Aalto University
School of Electrical Engineering

# CS-C3240 – Machine Learning D

## Non-Parametric methods

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# Learning goals

Understand the concepts of

- Decision trees
- Information score
- Estimation of error rates
- Pruning

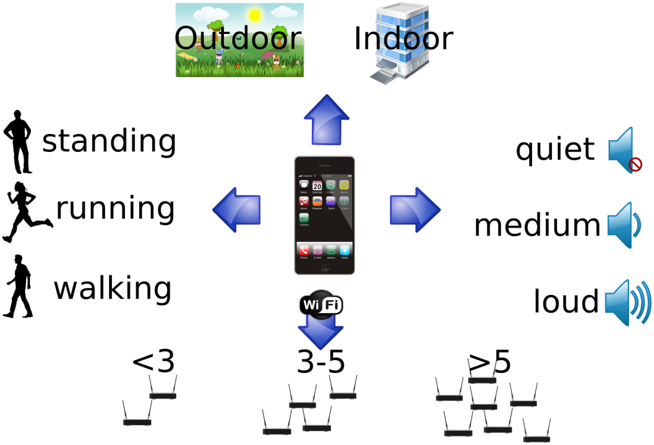
# Outline

Decision Trees

Optimizing the tree structure

Improving classification results

# Smartphone sensing:
# At work or not ?



# Decision trees

Assume that some training data was recorded and labelled for the two classes we consider in this example

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 1 | *<3* | *walking* | *quiet* | *outdoor* | Work |
| 2 | *<3* | *walking* | *quiet* | *outdoor* | Work |
| 3 | *3-5* | *walking* | *quiet* | *outdoor* | Work |
| 4 | *3-5* | *sitting* | *quiet* | *outdoor* | Work |
| 5 | *<3* | *sitting* | *quiet* | *indoor* | Work |
| 6 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 7 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 8 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 9 | *>5* | *walking* | *loud* | *indoor* | Work |
| 10 | *>5* | *standing* | *medium* | *indoor* | Work |
| 11 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 12 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 13 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 14 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 15 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 16 | *>5* | *sitting* | *loud* | *indoor* | Work |
| 17 | *<3* | *walking* | *quiet* | *indoor* | Not at work |
| 18 | *<3* | *walking* | *quiet* | *indoor* | Not at work |
| 19 | *<3* | *standing* | *quiet* | *indoor* | Not at work |
| 20 | *<3* | *walking* | *medium* | *indoor* | Not at work |
| 21 | *<3* | *walking* | *loud* | *outdoor* | Not at work |
| 22 | *<3* | *walking* | *medium* | *indoor* | Not at work |
| 23 | *<3* | *walking* | *medium* | *indoor* | Not at work |
| 24 | *3-5* | *walking* | *quiet* | *outdoor* | Not at work |
| 25 | *3-5* | *standing* | *quiet* | *outdoor* | Not at work |
| 26 | *3-5* | *standing* | *quiet* | *outdoor* | Not at work |
| 27 | *3-5* | *standing* | *loud* | *outdoor* | Not at work |
| 28 | *3-5* | *walking* | *loud* | *outdoor* | Not at work |
| 29 | *>5* | *sitting* | *loud* | *outdoor* | Not at work |
| 30 | *>5* | *sitting* | *loud* | *outdoor* | Not at work |

# Decision trees

A decision tree divides the examples from a dataset according to the features and classes observed for them

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 1 | *<3* | *walking* | *quiet* | *outdoor* | Work |
| 2 | *<3* | *walking* | *quiet* | *outdoor* | Work |
| 3 | *3-5* | *walking* | *quiet* | *outdoor* | Work |
| 4 | *3-5* | *sitting* | *quiet* | *outdoor* | Work |
| 5 | *<3* | *sitting* | *quiet* | *indoor* | Work |
| 6 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 7 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 8 | *3-5* | *sitting* | *quiet* | *indoor* | Work |
| 9 | *>5* | *walking* | *loud* | *indoor* | Work |
| 10 | *>5* | *standing* | *medium* | *indoor* | Work |
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| 12 | *>5* | *sitting* | *medium* | *indoor* | Work |
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| 14 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 15 | *>5* | *sitting* | *medium* | *indoor* | Work |
| 16 | *>5* | *sitting* | *loud* | *indoor* | Work |
| 17 | *<3* | *walking* | *quiet* | *indoor* | Not at work |
| 18 | *<3* | *walking* | *quiet* | *indoor* | Not at work |
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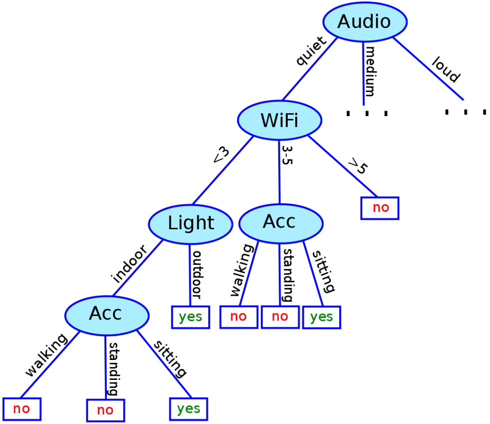
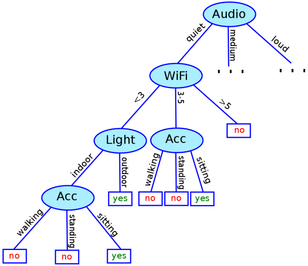


# Decision tree

How to generate such decision tree?

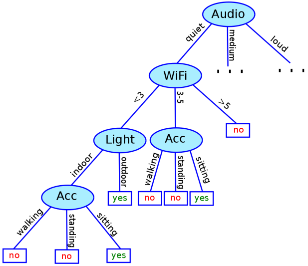


# Decision tree

## How to generate such decision tree?

First select a feature to split on and place it at the root node.

Then repeat this procedure for all child nodes



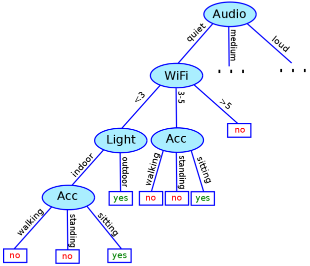
# Decision tree

## How to generate such decision tree?

**First** select a feature to split on and place it at the root node.

**Then** repeat this procedure for all child nodes

**How to determine the feature to split on?**



# Decision tree

| WiFi | yes | no | Accelerometer | yes | no | Audio | yes | no | Light | yes | no | At work yes | At work no |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $<3$ APs | 3 | 7 | walking | 4 | 8 | quiet | 8 | 5 | outdoor | 4 | 7 | 16 | 14 |
| [3, 5] | 5 | 5 | standing | 1 | 4 | medium | 6 | 3 | indoor | 12 | 7 | | |
| $>5$ APs | 8 | 2 | sitting | 11 | 2 | loud | 2 | 6 | | | | | |

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
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| 19 | <3 | *standing* | *quiet* | *indoor* | Not at work |
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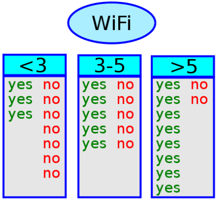
| 27 | 3-5 | *standing* | *loud* | *outdoor* | Not at work |
| 28 | 3-5 | *walking* | *loud* | *outdoor* | Not at work |
| 29 | >5 | *sitting* | *loud* | *outdoor* | Not at work |
| 30 | >5 | *sitting* | *loud* | *outdoor* | Not at work |

