MADS-ML – Machine Learning

Decision Trees

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Moodle (WiSe 2024/25)

"if-then-else"

Outline

Basics

Construction

Overfitting

Decision Trees in Python

Basic Idea 1/2

- think of the game 20 questions

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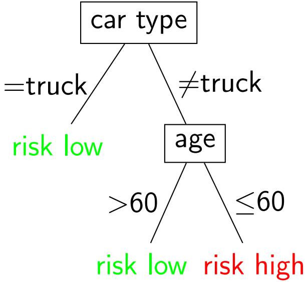
- think of the game 20 questions
- drawback of kNN: No explanation on how which features yield which decision

Motivation

ID	age	car type	risk
1	23	family	high
2	17	sports	high
3	43	sports	high
4	68	family	low
5	32	truck	low



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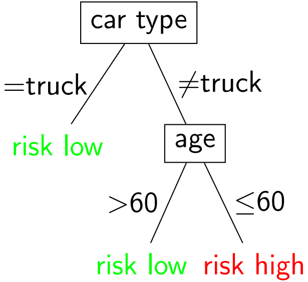

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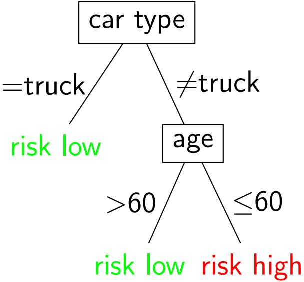

- decision trees find **explicit** knowledge
- decision trees provide **explanations** for their decisions (white box)

Rooted Trees

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Definition 2 (Rooted Tree)

A rooted tree is a graph in which one node is designated the **root**. The root induces a direction on the edges, i.e. all edges point away from the root.

Rooted Trees – Remarks

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- one node A with all its descendants forms another binary rooted tree, called the **branch** or **subtree** of A

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breadth of a tree: Number of leafs

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- Classification:
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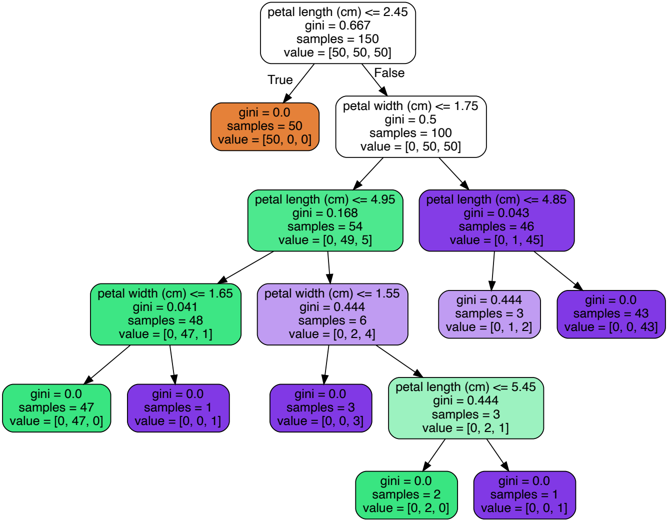
  - predict the class corresponding to that leaf.

An Example – The Iris Dataset (Features 2 and 3)



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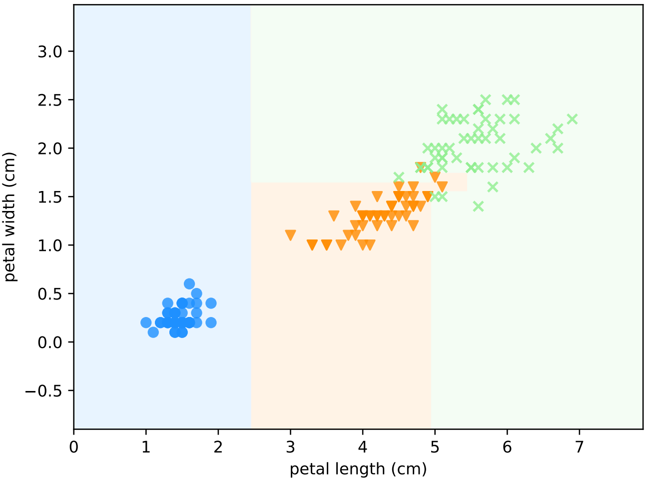

Remark: Notice the combination of rectangular regions!

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Abort criteria:

- all data instances in the current node belong to the same class
- no more split attributes available

Decision Tree: Example

day	forecast	temperature	humidity	wind	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

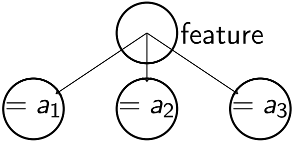
Is this a day to play tennis?

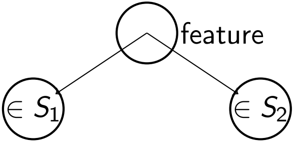
Let's try a split by forecast, . . .

