Machine Learning

Lecture 2: Decision Trees

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Reading material

Main reading

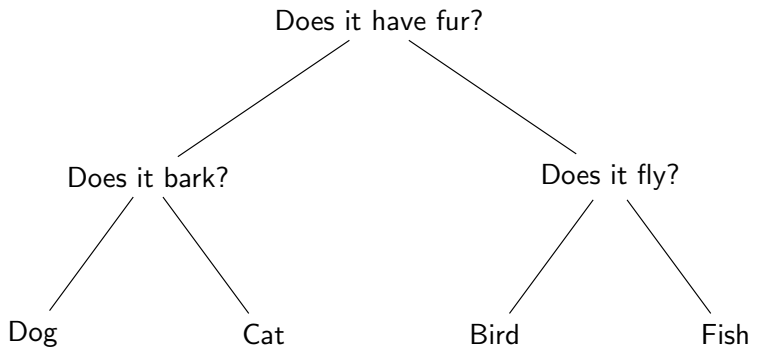
- "Machine Learning: A Probabilistic Perspective" by Murphy [ch. 16.2]

Extra reading

- "Pattern Recognition and Machine Learning" by Bishop [ch. 14.4]

Slides adapted from previous versions by W. Koepp & D. Korhammer. Also, some are inspired by *Understanding Random Forests* by G. Louppe.

The 20-Questions Game



Tennis dataset

Outlook	Temperature	Humidity	Windy	PlayTennis
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No

Goal: classification of unseen instances

Tennis dataset: decision tree

Outlook	Temperature	Humidity	Windy	PlayTennis
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
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Overcast	Hot	Normal	False	Yes
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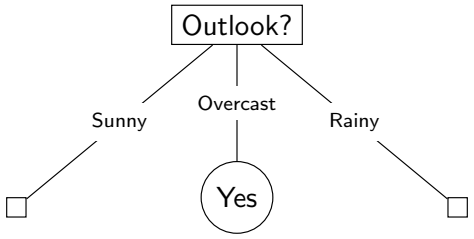
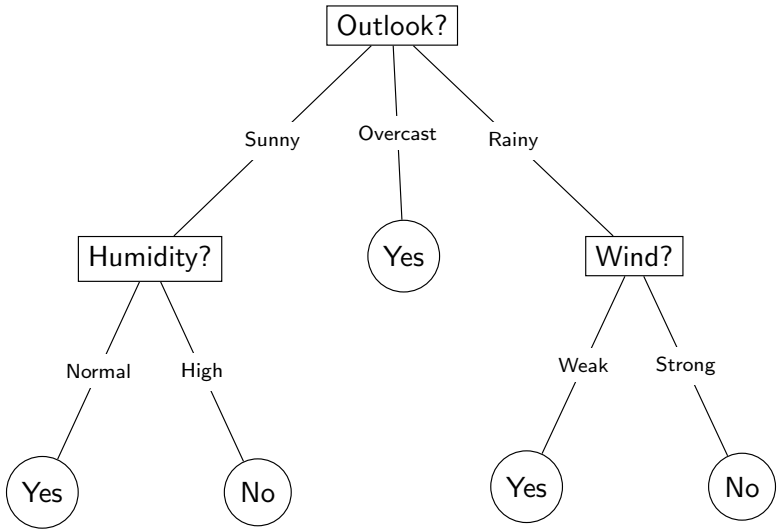
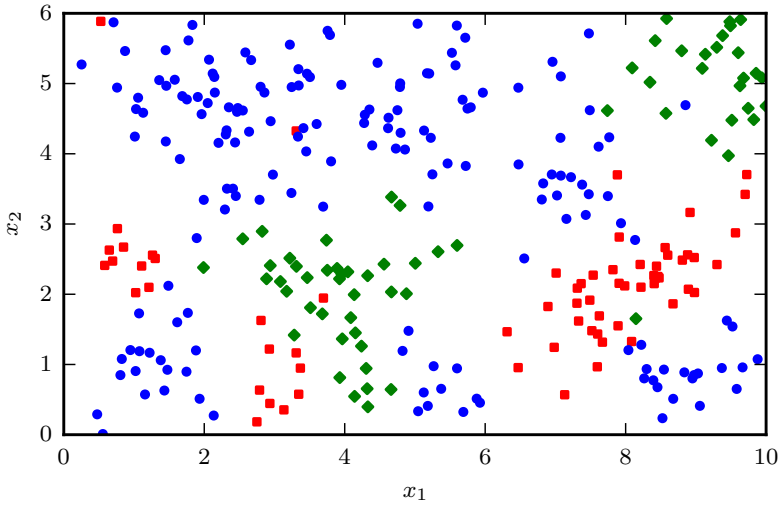