# Decision tree

| WiFi | | | Accelerometer | | | Audio | | | Light | | | At work | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | yes | no | | yes | no | | yes | no | | yes | no | yes | no |
| $<$3 APs | 3 | 7 | walking | 4 | 8 | quiet | 8 | 5 | outdoor | 4 | 7 | 16 | 14 |
| [3, 5] | 5 | 5 | standing | 1 | 4 | medium | 6 | 3 | indoor | 12 | 7 | | |
| $>$5 APs | 8 | 2 | sitting | 11 | 2 | loud | 2 | 6 | | | | | |



# Decision tree

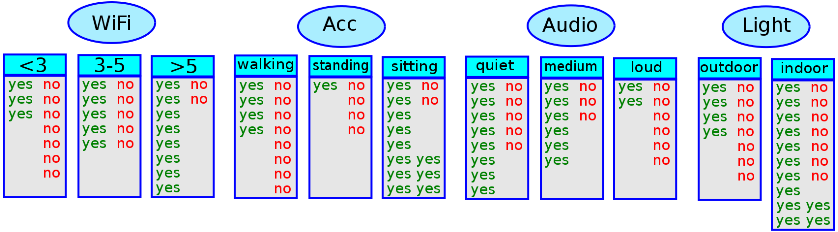
| WiFi | yes | no |
|---|---|---|
| <3 APs | 3 | 7 |
| [3, 5] | 5 | 5 |
| >5 APs | 8 | 2 |

| Accelerometer | yes | no |
|---|---|---|
| walking | 4 | 8 |
| standing | 1 | 4 |
| sitting | 11 | 2 |

| Audio | yes | no |
|---|---|---|
| quiet | 8 | 5 |
| medium | 6 | 3 |
| loud | 2 | 6 |

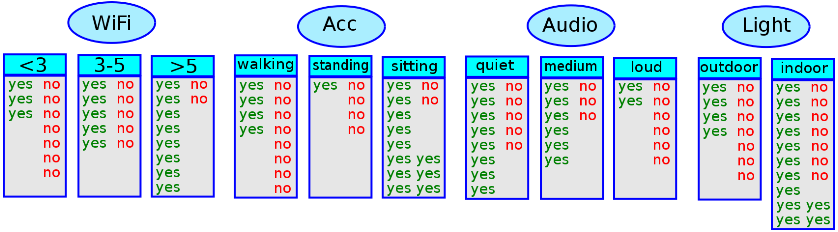
| Light | yes | no |
|---|---|---|
| outdoor | 4 | 7 |
| indoor | 12 | 7 |

| At work | |
|---|---|
| yes | no |
| 16 | 14 |



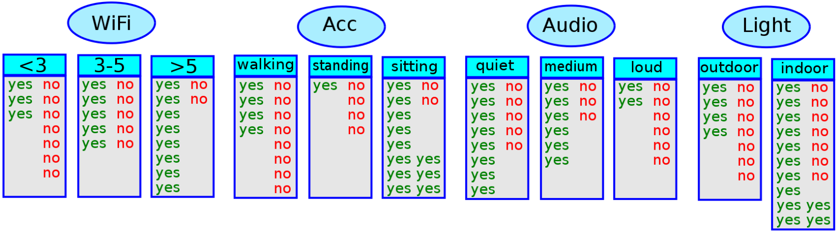

Which feature is the best choice to place at the root?

# Decision tree




We are interested in the gain in information when a particular choice is taken

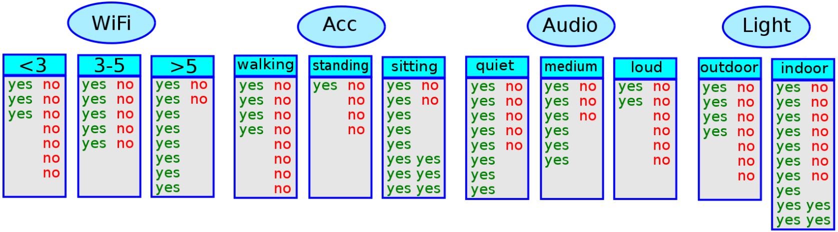
# Decision tree




We are interested in the gain in information when a particular choice is taken

The decision tree should decide for the split that promises maximum information gain.

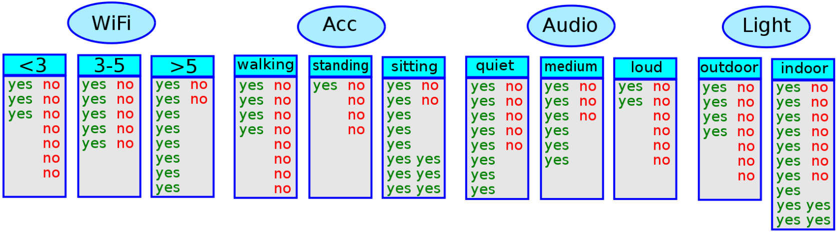
# Decision tree




Information gain can be estimated by the entropy of a value:

$$\mathcal{E}(p_1, p_2, \ldots, p_n) = -p_1 \log_2 p_1 - p_2 \log_2 p_2 \cdots - p_n \log_2 p_n$$

# Decision tree

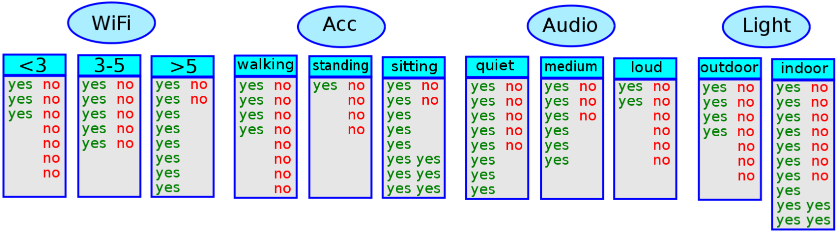



$$\mathcal{E}(p_1, p_2, \ldots, p_n) = \quad -p_1 \log_2 p_1 - p_2 \log_2 p_2 \cdots - p_n \log_2 p_n$$

## WiFi information value:

$$\mathcal{E}\left(\frac{3}{10}, \frac{7}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{5}{10}, \frac{5}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{8}{10}, \frac{2}{10}\right)\frac{10}{30} =$$

# Decision tree




$$\mathcal{E}(p_1, p_2, \ldots, p_n) = \quad -p_1 \log_2 p_1 - p_2 \log_2 p_2 \cdots - p_n \log_2 p_n$$

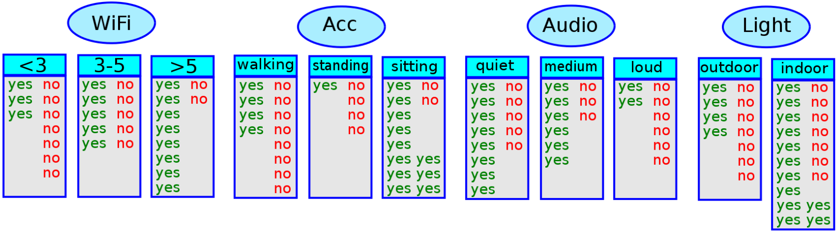
## WiFi information value:

$$\mathcal{E}\left(\frac{3}{10}, \frac{7}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{5}{10}, \frac{5}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{8}{10}, \frac{2}{10}\right)\frac{10}{30} = \quad \left(-\tfrac{3}{10}\log_2\tfrac{3}{10} - \tfrac{7}{10}\log_2\tfrac{7}{10}\right)\cdot\tfrac{10}{30}$$

$$+\left(-\tfrac{5}{10}\log_2\tfrac{5}{10} - \tfrac{5}{10}\log_2\tfrac{5}{10}\right)\cdot\tfrac{10}{30}$$

$$+\left(-\tfrac{8}{10}\log_2\tfrac{8}{10} - \tfrac{2}{10}\log_2\tfrac{2}{10}\right)\cdot\tfrac{10}{30}$$

