Nikita Kazeev

Decision Trees

2021

MLHEP 2021

HIGHER SCHOOL OF ECONOMICS
NATIONAL RESEARCH UNIVERSITY

LAMBDA • HSE

Yandex

SCHOOL OF DATA ANALYSIS

EPFL

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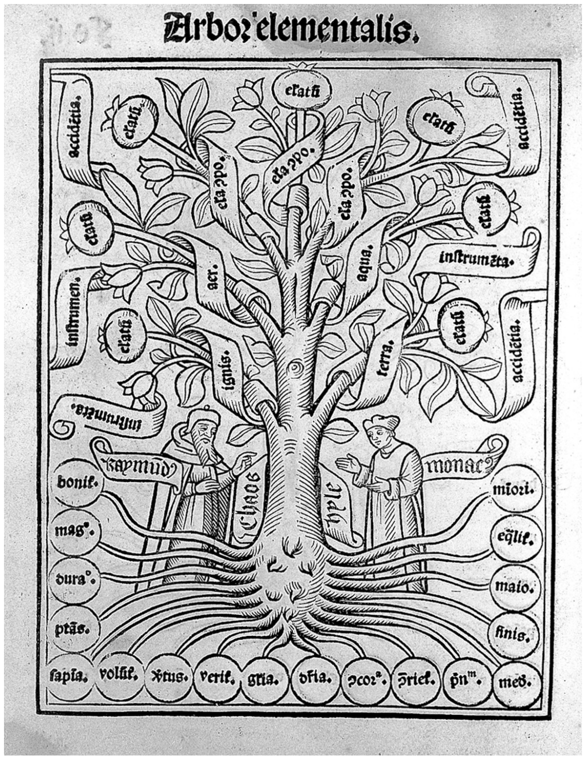
Schaffhausen Institute of Technology

Lecture overview

After the lecture, you will be able to:

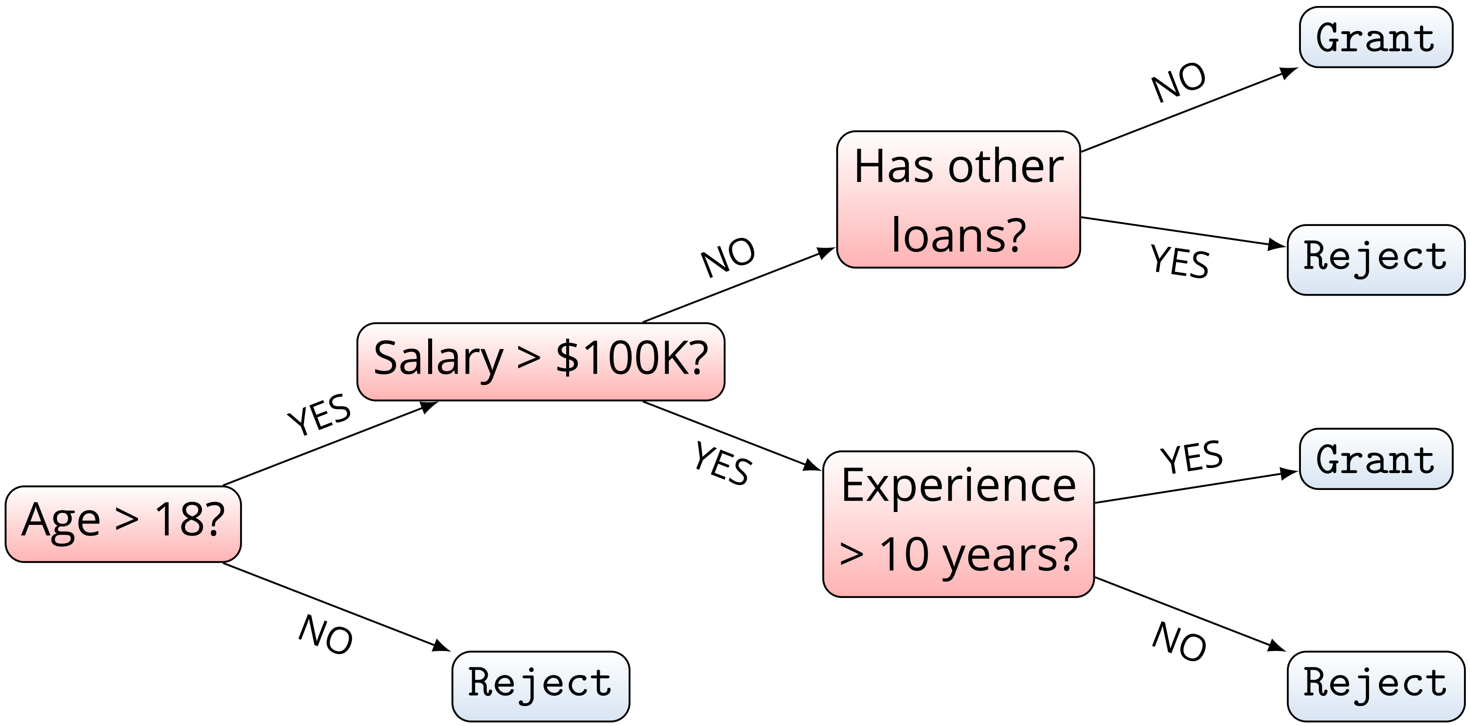
- Use the decision tree algorithm for classification and regression;
- Tune the algorithm parameters improve its performance.

Arbor Porphyrii



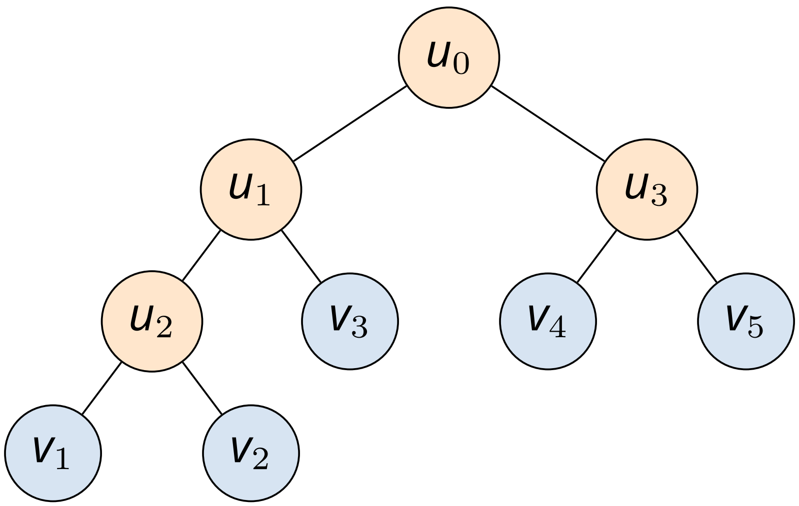
Picture credit: R. Lull, showing the Arbor Elementalis to monk

Decision making at a bank



Decision tree formalism

- Decision tree is a binary tree V
- Internal nodes $u \in V$: *predicates* $\beta_u : \mathcal{X} \to \{0, 1\}$
- Leaves $v \in V$: *predictions* $\beta_v : \mathcal{X} \to \mathcal{Y}$