Tennis dataset: final decision tree

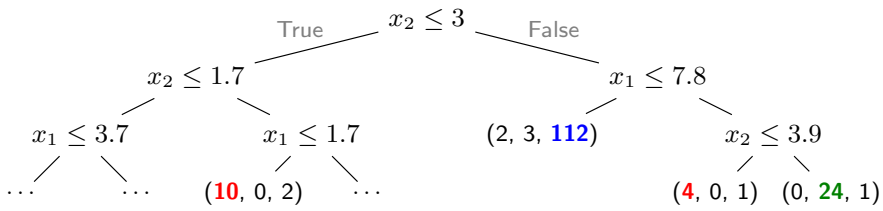


Numerical features



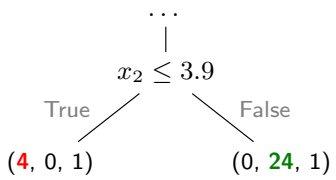
Example: data $\boldsymbol{X}$ with two *features* x_1 and x_2 and class labels y

Binary split



Simplest decision: binary split on a single feature, $x_i \leq a$
Distribution of classes in leaf: (red, green, blue)

Interpretation of a decision tree



- Node $\widehat{=}$ *feature* test $\rightarrow$ leads to decision boundaries.
- Branch $\widehat{=}$ different outcome of the preceding feature test.
- Leaf $\widehat{=}$ region in the input space and the distribution of *samples* in that region.

Decision trees partition the input space into cuboid regions.

Inference on decision trees

To classify a new sample $\boldsymbol{x}$:

- Test the attributes of $\boldsymbol{x}$ to find the region $\mathcal{R}$ that contains it and get the class distribution $\boldsymbol{n}_{\mathcal{R}} = (n_{c_1,\mathcal{R}}, n_{c_2,\mathcal{R}}, \ldots, n_{c_k,\mathcal{R}})$ for $C = \{c_1, \ldots, c_k\}$.
- The probability that a data point $\boldsymbol{x} \in \mathcal{R}$ should be classified belonging to class c is then:

$$p(y = c \mid \mathcal{R}) = \frac{n_{c,\mathcal{R}}}{\sum\limits_{c_i \in C} n_{c_i,\mathcal{R}}}$$

- A new unseen sample $\boldsymbol{x}$ is simply given the label which is most common[1] in its corresponding region:

$$\hat{y} = \arg\max_c \; p(y = c \mid \boldsymbol{x}) = \arg\max_c \; p(y = c \mid \mathcal{R}) = \arg\max_c \; n_{c,\mathcal{R}}$$

[1] Majority label, similar to kNN

Refresher: discrete probability theory

Given a jar that contains different colored balls $\{4, 10, 6\}$. What is the probability of randomly drawing a ball with a particular color (e.g. red)?

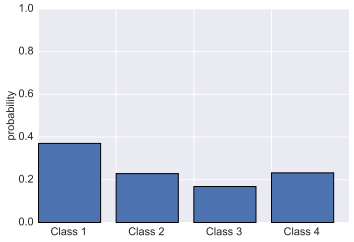
Intuitively: $p(\text{ball} = \textbf{red}) = \frac{\text{number of red balls}}{\text{total number of balls}} = \frac{4}{4+10+6} = \frac{4}{20} = 0.2$

Similarly: $p(\text{ball} = \textbf{green}) = 0.5, \quad p(\text{ball} = \textbf{blue}) = 0.3$

The probability mass function p assigns value to each possible outcome.

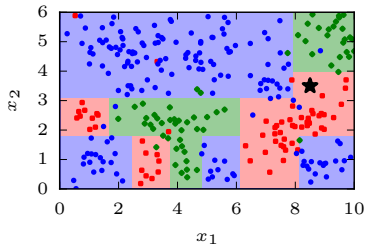
In general it has to hold:

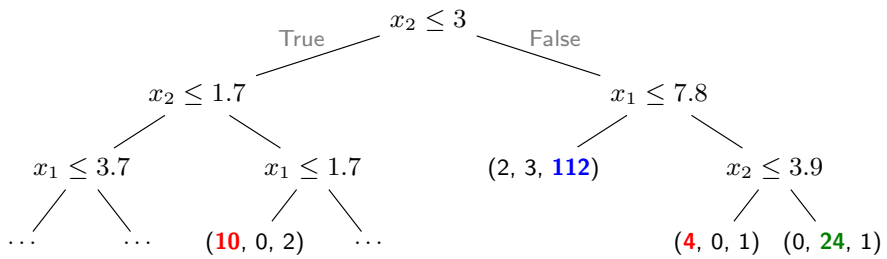
- $\forall x,\ p(X = x) \geq 0$
- $\sum_x p(X = x) = 1$