# Decision tree

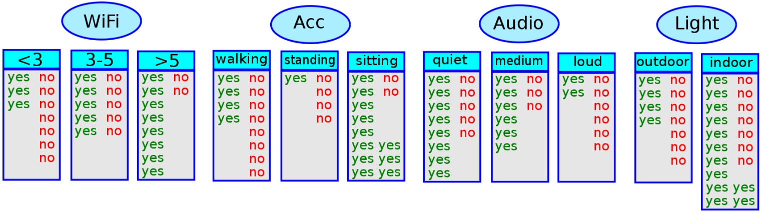



$$\mathcal{E}(p_1, p_2, \ldots, p_n) = \quad -p_1 \log_2 p_1 - p_2 \log_2 p_2 \cdots - p_n \log_2 p_n$$

## WiFi information value:

$$\begin{aligned}
\mathcal{E}\left(\frac{3}{10}, \frac{7}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{5}{10}, \frac{5}{10}\right)\frac{10}{30} + \mathcal{E}\left(\frac{8}{10}, \frac{2}{10}\right)\frac{10}{30} = \quad & \left(-\tfrac{3}{10}\log_2\tfrac{3}{10} - \tfrac{7}{10}\log_2\tfrac{7}{10}\right)\cdot\tfrac{10}{30} \\
& + \left(-\tfrac{5}{10}\log_2\tfrac{5}{10} - \tfrac{5}{10}\log_2\tfrac{5}{10}\right)\cdot\tfrac{10}{30} \\
& + \left(-\tfrac{8}{10}\log_2\tfrac{8}{10} - \tfrac{2}{10}\log_2\tfrac{2}{10}\right)\cdot\tfrac{10}{30} \\
\approx \quad & 0.868
\end{aligned}$$

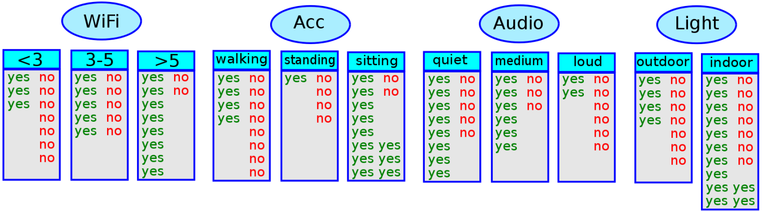
# Decision tree




Information value:

| | | |
|---|---|---|
| WiFi: | $\approx$ | 0.868 |
| Acc: | $\approx$ | ... |
| Audio: | $\approx$ | ... |
| Light: | $\approx$ | ... |

# Decision tree




Information value:

Information gain:

WiFi: $\approx$ 0.868

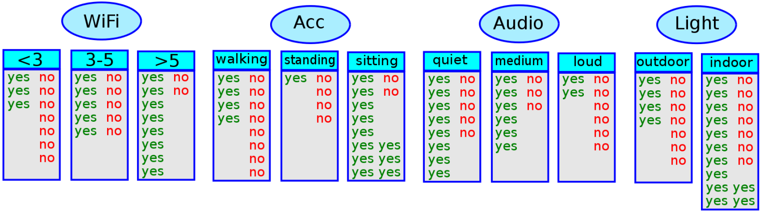
Acc: $\approx$ 0.756

Audio: $\approx$ 0.884

Light: $\approx$ 0.948

Initial information value (working [yes/no]): 0.997

# Decision tree




Information value:

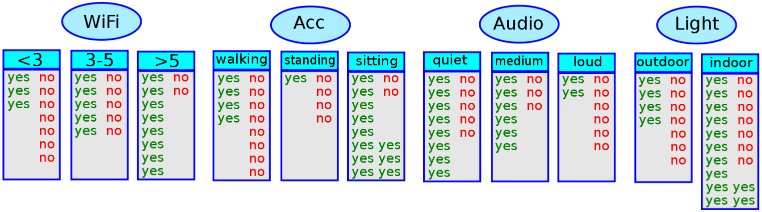
| | | |
|---|---|---|
| WiFi: | $\approx$ | 0.868 |
| Acc: | $\approx$ | 0.756 |
| Audio: | $\approx$ | 0.884 |
| Light: | $\approx$ | 0.948 |

Information gain:

| | | |
|---|---|---|
| WiFi: | $\approx$ | 0.129 |
| Acc: | $\approx$ | 0.241 |
| Audio: | $\approx$ | 0.113 |
| Light: | $\approx$ | 0.049 |

Initial information value (working [yes/no]): 0.997

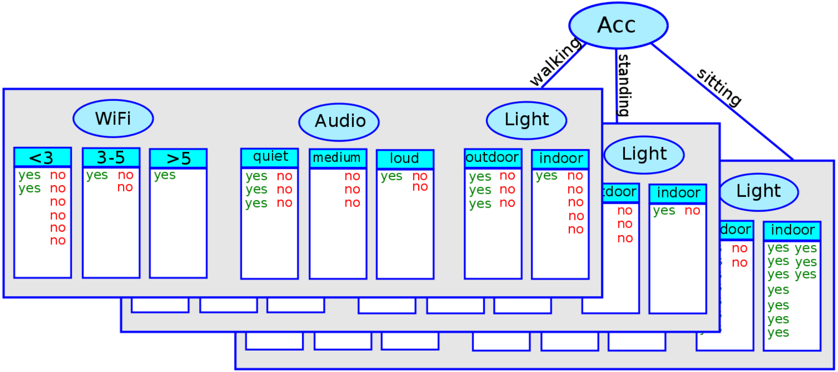
# Decision tree




| Information value: | | |
|---|---|---|
| WiFi: | $\approx$ | 0.868 |
| **Acc:** | $\approx$ | **0.756** |
| Audio: | $\approx$ | 0.884 |
| Light: | $\approx$ | 0.948 |

| Information gain: | | |
|---|---|---|
| WiFi: | $\approx$ | 0.129 |
| **Acc:** | $\approx$ | **0.241** |
| Audio: | $\approx$ | 0.113 |
| Light: | $\approx$ | 0.049 |

Initial information value (working [yes/no]): 0.997




Walking

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 1 | <3 | walking | quiet | outdoor | Work |
| 2 | <3 | walking | quiet | outdoor | Work |
| 3 | 3-5 | walking | quiet | outdoor | Work |
| 9 | >5 | walking | loud | indoor | Work |
| 17 | <3 | walking | quiet | indoor | Not at work |
| 18 | <3 | walking | quiet | indoor | Not at work |
| 20 | <3 | walking | medium | indoor | Not at work |
| 21 | <3 | walking | loud | outdoor | Not at work |
| 22 | <3 | walking | medium | indoor | Not at work |
| 23 | <3 | walking | medium | indoor | Not at work |
| 24 | 3-5 | walking | quiet | outdoor | Not at work |
| 28 | 3-5 | walking | loud | outdoor | Not at work |