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- Algorithm $h(\mathbf{x})$ starts at $u = u_0$
  - Compute $b = \beta_u(\mathbf{x})$
  - If u is a leaf, return b
  - If $b = 0$, $u \leftarrow \mathrm{LeftChild}(u)$
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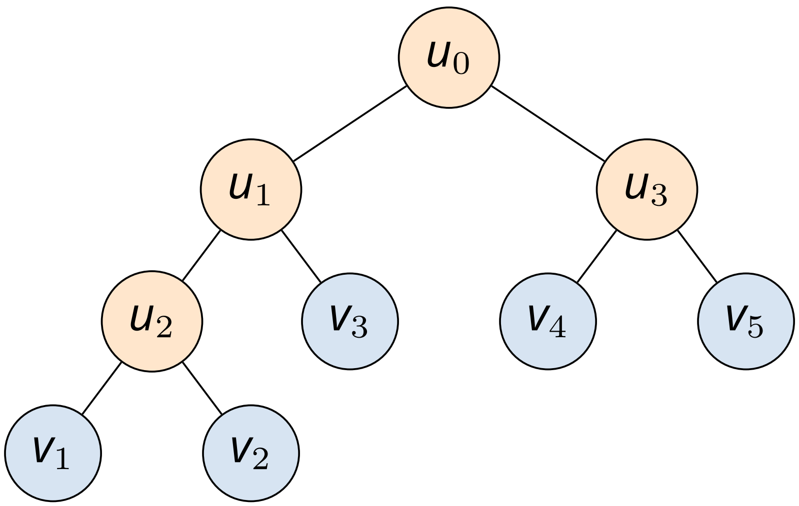

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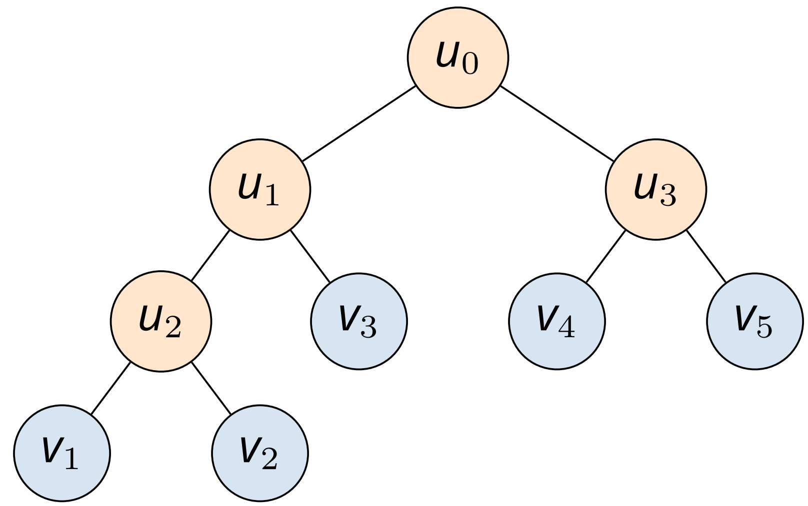
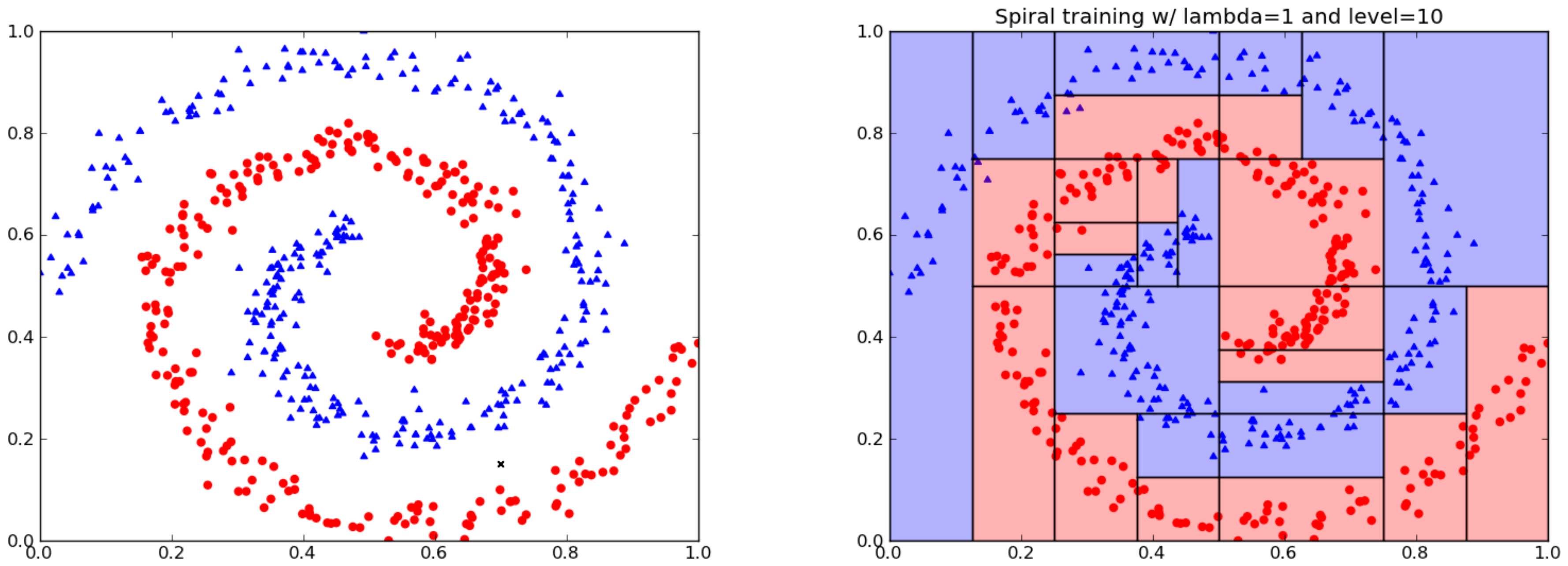
- In ML practice: $\beta_u(\mathbf{x}; j, t) = [\mathbf{x}^j < t]$



Decision surface



Picture credit: `https://www.classes.cs.uchicago.edu/archive/2015/winter/12200-1/assignments/pa5/index.html`

Decision tree training

- Greedy algorithm – on each iteration partition the data as if the split was final

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- There are two key components:
  - Split criterion to compare different ways to partition the data
  - Stopping condition to decide when to stop building the tree

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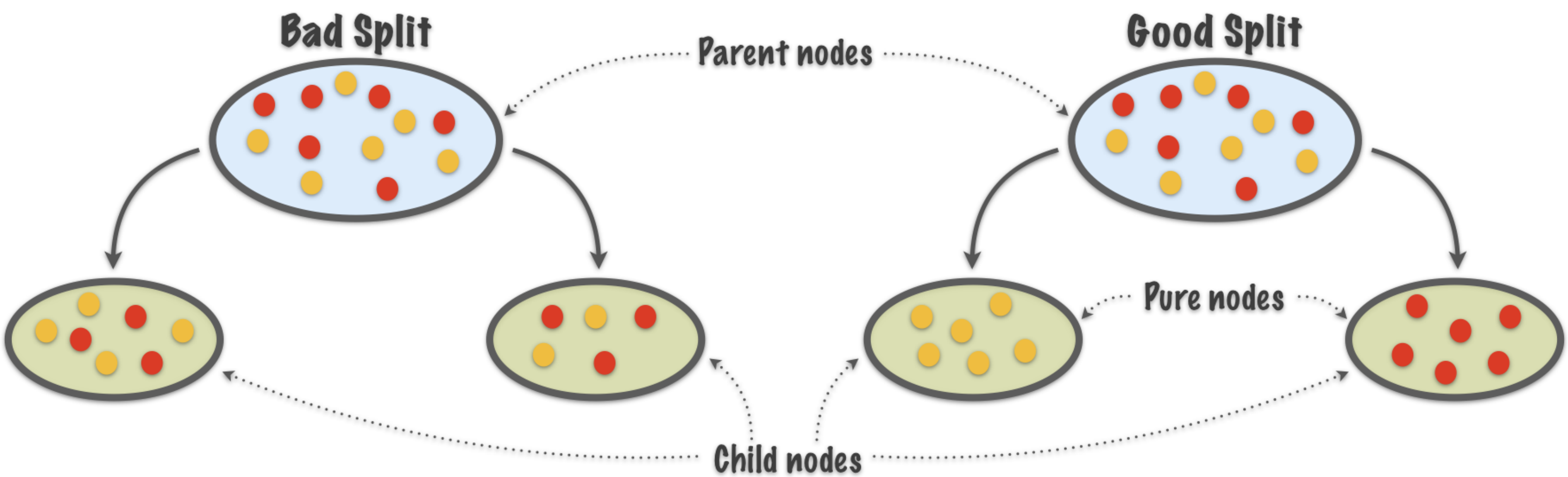
- Output: a decision tree V

