Trees

Statistical Learning

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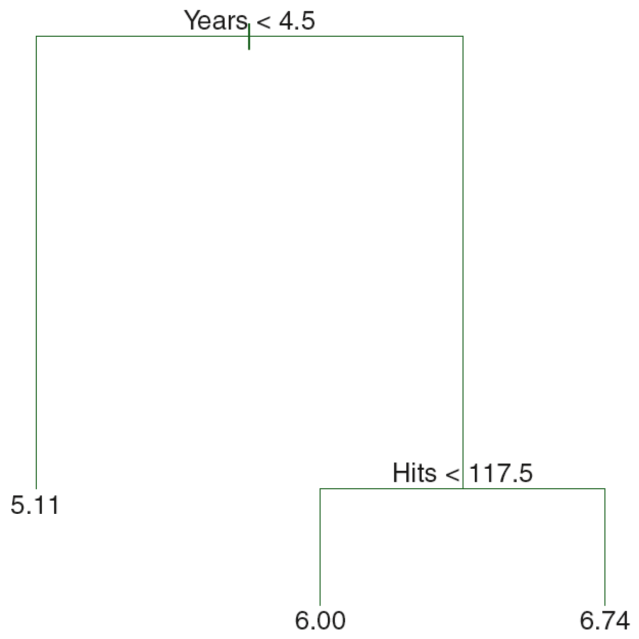
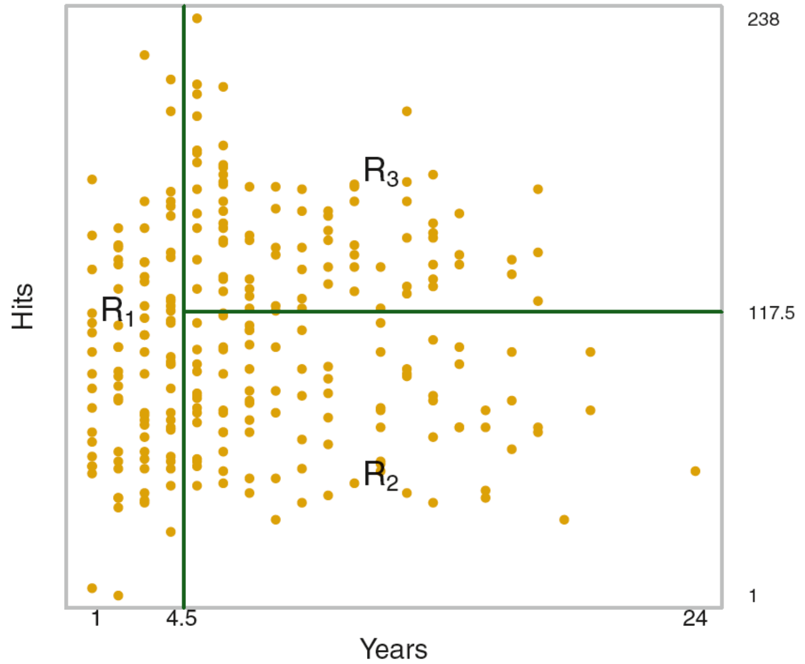
Background

- Stratify or segment the input space into a number of simple regions
- Splitting rules summarized in a decision tree
- Predictions of new observations: mean or mode of the training observations in the region
- Simple and useful for interpretation
- Not competitive with best supervised learning approaches
- Dramatic improvements when used in combination with bagging or boosting
- We focus the discussion on CART: classification and regression tree

Example

- Predicting the baseball player's salaries using regression trees
  - Inputs: years, hits, etc.
  - Output: salary (log-transformed)
    - R_1 mean log salary ($1,000) of $165,174 (5.107); R_2 $402,834; R_3 $845,346
  - Terminal nodes or leaves, internal nodes, branches
  - Easy to interpret, nice graphical representation





Regression Trees

- Two steps:
  - Divide the predictor space (set of possible values of X_1, ...X_p) into J distinct and non-overlapping regions, R_1, ..., R_J
  - For each observation that falls in R_j, the prediction will be the mean of the output values of the training observations in R_j

- How do we construct the regions, R_1, ..., R_J?
  - Regions are boxes (high dimensional rectangles)
  - Find boxes that minimize RSS:

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

    - Computationally infeasible to consider every partition into J boxes

Regression Trees (ii)

- Top-down greedy approach: recursive binary splitting
  - For each box, select the predictor X_j and the cutpoint *s* to minimize RSS within each region:

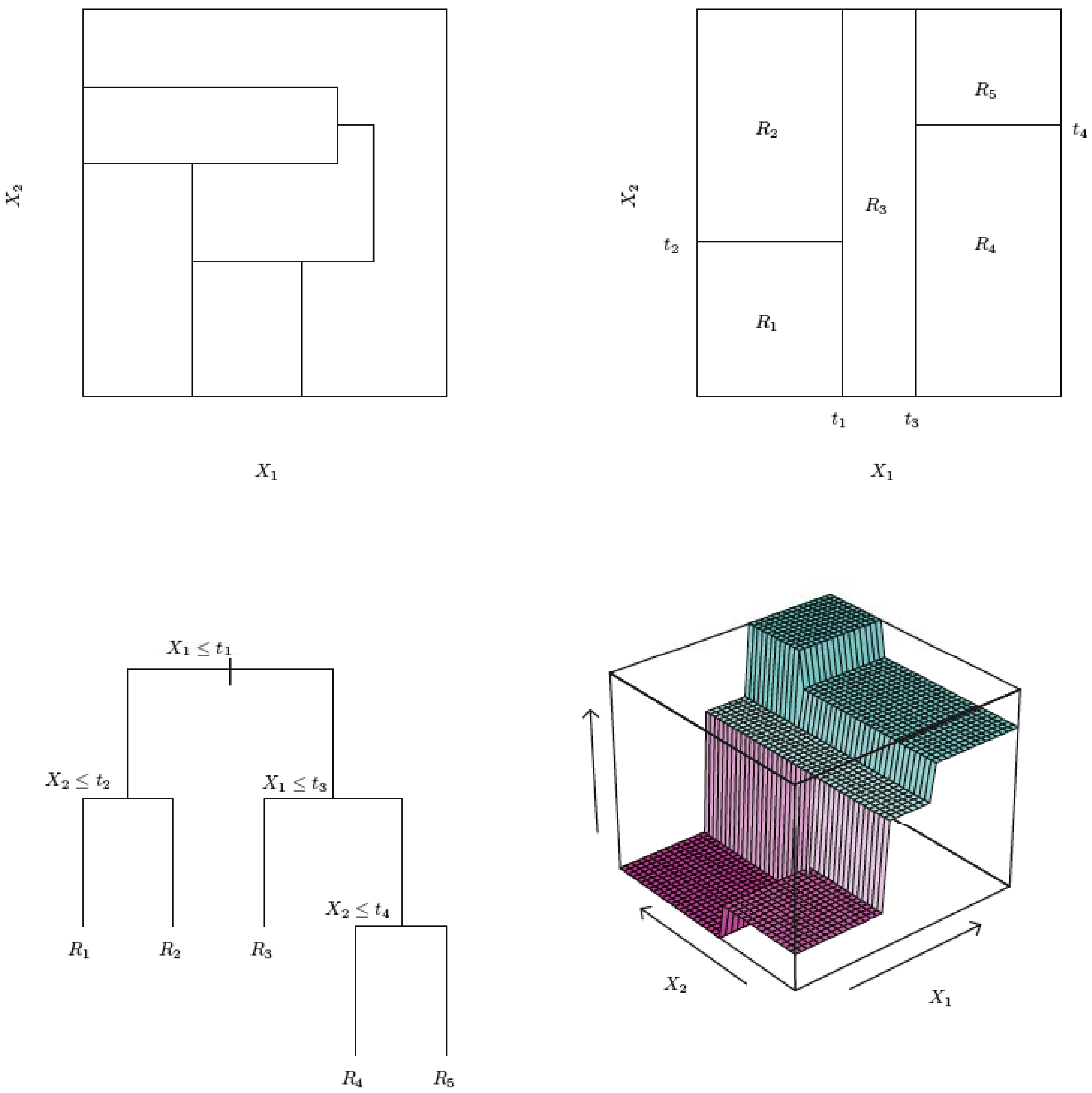
$$R_1(j,s) = \{X|X_j < s\} \text{ and } R_2(j,s) = \{X|X_j \geq s\}$$

$$\sum_{i:\ x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:\ x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

  - Continue until stopping criterion is reached: usually a minimum node size

- Predict the response of a new test observation using the mean of the training observations in the region
  - Predict the confidence: standard deviation

