Introduction to Data Science

Winter Semester 2019/20

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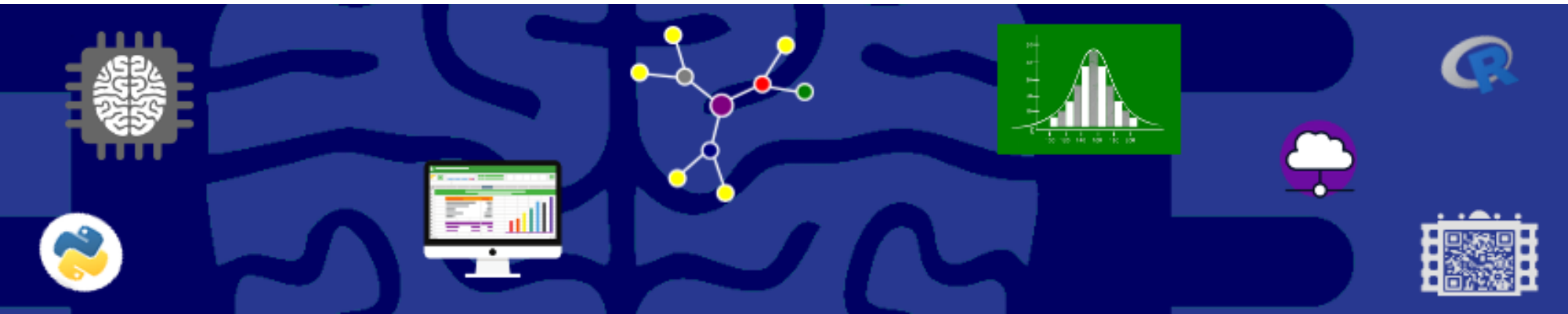
Lecture Slides



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Tree-Based Methods

Chapter overview

- In previous chapter, considered *piecewise* approximation for univariate models (piecewise constant, splines, etc.).
- Here: piecewise constant *multivariate approximation*.
- Much greater variety of possible domain partitions.
- **Recursive binary partitioning**: efficient representation using **binary trees**.
- Can be used for regression and classification.
- Refinements: **bagging**, **random forests**, **boosting**.

Contents

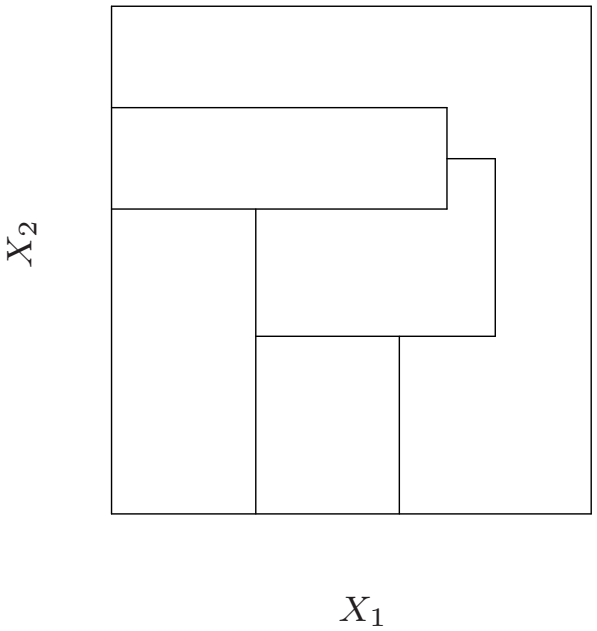
Tree-Based Methods

Basic idea

- Consider bivariate model

$$Y = f(X_1, X_2), \quad X_i \in [0, 1].$$

- Divide feature space into axis-aligned rectangles.
- Within each rectangle, predict Y as the mean of the observations it contains.

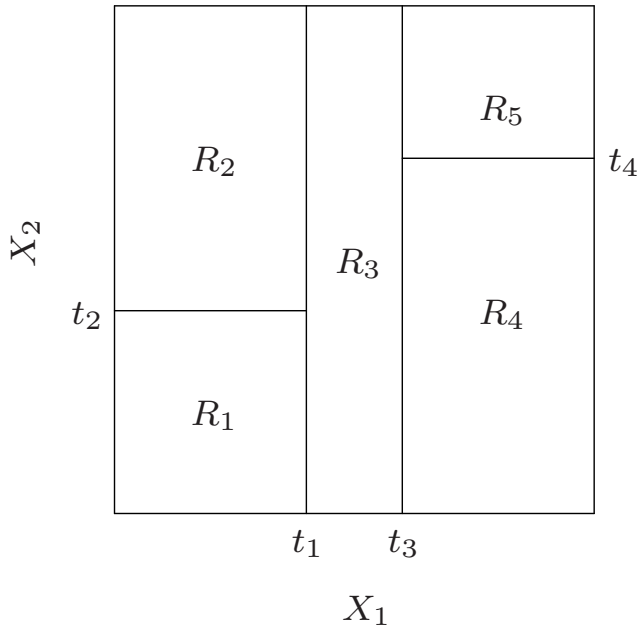


Tree-Based Methods

Basic idea

- Simpler structure: construct rectangles by **recursive binary partitioning**.
- Predicting $Y = \hat{y}_{R_m}$ in region R_m yields piecewise constant model

$$Y = \hat{f}(X) = \sum_{m=1}^{5} \hat{y}_{R_m} \mathbb{1}_{\{X \in R_m\}}$$



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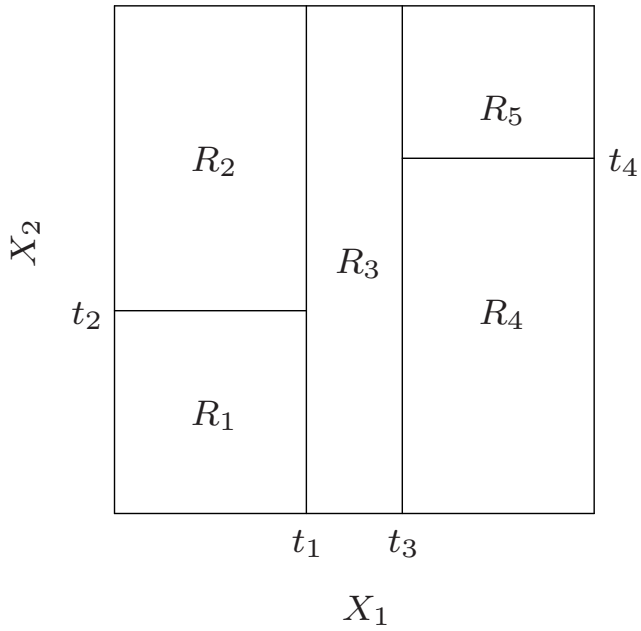

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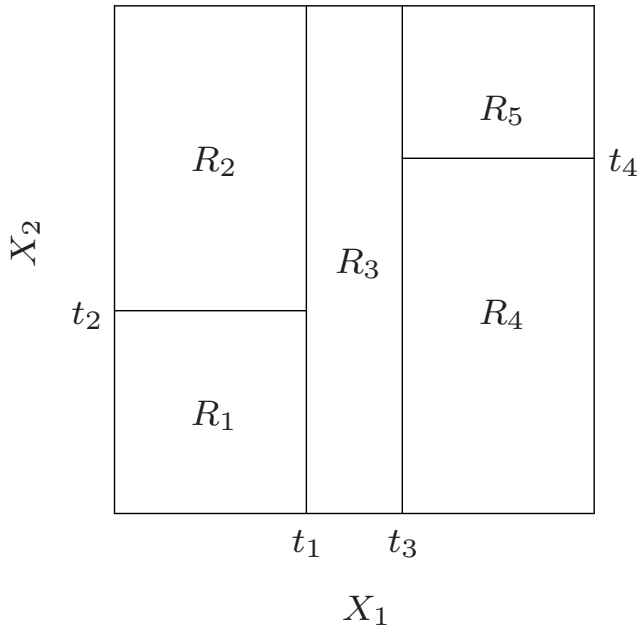

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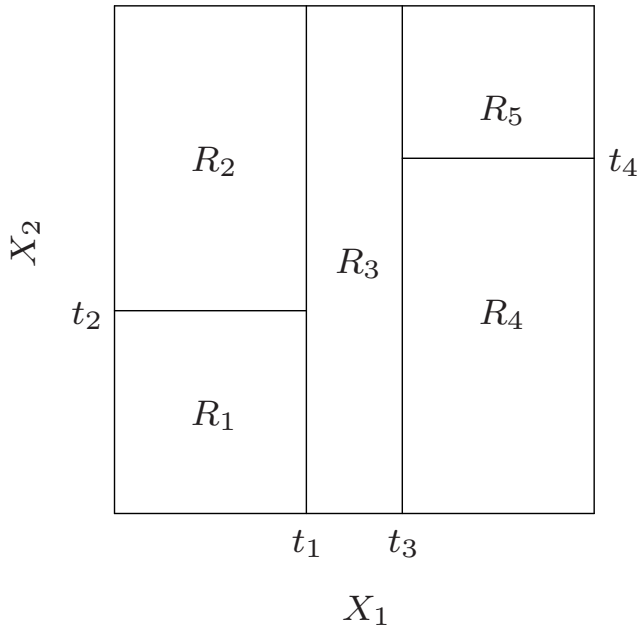

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  - Finally: region $X_1 > t_3$ is split at $X_2 = t_4$.

