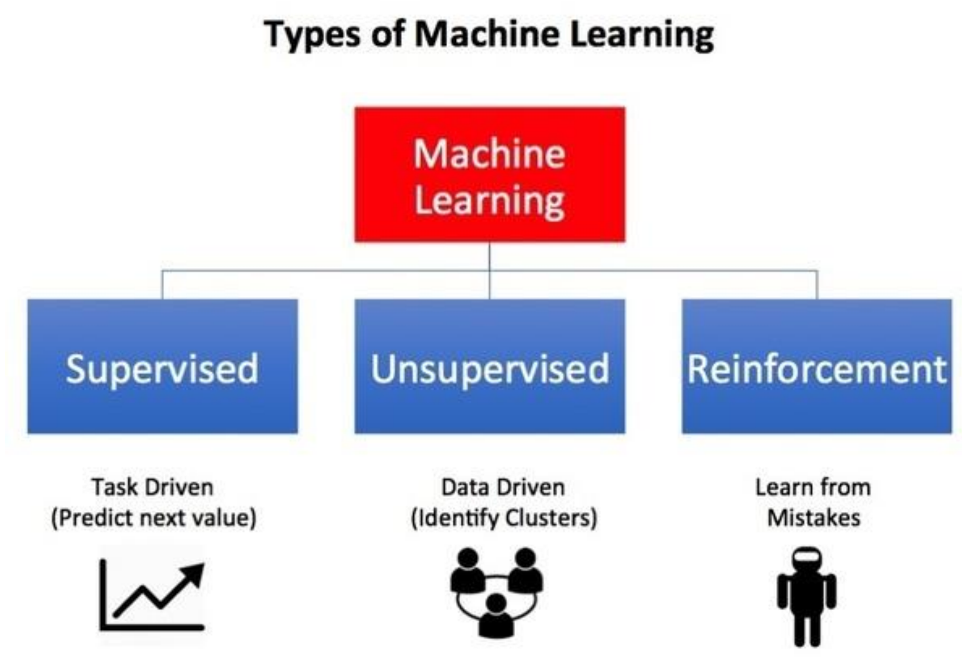
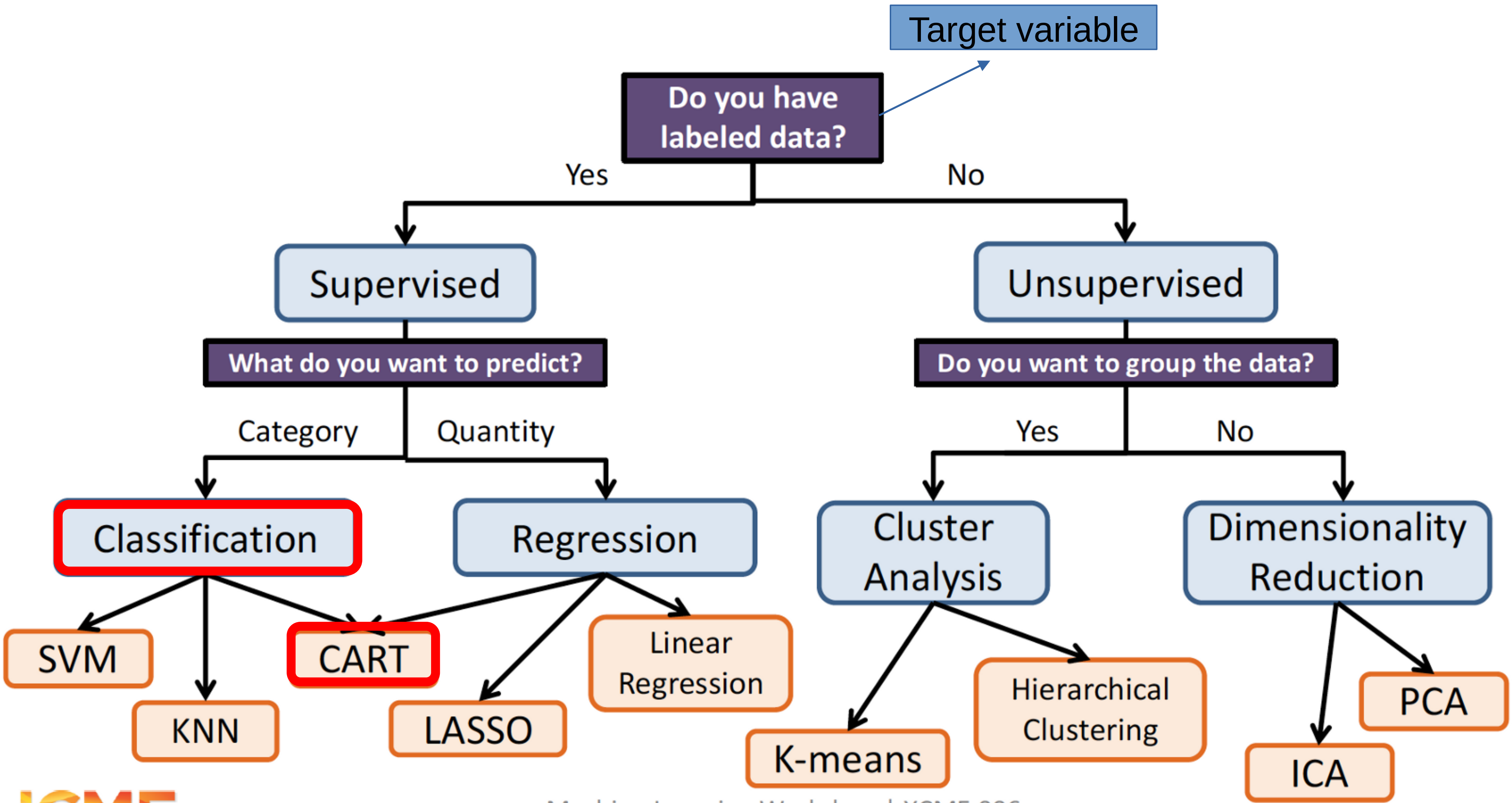


NOTA: Las líneas de código de R en esta presentación se muestran sobre un fondo gris

Oct	30	Aplazada (sesión de refuezo)
Nov	6	Presentación, introducción y perspectiva histórica
	8	Paradigmas, problemas canónicos y data challenges
	13	Reglas de asociación
	15	Práctica: Reglas de asociación
	20	Evaluación, sobreajuste y cross-validación
	22	Práctica: Cross-validación
	27	Árboles de clasificación
	29	Práctica: Árboles de clasificación
		T01. Datos discretos
Dic	4	Técnicas de vecinos cercano (k-NN)
	11	Práctica: Vecinos cercanos
	13	Reducción de dimensión lineal
	18	Práctica: LDA y PCA
	20	Reducción no lineal
		T02. Clasificación
Ene	8	Árboles de clasificación y regresión (CART)
	10	Práctica: CART
	15	Ensembles: Bagging and Boosting
	17	Práctica: Random forests
		T03. Predicción
	22	Práctica: Gradient boosting
	24a	Técnicas de agrupamiento
	24b	Práctica: Técnicas de agrupamiento
	29a	Práctica: El paquete CARET
	29b	Examen


Target variable
Do you have labeled data?
Yes
No
Supervised
Unsupervised
What do you want to predict?
Do you want to group the data?
Category
Quantity
Yes
No
Classification
Regression
Cluster Analysis
Dimensionality Reduction
SVM
KNN
CART
LASSO
Linear Regression
K-means
Hierarchical Clustering
PCA
ICA

Classification trees

PlayTennis dataset:
https://github.com/sjwhitworth/golearn/blob/master/examples/datasets/tennis.csv

Day	Outlook	Temperature	Humidity	Wind	Play Tennis
1	Sunny	Hot	High	Weak	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Weak	Yes
4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
10	Rain	Mild	Normal	Weak	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
14	Rain	Mild	High	Strong	No

Aim:

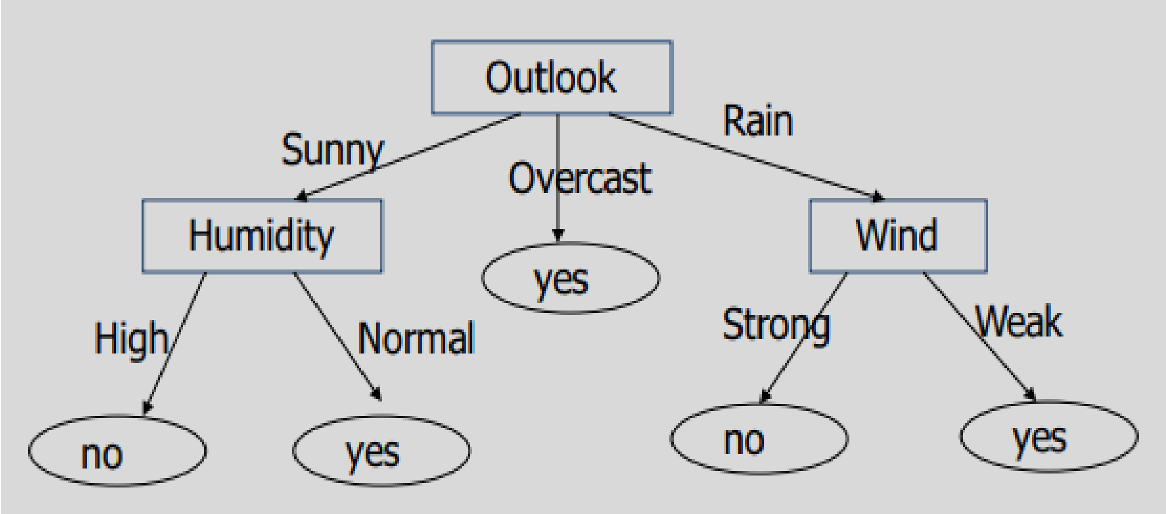
- To classify a **categorical** target variable (R factor) based on a set of **categorical or continuous** predictors

Structure:

- Each **node** corresponds to a test on an **attribute**
- Each **branch** corresponds to an attribute value
- Each **leaf** (terminal node) represents a final class
- Each **path** is a conjunction of attribute values

Key points:

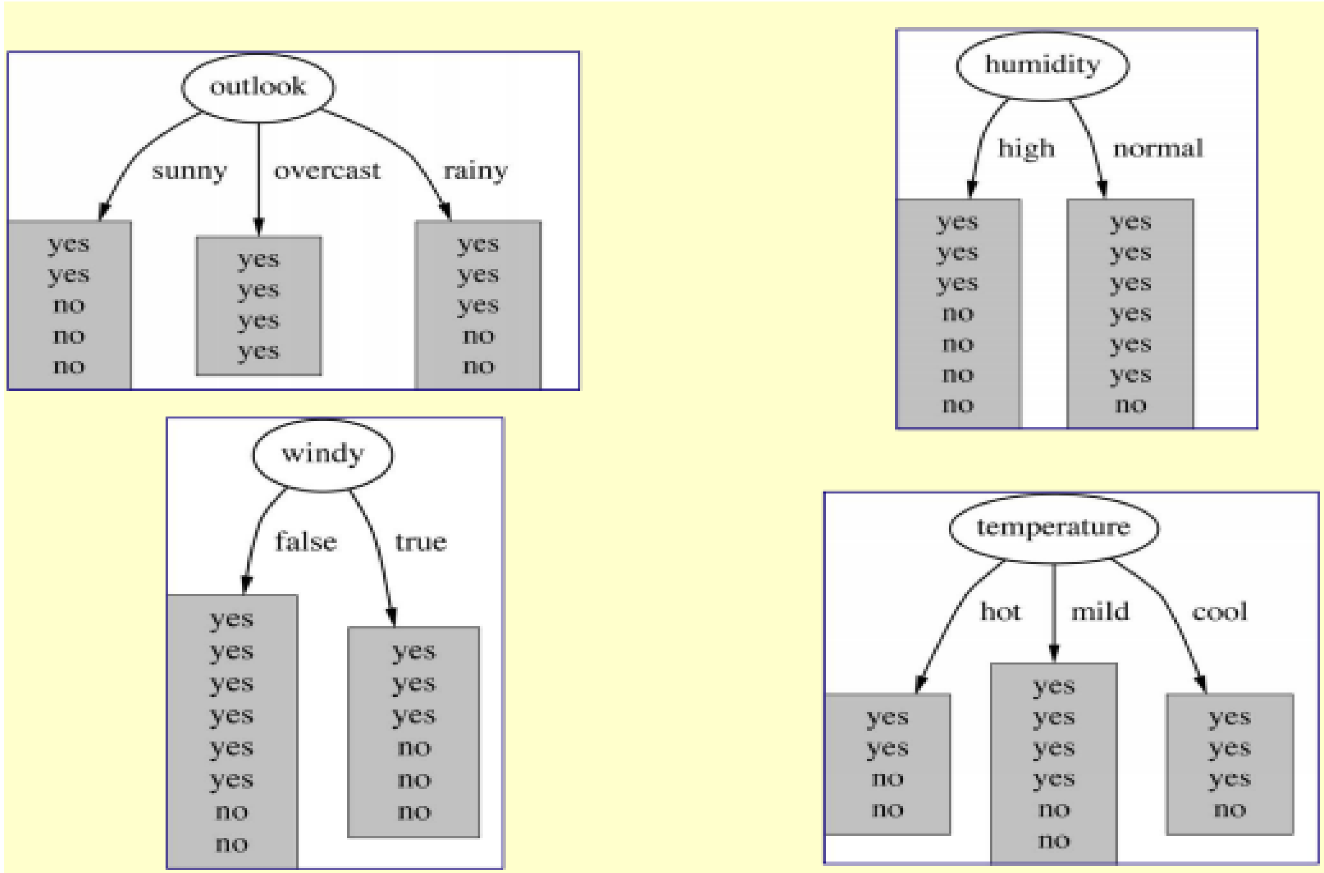
- Due to their intuitive representation, they are easy to assimilate by humans
- They can be constructed relatively fast as compared to other methods
- In general, they provide as good results as other more complex methods



Tree construction

There are several algorithms to build up the tree. However, the idea of all of them is the same: evaluate attribute according to its **power of separation**.