Example prediction

Classifcation of $\boldsymbol{x} = (8.5, 3.5)^T$

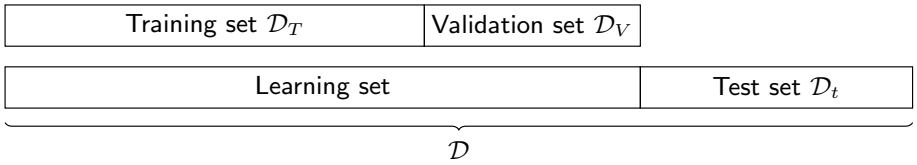




Optimal decision tree

Generalization: Find a DT that performs well on new (unseen) data.

Again, split the dataset:



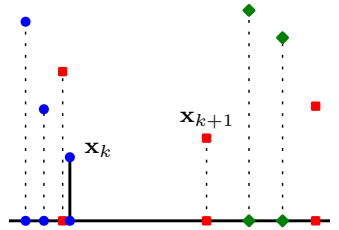
- build tree from training set $\mathcal{D}_T$,
- predict *validation set* labels $\hat{y}_i$ using the tree,
- evaluate by comparing predictions $\hat{y}_i$ to true labels y_i.
- pick the tree that performs the best on the validation set
- report final performance on the test set

Naive idea

Idea: Build all possible trees and evaluate how they perform on new data.

All combinations of features and values can serve as tests in the tree:

feature	tests
x_1	≤ 0.36457631
	≤ 0.50120369
	≤ 0.54139549
	$\leq \ldots$
x_2	≤ 0.09652214
	≤ 0.20923062
	$\leq \ldots$



In our simple example:
2 features $\times$ 300 unique values per feature
2 features $\times$ 299 possible thresholds per feature:
598 possible tests at the root node, slightly fewer at each descendant

Building the optimal decision tree is intractable

Iterating over all possible trees is possible only for very small examples because the number of trees quickly explodes.

Finding the optimal tree is *NP-complete*[2].

Instead: Grow the tree top-down and choose the best split node-by-node using a greedy heuristic on the *training data*.

[2]Optimal in the sense of minimizing the expected number of tests required to classify an unknown sample. Even the problem of identifying the root node in an optimal strategy is NP-hard. And several other aspects of optimal tree construction are known to be intractable.

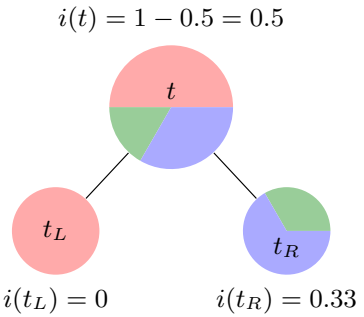
Example heuristic: misclassification rate

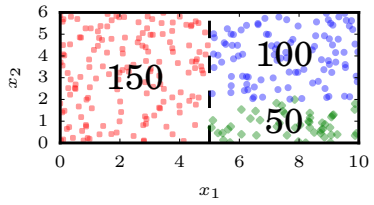
Split the node if it improves the misclassification rate (error) i_E at node t

$$i_E(t) = 1 - \max_c \; p(y = c \mid t)$$

The improvement when performing a split s of t into t_R and t_L for $i(t) = i_E(t)$ is given by

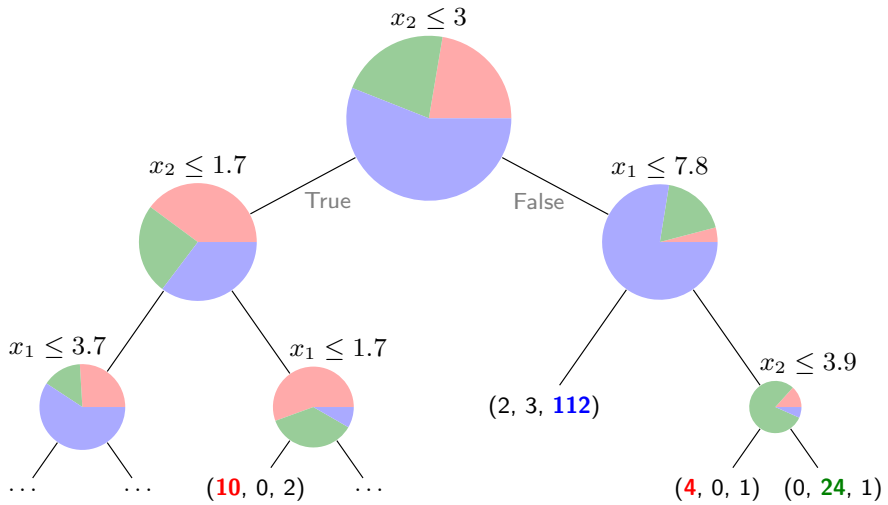
$$\Delta i(s,t) = i(t) - p_L \cdot i(t_L) - p_R \cdot i(t_R)$$