Split Types

Categorical Features:

- split condition of the form "feature $= a$" or "feature in $\in$ set"
- many possible subsets





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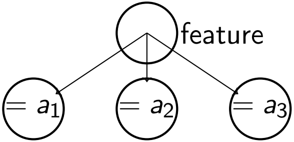

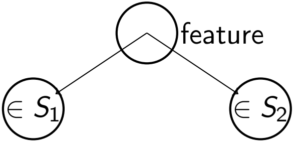

numerical features:

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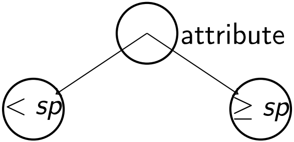

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- a measure of **information gain** that assesses the quality of a split
- a split of T into $T_1, T_2, \ldots, T_m$, that minimizes this measure

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  - It depends only on the largest class among the training instances, the distribution on the other classes is ignored.

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- $entropy(T) = 1$ for $k = 2$ with $p_i = \frac{1}{2}$.

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- maximizing information gain is equivalent to minimizing the subtrahend

$$\sum_{i=1}^{m} \frac{|T_i|}{|T|} \cdot entropy(T_i)$$

Split Strategy: Gini-Coefficient 1/2

- **Gini-Coefficient** for a set T of training instances w.r.t. a set of classes $c_1, c_2, \ldots, c_k$ is defined as:

$$gini(T) = \sum_{i=1}^{k} (p_i) \cdot (1 - p_i) = 1 - \sum_{i=1}^{k} p_i^2$$

- measures the expected risk of miss-classification (an element of class i occurs with probability p_i and is classified as not i with probability $1 - p_i$)
  - small gini-coefficient $\Leftrightarrow$ small risk
  - high gini-coefficient $\Leftrightarrow$ high risk

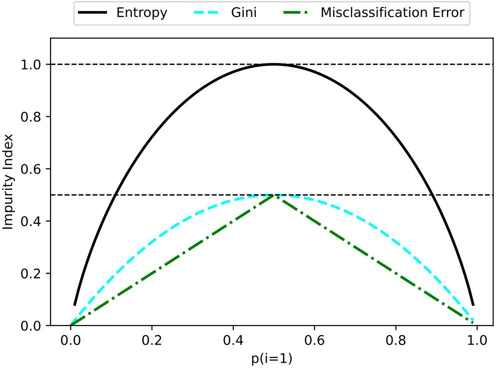
Split Strategy: Gini-Coefficient 2/2

- Let a split A create the partition $T_1, T_2, \ldots, T_m$ of T.
- The **Gini-Coefficient** of split A w.r.t. T is:

$$gini_A(T) = \sum_{i=1}^{m} \frac{|T_i|}{|T|} \cdot gini(T_i)$$

Gini vs. Entropy

- Entropy and Gini-Coefficient are similar
- Gini is computationally less expensive.
- Information gain is biased towards many-valued attributes



Split Strategies: Example – Tennis dataset

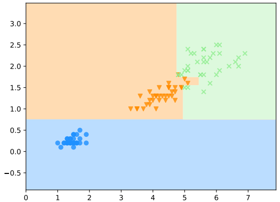
day	outlook	temp	humidity	wind	play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

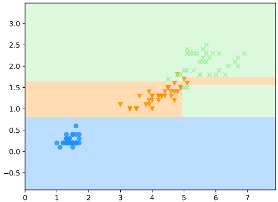
Compare a possible split by humidity to one by wind.

Notebook 04_1_decision_trees_information_gain_example

Stability of a tree

- Decision trees are very sensitive towards small changes in the training data
- Two different ways of sampling training data might create completely different trees.





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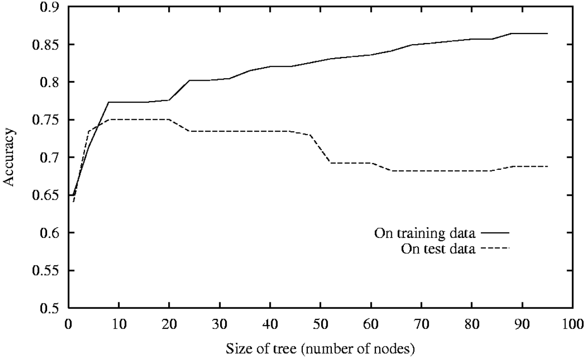
Decision Trees in Python

Problem: Overfitting[2]

Overfitting in the construction of a decision tree occurs, when a smaller tree (less depth) has

- a lower classification quality on the training data
- but a higher classification quality on the test data.



[1]

[1] source https://jmvidal.cse.sc.edu/talks/decisiontrees/allslides.html

[2] More detail on overfitting later

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- The tree would have learned the training data “by heart”
- Idea 1: Find criteria to stop the construction earlier
- Idea 2: Prune the tree after it has been constructed

Avoid Overfitting during Construction

- Choice of a *minimum support*: Minimum number of training instances to create further splits ($>> 1$)

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Avoid Overfitting during Construction

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➔ drawback: influence on overfitting not measured,
hyper-parameter has to be optimized on separate data subset (validation set).

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Error-Reduction-Pruning [Mitchell 1997]

- Split training set again into (a smaller) training and a test set.

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→ advantage: directly adress overfitting, drawback: need spearate data subset (validation set).

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Minimal cost-complexity pruning [Breiman, Friedman, Olshen & Stone 1984]

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Outline

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Construction

Overfitting

Decision Trees in Python

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sklearn.tree.DecisionTreeClassifier

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- parameters for stopping criteria and cost complexity pruning
- graphical output via graphviz[3]

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Notebook 04_2_plot_tree

Notebook 04_3_decision_tree_digits

Exercises 1–3