Best discriminating attribute



Many variants for attribute selection:

- from machine learning: **ID3** (**I**terative **D**ichotomizer), **C4.5** and **C5.0** (Quinlan 86, 93)
- from statistics: **CART** (**C**lassification **A**nd **R**egression **T**rees) (Breiman et al. 84)
- from pattern recognition: **CHAID** (**CH**i-squared **A**utomated **I**nteraction **D**etection) (Magidson 94)

Their main difference is the criterion followed to perform the division of the node (splitting)

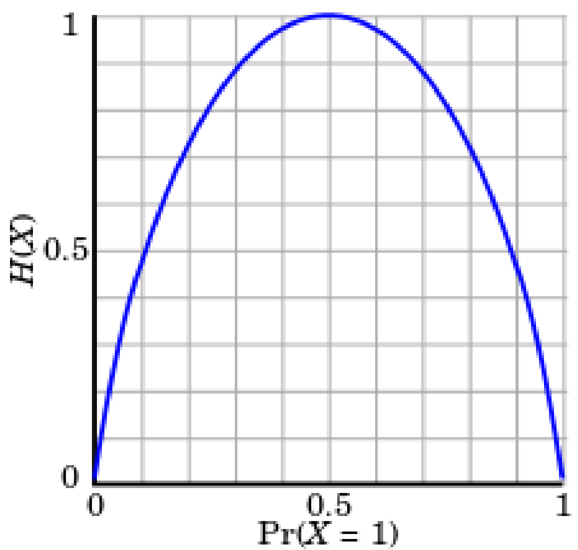
ID3 (the core algorithm)

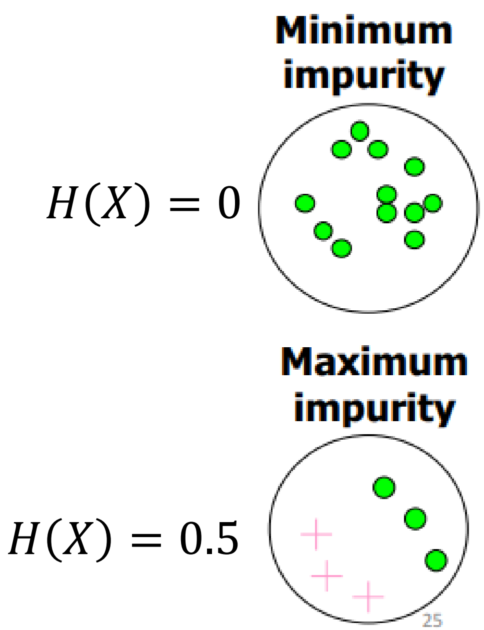
ID3 relies on the **information gain (IG)** to grow the tree. IG measures how important a given attribute is. The goal is to maximize the predictive power of the tree by reducing the uncertainty in the classified data (or **entropy, H)**. H can be seen as a measure of the **purity** of a node.

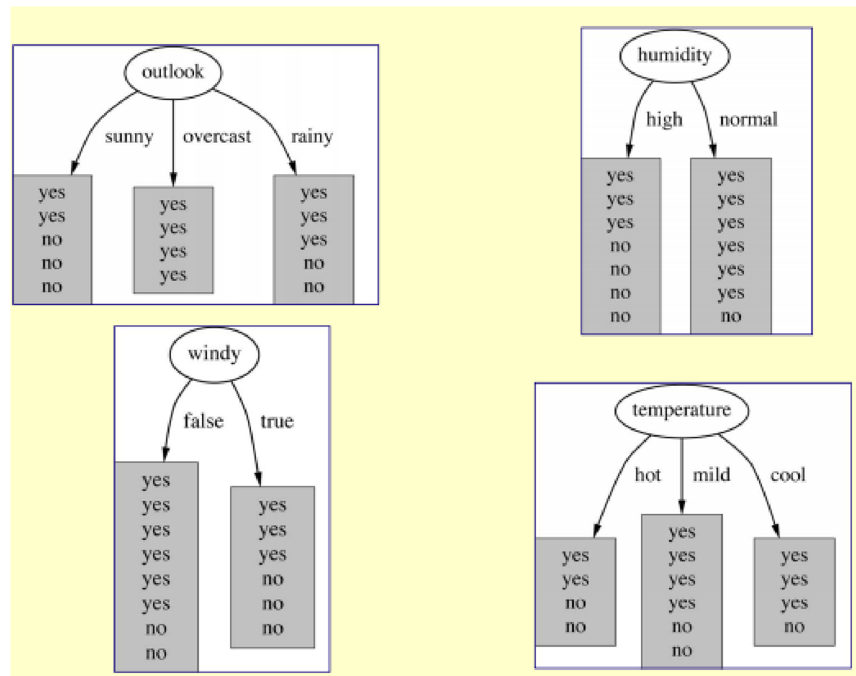
$$IG(X|Y) = H(X) - H(X|Y)$$

$$H(X) = -\sum_{X} p(x)\, log_2(p(x))$$

$$H(X|Y) = -\sum_{X}\sum_{Y} p(x,y)\, log_2(p(x|y))$$







Day	Outlook	Temperature	Humidity	Wind	Play Tennis
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4	Rain	Mild	High	Weak	Yes
5	Rain	Cool	Normal	Weak	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Weak	No
9	Sunny	Cool	Normal	Weak	Yes
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12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Weak	Yes
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$$H(PT) = -\frac{9}{14} log_2\left(\frac{9}{14}\right) - \frac{5}{14} log_2\left(\frac{5}{14}\right) = 0.940$$

Day	Outlook	Temperature	Humidity	Wind	Play Tennis
1	Sunny	Hot	High	***Weak***	No
2	Sunny	Hot	High	***Strong***	No
3	Overcast	Hot	High	***Weak***	Yes
4	Rain	Mild	High	***Weak***	Yes
5	Rain	Cool	Normal	***Weak***	Yes
6	Rain	Cool	Normal	***Strong***	No
7	Overcast	Cool	Normal	***Strong***	Yes
8	Sunny	Mild	High	***Weak***	No
9	Sunny	Cool	Normal	***Weak***	Yes
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11	Sunny	Mild	Normal	***Strong***	Yes
12	Overcast	Mild	High	***Strong***	Yes
13	Overcast	Hot	Normal	***Weak***	Yes
14	Rain	Mild	High	***Strong***	No

$$H(PT|Wind) = -p(Yes, Strong)\ log_2\big(p(Yes|Strong)\big) - p(No, Strong)\ log_2\big(p(No|Strong)\big)$$
$$-p(Yes, Weak)\ log_2(p(Yes|Weak)) - p(No, Weak)\ log_2(p(No|Weak))$$

Day	Outlook	Temperature	Humidity	Wind	Play Tennis
1	Sunny	Hot	High	***Weak***	No
2	Sunny	Hot	High	***Strong***	No
3	Overcast	Hot	High	***Weak***	Yes
4	Rain	Mild	High	***Weak***	Yes
5	Rain	Cool	Normal	***Weak***	Yes
6	Rain	Cool	Normal	***Strong***	No
7	Overcast	Cool	Normal	***Strong***	Yes
8	Sunny	Mild	High	***Weak***	No
9	Sunny	Cool	Normal	***Weak***	Yes
10	Rain	Mild	Normal	***Weak***	Yes
11	Sunny	Mild	Normal	***Strong***	Yes
12	Overcast	Mild	High	***Strong***	Yes
13	Overcast	Hot	Normal	***Weak***	Yes
14	Rain	Mild	High	***Strong***	No

$$H(PT|Wind) = -\frac{3}{14}log_2\left(\frac{3}{6}\right) - \frac{3}{14}log_2\left(\frac{3}{6}\right) - \frac{6}{14}log_2\left(\frac{6}{8}\right) - \frac{2}{14}log_2\left(\frac{2}{8}\right) = 0.892$$

$$H(PT) = -\frac{9}{14}log_2\left(\frac{9}{14}\right) - \frac{5}{14}log_2\left(\frac{5}{14}\right) = 0.940$$

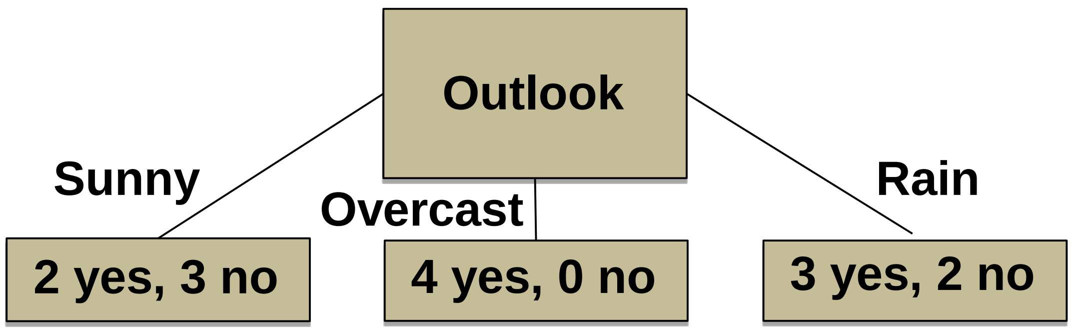
$$H(PT|Wind) = -\frac{3}{14}log_2\left(\frac{3}{6}\right) - \frac{3}{14}log_2\left(\frac{3}{14}\right) - \frac{6}{14}log_2\left(\frac{6}{8}\right) - \frac{2}{14}log_2\left(\frac{2}{14}\right) = 0.892$$

$$IG(PT|Wind) = 0.940 - 0.892 = 0.048$$

$$IG(PT|Humidity) = 0.151$$

$$\boxed{IG(PT|Outlook) = 0.246}$$ **Root node**

$$IG(PT|Temperature) = 0.029$$



$$H(PT) = -\frac{9}{14} log_2\left(\frac{9}{14}\right) - \frac{5}{14} log_2\left(\frac{5}{14}\right) = 0.940$$

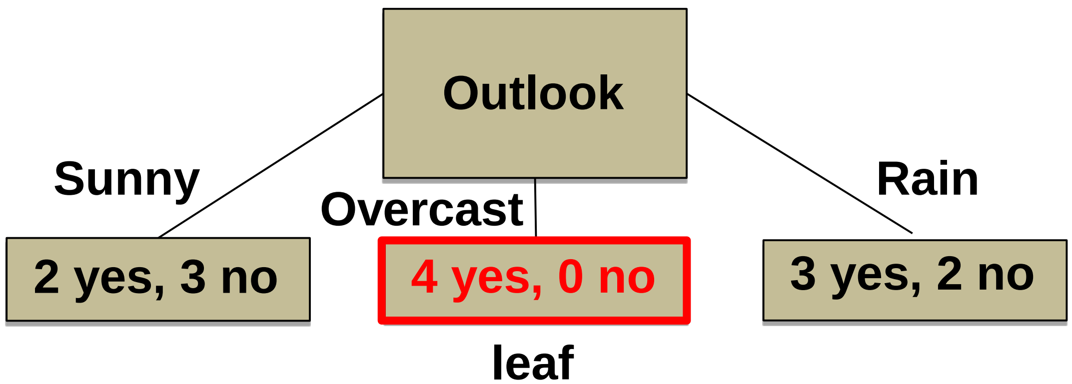
$$H(PT|Wind) = -\frac{3}{14} log_2\left(\frac{3}{6}\right) - \frac{3}{14} log_2\left(\frac{3}{14}\right) - \frac{6}{14} log_2\left(\frac{6}{8}\right) - \frac{2}{14} log_2\left(\frac{2}{14}\right) = 0.892$$