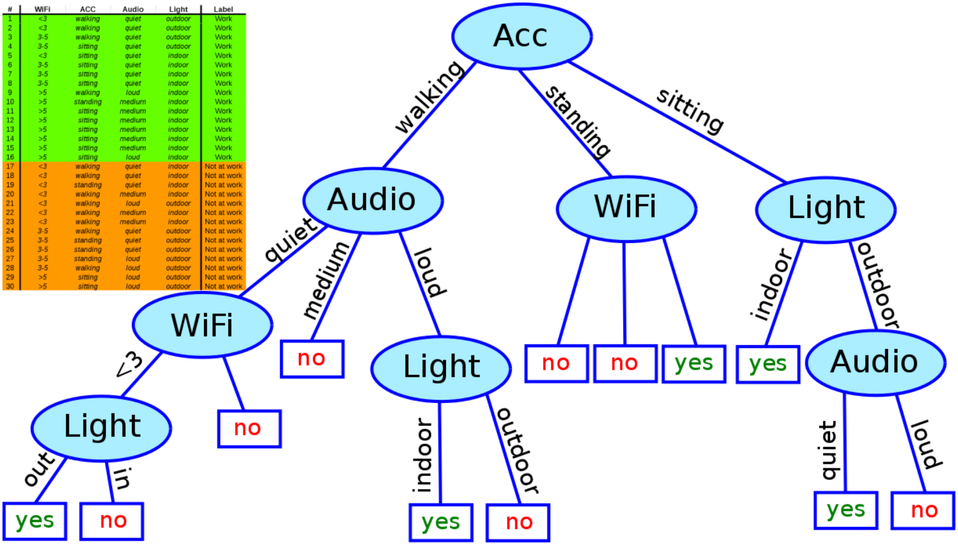
standing

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 10 | >5 | standing | medium | indoor | Work |
| 19 | <3 | standing | quiet | indoor | Not at work |
| 25 | 3-5 | standing | quiet | outdoor | Not at work |
| 26 | 3-5 | standing | quiet | outdoor | Not at work |
| 27 | 3-5 | standing | loud | outdoor | Not at work |

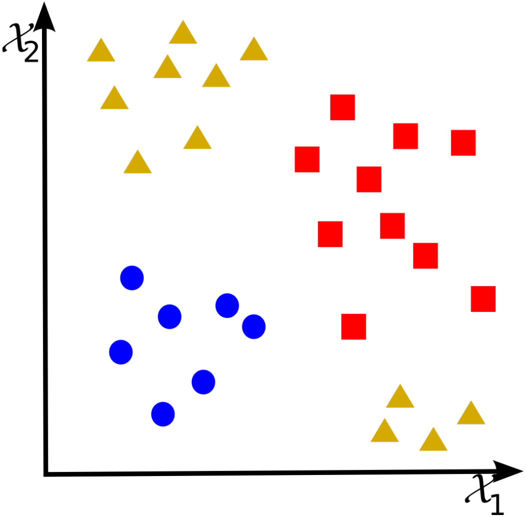
sitting

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 4 | 3-5 | sitting | quiet | outdoor | Work |
| 5 | <3 | sitting | quiet | indoor | Work |
| 6 | 3-5 | sitting | quiet | indoor | Work |
| 7 | 3-5 | sitting | quiet | indoor | Work |
| 8 | 3-5 | sitting | quiet | indoor | Work |
| 11 | >5 | sitting | medium | indoor | Work |
| 12 | >5 | sitting | medium | indoor | Work |
| 13 | >5 | sitting | medium | indoor | Work |
| 14 | >5 | sitting | medium | indoor | Work |
| 15 | >5 | sitting | medium | indoor | Work |
| 16 | >5 | sitting | loud | indoor | Work |
| 29 | >5 | sitting | loud | outdoor | Not at work |
| 30 | >5 | sitting | loud | outdoor | Not at work |

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 1 | <3 | walking | quiet | outdoor | Work |
| 2 | <3 | walking | quiet | outdoor | Work |
| 3 | 3-5 | walking | quiet | outdoor | Work |
| 4 | 3-5 | sitting | quiet | outdoor | Work |
| 5 | <3 | sitting | quiet | indoor | Work |
| 6 | 3-5 | sitting | quiet | indoor | Work |
| 7 | 3-5 | sitting | quiet | indoor | Work |
| 8 | 3-5 | sitting | quiet | indoor | Work |
| 9 | >5 | walking | loud | indoor | Work |
| 10 | >5 | standing | medium | indoor | Work |
| 11 | >5 | sitting | medium | indoor | Work |
| 12 | >5 | sitting | medium | indoor | Work |
| 13 | >5 | sitting | medium | indoor | Work |
| 14 | >5 | sitting | medium | indoor | Work |
| 15 | >5 | sitting | medium | indoor | Work |
| 16 | >5 | sitting | loud | indoor | Work |
| 17 | <3 | walking | quiet | indoor | Not at work |
| 18 | <3 | walking | quiet | indoor | Not at work |
| 19 | <3 | standing | quiet | indoor | Not at work |
| 20 | <3 | walking | medium | indoor | Not at work |
| 21 | <3 | walking | loud | outdoor | Not at work |
| 22 | <3 | walking | medium | indoor | Not at work |
| 23 | <3 | walking | medium | indoor | Not at work |
| 24 | 3-5 | walking | quiet | outdoor | Not at work |
| 25 | 3-5 | standing | quiet | outdoor | Not at work |
| 26 | 3-5 | standing | quiet | outdoor | Not at work |
| 27 | 3-5 | standing | loud | outdoor | Not at work |
| 28 | 3-5 | walking | loud | outdoor | Not at work |
| 29 | >5 | sitting | loud | outdoor | Not at work |
| 30 | >5 | sitting | loud | outdoor | Not at work |



# Graphical interpretation: Decision tree



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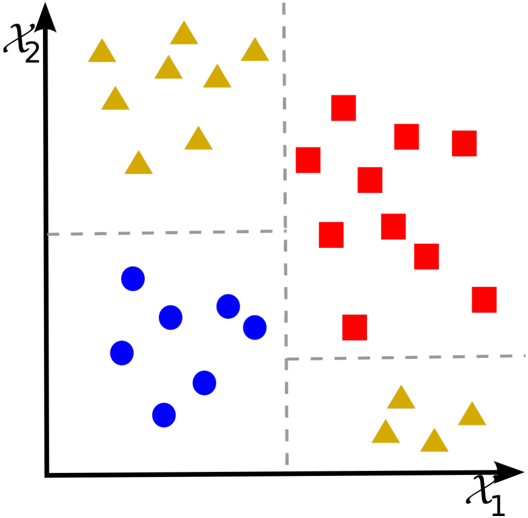
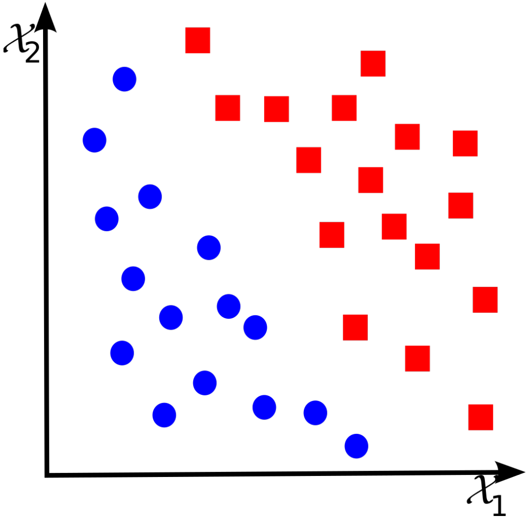