Tree-Based Methods

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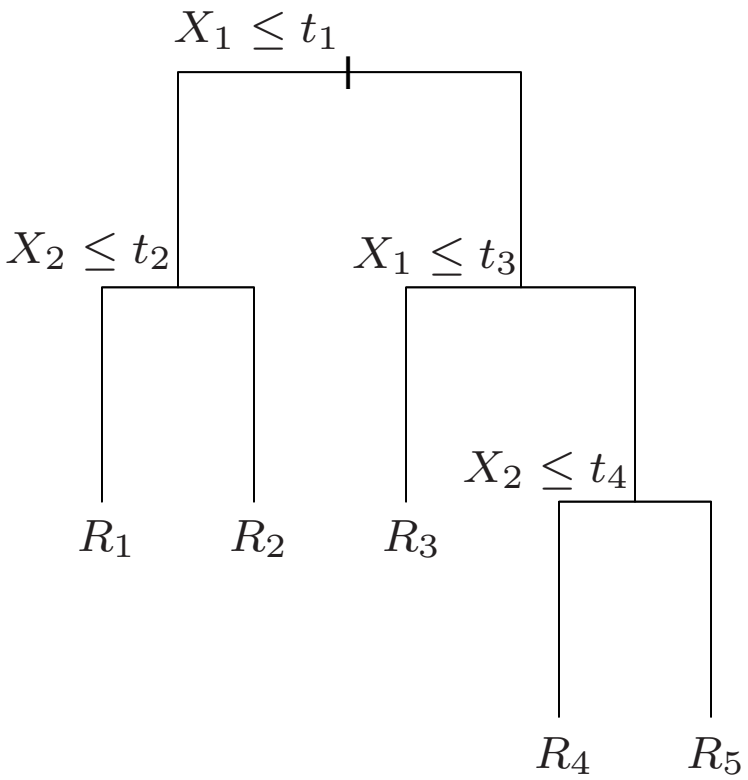

Recursive binary partition more conveniently represented by a binary tree; regions appear as **leaves**, internal nodes are the splits.

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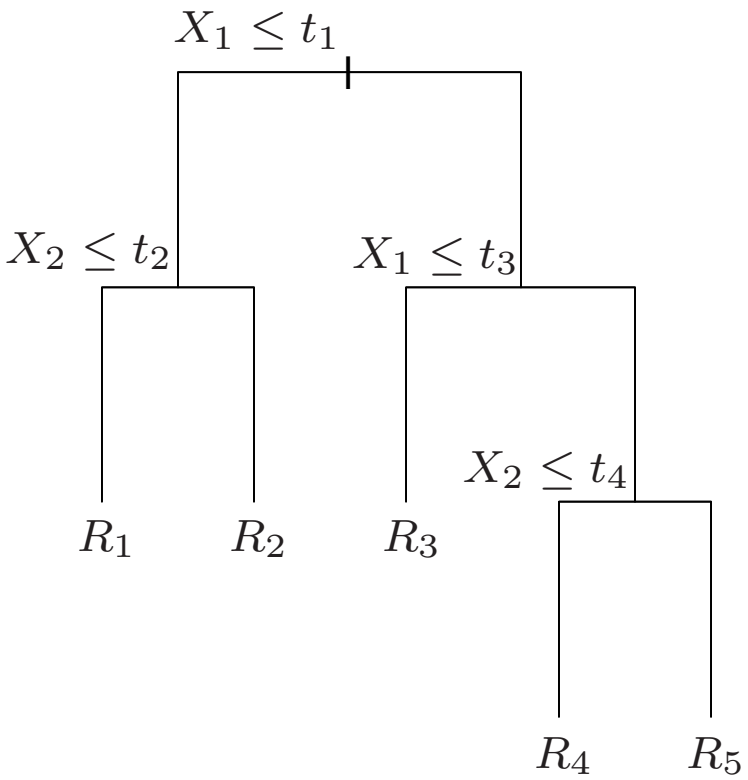

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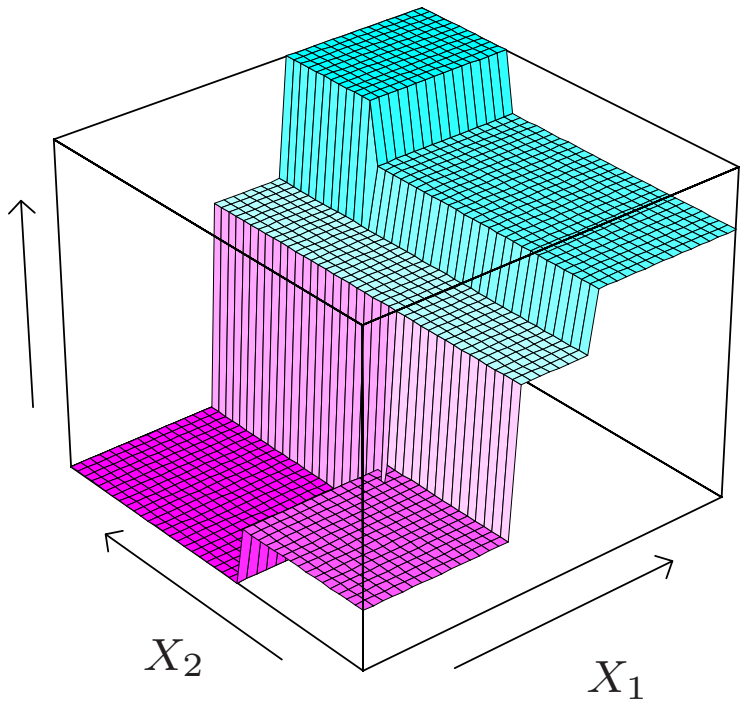

Equivalent representation as piecewise constant function.

Tree-Based Methods

Hitters example

- `Hitters` data set: predict baseball player's `Salary` based on

  `Years`: # years played in major leagues
  `Hits` : # hits made in previous year

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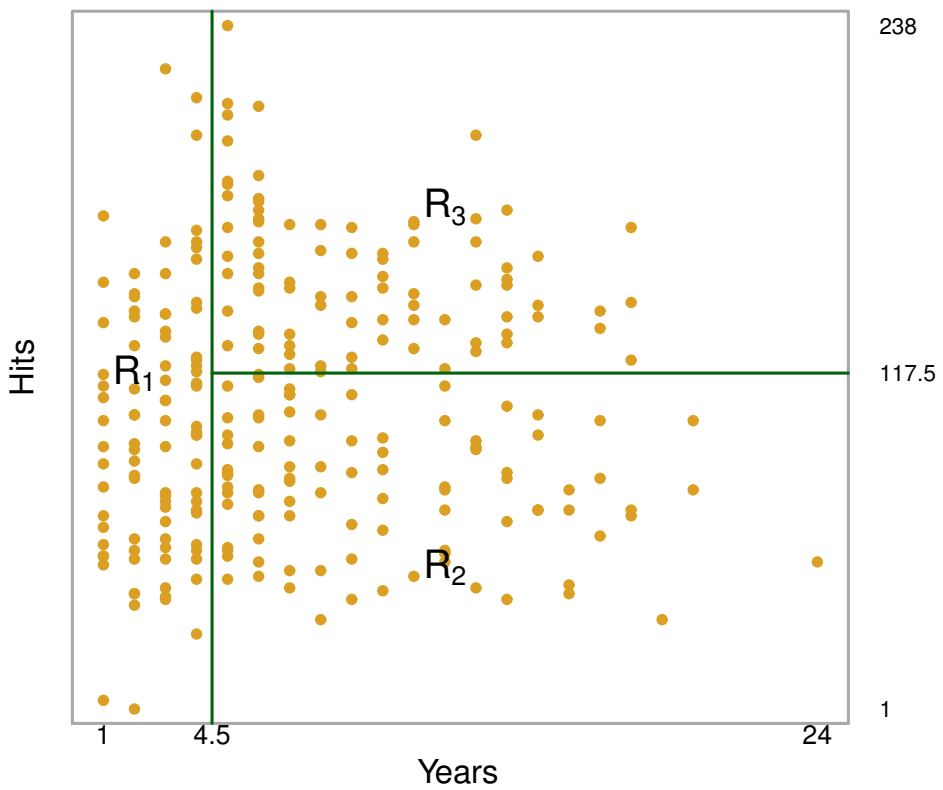
- First remove observations missing `Salary` values.
- Log-transform `Salary` values [k$] to make distribution more bell-shaped.