The idea: maximize purity



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- $H(R)$: impurity criterion
- Generally, $H(R) = \min_{c \in \mathcal{Y}} |R|^{-1} \sum_{(\mathbf{x}_i, y_i) \in R} L(y_i, c)$

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  - Cross-entropy: $H(R) = -\sum_{k=1}^{N} p_k \log p_k$

Stopping rules for decision tree learning

> What will happen if we build a decision tree to minimise the impurity to the greatest possible extent?

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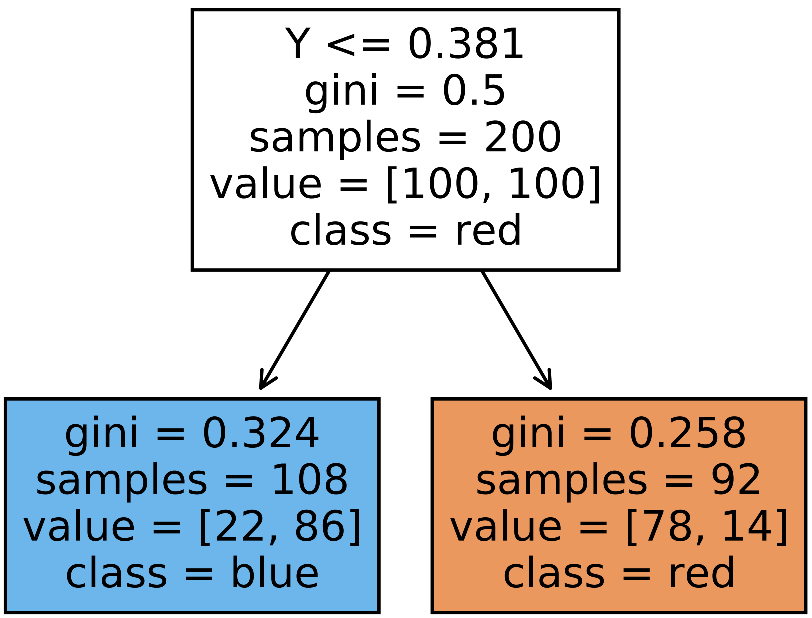
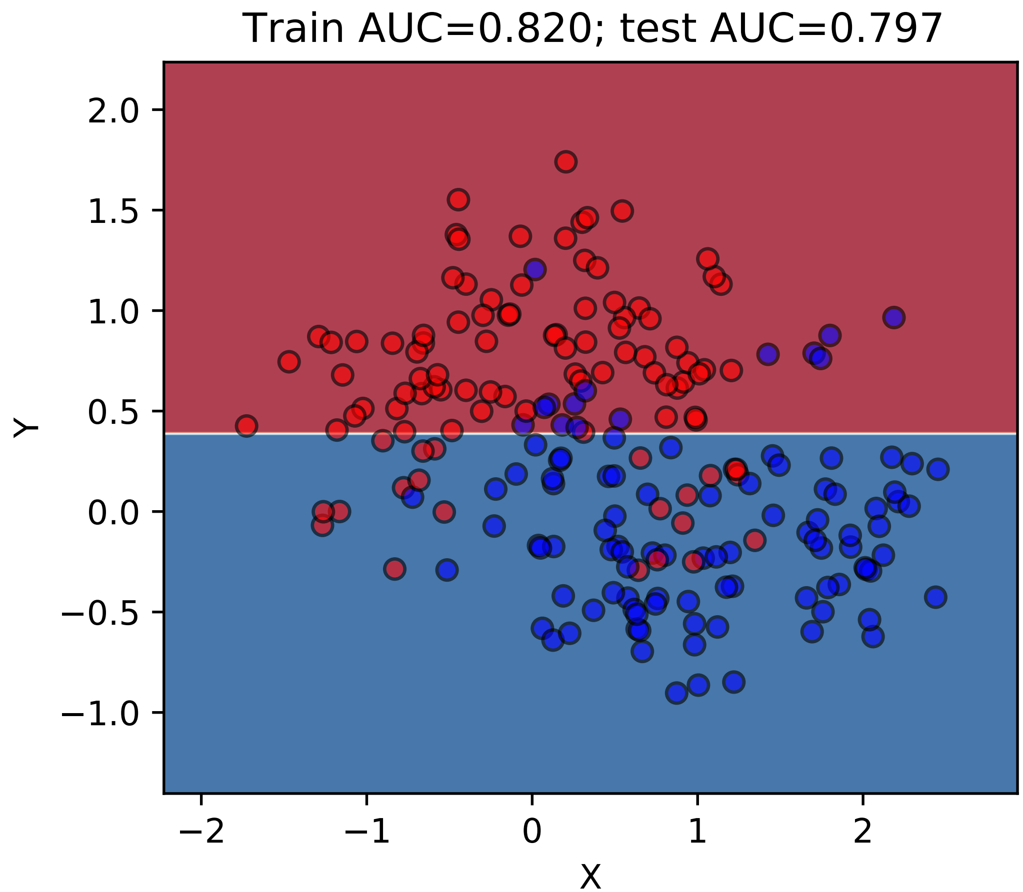
The tree will be built until all leaves are 100% pure, up to single-example leaves.

With decision trees, overfitting is easy!