$$IG(PT|Wind) = 0.940 - 0.892 = 0.048$$

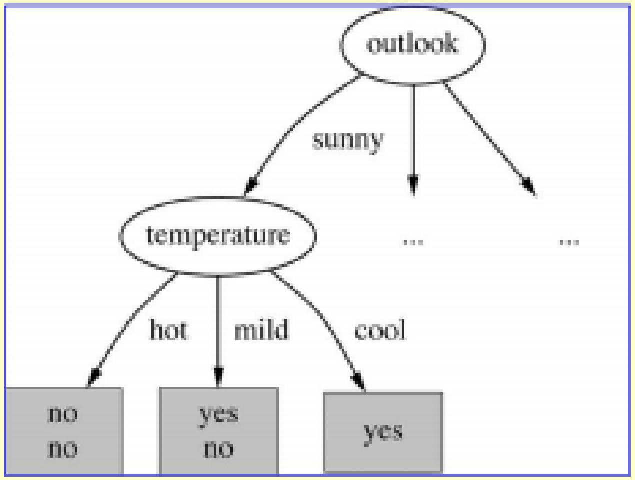
$$IG(PT|Humidity) = 0.151$$

$$\boxed{IG(PT|Outlook) = 0.246} \longleftarrow \textbf{Root node}$$

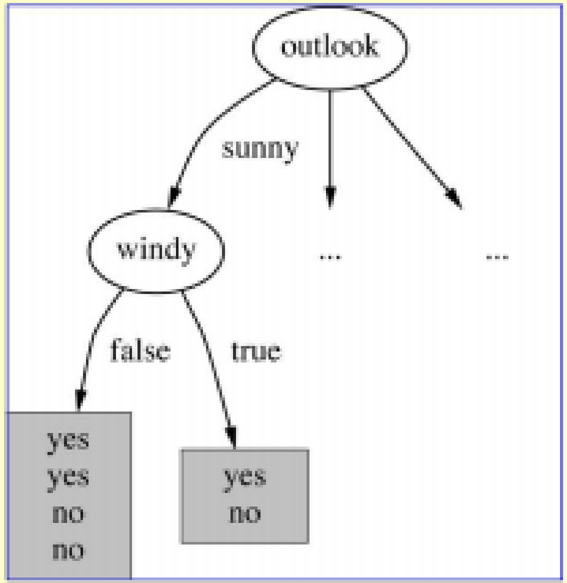
$$IG(PT|Temperature) = 0.029$$



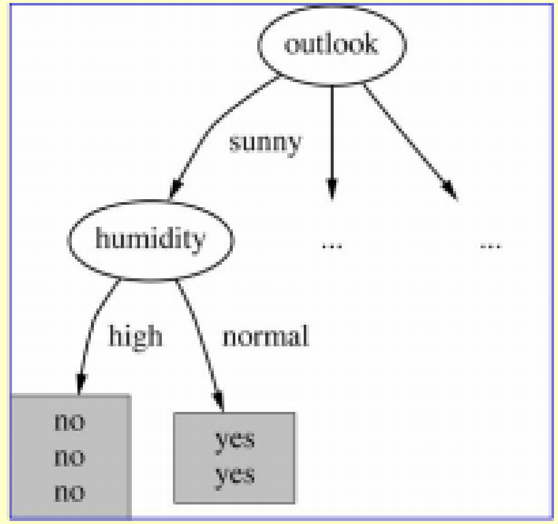
… continue to split…



Gain(Temperature) = 0.570



Gain(Wind) = 0.019

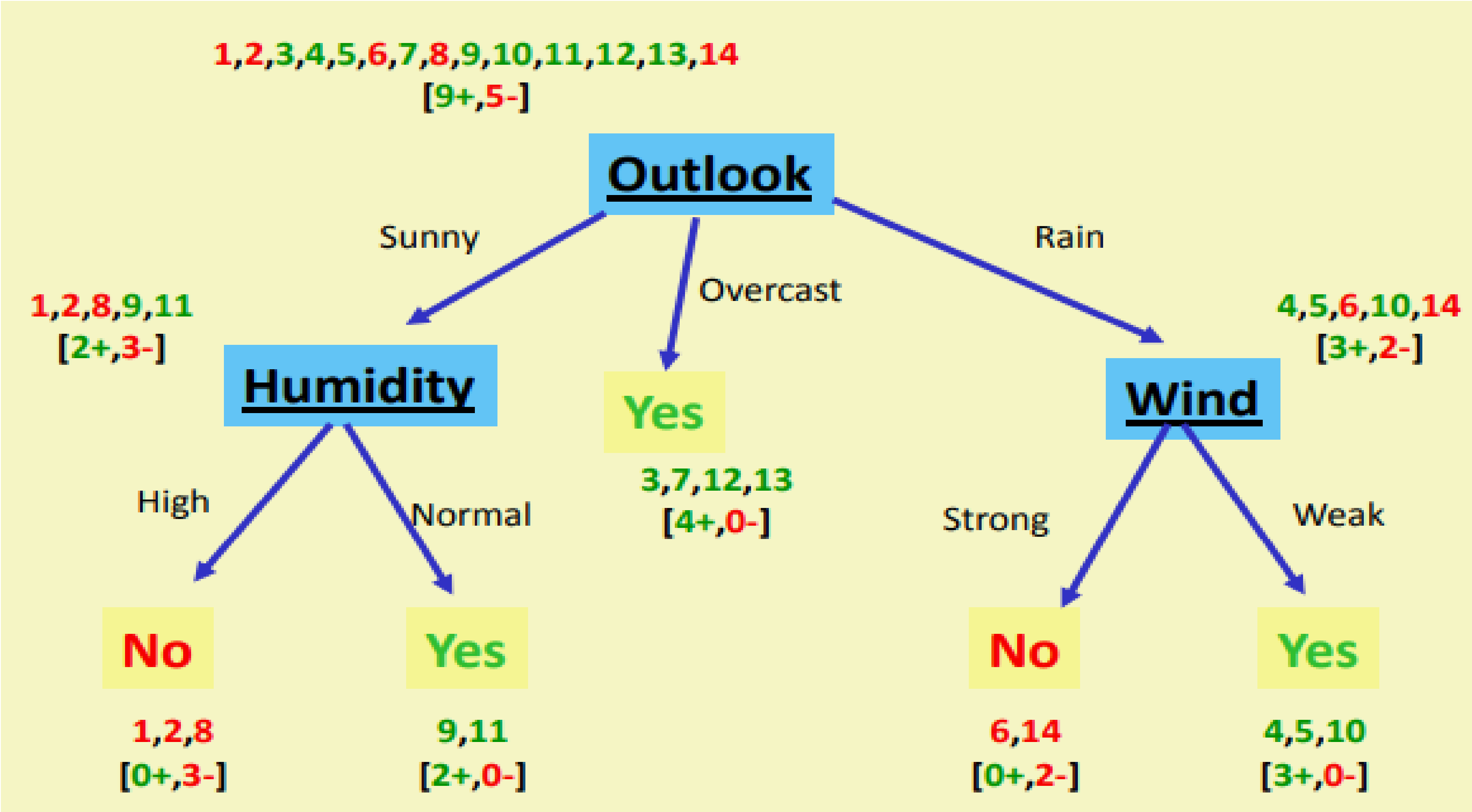


Gain(Humidity) = 0.970

next attribute chosen: Humidity

ID3 performs a **greedy search** in which the algorithm **never backtracks** to reconsider earlier choices. This type of search is likely not to be a globally optimum solution, but generally works well

… final tree!



- If some attributes are not useful for classification, they will not be selected to grow the tree. For this reason, decision trees often used as a pre-processing for other learning algorithms which suffers from the presence of irrelevant information
- For a sufficiently complex (i.e. large) tree, all instances can be correctly classified. However, this can lead to **overfitting** (we will see this later)

The C4.5 algorithm

The **information gain** is a measure that tends to prefer attributes with large number of possible values. To solve this, the successor of ID3, **C4.5** (Quinlan 93), uses the **gain ratio** as partitioning criterion. In addition, this new algorithm was improved to handle with missing data and continuous attributes (which are splitted into categories).

Gain ratio (GR): Takes into account the number and sizes of branches when choosing an attribute, penalizing those with many values and instances uniformly distributed.

$$GR = -\frac{IG}{Info} \qquad Info = -\sum_i \frac{|p_i|}{N} log_2 \frac{|p_i|}{N}$$

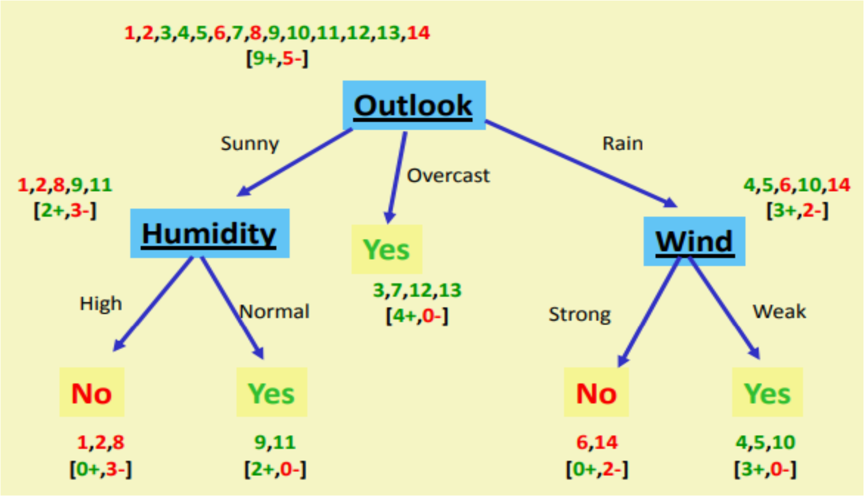
$$Info_{Outlook} = -\frac{5}{14} log_2\left(\frac{5}{14}\right) - \frac{5}{14} log_2\left(\frac{5}{14}\right) - \frac{4}{14} log_2\left(\frac{4}{14}\right) = 1.577$$

$$GR_{Outlook} = -\frac{IG_{Outlook}}{Info_{Outlook}} = \frac{0.246}{1.577} = \boxed{0.157}$$

attribute chosen

$$GR_{Humidity} = 0.152$$

$$GR_{Wind} = 0.049$$



C5.0 is just a more efficient implementation of C4.5 (faster computing times).
Most of the algorithms that have been developed for learning classification trees are variations of ID3 and its successors C4.5 and C5.0.

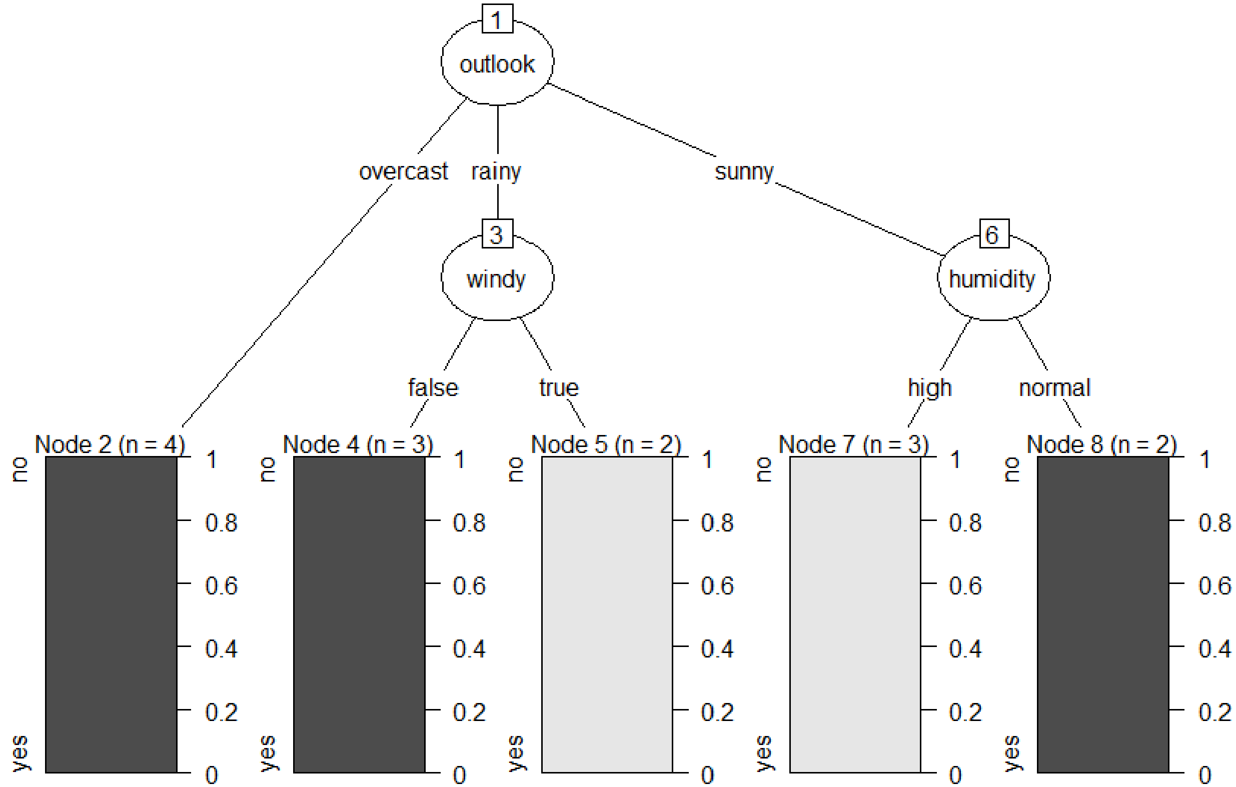
Tree construction in R

There are many packages in R to build classification tress: *tree*, *rpart*, *rpart2*, *C5.0*, etc.