Example



Tree Pruning

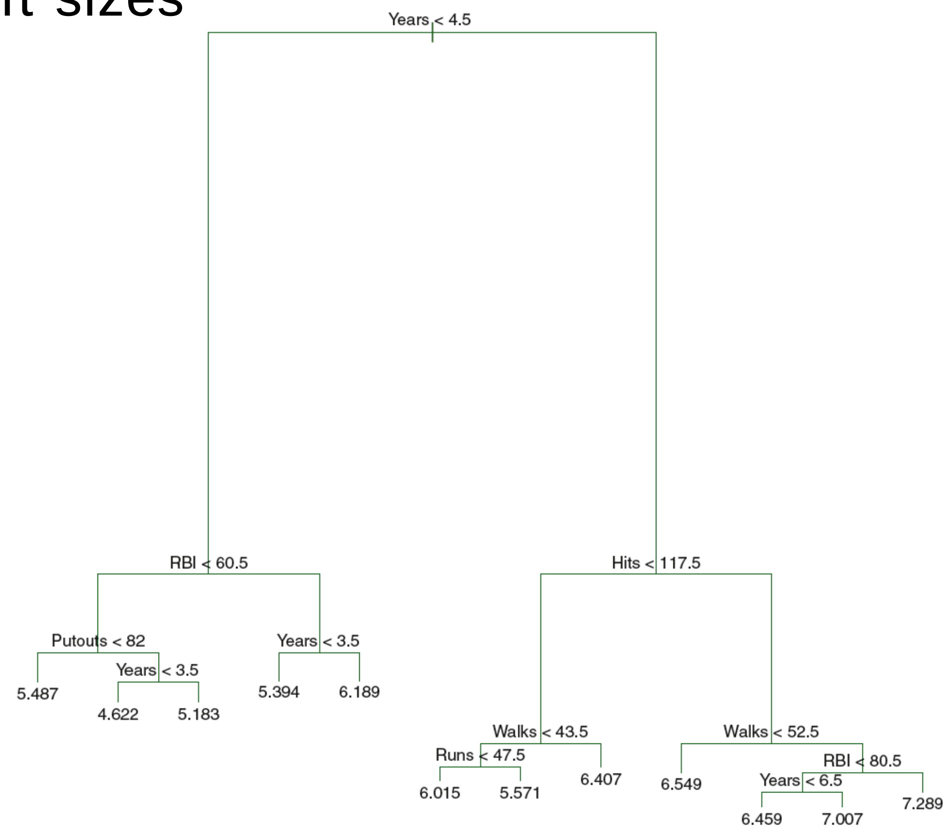
- The previous method generates complex trees: overfitting
- Smaller tree: lower variance, better interpretation, slightly higher bias
- One possible solution: build the tree so long as the decrease in RSS due to a split exceeds some threshold
  - Smaller trees, but short sighted strategy: a worthless split may be followed by a very good split later on
- A better strategy: grow a large tree, and prune it back
  - Best way to prune?
    - Cross-validation: extremely large number of subtrees
    - Cost complexity pruning (weakest link pruning)

Cost Complexity Pruning

- Collapse the internal node that produces the smallest per-node increase in:

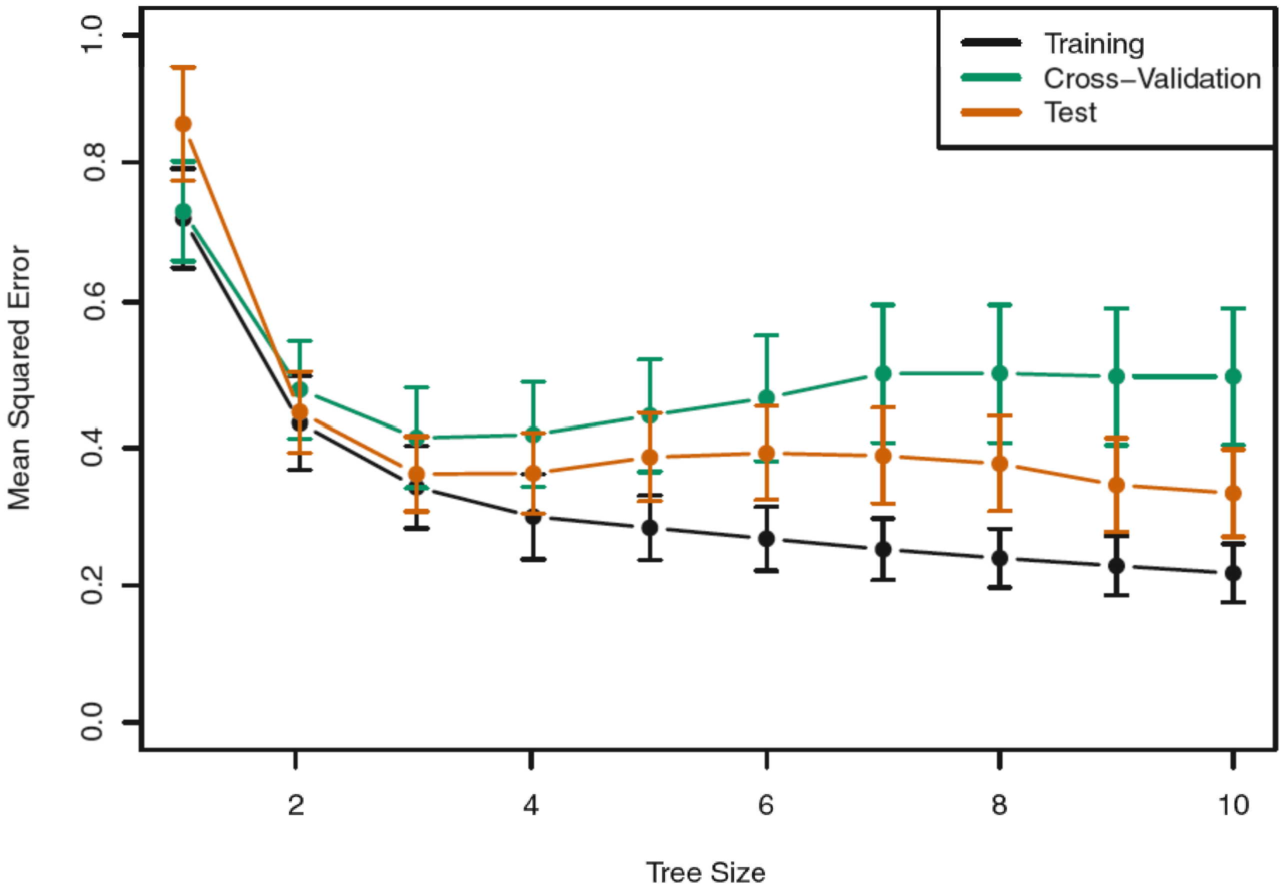
$$\sum_{m=1}^{|T|} \sum_{i:\, x_i \in R_m} (y_i - \hat{y}_{R_m})^2$$

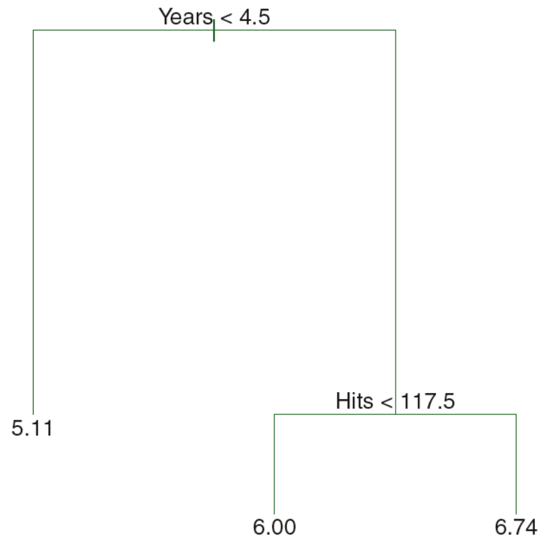
- Sequence of trees with different sizes
- Example: hitters data
  - Tree learned with 9 features
  - Training: 132 examples
  - Test: 131 examples
  - Unpruned tree



Example (hitters data)

- Six-fold cross-validation (number of examples multiple of 6)
- Minimum error: three node tree