# Graphical interpretation: Decision tree



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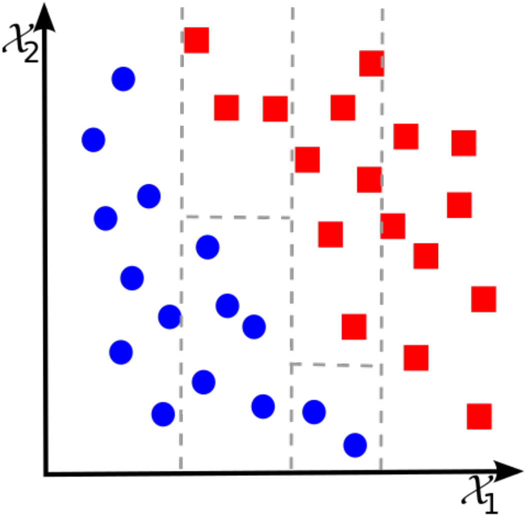

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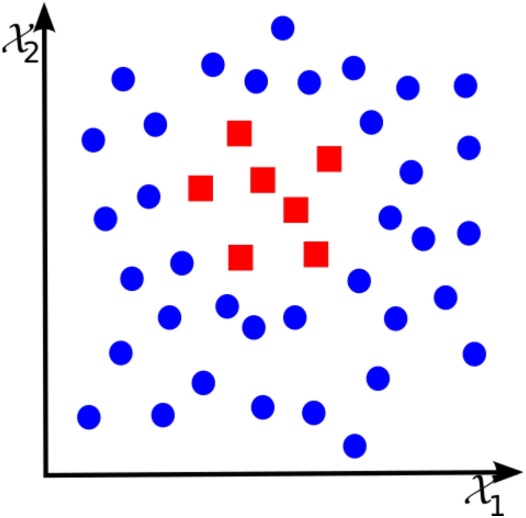

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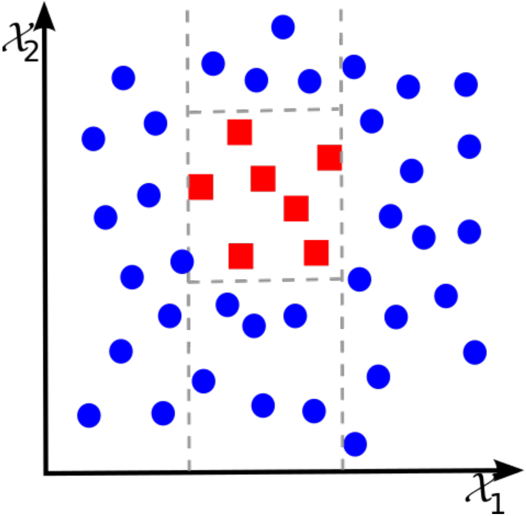


# Remark: An alternative to Information gain

## Gini impurity

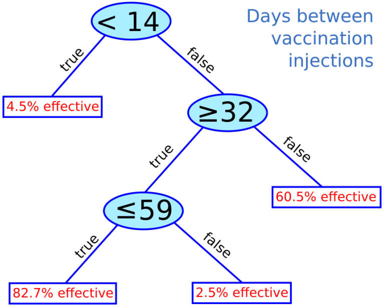
*Gini impurity* describes how often samples would be incorrectly labelled if labelled randomly according to the disctribution of labels in the subset. Let $p_i$ be the probability that a sample is correctly labelled. Gini impurity is then computed as

$$I_G = \sum_{i=1}^{n} p_i \cdot (1 - p_i)$$

# Regression trees

## Regression trees

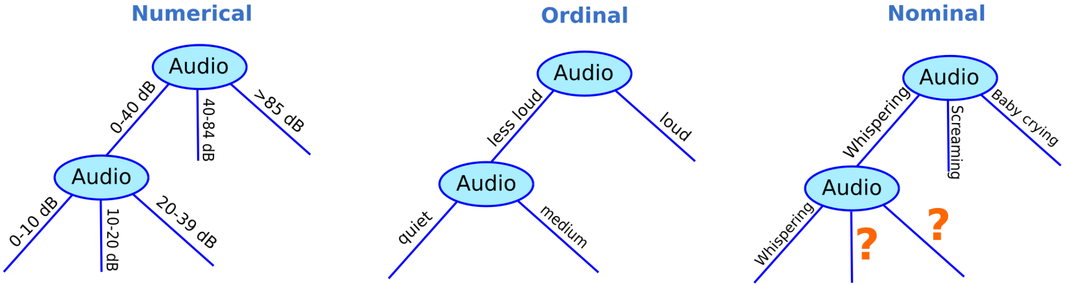
Decision trees where the target variable can take continuous values (typically real numbers) are called regression trees.



# Practical issues – numeric values

## Nominal feature values

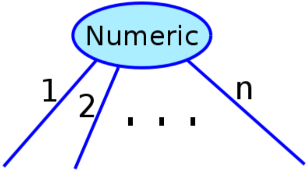
For nominal features, the decision tree splits on every possible value. Therefore, the information content of this feature is 0 after such branch has been conducted →Never branches on nominal features twice



# Practical issues – numeric values

## Numeric feature values

For numeric feature values, splitting on each possible value would lead to a very wide tree of small depth.



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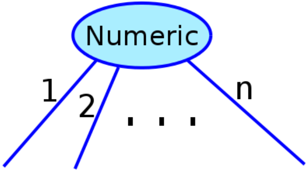


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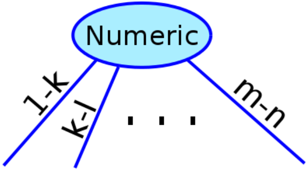
for numeric values, the tree is split into several intervals.



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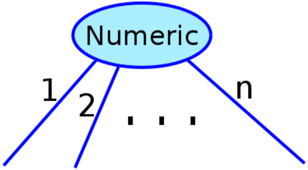


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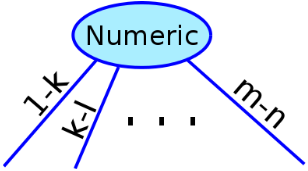
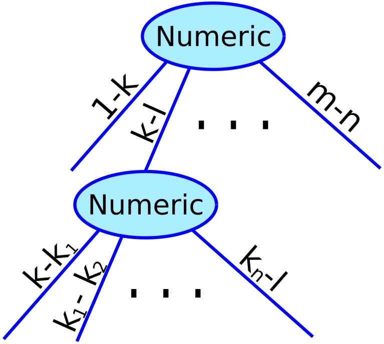



## Nested intervals possible



# Practical issues – Missing values

## Missing values in a data set

Missing values are common in real-world data sets

- participants in a survey refuse to answer
- malfunctioning sensors
- Biology: plants or animals might die before all variables have been measured
- ...