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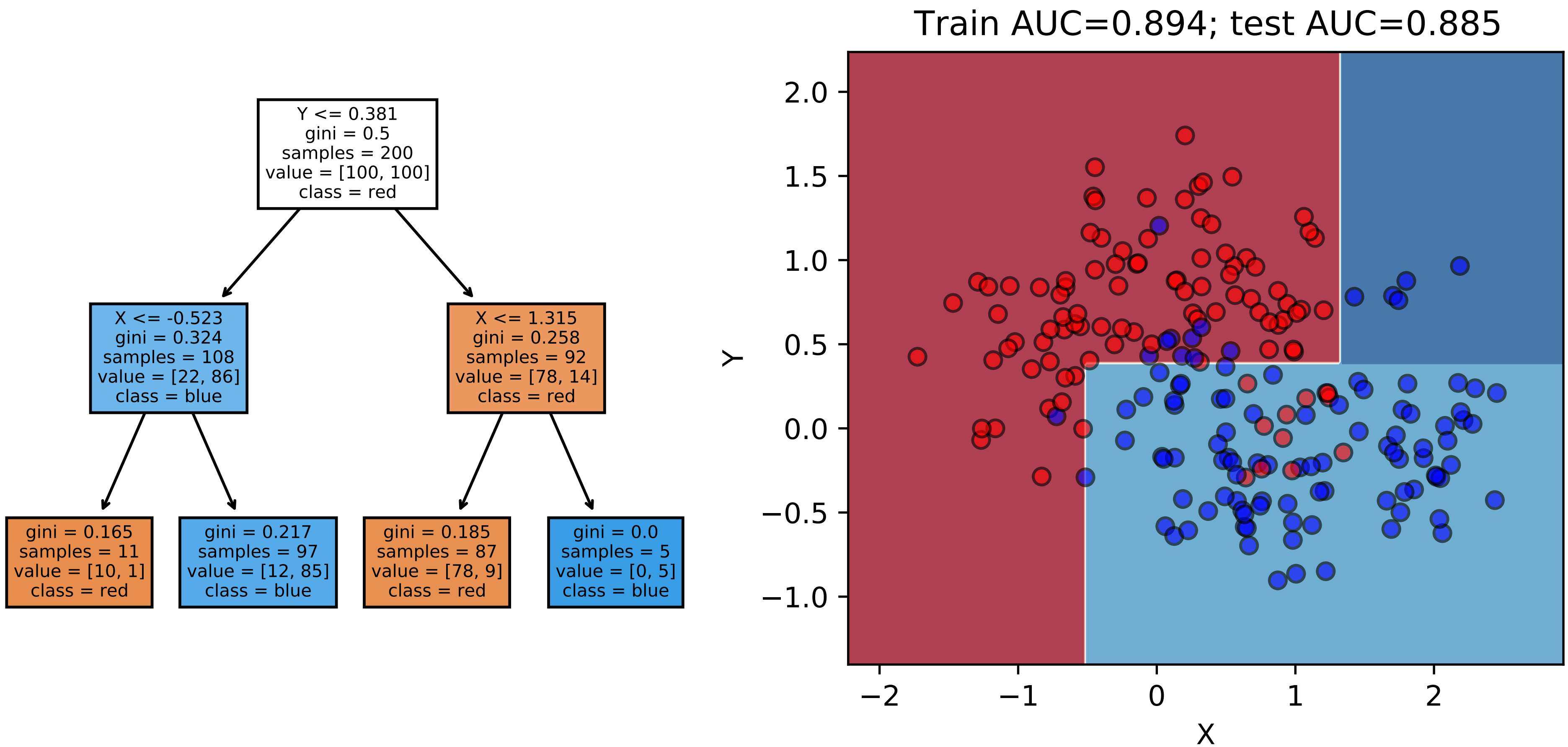

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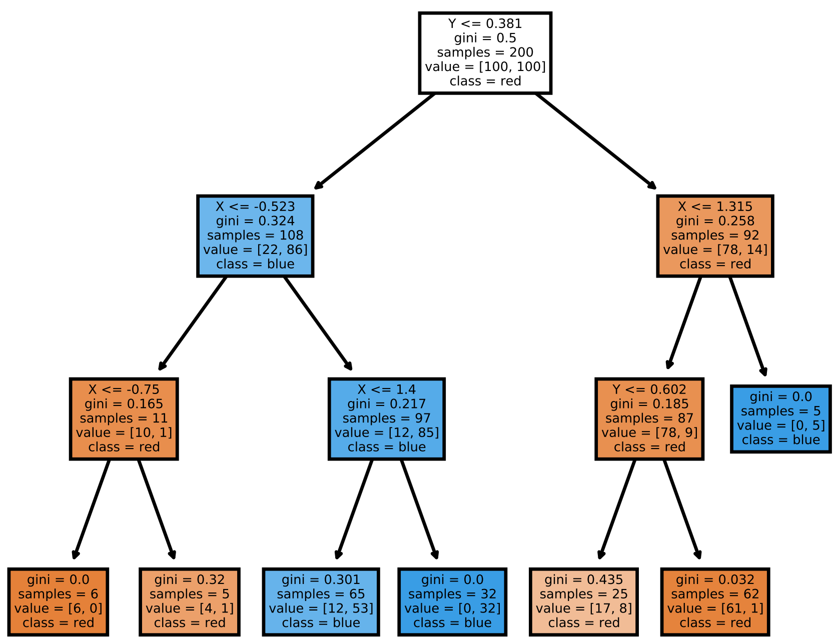

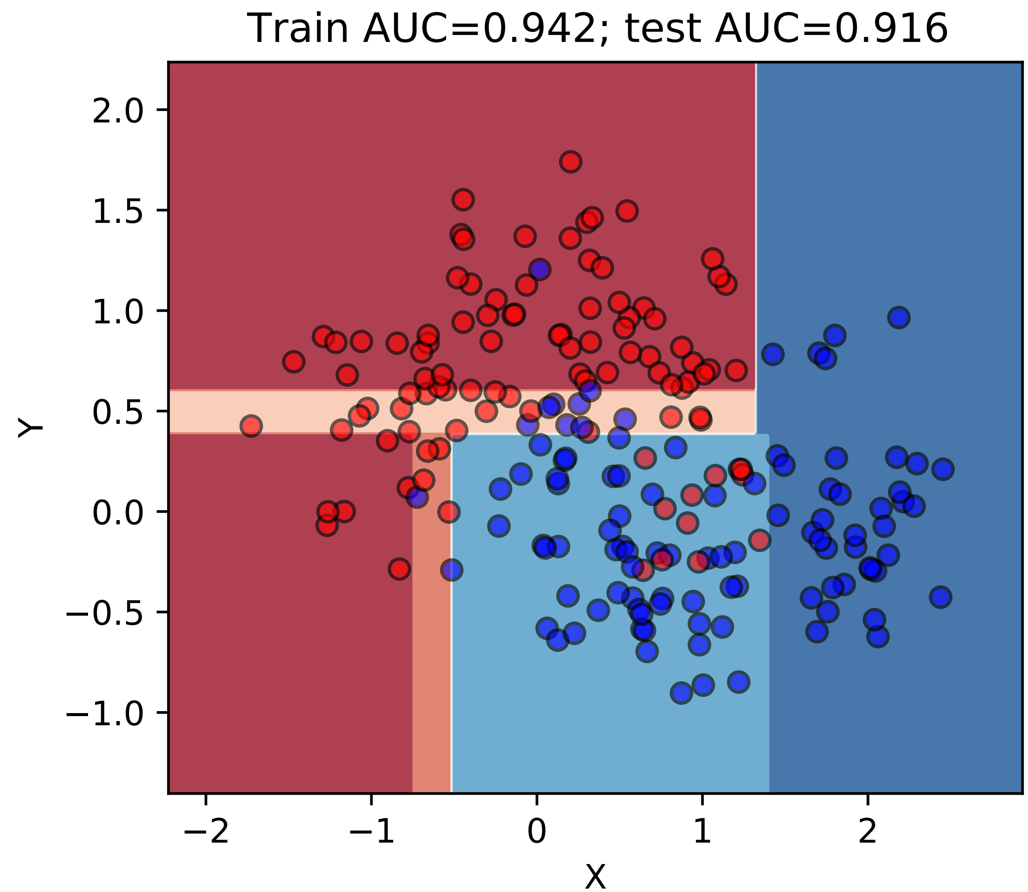

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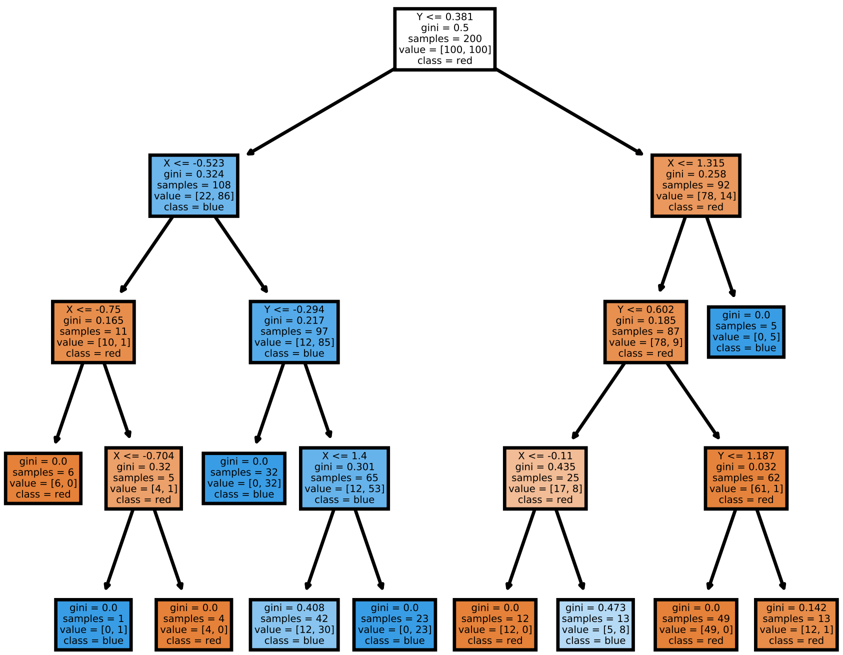