By repeatedly applying the heuristic

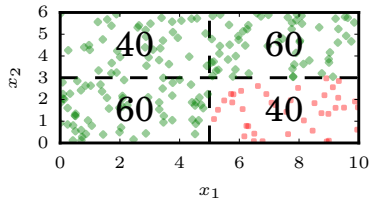
The distribution of labels becomes progressively more pure[3]...



[3]meaning we mostly have instances of the same class

Problems with misclassification rate

Problem 1: No split performed even though combining the two tests would result in perfect classification



no split: $i_E(t) = \frac{40}{200}$

$x_1 \leq 5$: $p_L \cdot i_E(t_L) + p_R \cdot i_E(t_R) = \frac{40}{200}$

$x_2 \leq 3$: $p_L \cdot i_E(t_L) + p_R \cdot i_E(t_R) = \frac{40}{200}$

Problem 2: No sensitivity to changes in class probability

Before split: $(400, 400)$
Split a: $\{(100, 300)\ ,\ (300, 100)\} \rightarrow i_E(t, a) = 0.25$
Split b: $\{(200, 400)\ ,\ (200, 0)\} \rightarrow i_E(t, b) = 0.25$

What is a suitable criterion

Use a criterion $i(t)$ that measures how *pure* the class distribution at a node t is. It should be

- **maximum** if classes are equally distributed in the node
- **minimum**, usually 0, if the node is pure
- **symmetric**

Impurity measures

With $\pi_c = p(y = c \mid t)$:

- Misclassification rate:

$$i_E(t) = 1 - \max_c \ \pi_c$$

- Entropy:

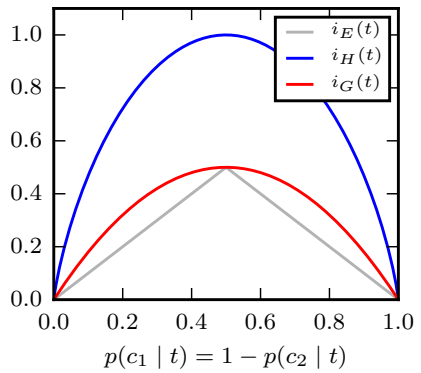
$$i_H(t) = -\sum_{c_i \in C} \pi_{c_i} \log \pi_{c_i}$$

(Note that $\lim_{x \to 0+} x \log x = 0$.)

- Gini index:

$$i_G(t) = \sum_{c_i \in C} \pi_{c_i}(1 - \pi_{c_i})$$
$$= 1 - \sum_{c_i \in C} \pi_{c_i}^2$$

For $C = \{c_1, c_2\}$:

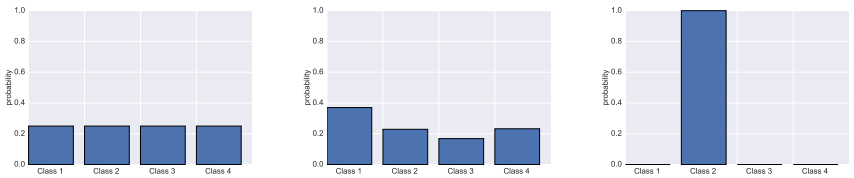


Shannon Entropy

Expected number of bits needed to encode a randomly drawn value from a distribution (under most efficient code)

For a discrete random variable X with possible values $\{x_1, \ldots, x_n\}$

$$\mathbb{H}(X) = -\sum_{i}^{n} p(X = x_i) \log_2 p(X = x_i)$$



$\mathbb{H} = 1.3863$ $\mathbb{H} = 1.3445$ $\mathbb{H} = 0$

Higher entropy → flatter histogram → sampled values less predictable
Lower entropy → peakier histogram → sampled values more predictable

Detour: Information Theory

Information theory is about encoding and transmitting information

We would like to encode four messages:

- m_1 = "There is free beer." $p(m_1) = 0.01$ → Code 111
- m_2 = "You have an exam." $p(m_2) = 0.02$ → Code 110
- m_3 = "You have a lecture." $p(m_3) = 0.30$ → Code 10
- m_4 = "Nothing happening." $p(m_4) = 0.67$ → Code 0

The code above is called a *Huffman Code*.

