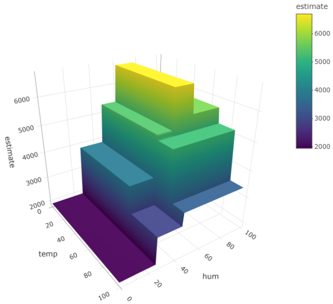
Interpretable Machine Learning

Rule-based Models

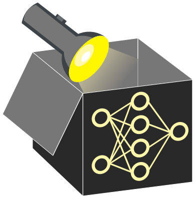


Learning goals

- Decision trees
- RuleFit
- Decision rules

DECISION TREES

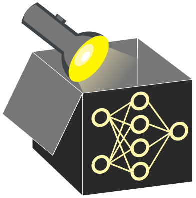
Breiman et al. (1984)



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 $\mathcal{R}_m$:

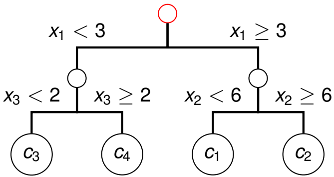
$$\hat{f}(x) = \sum_{m=1}^{M} c_m \mathbb{1}_{\{x \in \mathcal{R}_m\}}$$

DECISION TREES ▸ Breiman et al. (1984)

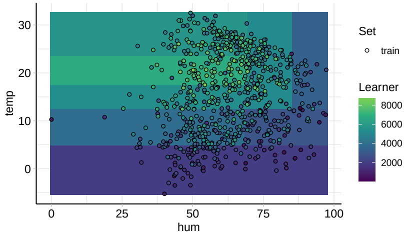


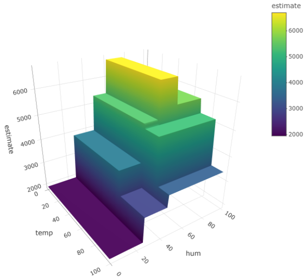
Idea of decision trees: Partition data into subsets based on cut-off values in features (found by minimizing a split criterion via greedy search) and predict constant mean c_m in leaf node $\mathcal{R}_m$:

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

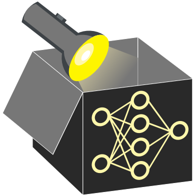


- Applicable to regression and classification
- Able to model interactions and non-linear effects
- Able to handle mixed feature spaces and missing values





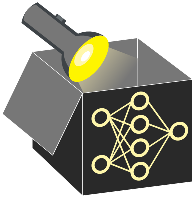
INTERPRETATION



- 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

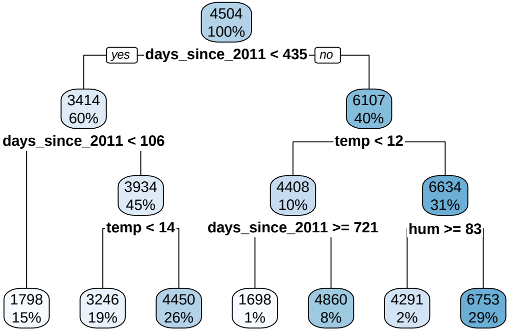
  $\rightsquigarrow$ e.g., variance for regression or Gini index for classification

DECISION TREES - EXAMPLE



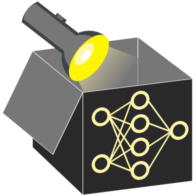
- Fit decision tree with tree depth of 3 on bike data
- E.g., mean prediction for the first 105 days since 2011 is 1798
  $\rightsquigarrow$ Applies to $\widehat{=}$15% of the data (leftmost branch)
- `days_since_2011`: highest feature importance (explains most of variance)

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)

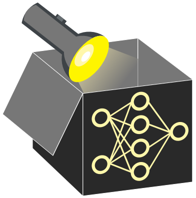


Problems with CART (Classification and Regression Trees):

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

UNBIASED RECURSIVE PARTITIONING

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



Problems with CART (Classification and Regression Trees):

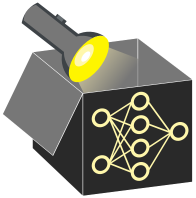
1. Selection bias towards high-cardinal/continuous features
2. Does not consider significant improvements when splitting ($\rightsquigarrow$ overfitting)