Tree-Based Methods

Hitters example



Observations of `Years` and `Hits` with partitioning arising from two splits.

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  $R_1 = \{X : \texttt{Years} < 4.5\}$.

Tree-Based Methods

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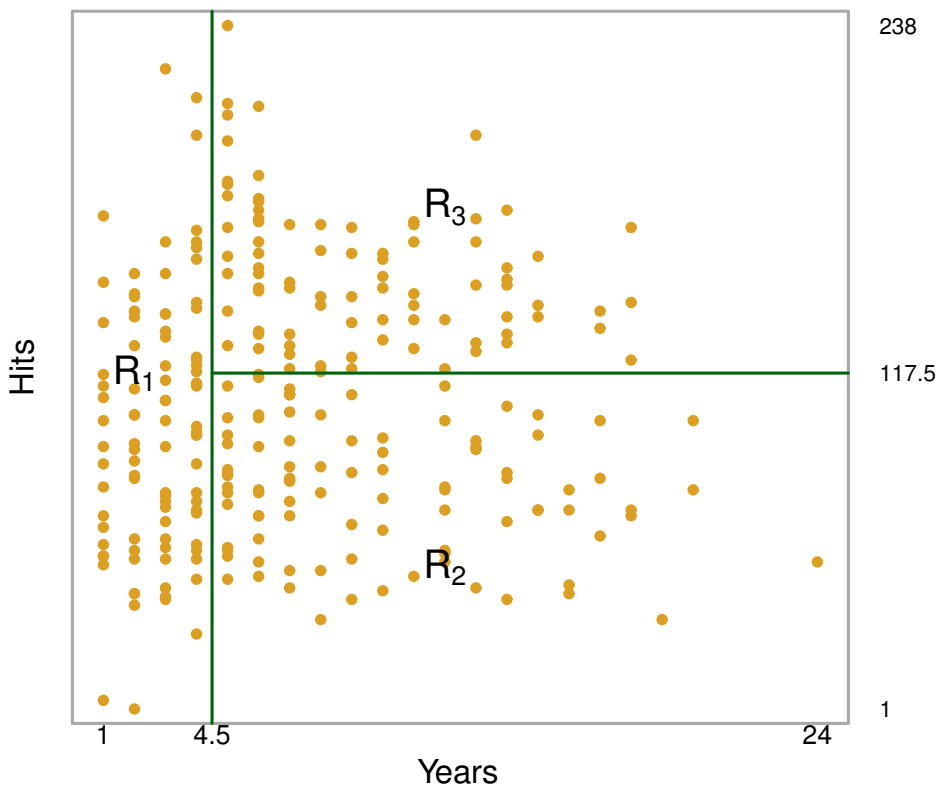

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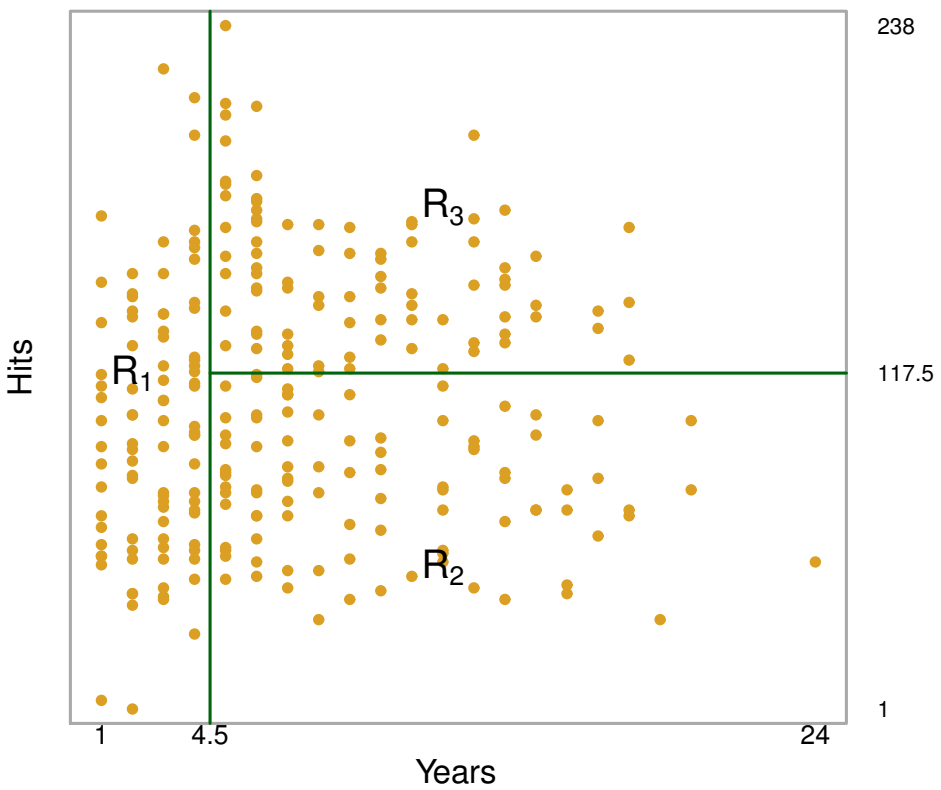

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- Predicted `Salary` in these regions:
  $R_1 : \$1000 \times \mathrm{e}^{5.107} = \$165,174,$
  $R_2 : \$1000 \times \mathrm{e}^{5.999} = \$402,838,$
  $R_3 : \$1000 \times \mathrm{e}^{6.740} = \$845,346.$

Tree-Based Methods

Hitters example

- Left **branch** contains R_1, right branch R_2 and R_3.

Regression tree resulting from these splits.

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- Advantages of tree: easily interpretable, nice graphical representation.
- Known as **CART**: classification and regression tree.

- **Goal:** Partition feature space into high-dimensional rectangles $\{R_m\}_{m=1}^M$ in such a way that

$$\text{RSS} = \sum_{m=1}^{M} \sum_{i \in R_m} (y_i - \hat{y}_{R_m})^2,$$

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- Top-down refers to starting with the entire feature space and recursively splitting regions (**recursive binary splitting**).
- **Greedy** approach refers to determining the locally best split without looking ahead and possibly choosing a split leading to a better tree in some future step.

- To construct first split, consider splitting along variable X_j at splitting point $X_j = s$ and define half-spaces

$$R_1(j,s) := \{X : X_j \leq s\}, \qquad R_2(j,s) := \{X : X_j > s\}. \tag{8.1}$$

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- Seek splitting variable index j and splitting point s which minimize

$$\min_{\hat{y}_{R_1}} \sum_{x_i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \min_{\hat{y}_{R_2}} \sum_{x_i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2. \tag{8.2}$$

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- For fixed j, s, the two minimizing values of $\hat{y}_{R_1}$ and $\hat{y}_{R_2}$ are clearly the sample means of the response observations in R_1 and R_2, respectively.
- For each j, the optimal splitting point s can be found very quickly; with best split (j, s), partition data into the resulting two subregions and continue splitting recursively.

Tree-Based Methods

Tree pruning

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  However, split with small RSS reduction may enable larger reduction in subsequent splits.
- Better strategy: grow very large tree T_0, then **prune** it back to obtain a **subtree**.
- Can compare different subtrees using **cross-validation**, but comparing all possible subtrees is infeasible.

Tree-Based Methods

Cost complexity pruning

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- To each $\alpha \geq 0$ there corresponds a subtree $T \subset T_0$ which minimizes

$$\sum_{m=1}^{|T|} \sum_{i:x_i \in R_m} (y_i - \hat{y}_{R_m})^2 + \alpha |T|, \tag{8.3}$$

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  where $|T|$ denotes the number of leaves of tree T. Tuning parameter α controls trade-off between fit to training data and tree complexity.
- $\alpha = 0$ corresponds to T_0. For $\alpha > 0$ (8.3) minimized by smaller tree T_α (can show this is unique).
- To find T_α use **weakest link pruning**: successively collapse internal node producing smallest per-node increase in $\sum_{m,i}(y_i - \hat{y}_{R_m})^2$, continue until single-node tree reached. Can show: this tree sequence must contain T_α.
- Select α using validation set or cross-validation.