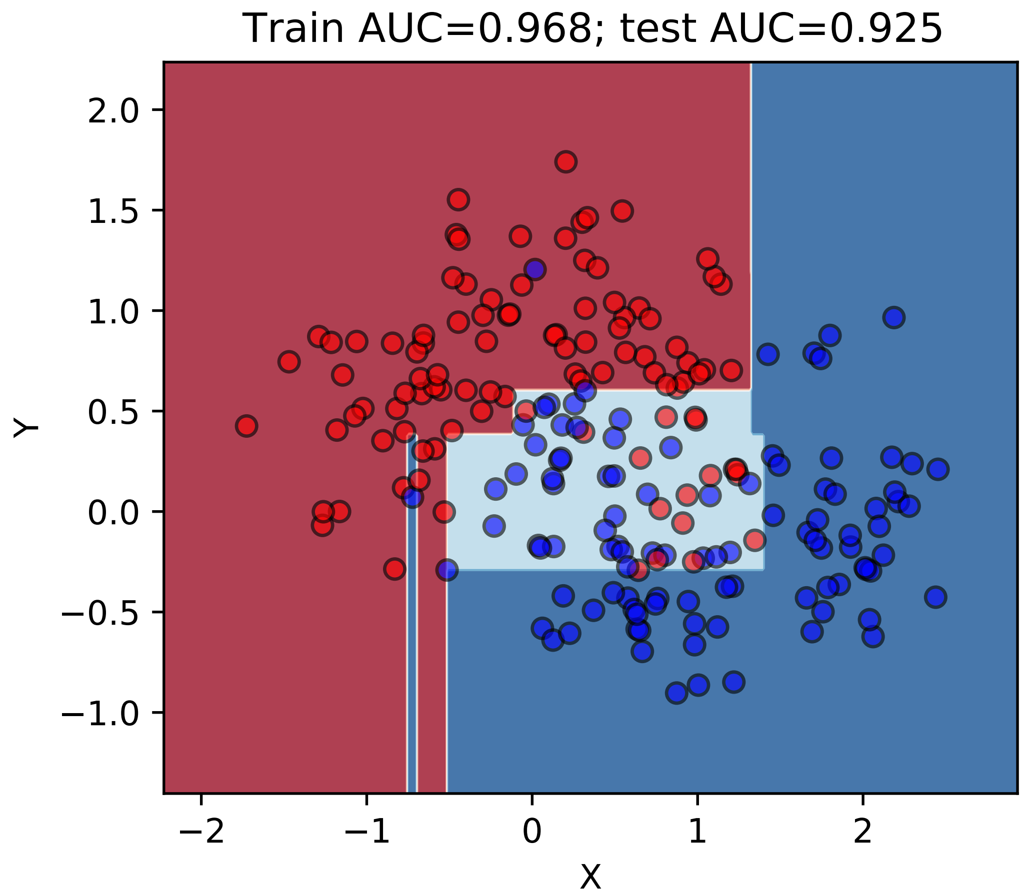

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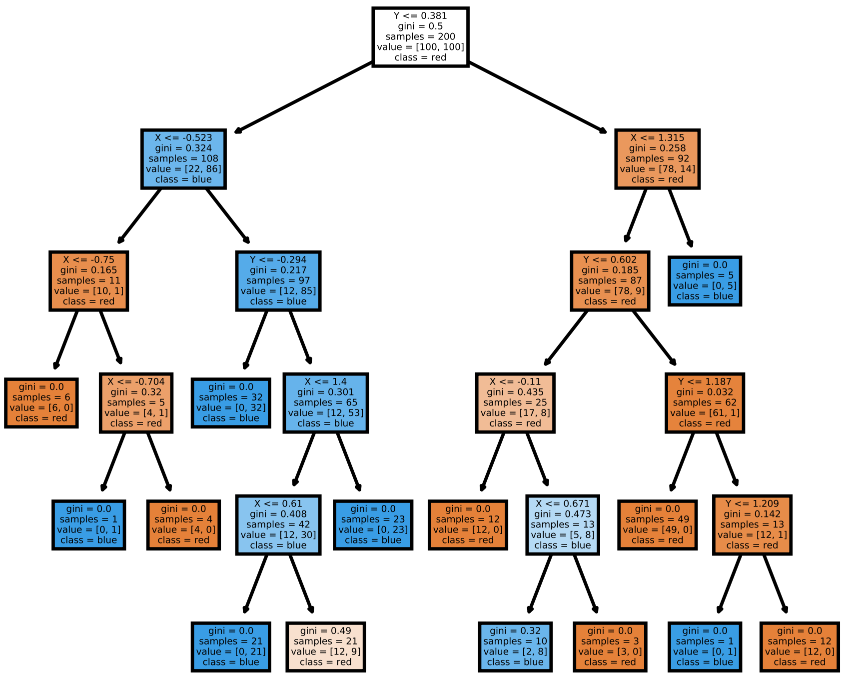