On average:

$$0.01 \times 3\,\text{bits} + 0.02 \times 3\,\text{bits} + 0.3 \times 2\,\text{bits} + 0.67 \times 1\text{bit} = 1.36\,\text{bits}$$

Gini Index

Measures how often a randomly chosen instance would be misclassified if it was randomly classified according to the class distribution

$$i_G(t) = \sum_{c_i \in C} \underbrace{\pi_{c_i}}_{\substack{\text{probability of} \\ \text{picking element}}} \cdot \underbrace{(1 - \pi_{c_i})}_{\substack{\text{probability is} \\ \text{misclassified}}}$$

Entropy vs Gini Index:

- It only matters in 2% of the cases which one you use. [4]
- Gini Index small advantage: no need to compute $\log$ which can be a bit faster

[4] See Raileanu LE, Stoffel K. Theoretical comparison between the gini index and information gain criteria.

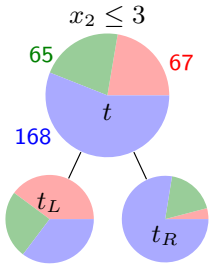
Building a decision tree

Compare all possible tests and choose the one where the improvement $\Delta i(s,t)$ for some splitting criterion $i(t)$ is largest

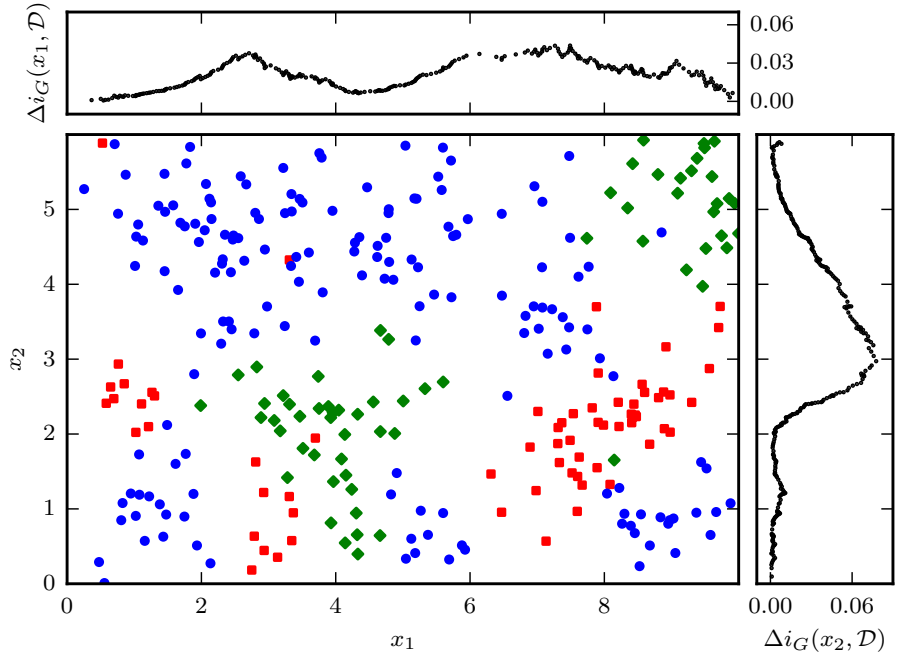
$$i_G(t) = 1 - \left(\frac{67}{300}\right)^2 - \left(\frac{65}{300}\right)^2 - \left(\frac{168}{300}\right)^2 \approx 0.5896$$

After testing $x_2 \leq 3$:

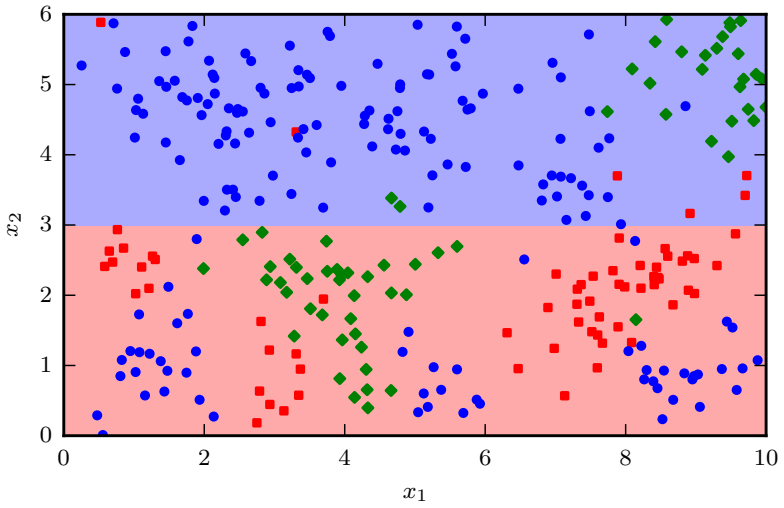
$i_G(t_L) \approx 0.6548$ and $i_G(t_R) \approx 0.3632$



$$\Rightarrow \Delta i_G(x_2 \leq 3, t) = i_G(t) - \frac{153}{300} \cdot i_G(t_L) - \frac{147}{300} \cdot i_G(t_R) \approx 0.07768$$