Use of C5.0 (based on GR):

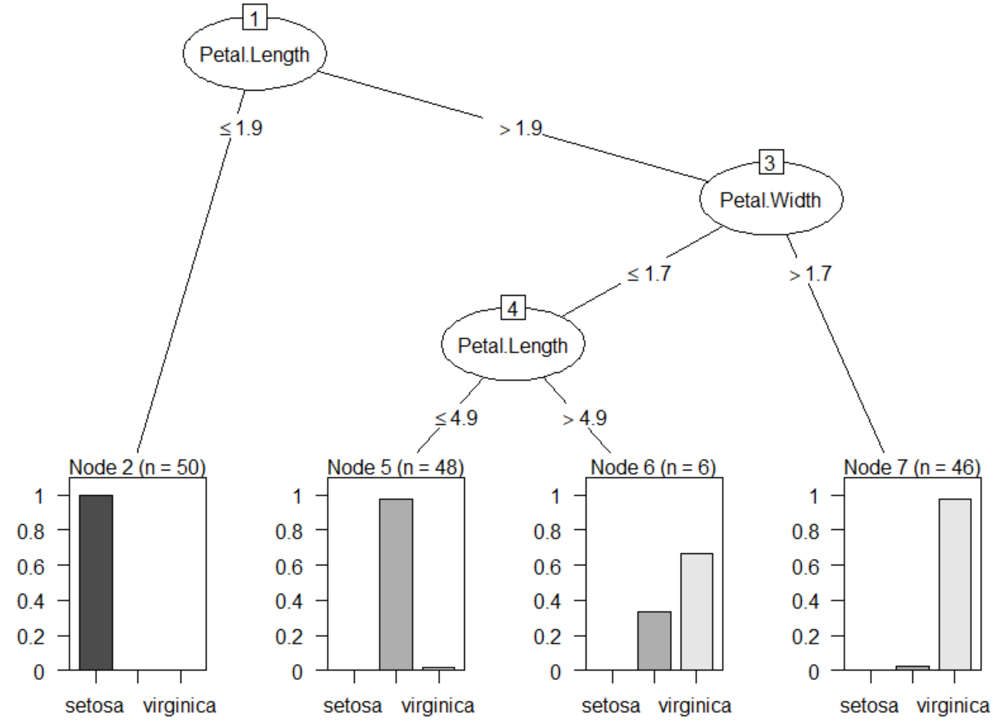
Example for playTennis (categorical attributes)

```
## read dataset
tennis = read.csv(“…/tennis.csv")
## grow the tree
library(C50)
t = C5.0(formula = play ~ .,
data = tennis)
## plot the tree
plot(t)
summary(t)

## percentage of training samples that
fall into all the terminal nodes after the split
C5imp(t)
        Overall
outlook   100.00
humidity   35.71
windy      35.71
temp        0.00
```

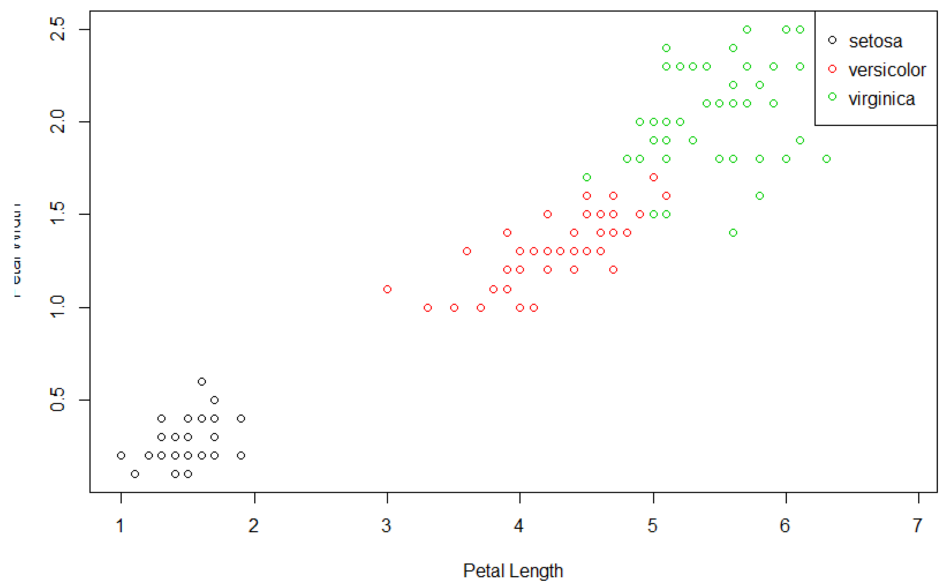


Example for iris (continuous attributes)

```
## continuous attributes are splitted into
categories based on thresholds
t = C5.0(formula = Species ~ ., data = iris)
plot(t)
summary(t)

## there are only two relevant predictors
t = C5.0(formula = Species ~ Petal.Length +
Petal.Width, data = iris)
plot(t)
summary(t)
```



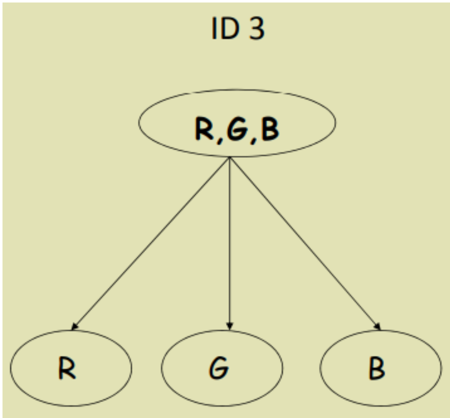

```
## the total space is partitioned according to the
thresholds determined by the tree
with(iris, plot(Petal.Length, Petal.Width, col = Species,
              xlab = "Petal Length", ylab = "Petal Width"))
legend("topright", levels(iris$Species), col =
1:length(levels(iris$Species)), pch = 1)
```

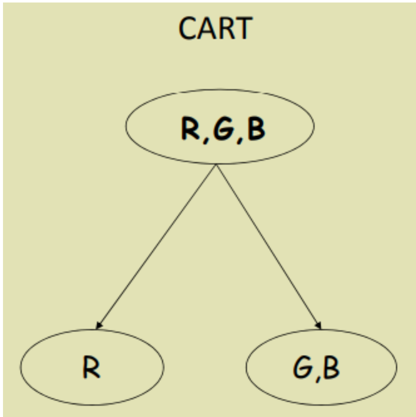


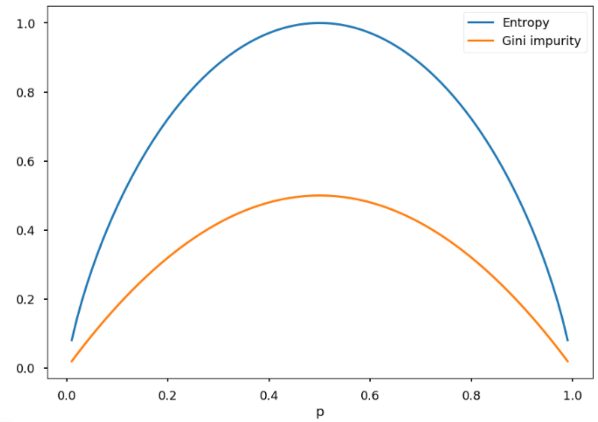
CART (Classification And Regression Trees)

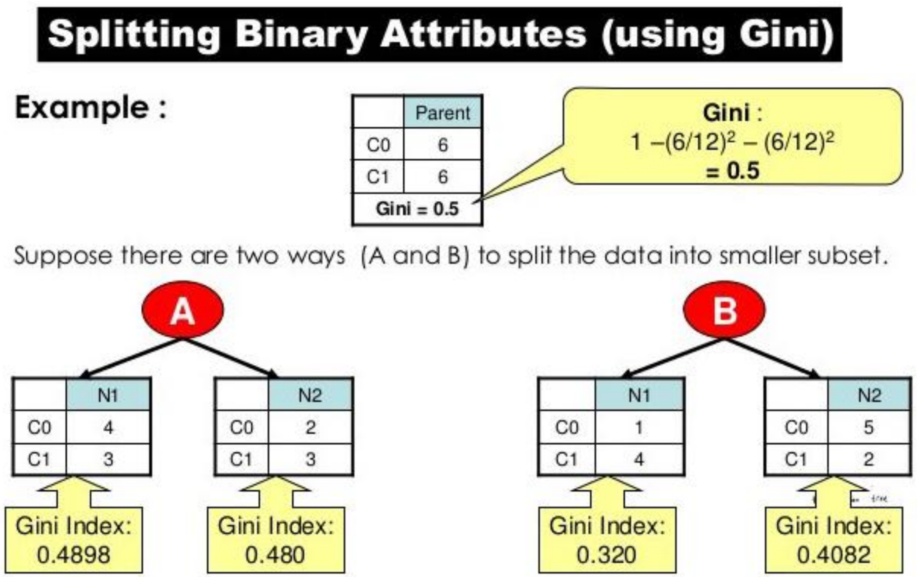
Splitting of **binary** attributes, based on the **Gini index** (another measure of the purity of the node). Lower Gini values are preferred (perfect index = 0).

$$GINI = 1 - \sum_{i=1}^{n} {p_i}^2$$

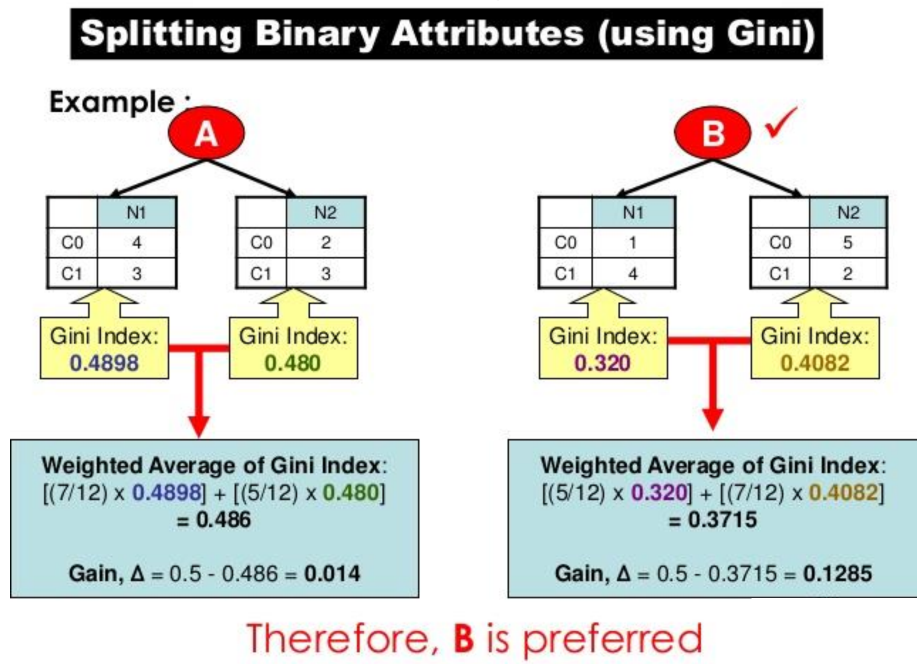








$$GINI_{N1} = 1 - \left(\frac{4}{7}\right)^2 - \left(\frac{3}{7}\right)^2 = 0.4898$$



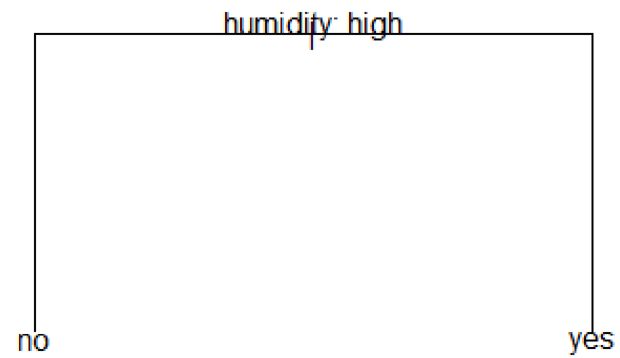
Tree construction in R

There are many packages in R to build classification tress: *tree*, *rpart*, *rpart2*, *C5.0*, etc.