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

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 ($\leadsto$ overfitting)

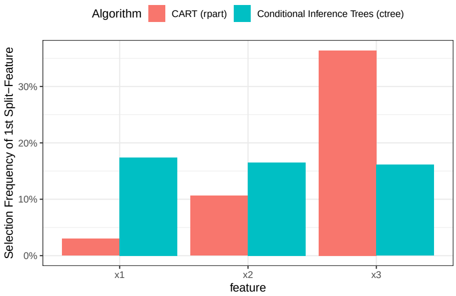
Unbiased recursive partitioning via conditional inference trees (`ctree`) or model-based recursive partitioning (`mob`):

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

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):

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

Which feature is selected in the first split?

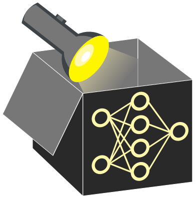


UNBIASED RECURSIVE PARTITIONING

Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Significance of split (p-value) given in each node
- Parametric model can be fitted in leave nodes
- `ctree` and `mob` differ in hypothesis test used for selecting the split feature

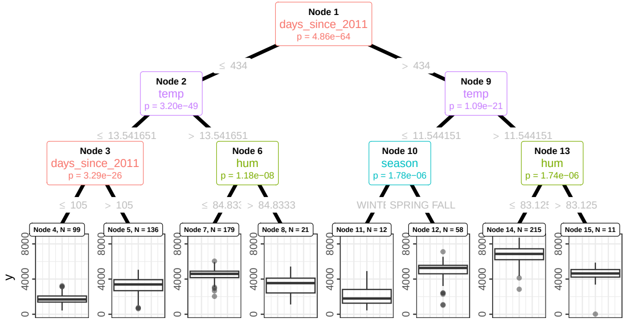
UNBIASED RECURSIVE PARTITIONING



Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Significance of split (p-value) given in each node
- Parametric model can be fitted in leave nodes
- `ctree` and `mob` differ in hypothesis test used for selecting the split feature

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

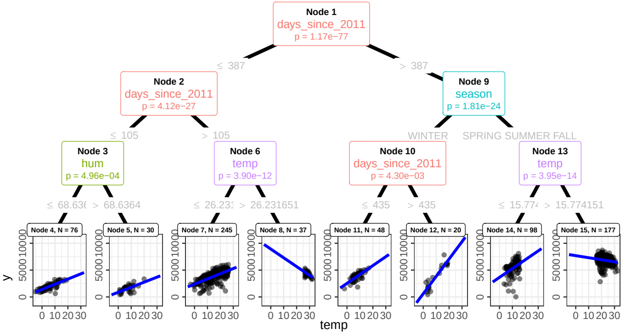


UNBIASED RECURSIVE PARTITIONING

Differences to CART:

- Two-step approach (1. find most significant split feature, 2. find best split point)
- Significance of split (p-value) given in each node
- Parametric model can be fitted in leave nodes
- `ctree` and `mob` differ in hypothesis test used for selecting the split feature

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

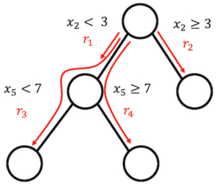


Train error (MSE): 758,844.0 (`ctree`), 742,244.4 (`mob`)

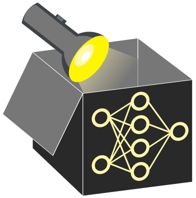
OTHER RULE-BASED MODELS

RuleFit ▸ Friedman and Popescu 2008

- Combination of LM and decision trees
- Allows for feature interactions and non-linearities

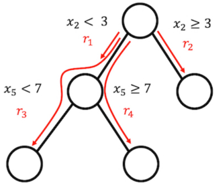


OTHER RULE-BASED MODELS



RuleFit ▸ Friedman and Popescu 2008

- Combination of LM and decision trees
- Allows for feature interactions and non-linearities



Decision Rules ▸ Holte 1993

- Simple "if – then" statements - very intuitive and easy-to-interpret
- Most methods work only for classification and categorical feat.

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

▸ Molnar 2022