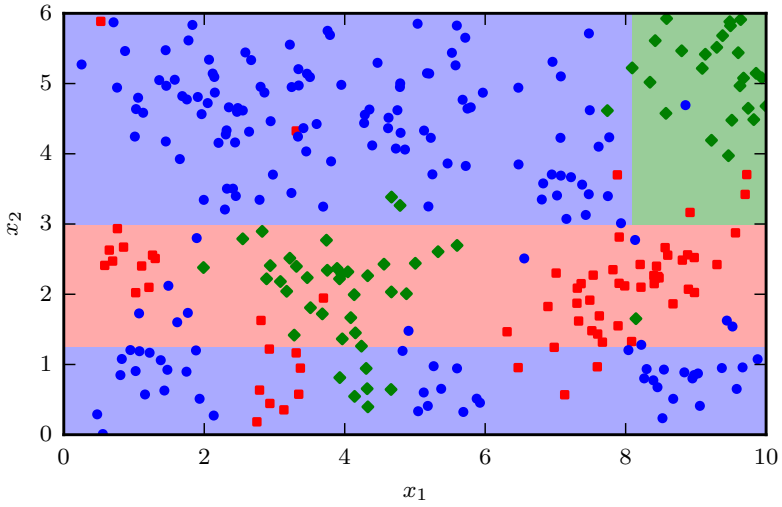


Decision boundaries at depth 1



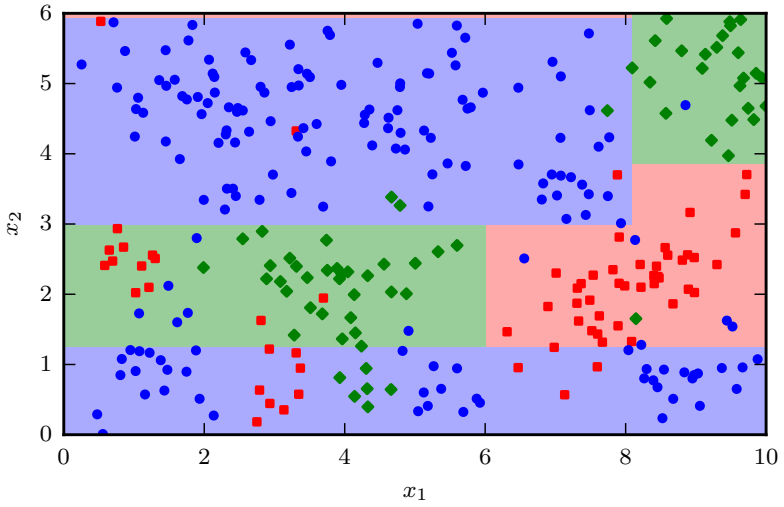
Accuracy on the whole data set: 58.3%

Decision boundaries at depth 2



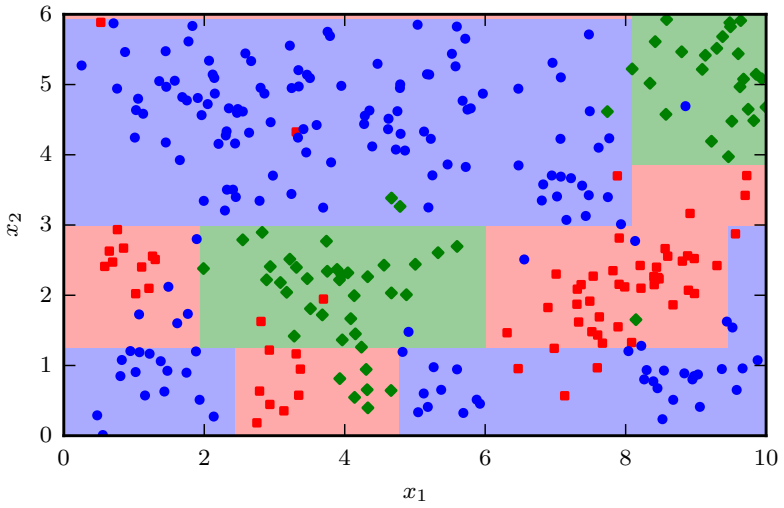
Accuracy on the whole data set: 77%

Decision boundaries at depth 3



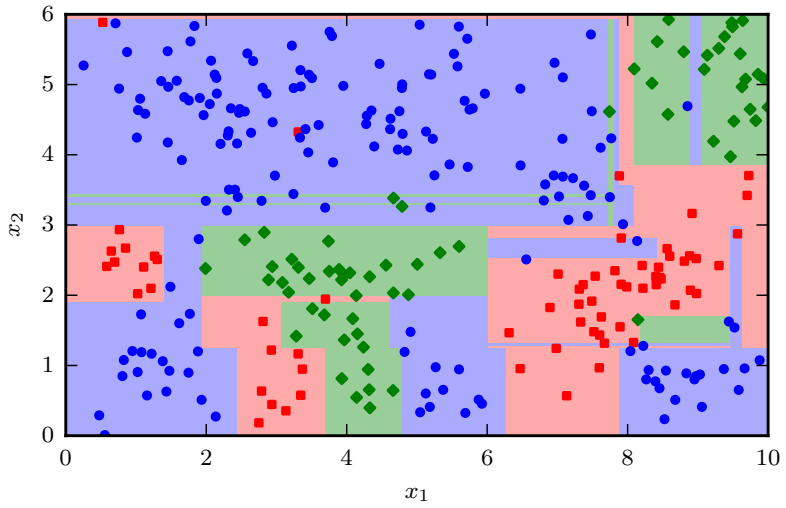
Accuracy on the whole data set: 84.3%

Decision boundaries at depth 4



Accuracy on the whole data set: 90.3%

Decision boundaries of a maximally pure tree



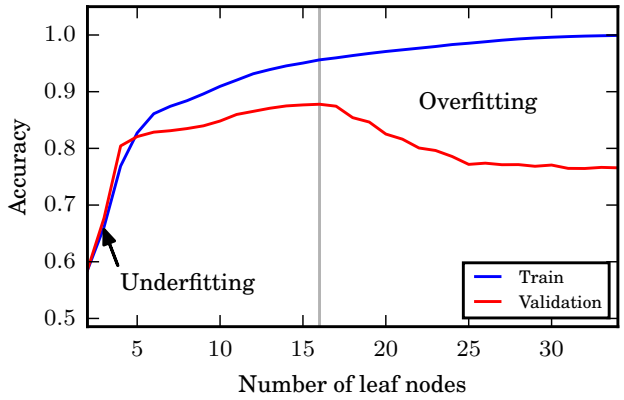
Accuracy on the whole data set: 100% → *Good generalization*?