Use of *tree* and *rpart* (CART; based on the Gini index):

<u>*Example for playTennis (categorical attributes)*</u>

```
## tree package
library(tree)
# default parameters
t = tree(formula = play ~ ., data = tennis)
plot(t)
text(t, pretty = F)
```



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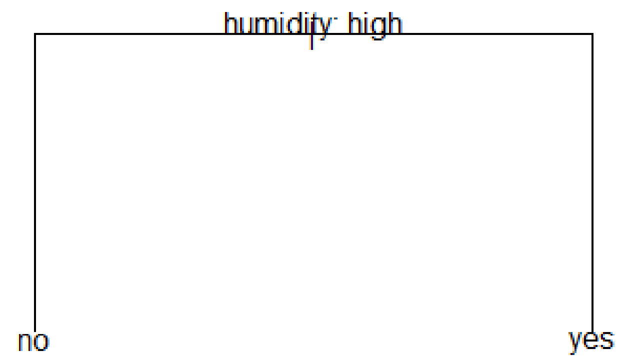
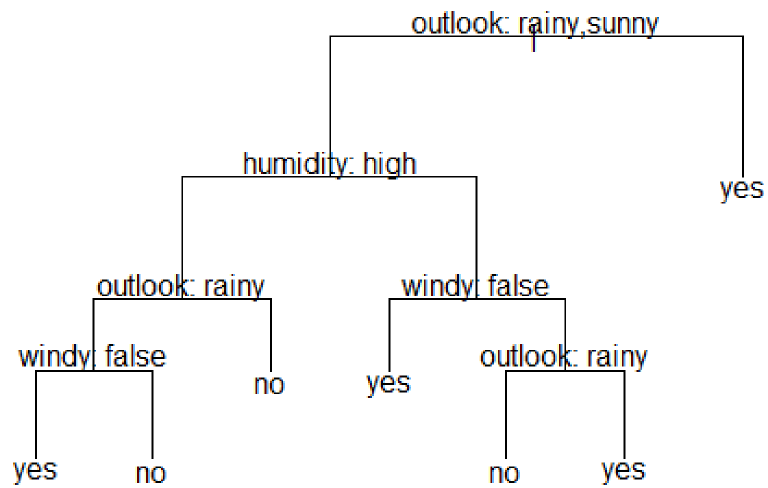



```
# user-defined parameters
t = tree(formula = play ~ ., data = tennis,
minsize = 1)
plot(t)
text(t, pretty = F)
```



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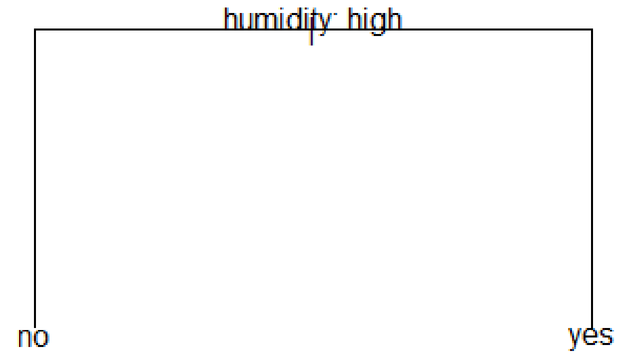
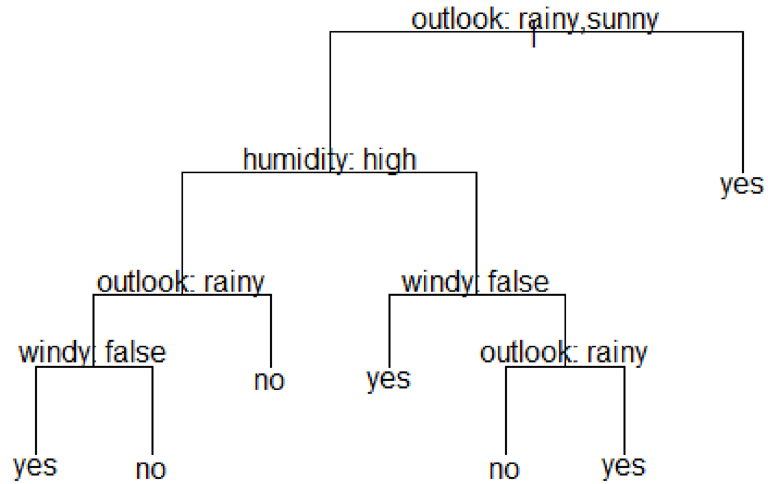


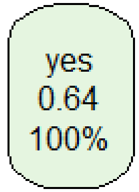
Documentation must be carefully read!!

```
# user-defined parameters
t = tree(formula = play ~ ., data = tennis,
minsize = 1)
plot(t)
text(t, pretty = F)
```

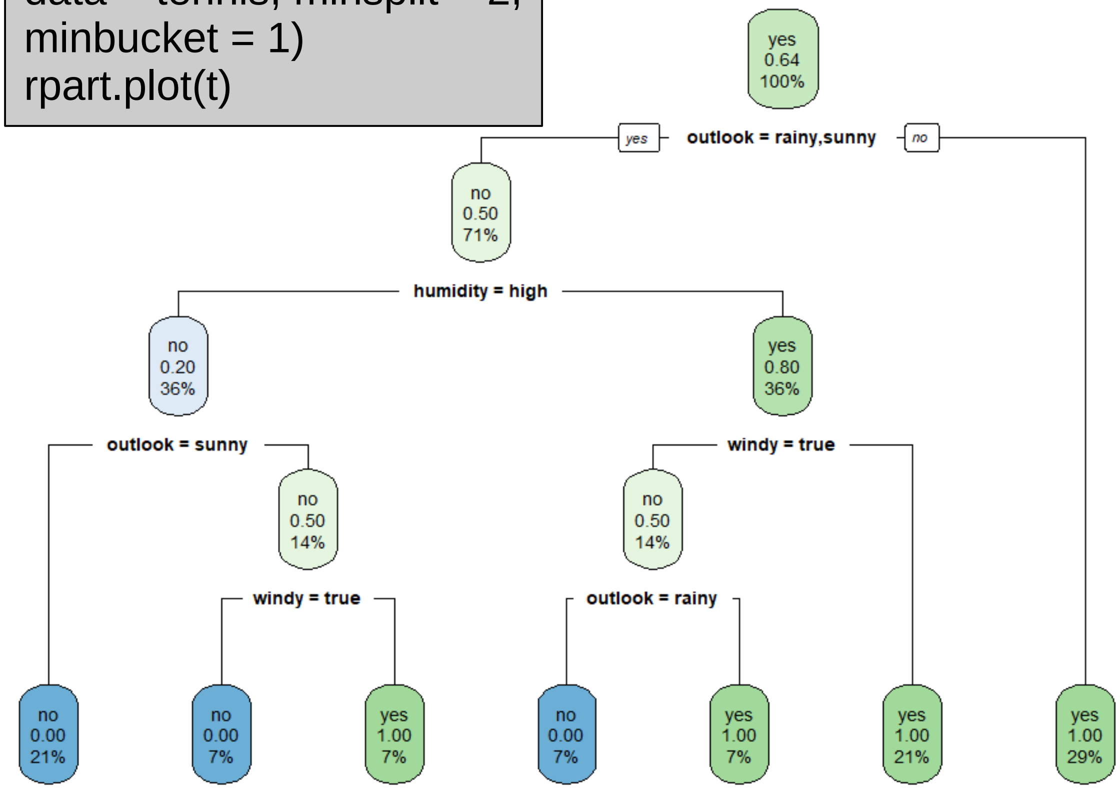


```
## rpart/rpart.plot packages
library(rpart)
# default parameters
t = rpart(formula = play ~ .,
data = tennis)
library(rpart.plot)
```

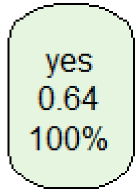
```
## rpart/rpart.plot packages
library(rpart)
# default parameters
t = rpart(formula = play ~ .,
data = tennis)
library(rpart.plot)
rpart.plot(t)
```



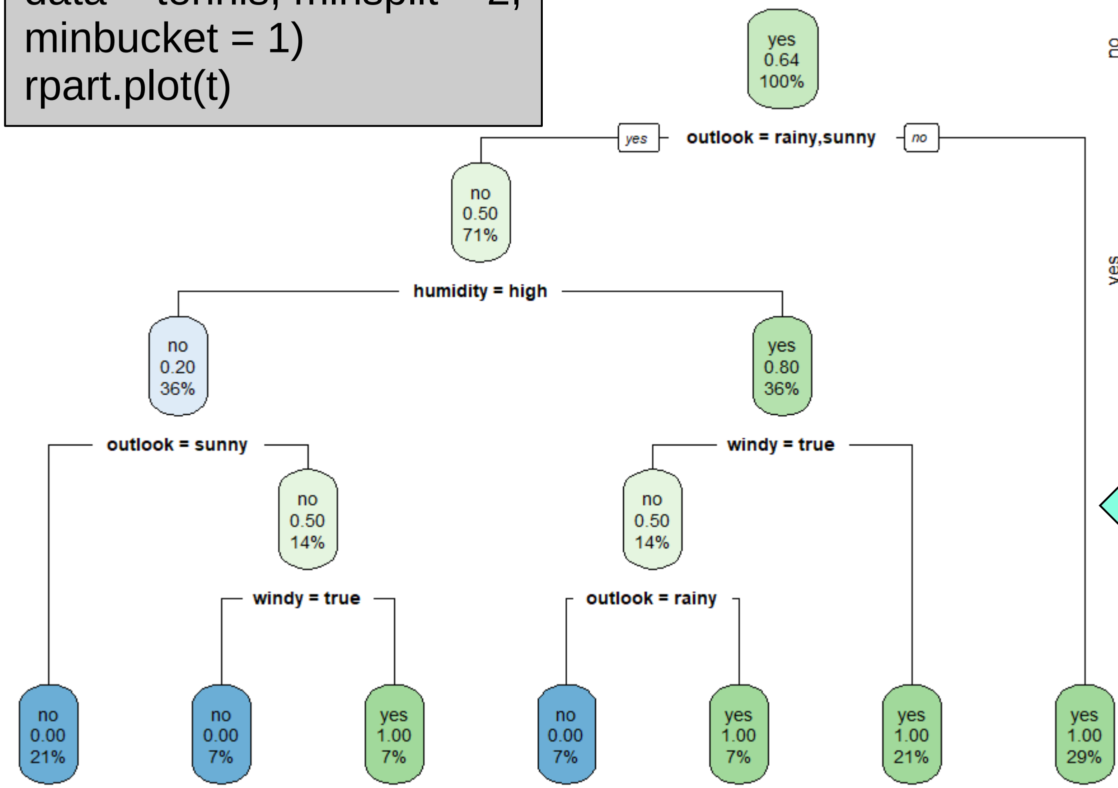

```
# user-defined parameters
t = rpart(formula = play ~ .,
data = tennis, minsplit = 2,
minbucket = 1)
rpart.plot(t)
```

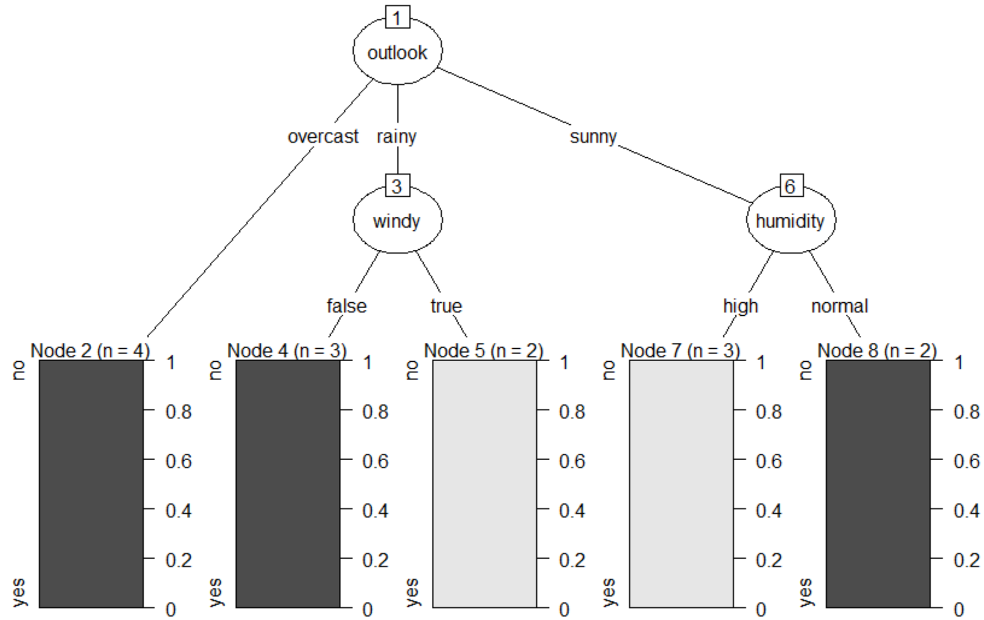


```
## rpart/rpart.plot packages
library(rpart)
# default parameters
t = rpart(formula = play ~ .,
data = tennis)
library(rpart.plot)
rpart.plot(t)
```



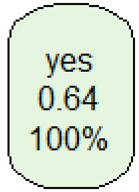

```
# user-defined parameters
t = rpart(formula = play ~ .,
data = tennis, minsplit = 2,
minbucket = 1)
rpart.plot(t)
```