Classification Trees

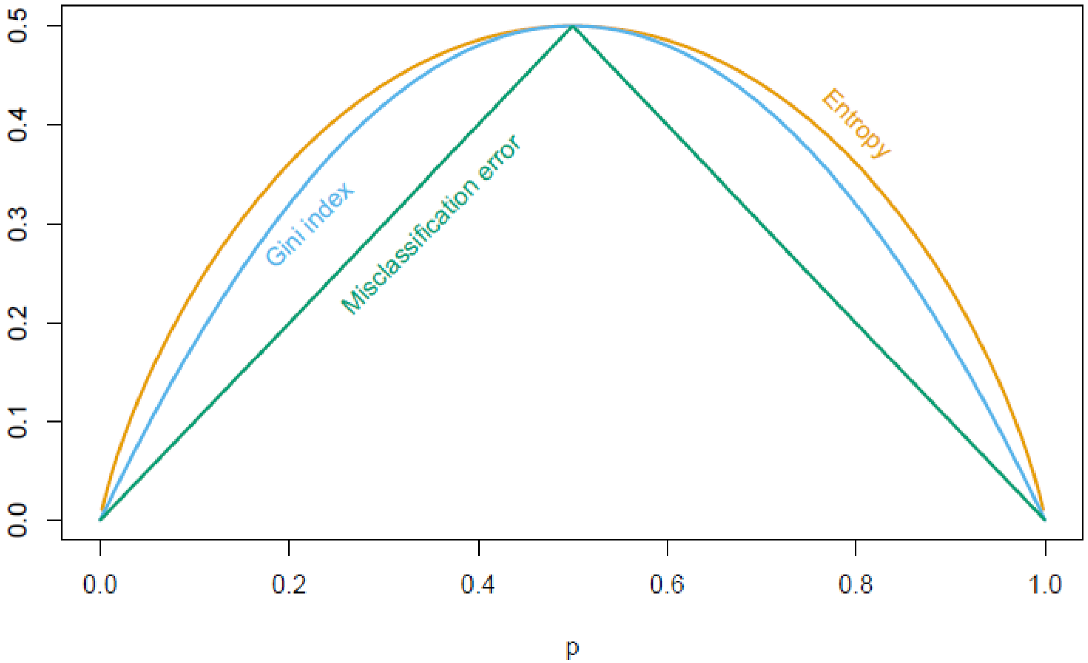
- Similar to a regression tree, but with qualitative response
- Predicted class: most commonly occurring class of training observations in the region to which it belongs
  - We are also interested in the class proportions among the training observations in that region
- Tree growing: recursive binary splitting (as in regression)
  - RSS cannot be used
  - A natural alternative: classification error rate
    - Fraction of the training observations of a region that do not belong to the most common class
    - $E = 1 - \max_k(\hat{p}_{mk})$ for the m-th region
    - Not sufficiently sensitive for tree-growing

Classification Trees (ii)

- Two other measures are preferable
- Gini index:
  - $$G = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$$
  - Total variance across the K classes
- Cross-entropy:
  - $$D = -\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}$$

Node impurity measures for two-class classification

Cross-entropy has been scaled



Classification Trees (iii)

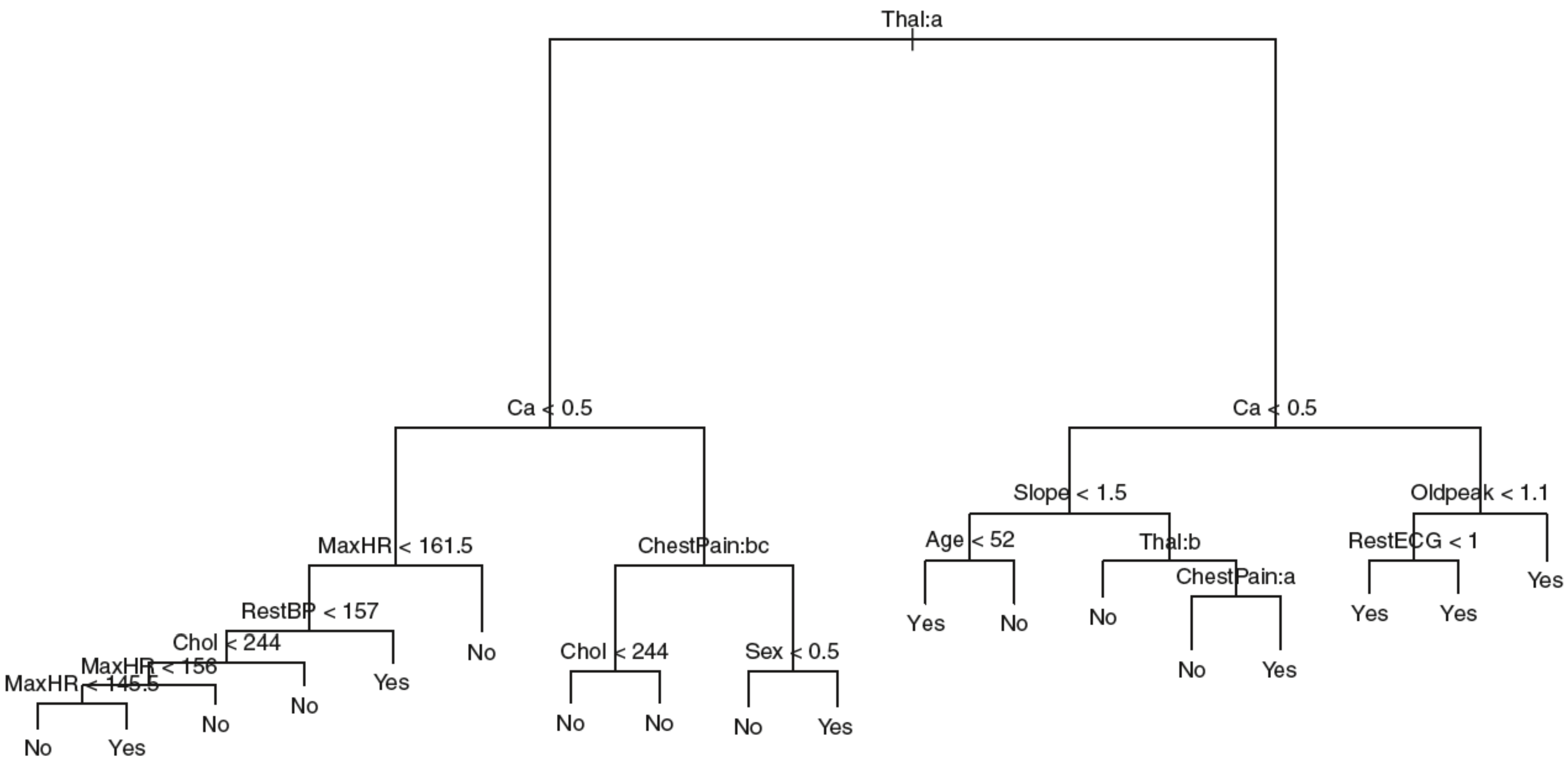
- We need to weight the node impurity measures by the number of observations in the two created child nodes