Overfitting

Overfitting typically occurs when we try to model the training data perfectly.

Overfitting means poor generalization! How can we spot overfitting?

- low training error, possibly 0
- validation error is comparably high

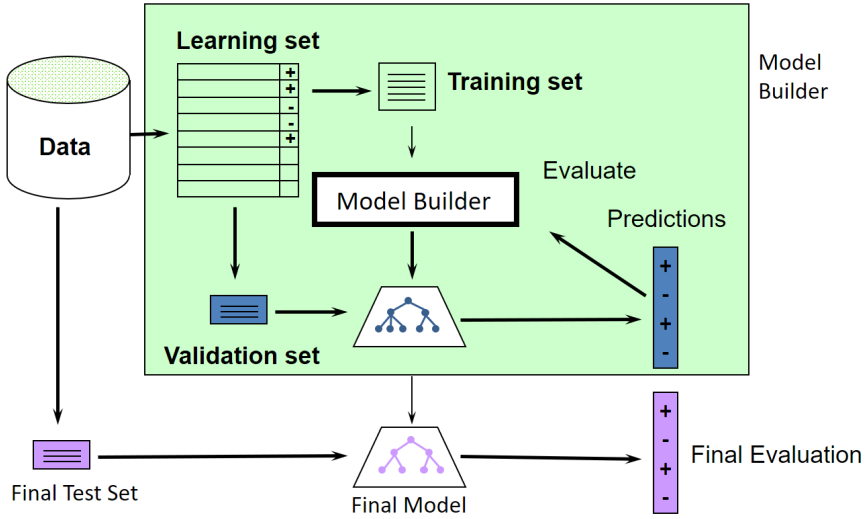


The training performance monotonically increases with every split.

The validation performance tells us how well our model generalizes, not the training performance!

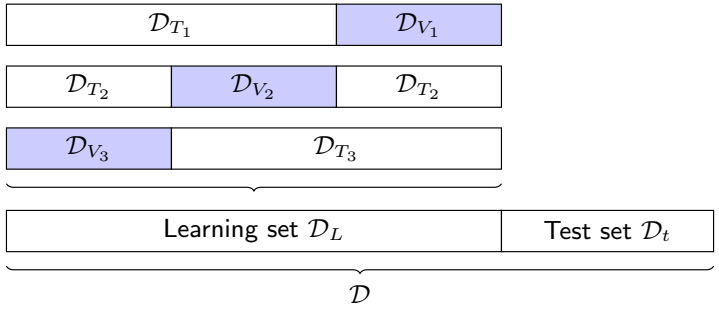
Good data science

How to do model selection / battle overfitting?