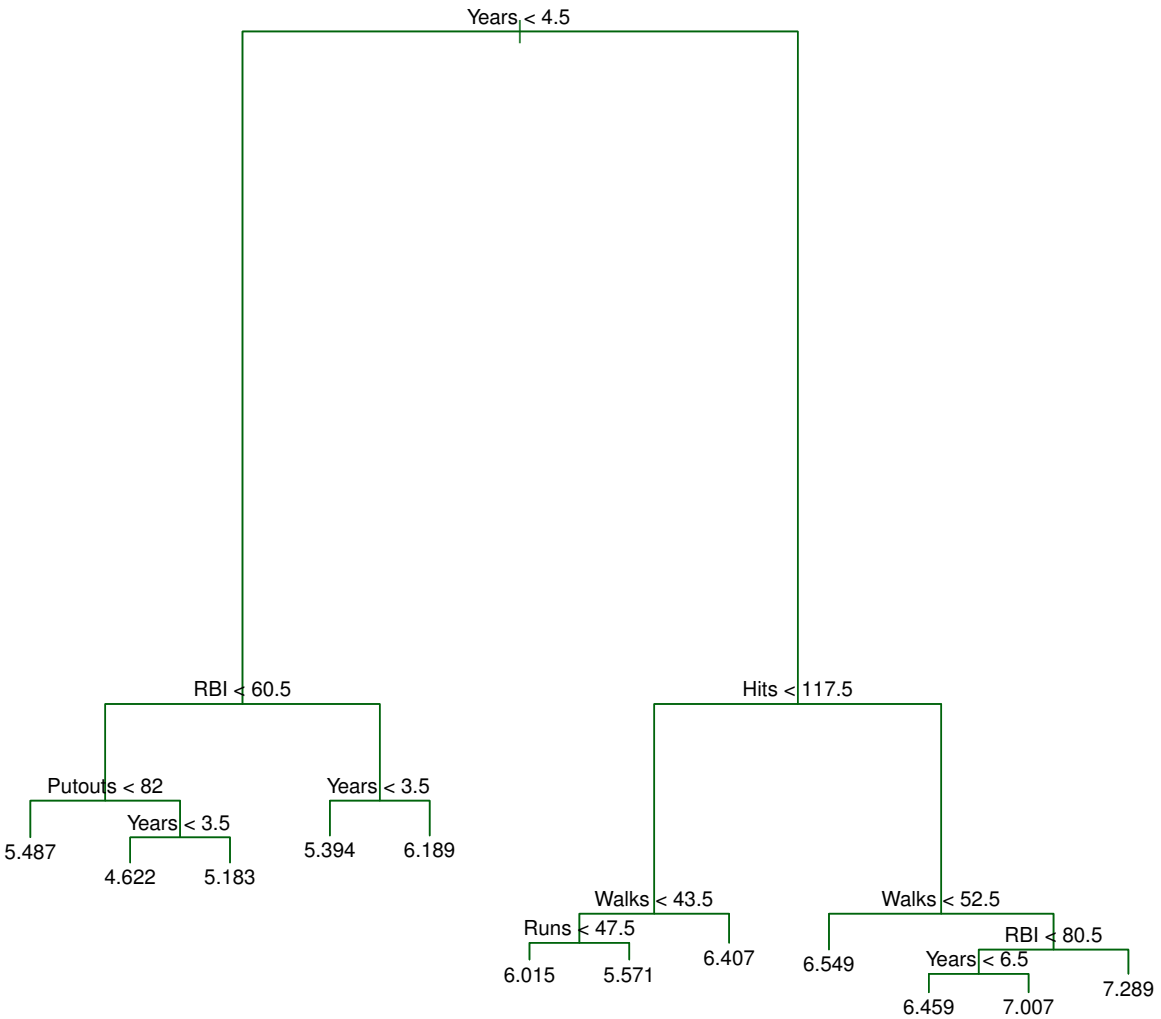
Algorithm 4: Regression tree.

1. Use recursive binary splitting to grow tree T_0 on the training data, stopping when each leaf contains fewer than some minimum number of observations.
2. Apply cost complexity pruning to T_0 to obtain sequence of best subtrees, as a function of α.
3. Use K-fold cross-validation to choose α: divide training observations into K folds. For each $k = 1, \ldots, K$:
   i. Repeat steps 1 and 2 on all but k-th fold of training data.
   ii. Evaluate test MSE on left out k-th fold, as function of α.

   Average MSE for each value of α, choode α minimizing average MSE.
4. Return subtree from Step 2 corresponding to minimizing α.

Tree-Based Methods

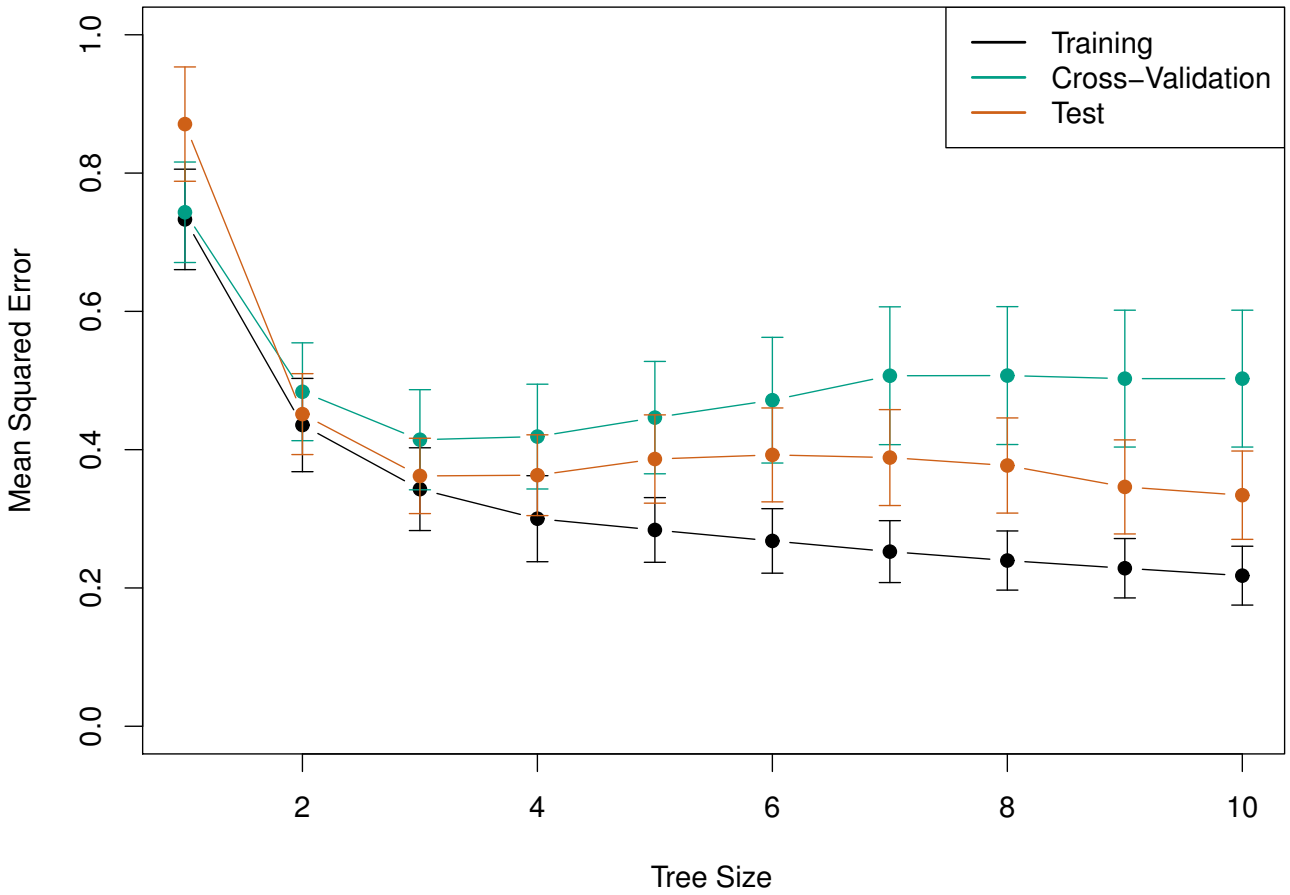
Hitters example revisited



- `Hitters` data set using nine features.
- Randomly divide data set into 132 training and 131 test observations.
- Grow tree on training data.
- Vary α to obtain subtrees T_α with different numbers of leaves.
- Perform 6−fold CV to estimate MSE of T_α as function of α.
- Unpruned tree shown on left.

Tree-Based Methods

Hitters example revisited



Training, CV and test MSEs for regression tree of `Hitters` data set as a function of α with bands indicating ± 1 standard error. CV MSE somewhat pessimistic, but reasonable estimate of test MSE.

Tree-Based Methods

Classification Trees

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- Grow classification tree using recursive binary splitting.
- In place of RSS, can use **classification error rate** E to determine optimal splits. This is simply the fraction of training observations not belonging to the most commonly occurring class, i.e.

$$E = 1 - \max_k \hat{p}_{m,k},$$

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  $\hat{p}_{m,k}$: proportion of training observations in R_m from k-th class.
- Classification error rate E not sensitive enough for tree-growing. Two other popular measures preferable:

- The **Gini index** is defined by

$$G = \sum_{k=1}^{K} \hat{p}_{m,k}(1 - \hat{p}_{m,k}) \tag{8.4}$$

and represents a measure of total variance across the K classes. Small if all $\hat{p}_{m,k}$ close to zero or one; indication of node *purity*, i.e., small value indicates node contains predominantly observations from a single class.