- For building the tree:
  - Gini index and cross-entropy are preferable: more sensitive to node purity

- For pruning the tree:
  - Any of the three approaches might be used
  - Classification error rate is preferable if prediction accuracy of the final pruned tree is the goal

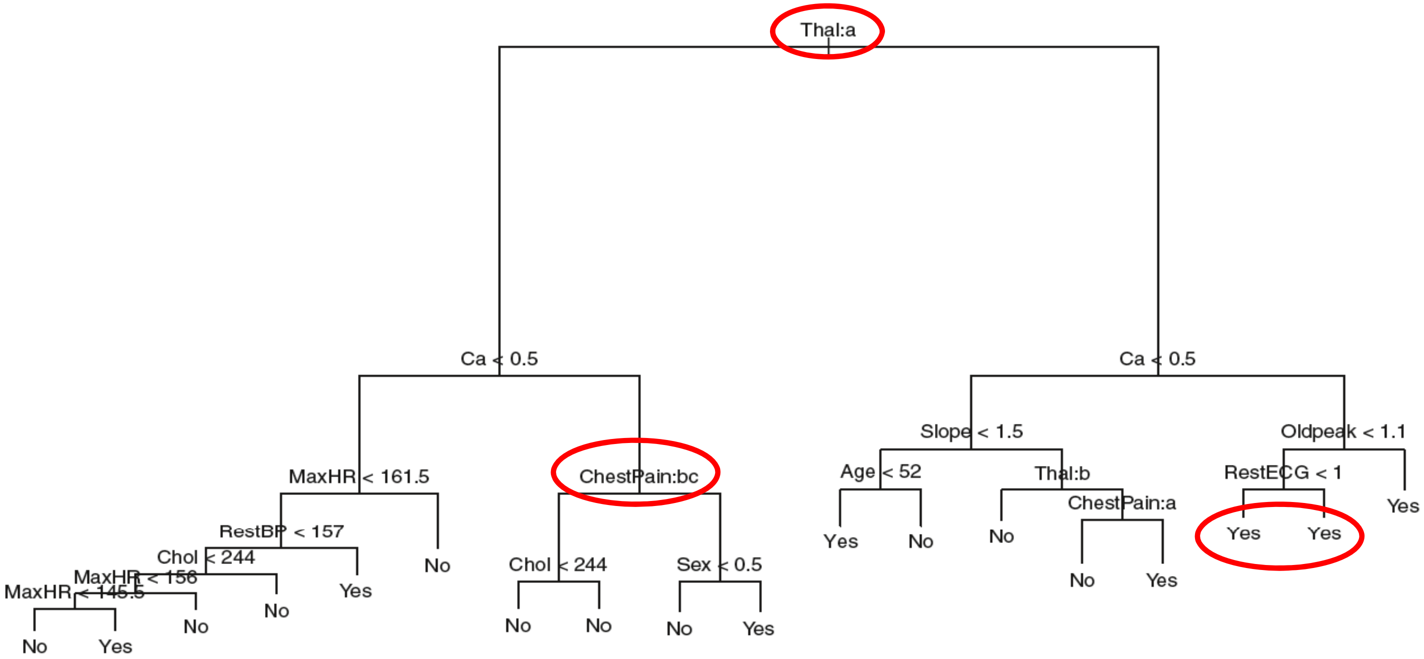
Example: Heart dataset

- Binary outcome (HD) for 303 patients
  - HD: Yes (heart disease) or No
- 13 predictors: Age, Sex, Chol (cholesterol measurement), Thal (Thalium stress test), ChestPain, ...
  - Categorical (qualitative) predictors: Sex, Thal, ChestPain