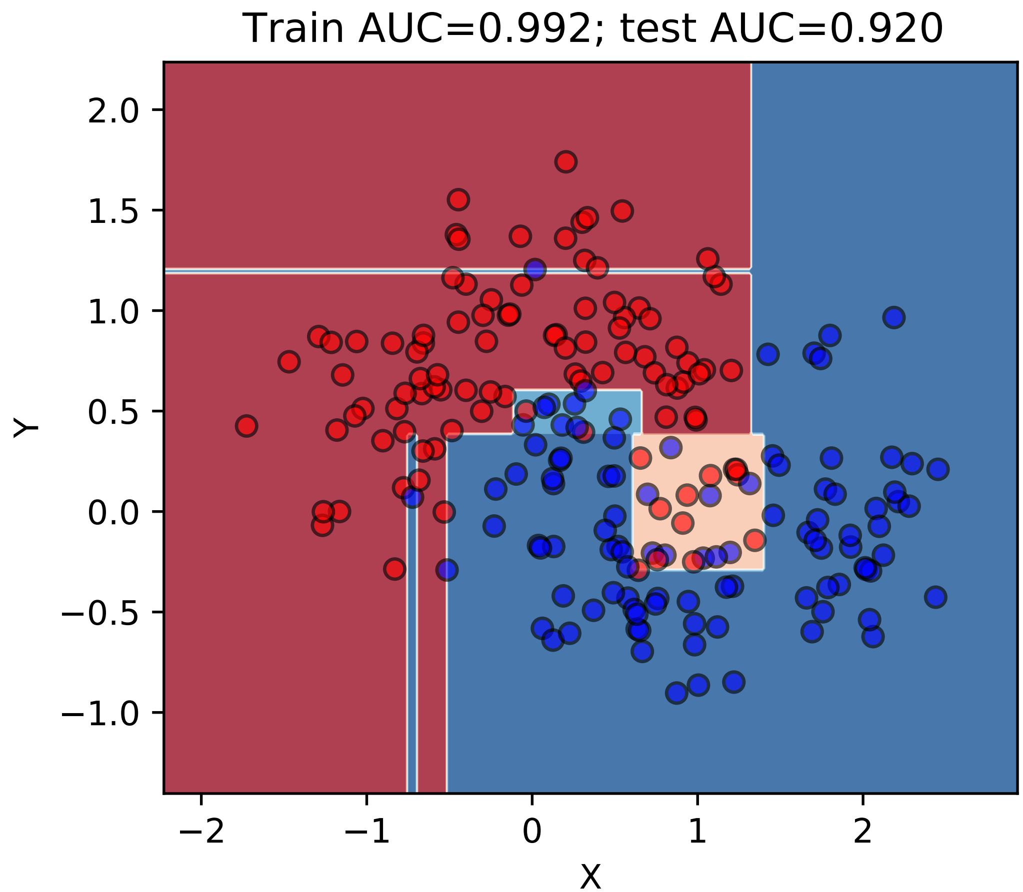

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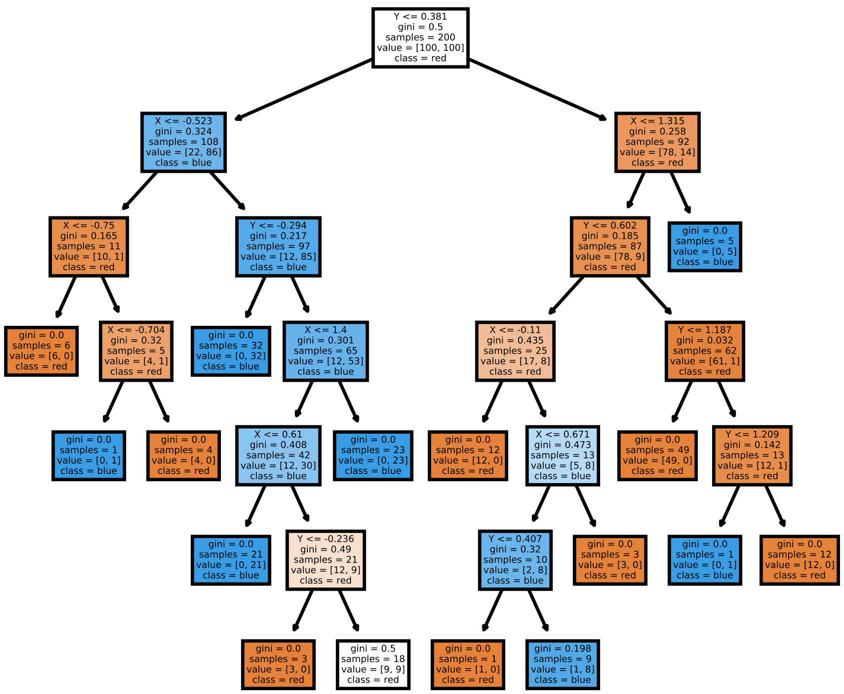

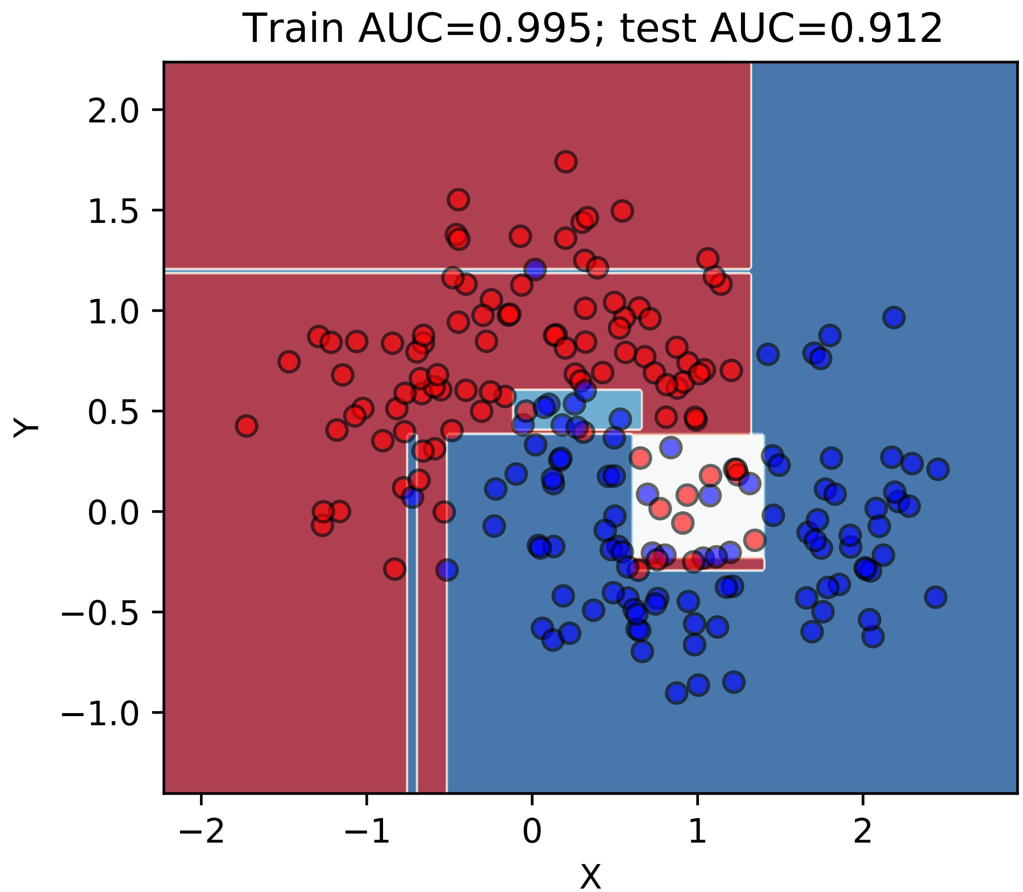

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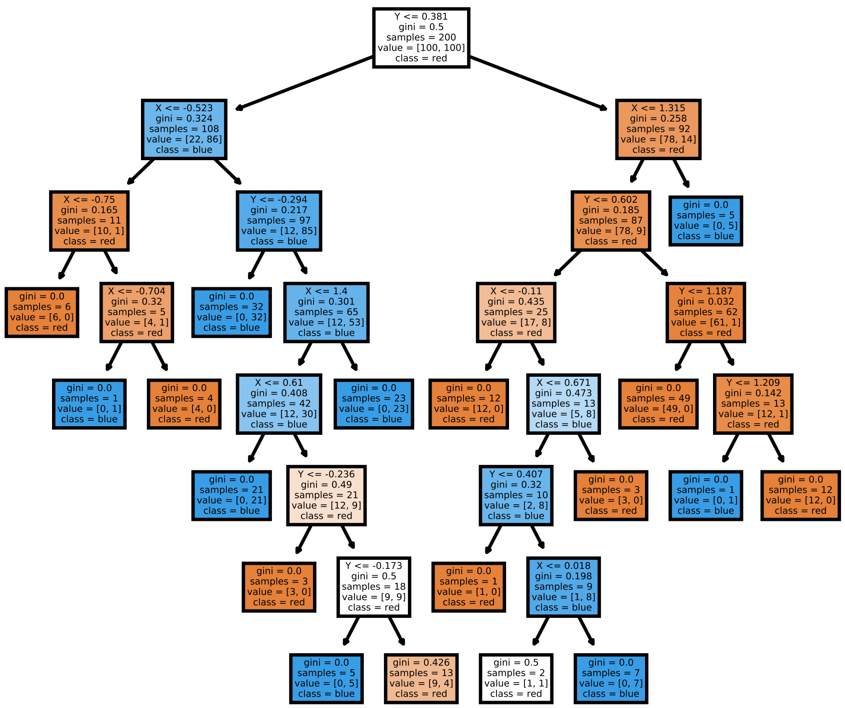