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- **Entropy** (or **deviance**) is defined by

$$D = -\sum_{k=1}^{K} \hat{p}_{m,k} \log \hat{p}_{m,k}. \tag{8.5}$$

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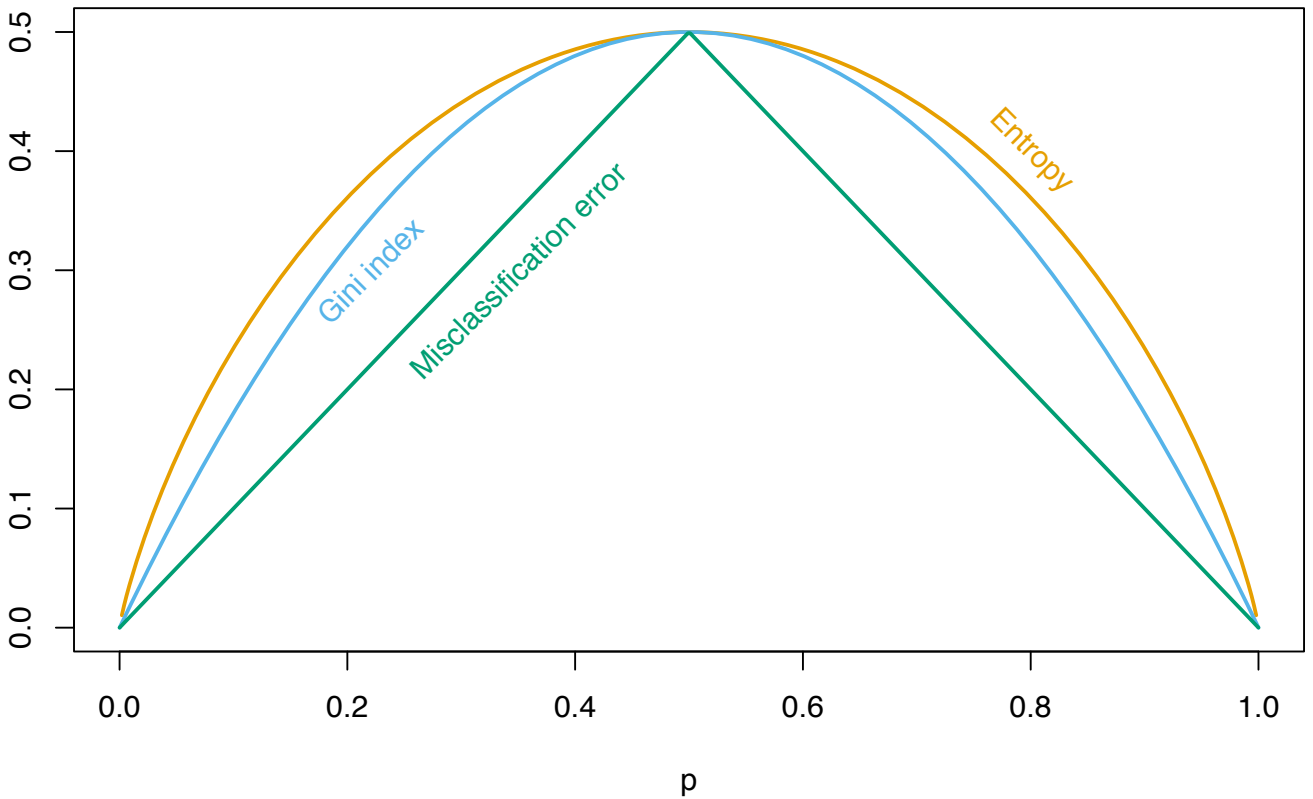
- Any of E, G or D can be used to build the tree, but pruning should be done using E to maximize prediction accuracy of final pruned tree.

Tree-Based Methods

Gini index and entropy



Node purity measures for two-class classification as a function of proportion p in class 2. Entropy has been scaled to pass through $(0.5, 0.5)$. For two classes, if p denotes the proportion in class 2, the three measures are $1 - \max(p, 1-p)$, $2p(1-p)$ and $-p\log p - (1-p)\log(1-p)$.

Tree-Based Methods

Heart example

- `Heart` data set: binary response `HD` for 303 patients who presented with chest pain.
- Response `Yes` indicates presence of heart disease (based on angiographic test), `No` indicates absence of heart disease.
- 13 predictors including `Age`, `Sex`, `Chol` (cholesterol measurement), and further heart and lung function measurements.
- Cross-validation results in tree with six leaves.

Tree-Based Methods

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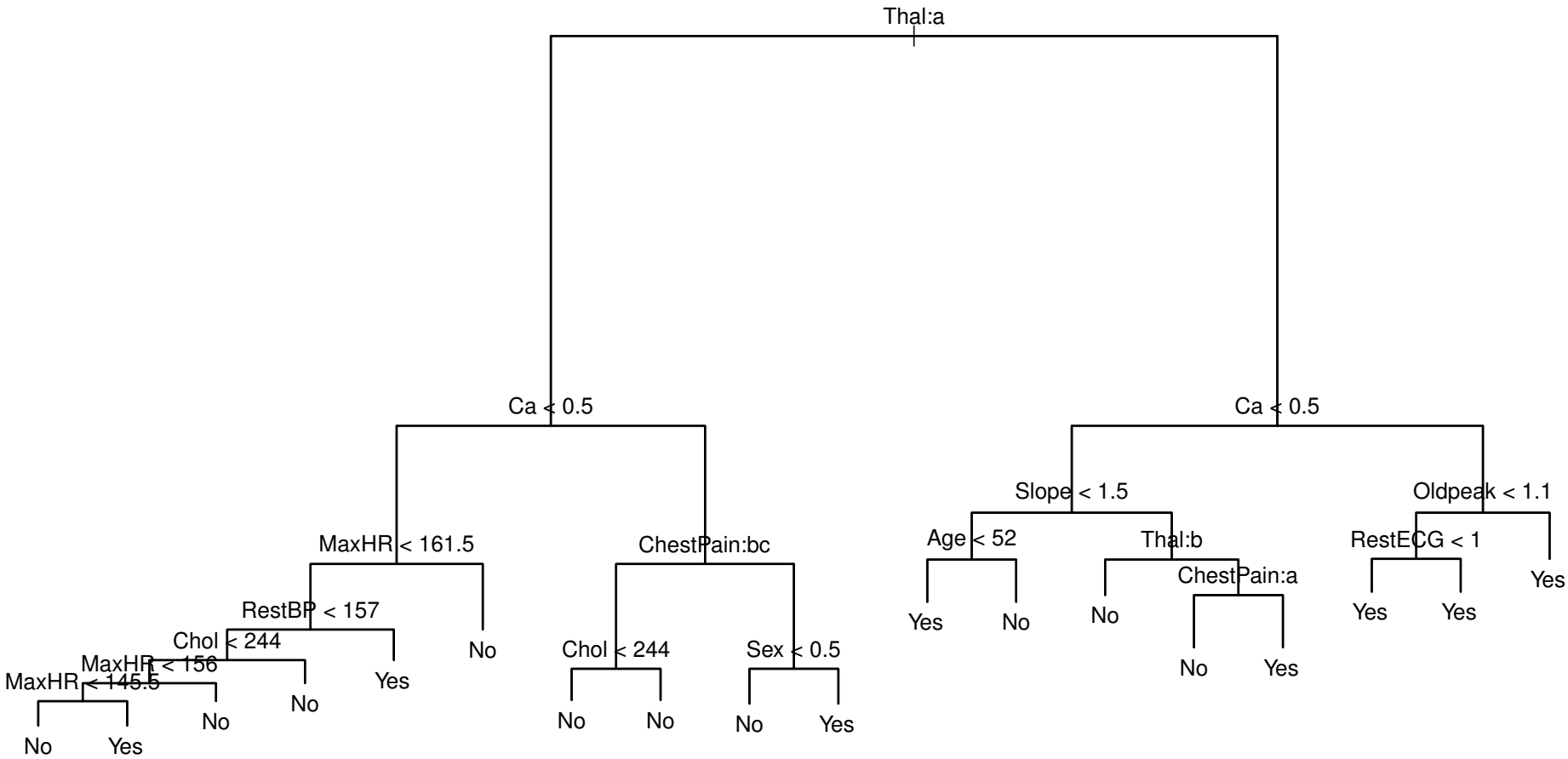
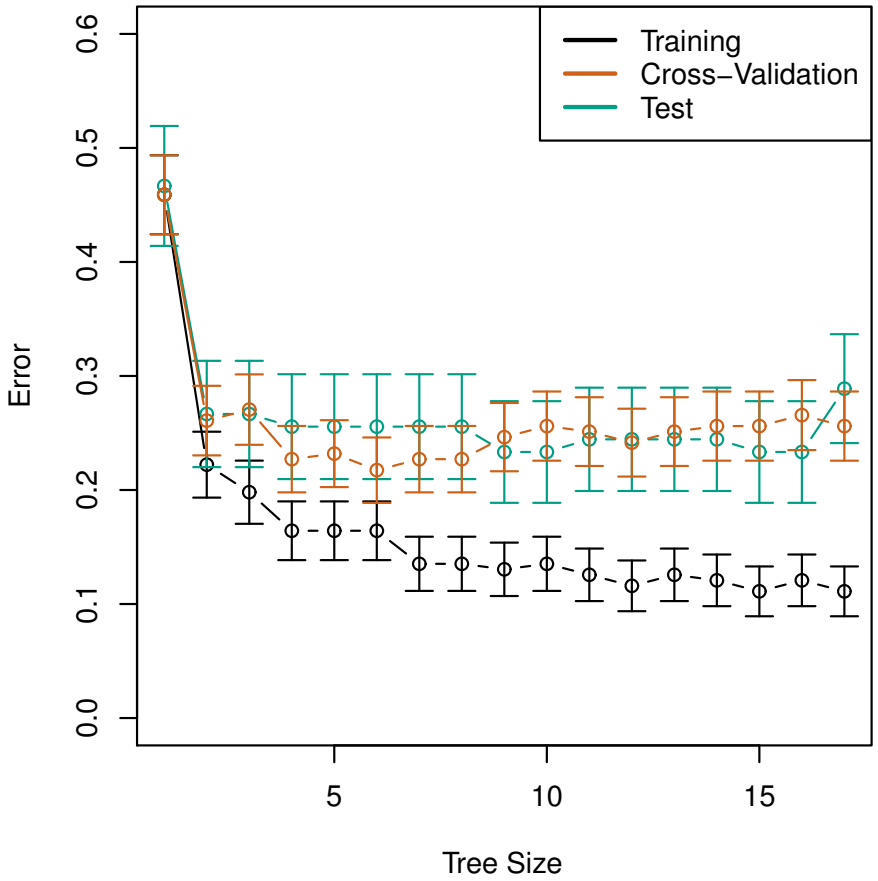
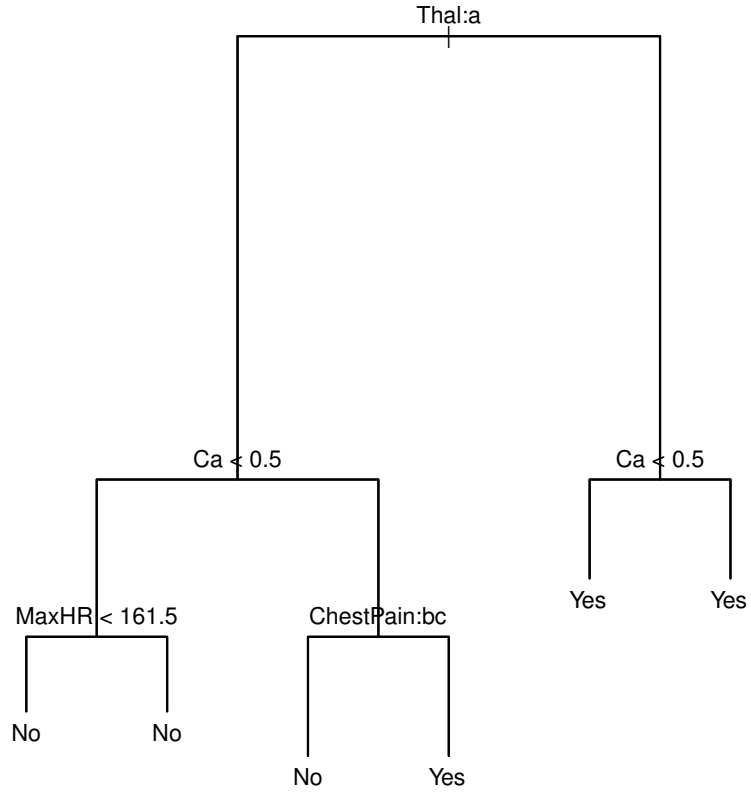