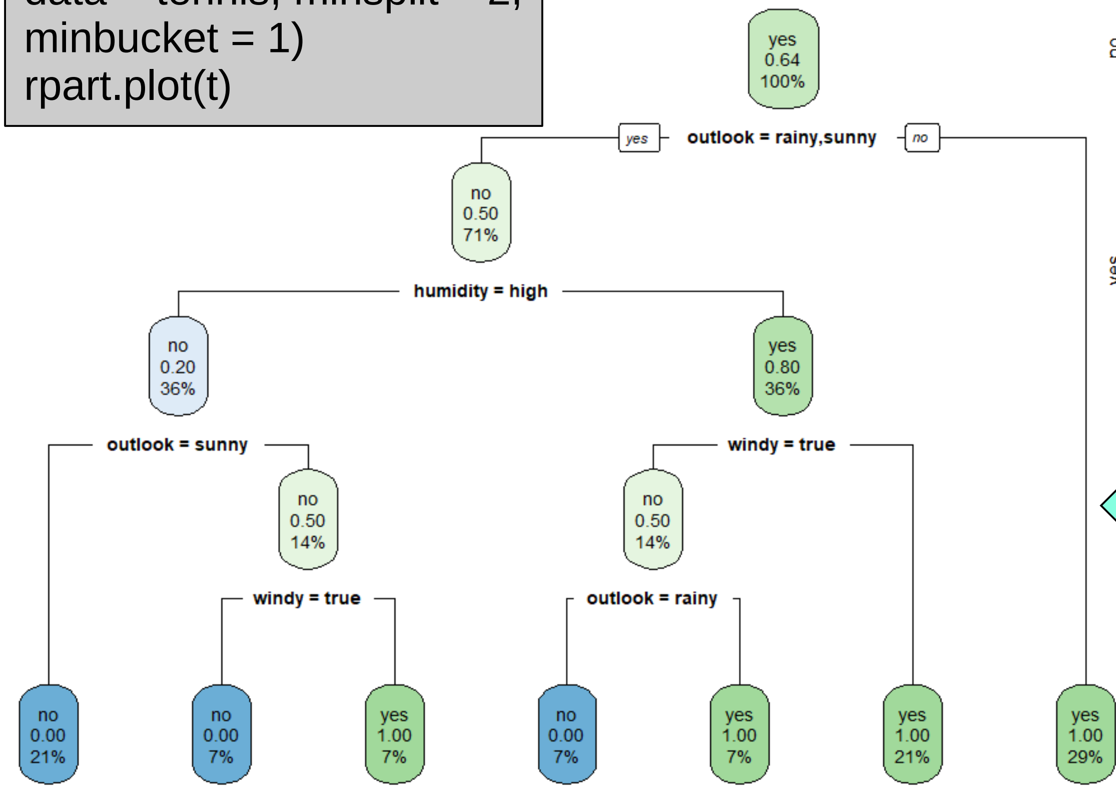


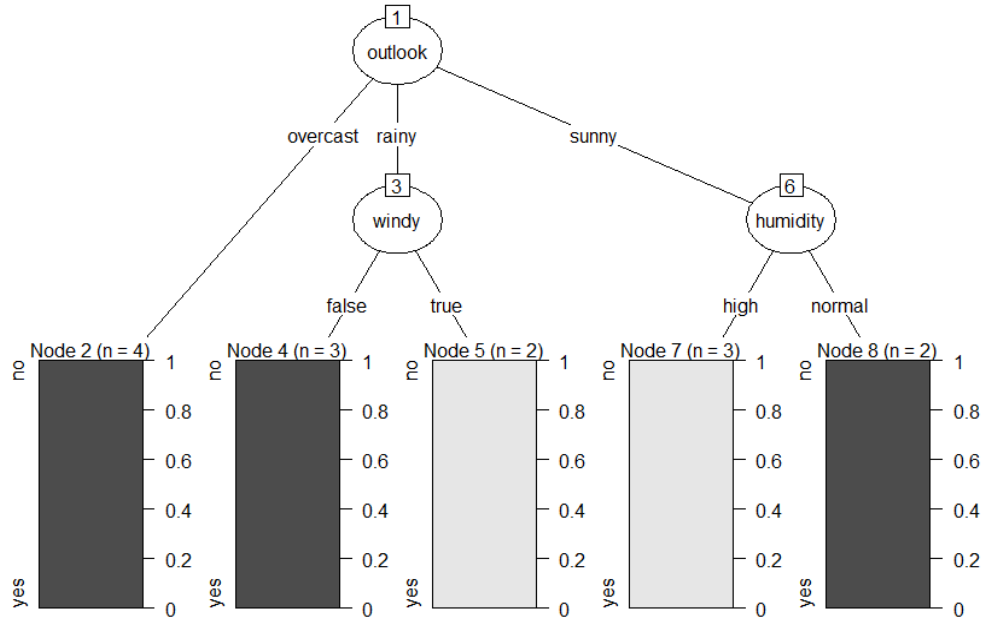
Compare with the result obtained with the *C50* package: **which are the differences?**

```
## rpart/rpart.plot packages
library(rpart)
# default parameters
t = rpart(formula = play ~ .,
data = tennis)
library(rpart.plot)
rpart.plot(t)
```




```
# user-defined parameters
t = rpart(formula = play ~ .,
data = tennis, minsplit = 2,
minbucket = 1)
rpart.plot(t)
```



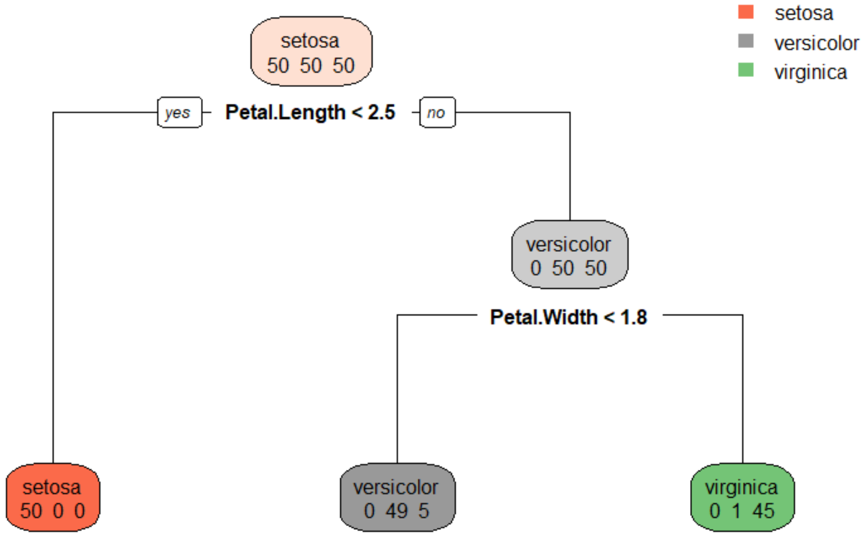


Compare with the result obtained with the *C50* package: **which are the differences?**

Documentation must be carefully read!!

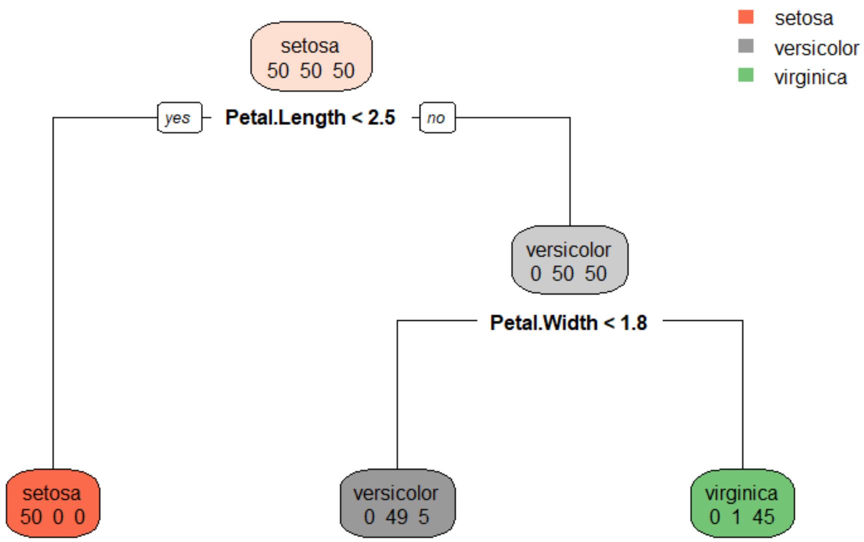
Example for iris (continuous attributes)

```
# default parameters
t = rpart(formula = Species ~ ., data = iris)
rpart.plot(t, extra = 1)
```

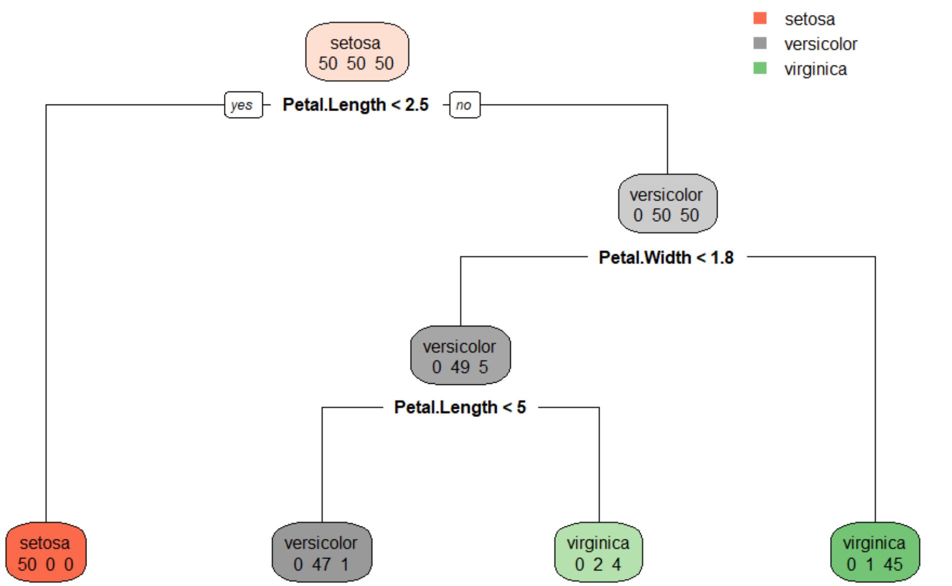


Example for iris (continuous attributes)

```
# default parameters
t = rpart(formula = Species ~ ., data = iris)
rpart.plot(t, extra = 1)
```

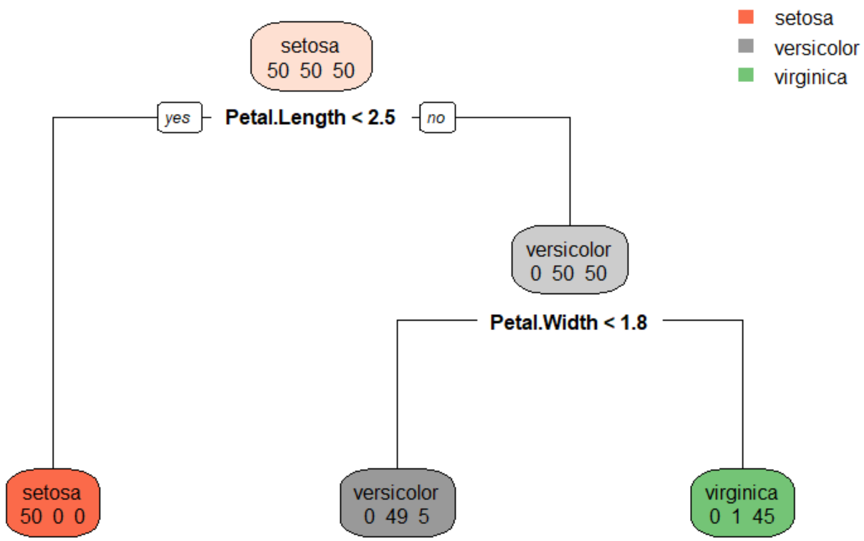



```
# user-defined parameters
t = rpart(formula = Species ~ ., data = iris,
minsplit = 2, minbucket = 1)
rpart.plot(t, extra = 1)
```

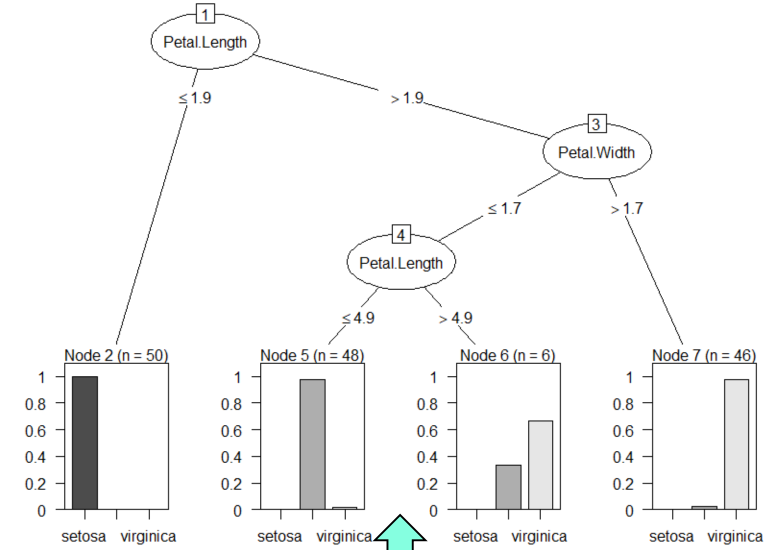


Example for iris (continuous attributes)

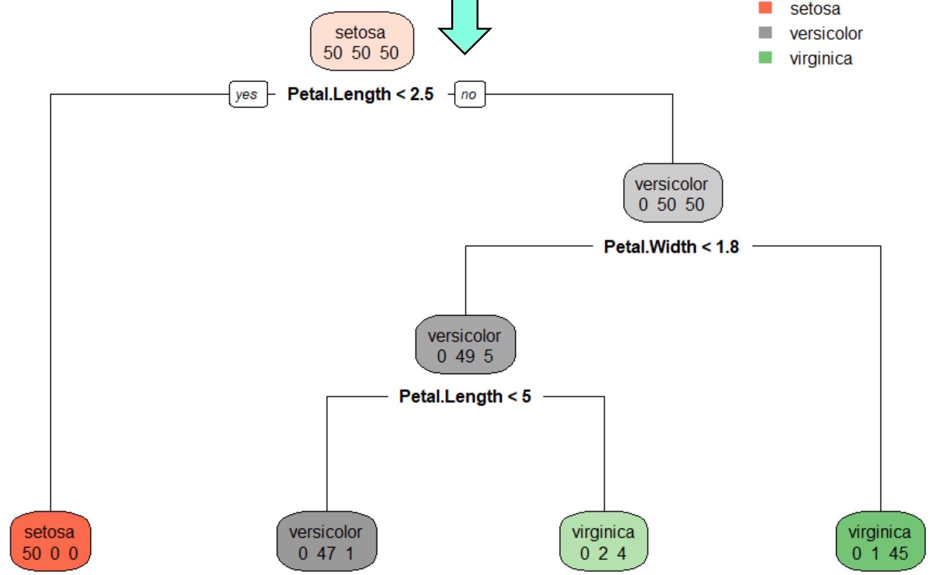
```
# default parameters
t = rpart(formula = Species ~ ., data = iris)
rpart.plot(t, extra = 1)
```




```
# user-defined parameters
t = rpart(formula = Species ~ ., data = iris,
minsplit = 2, minbucket = 1)
rpart.plot(t, extra = 1)
```