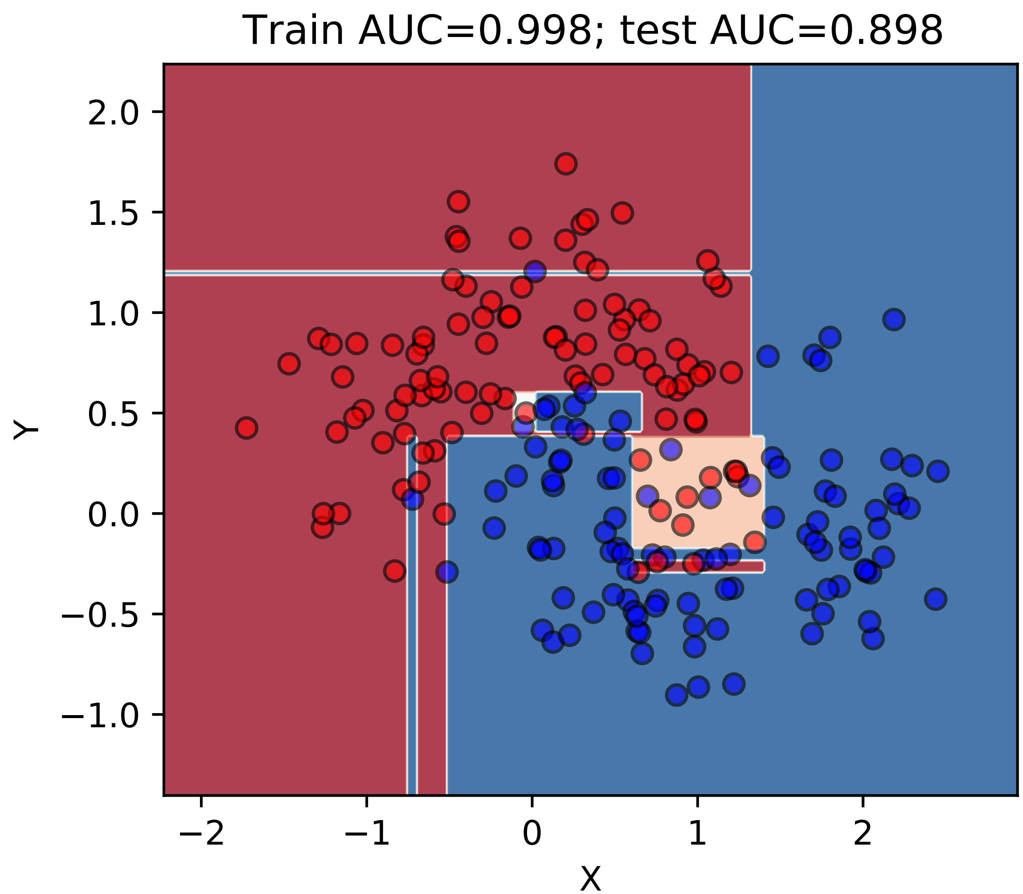

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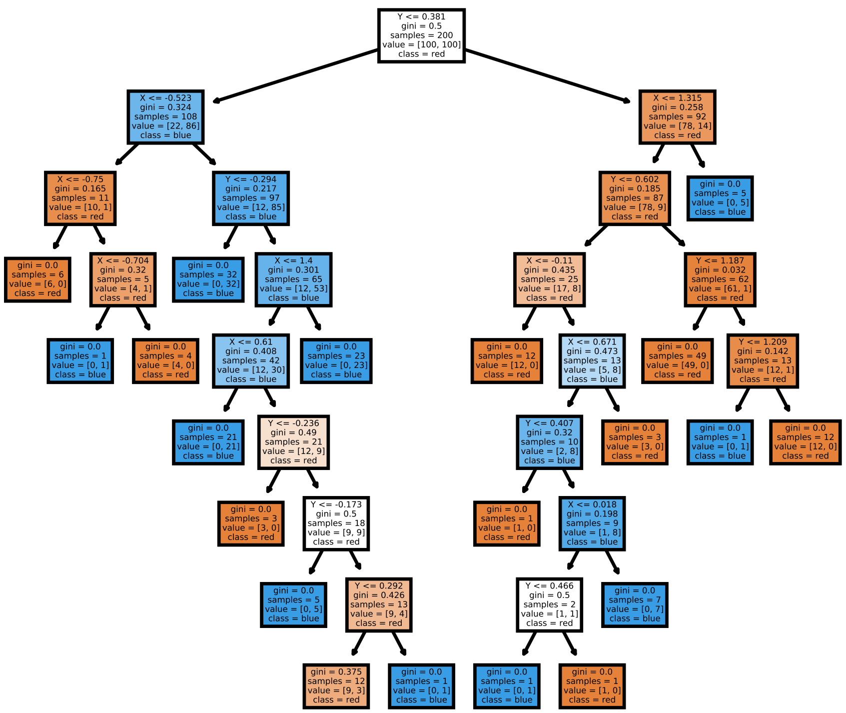

