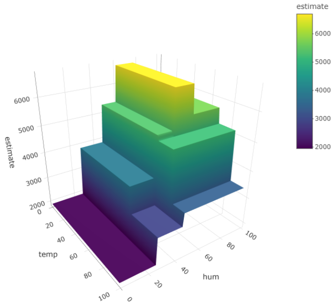
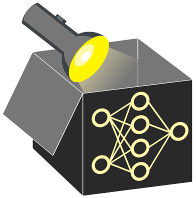
Interpretable Machine Learning

Rule-based Models

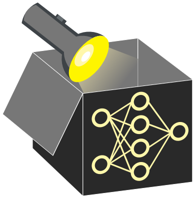


Learning goals

- Decision trees
- RuleFit
- Decision rules



DECISION TREES ▸ Breiman et al. (1984)



Idea of decision trees: Partition data into subsets based on cut-off values in features (found by minimizing a split criterion via greedy search) and predict constant mean c_m in leaf node $\mathcal{R}_m$:

$$\hat{f}(x) = \sum_{m=1}^{M} c_m \mathbb{1}_{\{x \in \mathcal{R}_m\}}$$

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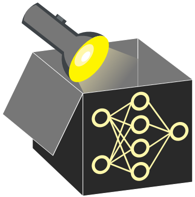

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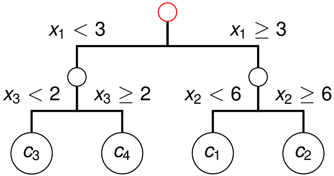
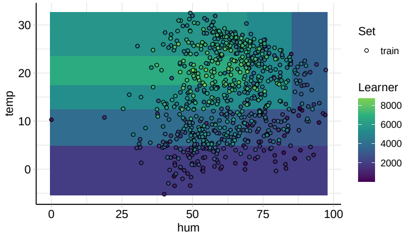
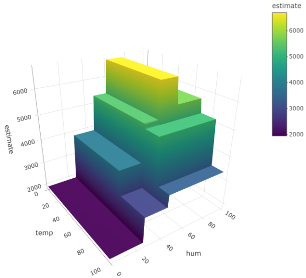
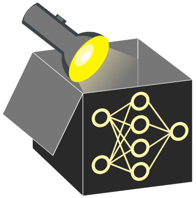


- Applicable to regression and classification
- Able to model interactions and non-linear effects
- Able to handle mixed feature spaces and missing values





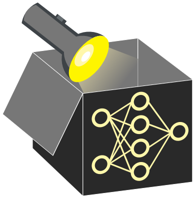
INTERPRETATION



- Directly by following the tree structure (i.e., sequence of decision rules)
- Importance of x_j: Aggregate "improvement in split criterion" over all splits where x_j was involved

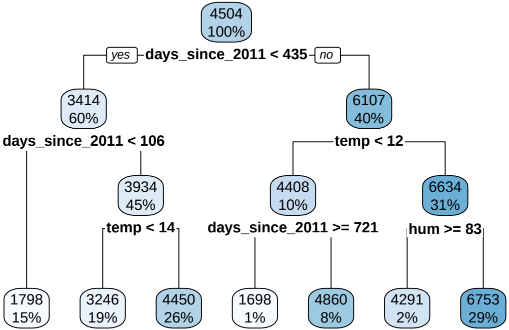
  $\leadsto$ e.g., variance for regression or Gini index for classification

DECISION TREES - EXAMPLE



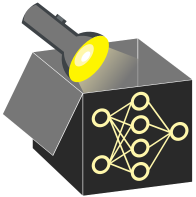
- Fit decision tree with tree depth of 3 on bike data
- E.g., mean prediction for the first 105 days since 2011 is 1798
  $\rightsquigarrow$ Applies to $\hat{=}15\%$ of the data (leftmost branch)
- $\mathrm{days\_since\_2011}$: highest feature importance (explains most of variance)

Feature	Importance
days_since_2011	79.53
temp	17.55
hum	2.92



UNBIASED RECURSIVE PARTITIONING

▸ Hothorn et al. (2006) ▸ Zeileis et al. (2008) ▸ Strobl et al. (2007)



Problems with CART (Classification and Regression Trees):

1. Selection bias towards high-cardinal/continuous features
2. Does not consider significant improvements when splitting ($\rightsquigarrow$ overfitting)

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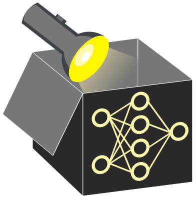

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Unbiased recursive partitioning via conditional inference trees (ctree) or model-based recursive partitioning (mob):