Only touch the test set once at the end to report final performance!

K-fold Cross-Validation



- Split your learning data into K folds (10-fold CV is common).
- Use $K-1$ folds for training and the remaining for evaluation.
- Average over all folds to get an estimate
  - of the error for a setting of your *hyper-parameters*
  - or the model for your model selection
- Try different settings for your hyper-parameters.
- Use all your training data and the best hyper-parameters for final training (and testing) of your model.

The extreme case - LOOCV

In *leave-one-out-cross validation* (LOOCV) we train on all but one sample.

If we have N samples, this is the same as N-fold cross-validation.

LOOCV is interesting if we do not have a lot of data and we want to use as much of it for training as possible but still get a good estimate of model performance.

But it also means that we need to train our model N times...

If we have sufficiently large amounts of data and training our model is computationally expensive, we better stick to lower numbers of K or a single validation set.

Back to ...

... Decision Trees

Stopping criterion

We are recursively splitting the data, thereby growing the DT.

When to stop growing?

Possible stopping (or *pre-pruning*) criteria:

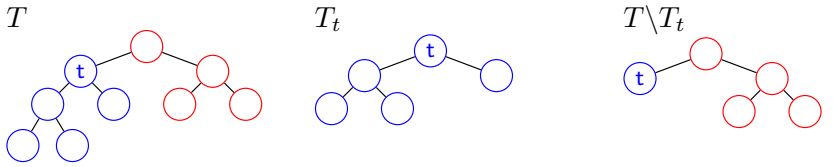
- distribution in branch is *pure*, i.e $i(t) = 0$
- maximum depth reached
- number of samples in each branch below certain threshold t_n
- benefit of splitting is below certain threshold $\Delta i(s,t) < t_\Delta$
- accuracy on the validation set

Or we can grow a tree maximally and then (post-)prune it.

Reduced error pruning

Let T be our decision tree and t one of its inner nodes.

Pruning T w.r.t. t means deleting all descendant nodes of t (but not t itself). We denote the pruned tree $T\backslash T_t$.

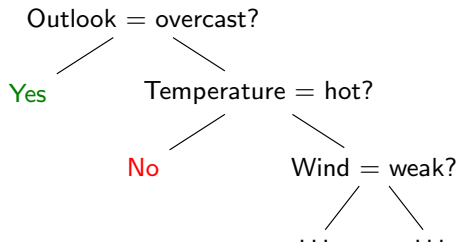


- Use validation set to get an error estimate: $\text{err}_{\mathcal{D}_V}(T)$.
- For each node t calculate $\text{err}_{\mathcal{D}_V}(T\backslash T_t)$
- Prune tree at the node that yields the highest error reduction.
- Repeat until for all nodes t: $\text{err}_{\mathcal{D}_V}(T) < \text{err}_{\mathcal{D}_V}(T\backslash T_t)$.

After pruning you may use both training and validation data to update the labels at each leaf.

Decision trees with categorical features

Day	Outlook	Temperature	Humidity	Wind	Play Tennis?
D1	sunny	hot	high	weak	No
D2	sunny	hot	high	strong	No
...					

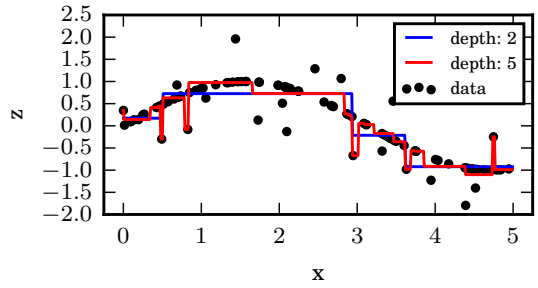


Different algorithm variants (ID3, C4.5, CART) handle these things differently.

Decision trees for regression

For regression (if y_i is a real value rather than a class):

- At the leaves compute the mean (instead of the mode) over the outputs.
- Use the mean-squared-error as splitting heuristic.



Considerations

- Human interpretable
- Can handle any combination of numerical and categorical features and targets
- Extensions (e.g. random forests, boosted trees) have very competitive performance (e.g. Kaggle competitions)
- Compared to k-NN:
  - Much better complexity w.r.t. memory/storage and inference
  - More flexible decision function

What we learned

- Interpretation and building of Decision Trees
- Impurity functions / Splitting heuristics
- Overfitting
- Good data science