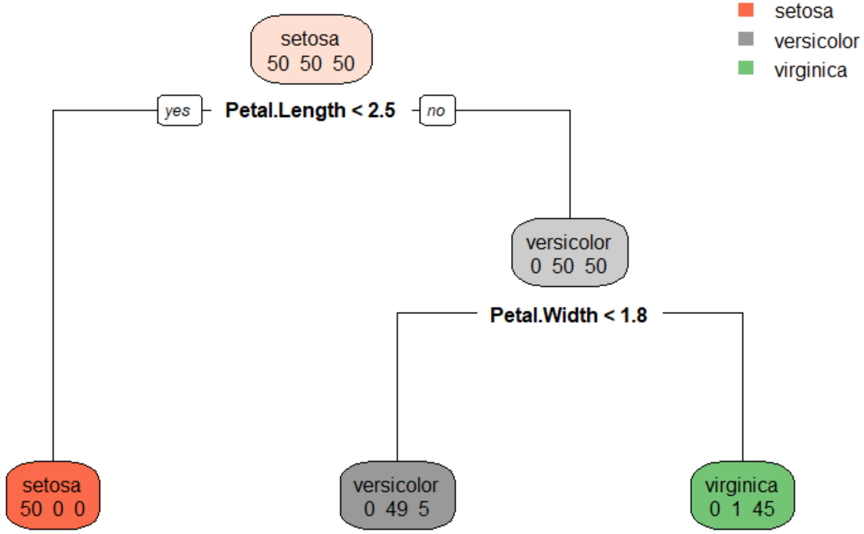


Compare with the result obtained with the *C50* package: **which are the differences?**



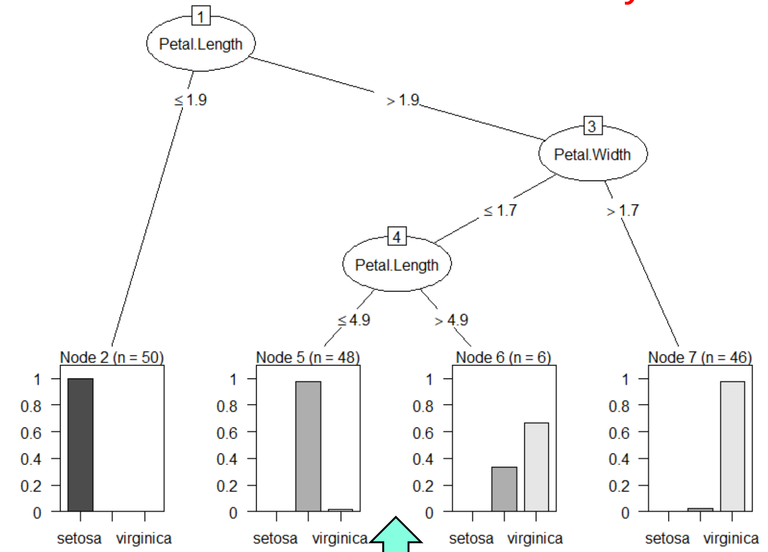
Example for iris (continuous attributes)

```
# default parameters
t = rpart(formula = Species ~ ., data = iris)
rpart.plot(t, extra = 1)
```

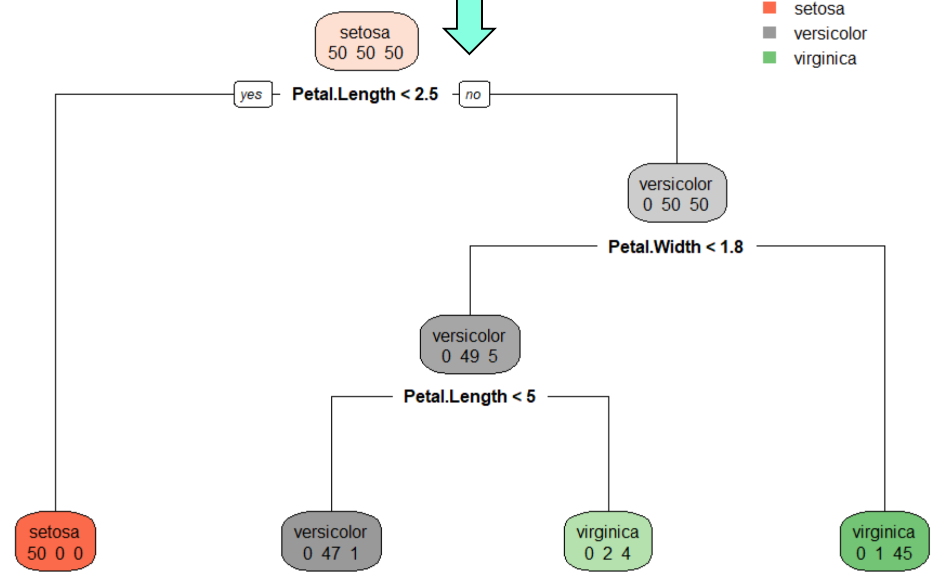



```
# user-defined parameters
t = rpart(formula = Species ~ ., data = iris,
minsplit = 2, minbucket = 1)
rpart.plot(t, extra = 1)
```

Documentation must be carefully read!!

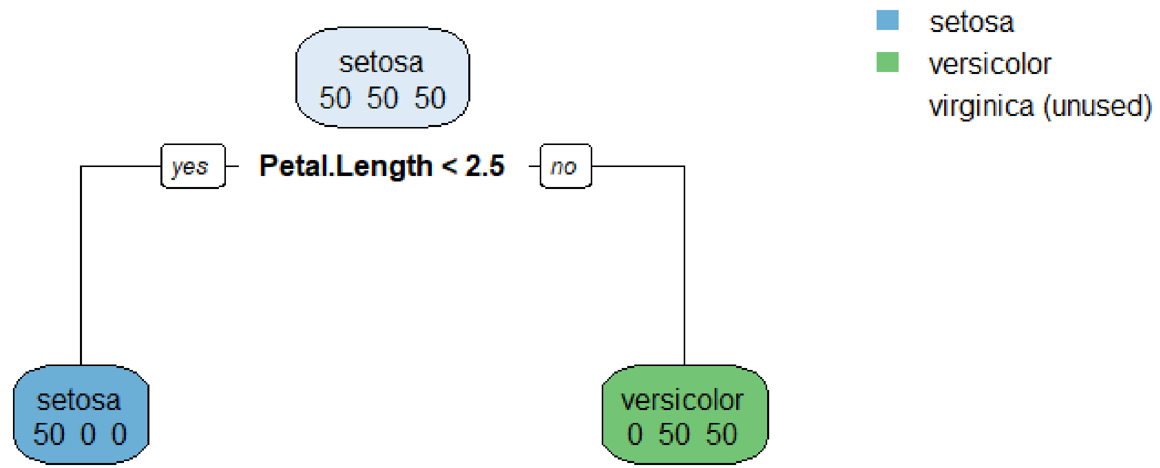


Compare with the result obtained with the *C50* package: **which are the differences?**

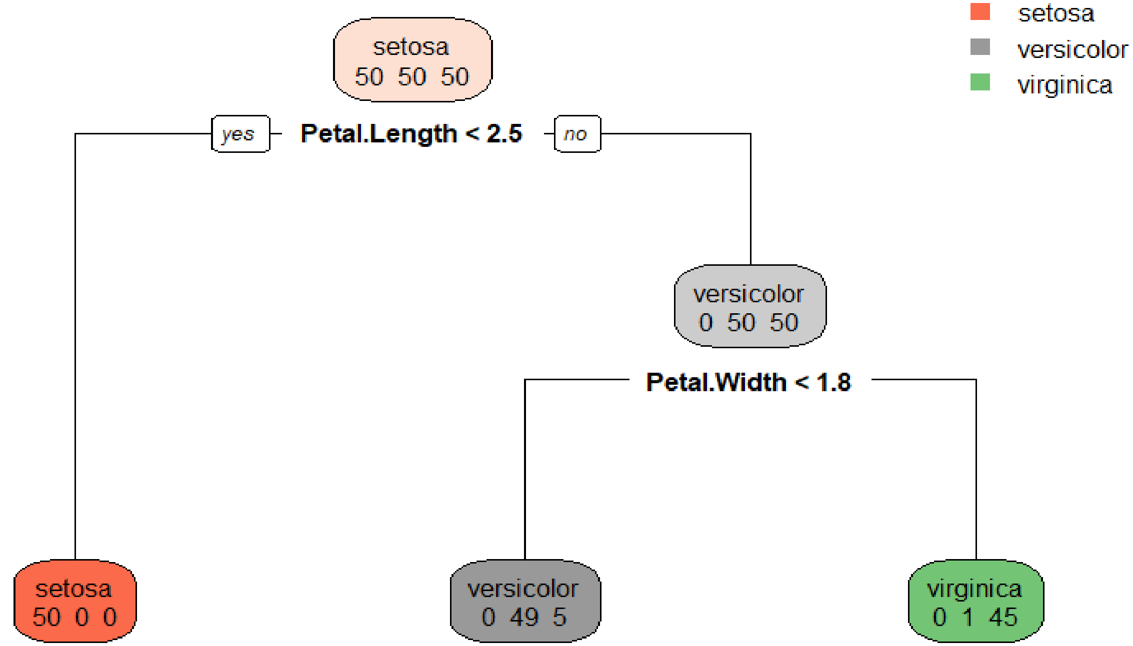


```
summary(t)
Call:
rpart(formula = Species ~ ., data = iris, minsplit = 2, minbucket = 1)
  n= 150

    CP nsplit rel error xerror       xstd
1 0.50      0      1.00   1.22 0.04772141
2 0.44      1      0.50   0.70 0.06110101
3 0.02      2      0.06   0.11 0.03192700
4 0.01      3      0.04   0.10 0.03055050

Variable importance
 Petal.Width Petal.Length Sepal.Length  Sepal.Width
          34           32           20           14

Node number 1: 150 observations,    complexity param=0.5
  predicted class=setosa      expected loss=0.6666667  P(node) =1
    class counts:    50    50    50
   probabilities: 0.333 0.333 0.333
  left son=2 (50 obs) right son=3 (100 obs)
  Primary splits:
      Petal.Length < 2.45 to the left,  improve=50.00000, (0 missing)
      Petal.Width  < 0.8  to the left,  improve=50.00000, (0 missing)
      Sepal.Length < 5.45 to the left,  improve=34.16405, (0 missing)
      Sepal.Width  < 3.35 to the right, improve=19.03851, (0 missing)
  Surrogate splits:
      Petal.Width  < 0.8  to the left,  agree=1.000, adj=1.00, (0 split)
      Sepal.Length < 5.45 to the left,  agree=0.920, adj=0.76, (0 split)
      Sepal.Width  < 3.35 to the right, agree=0.833, adj=0.50, (0 split)

Node number 2: 50 observations
  predicted class=setosa      expected loss=0  P(node) =0.3333333
    class counts:    50     0     0
   probabilities: 1.000 0.000 0.000

Node number 3: 100 observations,    complexity param=0.44
  predicted class=versicolor  expected loss=0.5  P(node) =0.6666667
    class counts:     0    50    50
   probabilities: 0.000 0.500 0.500
  left son=6 (54 obs) right son=7 (46 obs)
  Primary splits:
      Petal.Width  < 1.75 to the left,  improve=38.969400, (0 missing)
      Petal.Length < 4.75 to the left,  improve=37.353540, (0 missing)
      Sepal.Length < 6.15 to the left,  improve=10.686870, (0 missing)
      Sepal.Width  < 2.45 to the left,  improve= 3.555556, (0 missing)
  Surrogate splits:
      Petal.Length < 4.75 to the left,  agree=0.91, adj=0.804, (0 split)
      Sepal.Length < 6.15 to the left,  agree=0.73, adj=0.413, (0 split)
      Sepal.Width  < 2.95 to the left,  agree=0.67, adj=0.283, (0 split)

Node number 6: 54 observations,    complexity param=0.02
  predicted class=versicolor  expected loss=0.09259259  P(node) =0.36
    class counts:     0    49     5
   probabilities: 0.000 0.907 0.093
  left son=12 (48 obs) right son=13 (6 obs)
  Primary splits:
      Petal.Length < 4.95 to the left,  improve=4.4490740, (0 missing)
      Sepal.Length < 7.1  to the left,  improve=1.6778480, (0 missing)
      Petal.Width  < 1.35 to the left,  improve=0.9971510, (0 missing)
      Sepal.Width  < 2.65 to the right, improve=0.2500139, (0 missing)

Node number 7: 46 observations
  predicted class=virginica   expected loss=0.02173913  P(node) =0.3066667
    class counts:     0     1    45
   probabilities: 0.000 0.022 0.978

Node number 12: 48 observations
  predicted class=versicolor  expected loss=0.02083333  P(node) =0.32
    class counts:     0    47     1
   probabilities: 0.000 0.979 0.021

Node number 13: 6 observations
  predicted class=virginica   expected loss=0.3333333  P(node) =0.04
    class counts:     0     2     4
   probabilities: 0.000 0.333 0.667
```

```
# user-defined parameters: "maxpdepth"
t = rpart(formula = Species ~ ., data = iris,
maxdepth = 1)
rpart.plot(t, extra = 1)
```