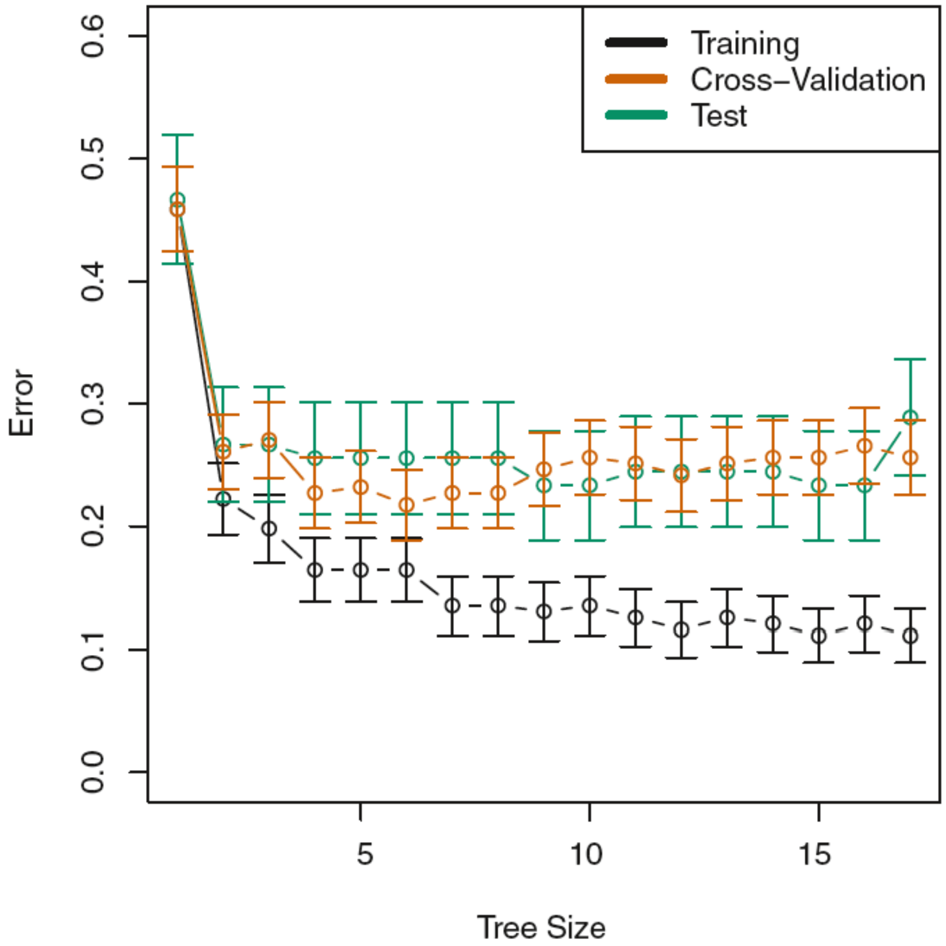


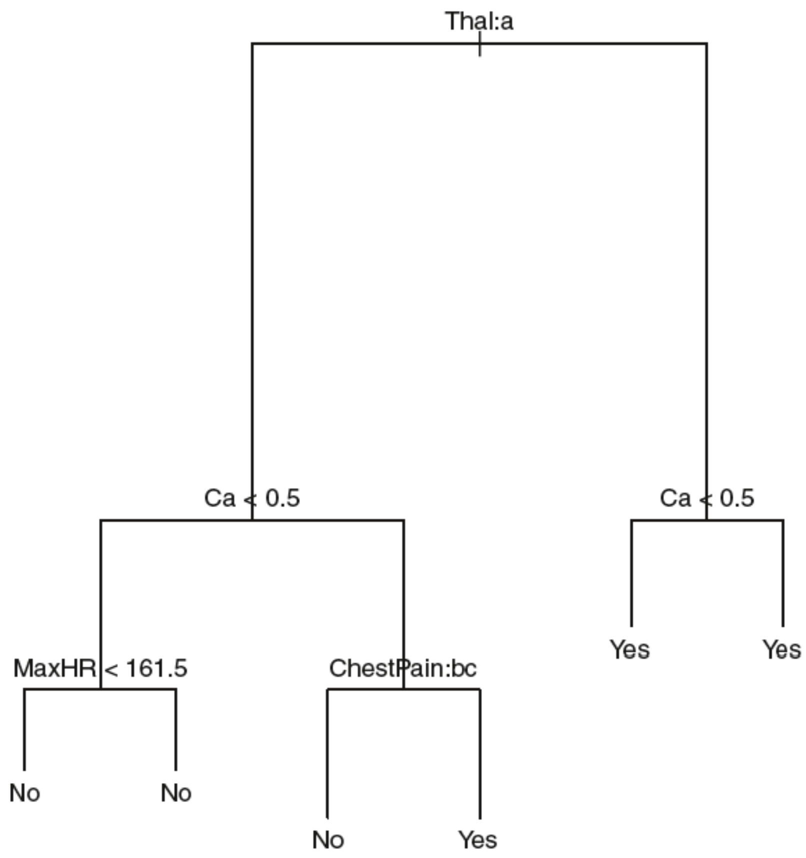
Example: Heart dataset (ii)