1. Separate selection of **feature used for splitting** and **split point**
2. Hypothesis test as stopping criteria

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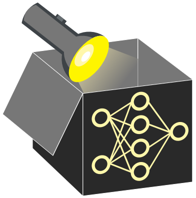

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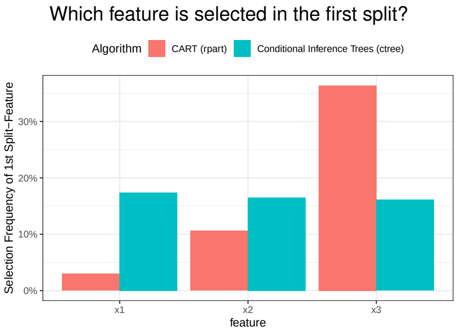
Example (selection bias):
Simulate data ($n = 200$) with $Y \sim N(0, 1)$ and 3 features of different cardinality independent from Y (repeat 500 times):

- $X_1 \sim Binom(n, \frac{1}{2})$
- $X_2 \sim M(n, (\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}))$
- $X_3 \sim M(n, (\frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}, \frac{1}{8}))$



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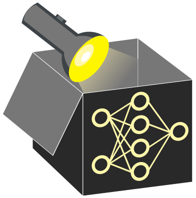

Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Parametric model (e.g. LM instead of constant) can be fitted in leave nodes
- Significance of split (p-value) given in each node
- ctree and mob differ in hypothesis test used for selecting the split feature (independence test vs. fluctuation test) and how to find the best split point

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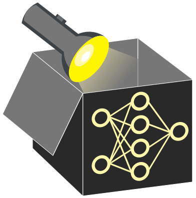

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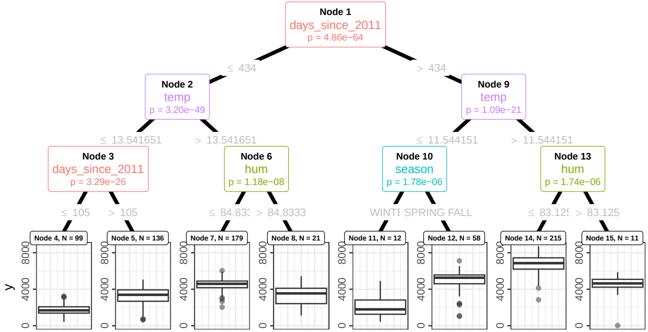
Example (ctree): Bike data (constant model in final nodes)



Train error (MSE):
758,844.0 (ctree)
742,244.4 (mob)

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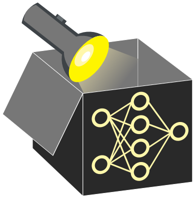

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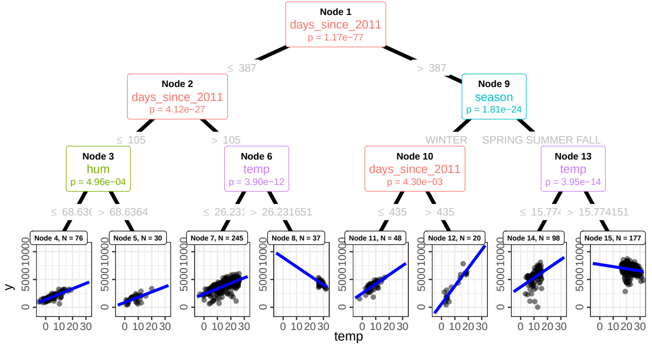
Example (mob): Bike data (linear model with temp in final nodes)



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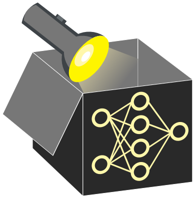
OTHER RULE-BASED MODELS



Decision Rules ▸ Holte 1993

- (Chaining of) simple “if – then” statements
  $\rightsquigarrow$ very intuitive and easy-to-interpret
- Most methods work only for classification and categorical features

IF `size=small` THEN `value=low`
IF `size=medium` THEN `value=medium`
IF `size=big` THEN `value=high`

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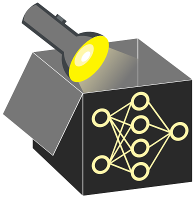

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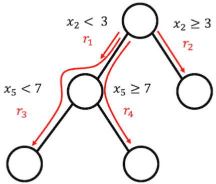
RuleFit ▸ Friedman and Popescu 2008

- Combination of LM and decision trees
- Uses (many) decision trees to extract important decision rules r_1, r_2, r_3, r_4 which are used as features in a (regularized) LM
- Allows for feature interactions and non-linearities



▸ Molnar 2022