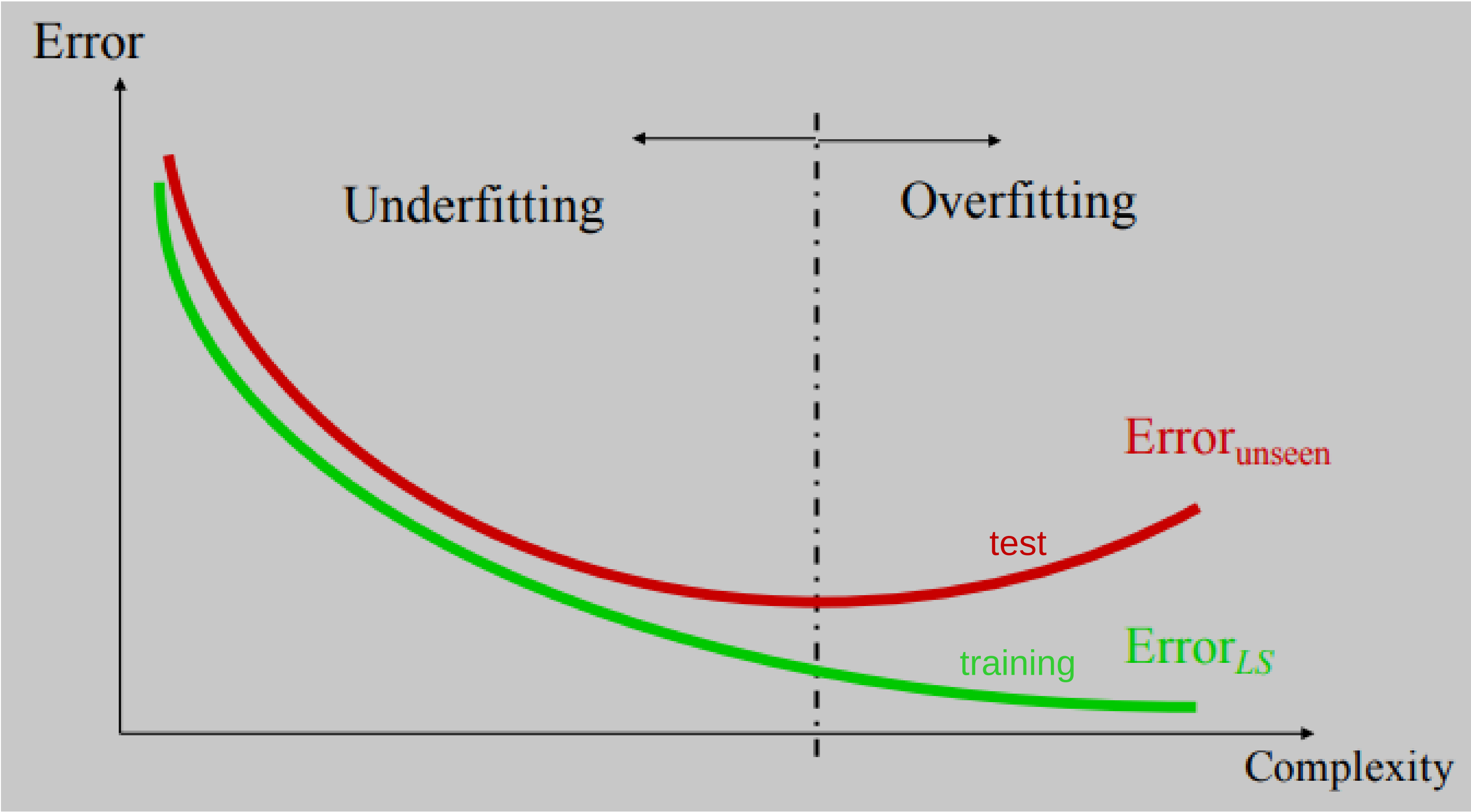



```
# user-defined parameters: "maxpdepth"
t = rpart(formula = Species ~ ., data = iris,
maxdepth = 2)
rpart.plot(t, extra = 1)
```



Overfitting

A large tree (i.e. with many terminal nodes) may tend to overfit the training data, leading to poor performance in the test set. Generally, we can improve this behavior by **pruning** the tree, i.e., cutting off some of the terminal nodes.

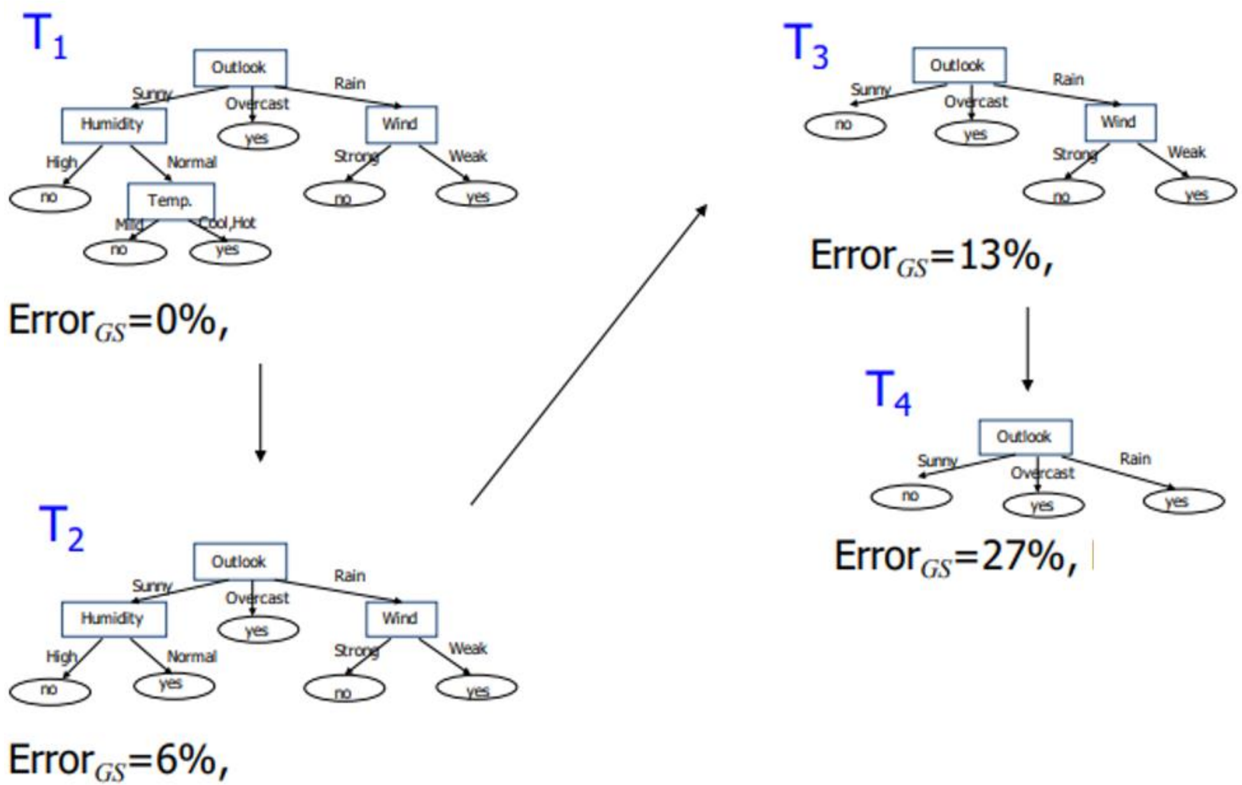


How can we avoid overfitting?

Pre-pruning: stop growing the tree before it reaches the point at which it perfectly classifies the learning sample. *Procedure:*
Stop splitting a node if:

- The number of objects is too small
- The impurity is low enough

This approach leads to small trees but can remove relevant splits



Post-pruning: allow the tree to overfit and then, one finalized, remove the less useful nodes. In general, this is preferred option. *Procedure:*
Compute a sequence of trees {T1, T2, …} where T1 is the complete tree. T2 is obtained by removing from T1 the node that less increases the error. Sometimes, this process is guided based on some **cost-complexity** criterion (e.g. in medicine)

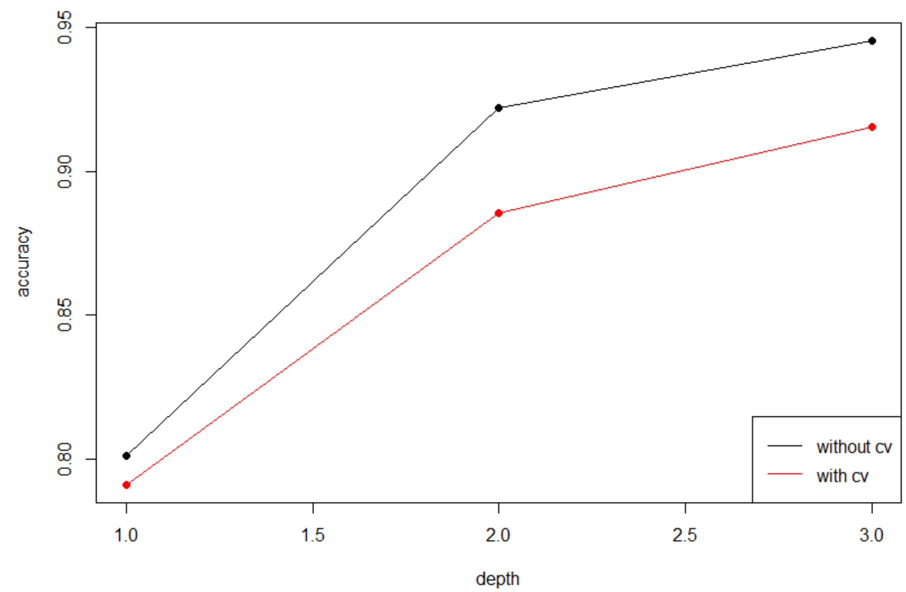
The question is: **where to stop?** In practice, it is usual to split the learning dataset into two subsets: a **training sample** for growing the tree and a **test sample** for evaluating its generalization error (e.g. hold-out **cross-validation**).

Post-pruning in R

Example for cars (dataset included in the caret package)

```
## exploring the dataset
library(caret)
data("cars")
summary(cars)
## convert continuous variable "Price" to categorical
cars$Price = as.factor(ifelse(cars$Price >= 22000, "E", "C"))

## 50% of dataset for training and the other 50% for test
n = dim(cars)[1]
set.seed(2)
indtrain = sample(1:n, round(0.5*n))
indtest = setdiff(1:n, indtrain)
dataset.train = cars[indtrain, ]
dataset.test = cars[indtest, ]

## performance without cross-validation, for increasingly complex
configurations of the tree
acc.nocv = c()
for (md in 1:3) {  # maximum depth allowed for the tree
# learning the tree
t = rpart(formula = Price ~ ., data = dataset.train, maxdepth = md)
# applying learnt tree to predict
pred = predict(t, dataset.train, type = "class")
# performance evaluation
acc.nocv[md] = sum(diag(table(pred, dataset.train$Price))) /
length(indtrain)
}
```

```
## performance with cross-validation, for increasingly complex
configurations of the tree
acc.cv = c()
for (md in 1:3) {  # maximum depth allowed for the tree
# learning the tree
t = rpart(formula = Price ~ ., data = dataset.train, maxdepth = md)
# applying learnt tree to predict
pred = predict(t, dataset.test, type = "class")
# performance evaluation
acc.cv[md] = sum(diag(table(pred, dataset.test$Price))) / length(indtest)
}

## plotting results
matplot(cbind(acc.nocv, acc.cv), type = "o", pch = 19, lty = 1, col =
c("black", "red"),
        xlab = "depth", ylab = "accuracy")
legend("bottomright", c("without cv", "with cv"), lty = 1, col = c("black",
"red"))
grid()
```



Example for cars (using caret)

Caret tremendously simplifies the model fitting process, allowing for automatized cross-validation

```
## 50% of the dataset for cross-validation and
## 50% for test
indtrain = createDataPartition(y = cars$Price, p = 0.5,
list = FALSE)
dataset.train = cars[indtrain,]
dataset.test = cars[-indtrain,]
# 10 folds
trctrl = trainControl(method = "cv", number = 10)
## caret automatically tries different values of the
## method parameter (5 in this case, internally selected)
t = train(Price ~ ., data = dataset.train,
          method = "rpart2",
          trControl = trctrl,
          tuneLength = 5)
plot(t)

## prediction
pred = predict(t, newdata = dataset.test)
## evaluation
sum(diag(table(pred, dataset.test$Price))) /
dim(dataset.test)[1]
```

To check the parameters handled by caret:
http://topepo.github.io/caret/index.html