`Heart` data set: unpruned tree.

Tree-Based Methods

Heart example





`Heart` data set. Left: training, CV and test MSE for different sizes of pruned tree. Right: pruned tree corresponding to minimal CV MSE.

Tree-Based Methods

Heart example, qualitative predictors

- `Heart` data set contains a number of *qualitative* predictor variables such as `Sex`, `Thal` (Thallium stress test) and `ChestPain`.
- Splitting along one of these variables: assign some of the qualitative values to one branch, remaining values to other branch.
- In previous image: some internal nodes split quantitative variables.
- Top internal node splits `Thal`. Text `Thal:a` indicates left branch consists of observations with first value of `Thal` (normal), right consists of remaining values (fixed or reversible defects).
- Text `ChestPain:bc` on third split on left indicates left branch contains observations with second and third values of `ChestPain` variable (whose possible values are *typical angina*, *atypical angina*, *non-anginal pain* and *asymptomatic*).

Tree-Based Methods

Heart example, leaves with identical values

- Some leaves in `Heart` classification tree have the same predicion values.
- Example: split `RestECG` < 1 near bottom right of unpruned tree, both subregions predict response value `Yes`. Why perform split in the first place?

Tree-Based Methods

Heart example, leaves with identical values

- Some leaves in `Heart` classification tree have the same predicion values.
- Example: split `RestECG` < 1 near bottom right of unpruned tree, both subregions predict response value `Yes`. Why perform split in the first place?
- Split made to increase *node purity*.
- All 9 observations in right branch have leaf response value `Yes`. In left branch, 7/11 have response value `Yes`.
- Importance of node purity: given test observation belonging to region on right branch, then response certaionly `Yes`. For test observation on left branch, pobably `Yes`, but with much less certainty.
- Even though `RestECG` < 1 does not reduce classification error, it improves the Gini index and entropy, which are more sensitive to node purity.

- Prediction model of linear regression vs. regression tree

$$f(X) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p, \qquad f(X) = \sum_{m=1}^{M} \hat{\boldsymbol{y}}_{R_m} \mathbb{1}_{\{X \in R_m\}}$$

with regression coefficients $\{\beta_j\}_{j=0}^{p}$ and partition of feature space into rectangular regions R_m.

Tree-Based Methods

Trees vs. linear models

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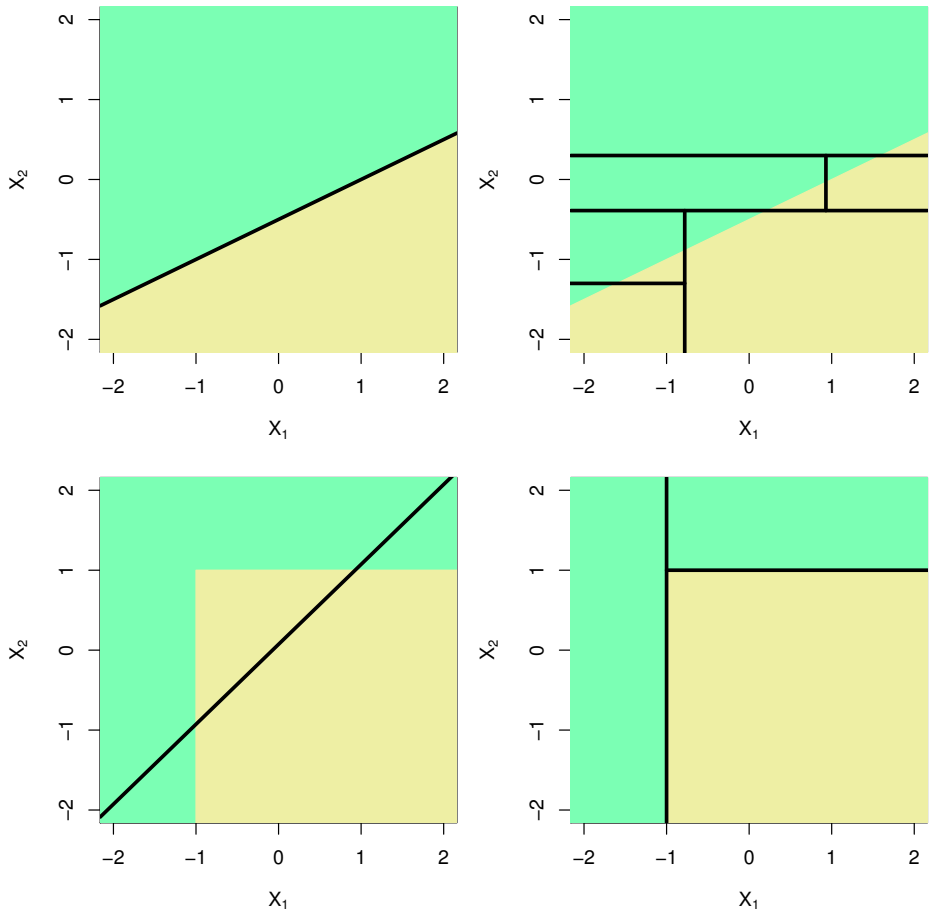
- If feature-response relation close to linear, linear regression model likely superior.
  Otherwise, tree-based models may outperform linear regression.
- Relative performances can be assessed by estimating test MSE via CV or validation set approach.
- Other considerations may also be relevant in comparison, such as interpretability or visualization.