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
| 1 | <3 | *walking* | *quiet* | *outdoor* | Work |
| 2 | <3 | *walking* | *quiet* | *outdoor* | Work |
| 3 | <3 | *walking* | *quiet* | *outdoor* | Work |
| 4 | 3-5 | *sitting* | *quiet* | -- | Work |
| 5 | 3-5 | *sitting* | *quiet* | *indoor* | Work |
| 6 | 3-5 | *sitting* | -- | *indoor* | Work |
| 7 | 3-5 | *sitting* | *quiet* | *indoor* | Work |
| 8 | 3-5 | *sitting* | *quiet* | *indoor* | Work |
| 9 | >5 | *walking* | *loud* | *indoor* | Work |
| 10 | >5 | *standing* | -- | *indoor* | Work |
| 11 | >5 | *sitting* | *medium* | *indoor* | Work |
| 12 | >5 | *sitting* | *medium* | *indoor* | Work |
| 13 | -- | *sitting* | *medium* | *indoor* | Work |
| 14 | >5 | *sitting* | *medium* | *indoor* | Work |
| 15 | >5 | *sitting* | *medium* | *indoor* | Work |
| 16 | >5 | *sitting* | *loud* | *indoor* | Work |
| 17 | <3 | *walking* | -- | *indoor* | Not at work |
| 18 | <3 | *walking* | *quiet* | -- | Not at work |
| 19 | <3 | *standing* | *quiet* | *indoor* | Not at work |
| 20 | <3 | *walking* | *medium* | *indoor* | Not at work |
| 21 | -- | *walking* | *loud* | *outdoor* | Not at work |
| 22 | <3 | *walking* | *medium* | *indoor* | Not at work |
| 23 | <3 | *walking* | *medium* | *indoor* | Not at work |
| 24 | 3-5 | *walking* | *quiet* | *outdoor* | Not at work |
| 25 | 3-5 | *standing* | *quiet* | *outdoor* | Not at work |
| 26 | 3-5 | -- | *quiet* | *outdoor* | Not at work |
| 27 | 3-5 | *standing* | *loud* | *outdoor* | Not at work |
| 28 | 3-5 | *walking* | *loud* | *outdoor* | Not at work |
| 29 | >5 | *sitting* | *loud* | -- | Not at work |
| 30 | -- | *sitting* | *loud* | *outdoor* | Not at work |

# Practical issues – Missing values

## Missing values in a data set

Missing values are common in real-world data sets

- participants in a survey refuse to answer
- malfunctioning sensors
- Biology: plants or animals might die before all variables have been measured
- ...

Most machine learning schemes assume no significance in the fact that a certain value is missing.

| # | WiFi | ACC | Audio | Light | Label |
|---|---|---|---|---|---|
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| 5 | 3-5 | sitting | quiet | indoor | Work |
| 6 | 3-5 | sitting | -- | indoor | Work |
| 7 | 3-5 | sitting | quiet | indoor | Work |
| 8 | 3-5 | sitting | quiet | indoor | Work |
| 9 | >5 | walking | loud | indoor | Work |
| 10 | >5 | standing | -- | indoor | Work |
| 11 | >5 | sitting | medium | indoor | Work |
| 12 | >5 | sitting | medium | indoor | Work |
| 13 | -- | sitting | medium | indoor | Work |
| 14 | >5 | sitting | medium | indoor | Work |
| 15 | >5 | sitting | medium | indoor | Work |
| 16 | >5 | sitting | loud | indoor | Work |
| 17 | <3 | walking | -- | indoor | Not at work |
| 18 | <3 | walking | quiet | -- | Not at work |
| 19 | <3 | standing | quiet | indoor | Not at work |
| 20 | <3 | walking | medium | indoor | Not at work |
| 21 | -- | walking | loud | outdoor | Not at work |
| 22 | <3 | walking | medium | indoor | Not at work |
| 23 | <3 | walking | medium | indoor | Not at work |
| 24 | 3-5 | walking | quiet | outdoor | Not at work |
| 25 | 3-5 | standing | quiet | outdoor | Not at work |
| 26 | 3-5 | -- | quiet | outdoor | Not at work |
| 27 | 3-5 | standing | loud | outdoor | Not at work |
| 28 | 3-5 | walking | loud | outdoor | Not at work |
| 29 | >5 | sitting | loud | -- | Not at work |
| 30 | -- | sitting | loud | outdoor | Not at work |

# Practical issues – Missing values

The absence of data might already hold valuable information!

[1] Witten et al., Data Mining, Morgan Kaufmann, 2011

# Practical issues – Missing values

The absence of data might already hold valuable information!

## Example

People analyzing medical databases have noticed that cases may, in some circumstances, be diagnosable simply from the tests that a doctor decides to make – regardless of the outcome of the tests[1]

[1] Witten et al., Data Mining, Morgan Kaufmann, 2011

# New feature for missing values

- Add binary feature describing whether the value is missing or not
- split the instance at the missing feature:
  1. propagate all instances (weighted with the respective frequency observed from training samples) down to the leaves
  2. combine the results at the leaf nodes given the weighting of the instances


| # | WiFi | ACC | Audio | Light | Label |
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| 16 | >5 | sitting | loud | indoor | Work |
| 17 | <3 | walking | -- | indoor | Not at work |
| 18 | <3 | walking | quiet | -- | Not at work |
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| 27 | 3-5 | standing | loud | outdoor | Not at work |
| 28 | 3-5 | walking | loud | outdoor | Not at work |
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| 30 | -- | sitting | loud | outdoor | Not at work |

# Outline

Decision Trees

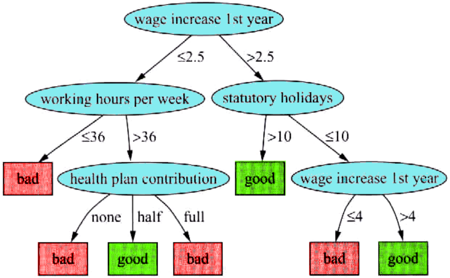
Optimizing the tree structure

Improving classification results

# Optimizing the tree structure

## Motivation

Fully expanded decision trees often contain unnecessary structure that should be simplified before deployment



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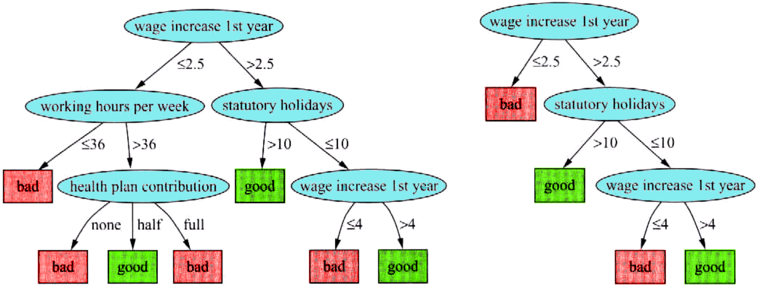

# Confidence on a prediction

Assume we measure the error of a classifier on a test set and estimate a numerical error rate of $q'$ (a success rate of $p' = (1 - q')$).

What can we say about the true success rate $p$?

- It will be close to $p'$,
- but how close? (within 5% or 10% ?)

This depends on the size of the test set

Naturally, we are more confident on $p'$ when it based based on a large number of evaluations.

# Confidence on a prediction

In statistics, a succession of independent events that either succeed or fail is called a Bernoulli process

## Bernoulli process

A Bernoulli process is a repeated coin flipping, possibly with an unfair coin

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Assume that out of $n$ events, $s$ are successful.