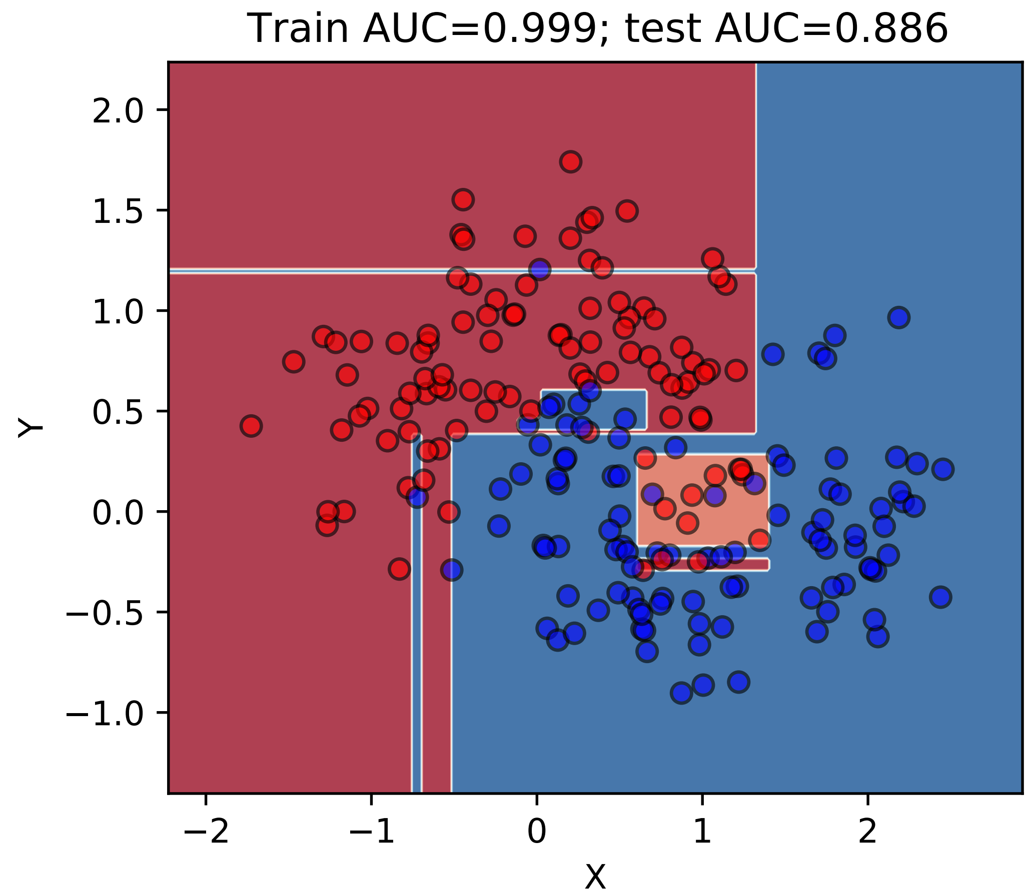

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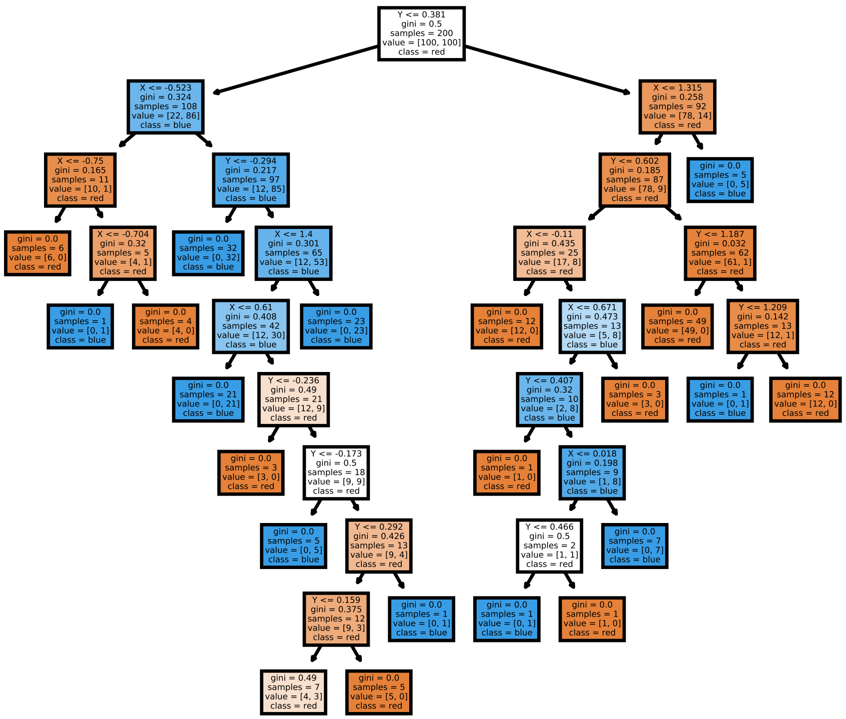

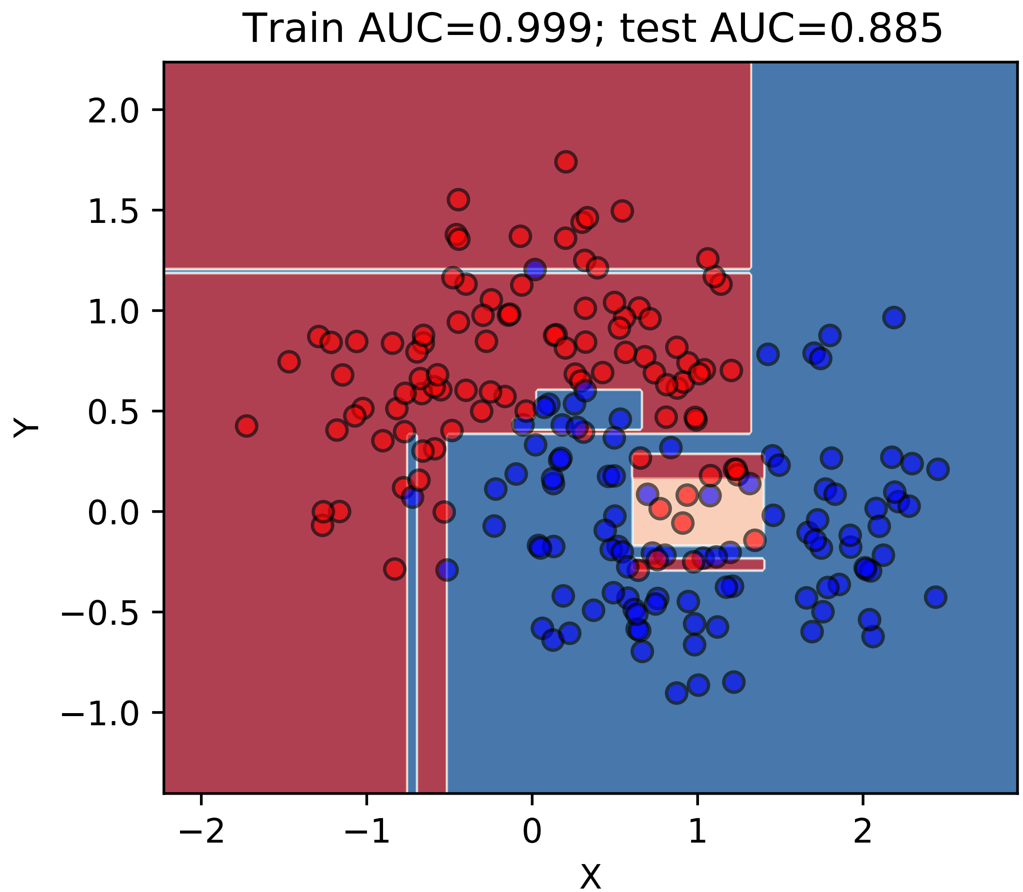

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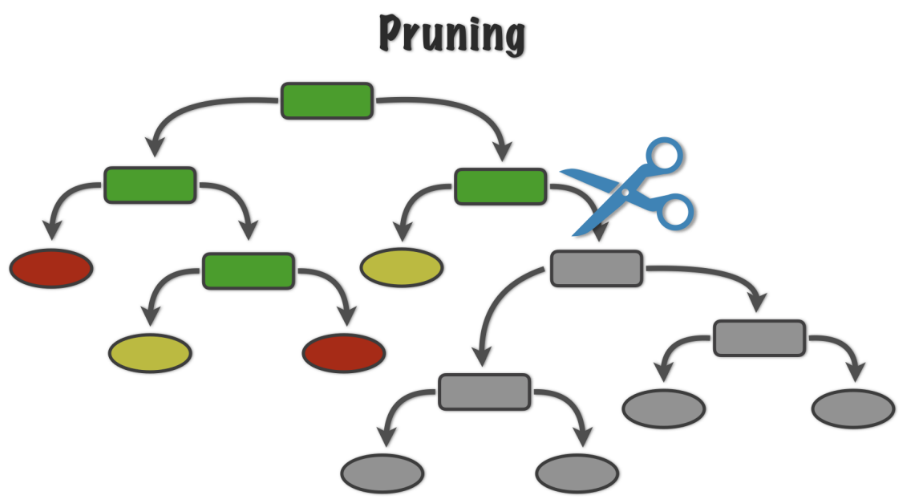
  - Constrain quality improvement
    (stop when improvement gains drop below a defined threshold)
- Typically selected via exhaustive search and cross-validation

Decision tree pruning



Picture credit: `https://alanjeffares.wordpress.com/tutorials/decision-tree/`

- Learn a large tree (effectively overfit the training set)
- Remove the least important nodes
- Often leads to better results than simply learning a smaller tree. Why?

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  - ... require little preprocessing, don't depend on the features' scale
- The bad thing:
  - sub par performance. But that can be improved with ensembles, stay tuned for the next lecture!

Acknowledgements

These slides are based on the slides for for the previous edition of the MLHEP school by Alexey Artemov.