Tree-Based Methods

Trees vs. linear models: example



Top row: 2D classification example with linear decision boundary (shaded regions), linear regression model superior. Bottom row: nonlinear)(piecewise constant) decision boundary captured perfectly by tree-based method,

Tree-Based Methods

Advantages and shortcomings of trees

+ Easy to explain (more so than linear regression).
+ Some argue decision trees more closely mimick human decision-making than linear regression/classification techniques (also widely used outside of statistical learning).
+ Trees, particularly small ones, easily displayed graphically, easily interpreted by non-experts.
+ Can handle qualitative predictors without introducing dummy variables.
- Prediction accuracy generally not as good as classical regression and classification techniques.
- Robustness (stability w.r.t. small data changes) often lacking.

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Some of these disadvantages addressed by bagging, random forests, boosting.

Contents

- Recall the **bootstrap** approach introduced in Chapter 5 for randomly generating subsamples of a set of observations for estimating statistical quantities without collecting additional data.

- Recall the **bootstrap** approach introduced in Chapter 5 for randomly generating subsamples of a set of observations for estimating statistical quantities without collecting additional data.
- Here we revisit the bootstrap to show how it can be used as a **variance-reduction technique** for any statistical learning method.
- This is particularly relevant for decision trees, which tend to possess high variance.
- **Bagging**: **b**ootstrap **agg**regation.
- Variance can be reduced by averaging observations: for $\{X_k\}_{k=1}^N$ i.i.d. RV with variance σ^2, variance of $\overline{X} = (X_1 + \cdots + X_N)/N$ is σ^2/N.
- **Idea:** Collect N training sets, construct prediction model $\hat{f}_k$ for each, and average these to aggregate model

$$\hat{f}_{\text{avg}}(x) = \frac{1}{N}\sum_{k=1}^{N} \hat{f}_k(x).$$

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Tree-Based Methods

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- For (regression) decision trees: grow (unpruned) tree for each resampled data set and average them.
- For classification trees: replace average with **majority vote**, i.e., for each new predictor observation, have aggregate model predict that class occurring most commonly across all decision trees $\hat{f}_k^*$.

Tree-Based Methods

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- For i-th observation: predict response using all trees for which it was OOB. Take average (regression) or majority vote (classification) to obtain aggregated prediction for all n observations, compare with response observation, i.e., MSE (regression) or classification error (classification), to obtain error estimate.

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- Can show: for N_b sufficiently large, OOB error estimate virtually equivalent to LOOCV error estimate.
  This is a great benefit when performing bagging on large data sets, where CV would be computationally burdensome.

Tree-Based Methods

Measuring variable importance

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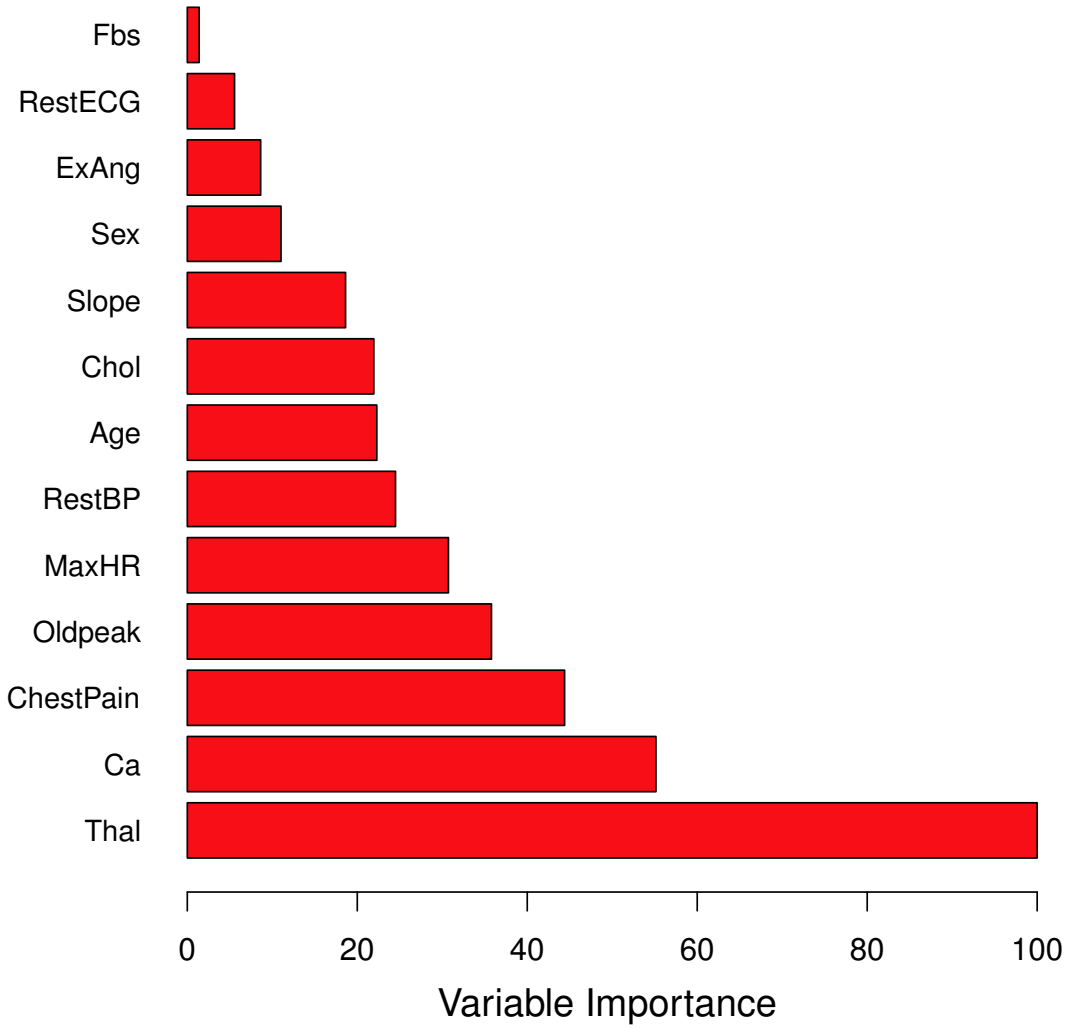
- Crucial interpretation element: which predictor variables most important?
- For regression trees, overall summary of importance of each predictor can be obtained by recording total amount RSS decreases when split performed along this variable, then averaging over all trees.
- For classification trees: record totel Gini index reduction due to splits along each predictor per tree, then average over all trees.
- Large value indicates important predictor variable.

Tree-Based Methods

Measuring variable importance: Heart data set



`Heart` data set. Variable importance (relative to maximum) in terms of mean decrease in Gini index.

Tree-Based Methods

Random forests

- Improve over bagging by "**decorrelating**" trees.
- Build decision trees on bootstrapped samples as in bagging.
- When choosing next predictor variable to split, restrict selection to $m < p$ randomly chosen variables instead of full set of p predictors.
  New set of m splitting candidates chosen at each splitting step.
- Common choice: $m \approx \sqrt{p}$. Smaller m called for in case of many correlated predictors.
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- **Rationale:** strongly dominant variables will be used in splitting for majority of bagged trees, leading to similarity among these trees, and thereby strong correlations.
  This limits the variance reduction from averaging.
- On average, $(p-m)/p$ splits will not even consider a given strong predictor.
- This mechanism results in a decorrelation of the trees, making their average less variable, hence more reliable.