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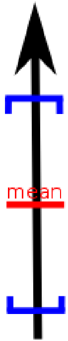


**Assume** that out of $n$ events, $s$ are successful.

**Then** we have an observed success rate of $p' = \frac{s}{n}$

## Confidence Interval

The true success rate $p$ lies within an interval with a specified confidence

# Confidence on a prediction

($\sigma$ and $\mu$ are the standard deviation and mean of $p'$)

The probability that a random variable $\overline{p} = \frac{p'-\mu}{\sigma}$, with zero mean and unit variance, lies within a certain confidence range of width $2z$ is

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Confidence limits for the normal distribution are e.g.

| $\mathcal{P}[\overline{p} \geq z]$ | 0.001 | 0.005 | 0.01 | 0.05 | 0.1 | 0.2 | 0.4 |
|---|---|---|---|---|---|---|---|
| z | 3.09 | 2.58 | 2.33 | 1.65 | 1.28 | 0.84 | 0.25 |

Standard assumption in such tables on the random variable:

| | |
|---|---|
| mean | 0 |
| variance | 1 |

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| $\mathcal{P}[\overline{p} \geq z]$ | 0.001 | 0.005 | 0.01 | 0.05 | 0.1 | 0.2 | 0.4 |
|---|---|---|---|---|---|---|---|
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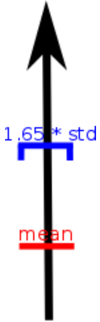


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**Interpretation**

E.g. $\mathcal{P}[\overline{p} \geq z] = 0.05$ implies that there is a 5% chance that $\overline{p}$ lies more than 1.65 standard deviations above the mean.

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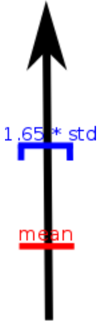


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**Interpretation**

E.g. $\mathcal{P}[\overline{p} \geq z] = 0.05$ implies that there is a 5% chance that $\overline{p}$ lies more than 1.65 standard deviations above the mean.

Since the distribution is symmetric, the chance that $\overline{p}$ lies more than 1.65 standard deviations from the mean is 10%:

$$\mathcal{P}[-1.65 \leq \overline{p} \leq 1.65] = 0.9$$

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In order to apply this to the random variable $p'$, we have to reduce it to have zero mean and unit variance.

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$\rightarrow$ subtract mean $\mu$ & divide by standard deviation $\sigma = \sqrt{\frac{\sum_{i=1}^{n}(p'-\mu)^2}{n}}$

This leads to

$$\mathcal{P}\left[-z < \frac{p' - \mu}{\sqrt{\frac{\sum_{i=1}^{n}(p'-\mu)^2}{n}}} < z\right] = c$$

# Confidence on a prediction

To find confidence limits $z$, given a target confidence value $c$:

- consult a table with confidence limits for the normal distribution

**Table 5.1** Confidence Limits for the Normal Distribution

| $Pr[X \geq z]$ | $z$ |
|---|---|
| 0.1% | 3.09 |
| 0.5% | 2.58 |
| 1% | 2.33 |
| 5% | 1.65 |
| 10% | 1.28 |
| 20% | 0.84 |
| 40% | 0.25 |

# Confidence on a prediction

To find confidence limits $z$, given a target confidence value $c$:

- consult a table with confidence limits for the normal distribution
- since one-sided *success* probabilities (not *error*-) are displayed, we have to subtract $Pr[X \geq z] = c$ from 1 and divide by two:

$$z = \frac{1 - c}{2}$$

# Confidence on a prediction

$$\mathcal{P}\left[-z < \frac{p' - \mu}{\sqrt{\frac{\sum_{i=1}^{n}(p'-\mu)^2}{n}}} < z\right] = c$$

- Then, write inequality above as equality, invert it to find an expression for $\mu$ and solve a quadratic equation to yield

$$\mu = \frac{\left(p' + \frac{z^2}{2n} \pm z\sqrt{\frac{p'}{n} - \frac{p'^2}{n} + \frac{z^2}{4n^2}}\right)}{1 + \frac{z^2}{n}}$$

The resulting two values are the upper and lower confidence boundaries

# Confidence on a prediction

## Example

$$p' = 0.75;\ n = 1000,\ c = 0.8\ (z = 1.28) \quad \rightarrow \quad [0.732, 0.767]$$
$$p' = 0.75;\ n = 100,\ c = 0.8\ (z = 1.28) \quad \rightarrow \quad [0.691, 0.801]$$

Note that the assumptions taken are only valid for large $n$

# Optimization – Noisy data

Fully expanded decision trees often contain unnecessary structure that should be simplified before deployment

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## Pruning

**Prepruning** Trying to decide through the tree-building process when to stop developing subtrees

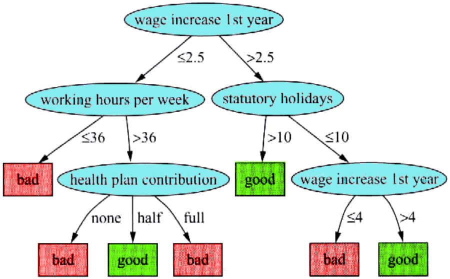
- Might speed up tree creation phase
- Difficult to spot dependencies between features at this stage (features might be meaningful together but not on their own)

**Postpruning** Simplification of the decision tree after the tree has been created

# Postpruning – subtree replacement

Select some subtrees and replace them with single leaves

- Will reduce accuracy on the training set
- May increase accuracy on independently chosen test set (reduction of noise)



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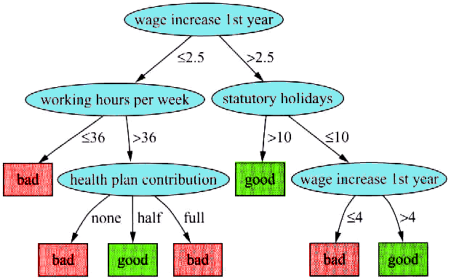
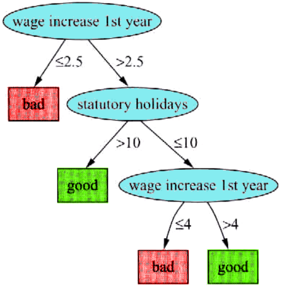
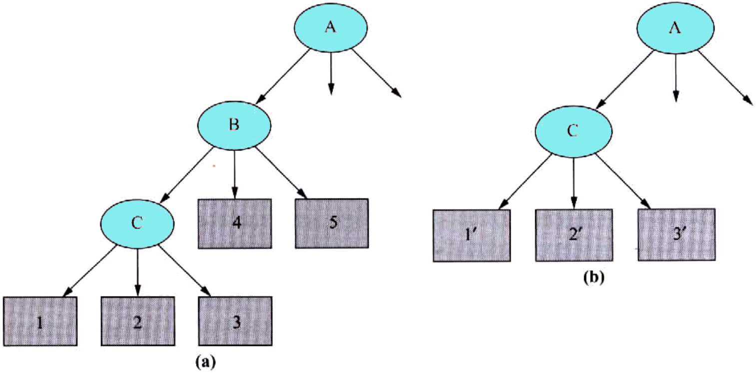


# Optimization – Noisy data

## Postpruning – subtree raising

Complete subtree is raised one level and samples at the nodes of the subtree have to be recalculated



# Optimization – Estimating error rates

When should we raise or replace subtrees?

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When should we raise or replace subtrees?

## Estimating error rates

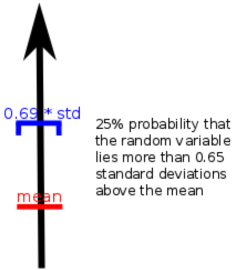
Raise the tree, when the estimated error rate of an expanded tree (considering all leaf nodes) would exceed the estimated error rate of a raised subtree.