- ChestPain: (a) typical angina, (b) atypical angina, (c) non-anginal pain, (d) asymptomatic
- RestECG: increased node purity
  - Improves Gini index and cross-entropy
  - Classification error not improved
  - Right-hand leaf: 9/9 observations with response value Yes
  - Left-hand leaf: 7/11 observations with response value Yes



- Best tree: six nodes





Categorical predictors

- q values: $2^{q-1}-1$ possible partitions into two groups
- In a two-class problem: order the predictor classes according to the proportion falling in outcome class 1
  - Then split as an ordered predictor
  - Optimal split in terms of Gini index and cross-entropy
- This also holds for regression (RSS)
  - Order the categories by increasing mean of the outcome
- For multi-category outcomes no such simplifications are possible
- Try to avoid variables with large q: overfitting

Trees vs. Linear Models

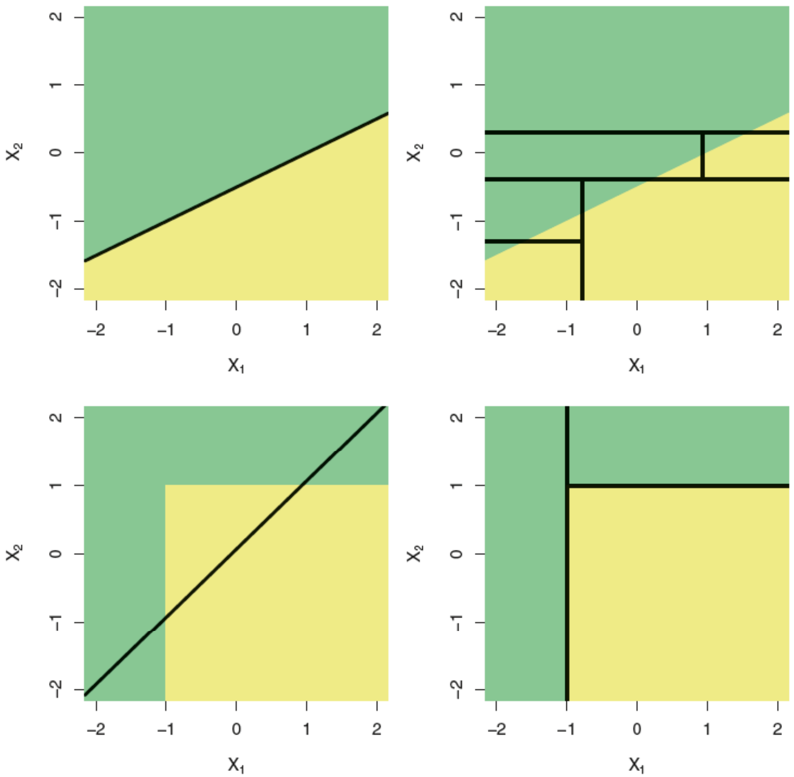
- Linear regression: $f(X) = \beta_0 + \sum_{j=1}^{p} X_j \beta_j$

- Regression trees: $f(X) = \sum_{m=1}^{M} c_m \cdot 1_{(X \in R_m)}$

- A two-dimensional classification example:

Linear model is better

Tree is better



Advantages and Disadvantages of trees

- Pros:
  - Easy to explain
  - More closely mirror human decision-making
  - Can be displayed graphically, and are easily interpreted
  - Can handle qualitative predictors without the need to create dummy variables

- Cons:
  - Predictive accuracy is lower than other approaches

Bibliography

- G. James, D. Witten, T. Hastie, y R. Tibshirani, An Introduction to Statistical Learning with Applications in R. Springer, 2013.
  - Chapter 8, Sec. 8.1.

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  - Chapter 9, Sec. 9.2.