# Estimating error rates – success probability

Given a confidence $c$ we find a confidence limit $z$ (for $c = 25\% \rightarrow z = 0.69$) such that

$$\mathcal{P}\left[\frac{q' - \mu_{q'}}{\sqrt{\frac{q'(1-q')}{n}}} > z\right] = c$$

(with the observed error rate $q' = \frac{e}{n}$)



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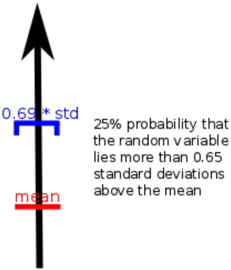



(with the observed error rate $q' = \frac{e}{n}$)

- This leads to a pessimistic error rate $\mu_{q'}$ as an upper confidence limit for $q$ (solving the equation for q):

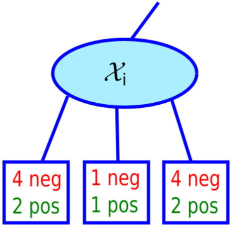
$$\mu_{q'} = \frac{q' + \frac{z^2}{2n} + z\sqrt{\frac{q'}{n} - \frac{q'^2}{n} + \frac{z^2}{4n^2}}}{1 + \frac{z^2}{n}}$$

## Example

Lower left leaf ($e = 2, n = 6$) Utilising the formula for $\mu_{q'}$, we obtain
$q' = 0.33$ and $\mu_{q'} = 0.47$

Minimizing the error:

Majority vote at the parent node F1 vs. majority votes at the leaves ?



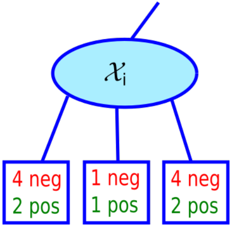
# Example

Lower left leaf ($e = 2, n = 6$) Utilising the formula for $\mu_{q'}$, we obtain
$q' = 0.33$ and $\mu_{q'} = 0.47$

Center leaf($e = 1, n = 2$) $\mu_{q'} = 0.72$

Minimizing the error:

Majority vote at the parent node F1 vs. majority votes at the leaves ?



## Example

Lower left leaf ($e = 2, n = 6$) Utilising the formula for $\mu_{q'}$, we obtain $q' = 0.33$ and $\mu_{q'} = 0.47$

Center leaf($e = 1, n = 2$) $\mu_{q'} = 0.72$

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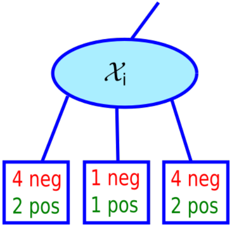

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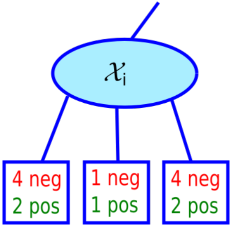

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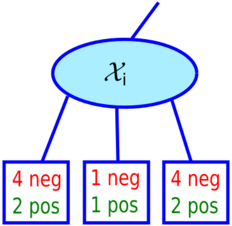
**Error estimate for parent node** $q' = \frac{5}{14} \rightarrow \mu_{q'} = 0.46$
$0.46 < 0.51 \Rightarrow$ prune children away

Minimizing the error:

Majority vote at the parent node F1 vs. majority votes at the leaves ?



# Outline

Decision Trees

Optimizing the tree structure

Improving classification results

# Bottom-line: Decision trees

## Strengths

- Simple, intuitive approach
- Robust to the inclusion of irrelevant features
- Invariant under transformation of features, e.g. scaling

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- Simple, intuitive approach
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## Weaknesses

- Tendency to overfit
- Often complex, deep trees even for simple linearly separable classes

# Improving classification results

## C4.5 – design decisions ($\rightarrow$ heuristic)

**Postpruning – Confidence value** $c = 25\%$

**Postpruning – Split Threshold** Candidate splits on a numeric feature are only considered when at least $\min(10\%, 25)$ of all training samples are cut off by the split

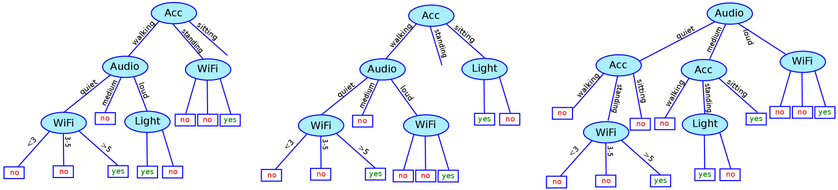
**Prepruning with information gain** Given $u$ candidate splits on a certain numeric attribute, $\log_2 \frac{u}{n}$ is subtracted from the information gain

- in order to prevent overfitting
- Negative information gain $\rightarrow$ tree-construction will stop

# Improving classification results

## Tree bagging

Bootstrap aggregating, or bagging builds several 100 or 1000 trees from random subsets of the training set (*random samples with replacement*)

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Reduces variance without affecting bias

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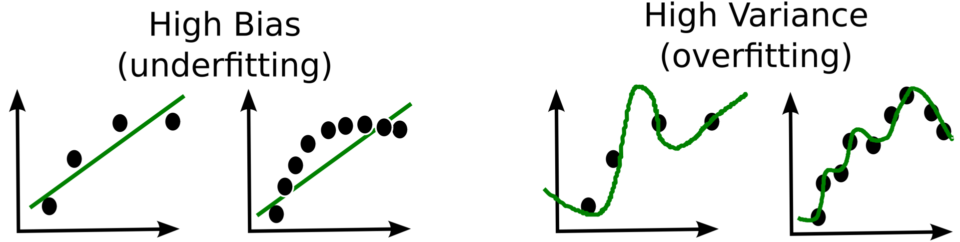


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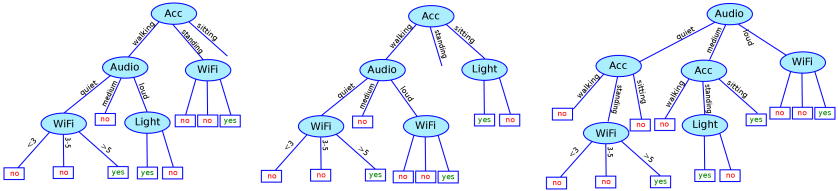
# Improving classification results

## Random forests

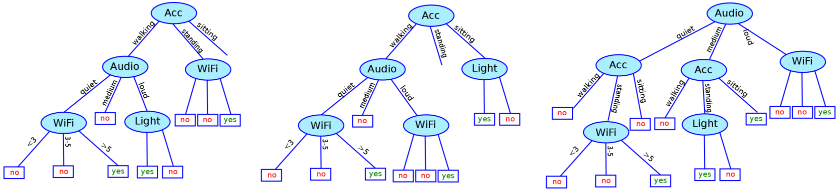
Random forests exploit *Tree bagging* and in addition use a random subset of features at each candidate split in order to reduce the impact of strong features. (Strong features may lead to dependent trees and thus impair the benefits of Tree bagging)



# Improving classification results

## Extra Trees

A way to generate extremely randomized trees is to build a *Random forest* but in addition for each feature split exploit random decision (based on *information gain* or *Gini impurity*) instead of deterministic choice.



# Questions?

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# Literature

I.H. Witten, E. Frank, M.A. Hall: Data Mining – Practical Machine Learning Tools and Techniques, Morgan Kaufmann, 2011.