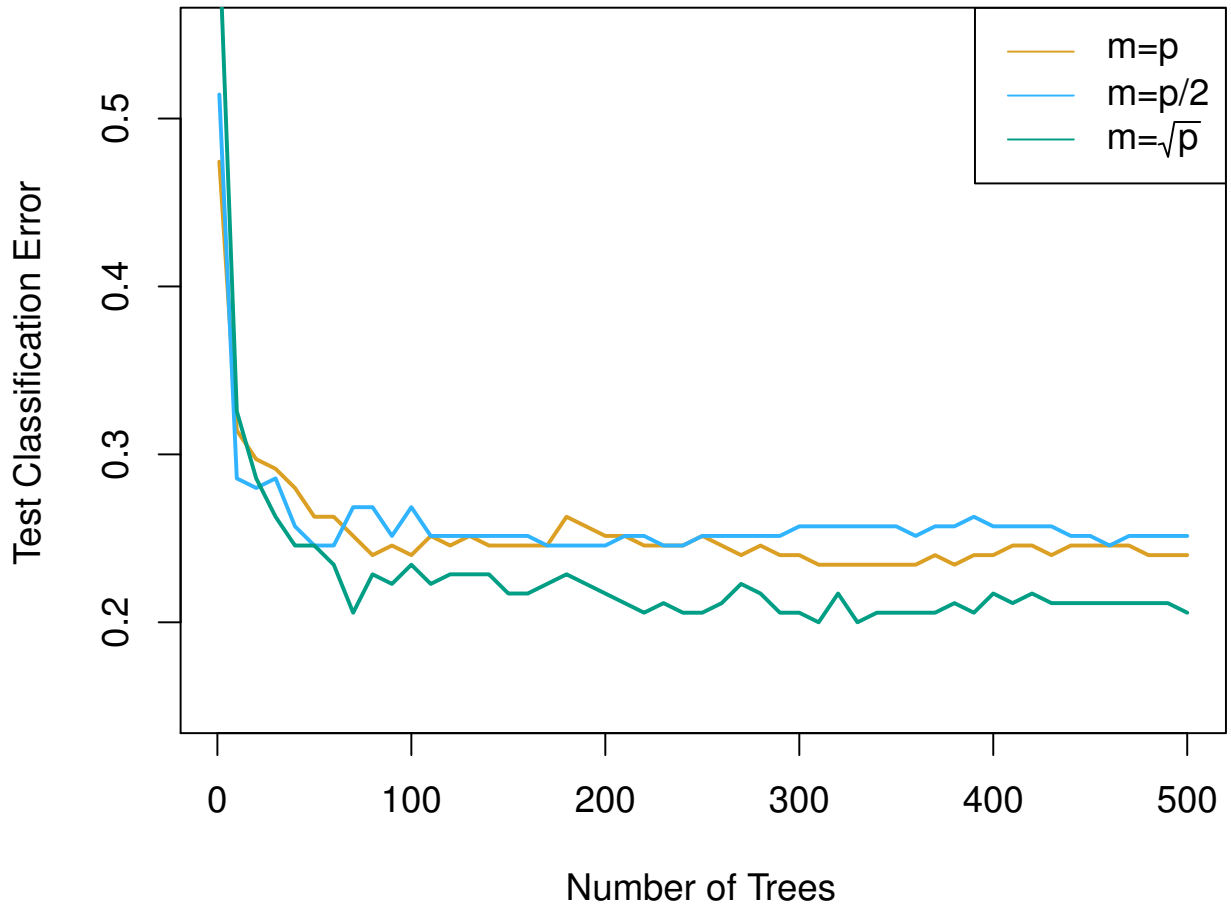
Tree-Based Methods

Random forests: gene expression example

- High-dimensional biological data set: expression measurements for 4,718 genes on tissue samples from 349 patients.
- Human genome contains $\approx 20,000$ genes.
- Individual genes have varying levels of **expression** (activity) in different body cells, tissue or biological conditions.
- Here: each patient sample assigned to one of 15 classes (normal or one of 14 cancer types).
- Goal: predict cancer type using random forests based on 500 genes with largest variance in training set.
- Random division into training and test set.
- Random forests applied for 3 different values of m.

Tree-Based Methods

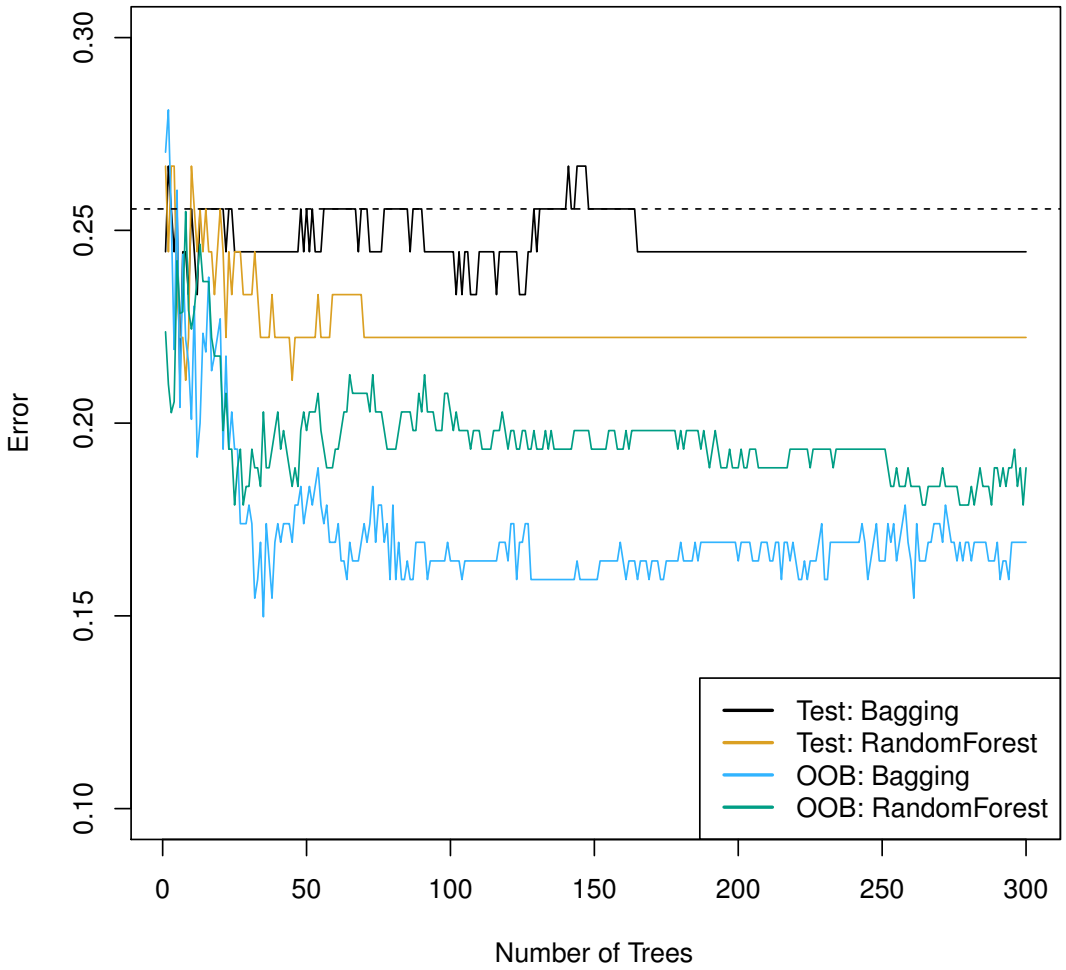
Random forests: gene expression example



Random forests for 15-class gene expression with $p = 500$: test error against # trees. Single tree has classification error rate of 45.7%. Null rate (always assign to dominant class) is 75.4%. As for bagging, no danger of overfitting as # trees increases.

Tree-Based Methods

Bagging vs. random forests: Heart data set



Test error against number N_b of bootstrapped data sets. Random forests used $m = \sqrt{p}$. Dashed line: error of single classification tree. Solid green/blue: OOB errors considerably lower.

- **Boosting:** general approach for improving predictions of statistical learning methods, here in context of decision trees.
- Basic approach as in bagging, but trees grown **sequentially** using information from previously generated trees.
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- Basic approach as in bagging, but trees grown **sequentially** using information from previously generated trees.
- No bootstrap sampling; instead, each tree fit to a modified version of original data set.
- Prodedure: begin with tree fit to original data.
- Fit next tree to **residuals** of first model in place of observation responses. Then add this tree to the first, as a **model correction**.
- Each tree can be small (few leaves) determined by parameter d in the algorithm.
  By fitting small trees to residuals, $\hat{f}$ is slowly improved in areas where it previously didn't perform well.
- Boosting for classification trees slightly more complicated.

Tree-Based Methods

Tuning parameters in boosting

1. # trees N_b. Overfitting is possible with boosting, although it sets in slowly. Selection using CV.

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2. Shrinkage parameter $\lambda > 0$ (small) determining learning rate.
   Typical values 10^{-2} or 10^{-3}.
   Very small λ can require very large N_b for good prediction.
3. # splits d per tree, controls complexity of boosted ensemble.
   Can also use $d = 1$ ("stump") with single split, leads to an **additive model**.
   Since d splits can involve at most d variables, it controls the **interaction order** of the boosted model.

Algorithm 5: Boosting for regression trees.

1. Set $\hat{f}(x) \equiv 0$ and $r_i = y_i$, $i = 1, \ldots, n$ (entire training set).
2. **for** $k = 1$ **to** N_n **do**

   Fit a tree $\hat{f}_k$ with d splits $(d+1)$ leaves to training data (X, r)

   Update $\hat{f}_k$ by adding damped version of new tree:

   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}_k(x)$$

   Update residuals

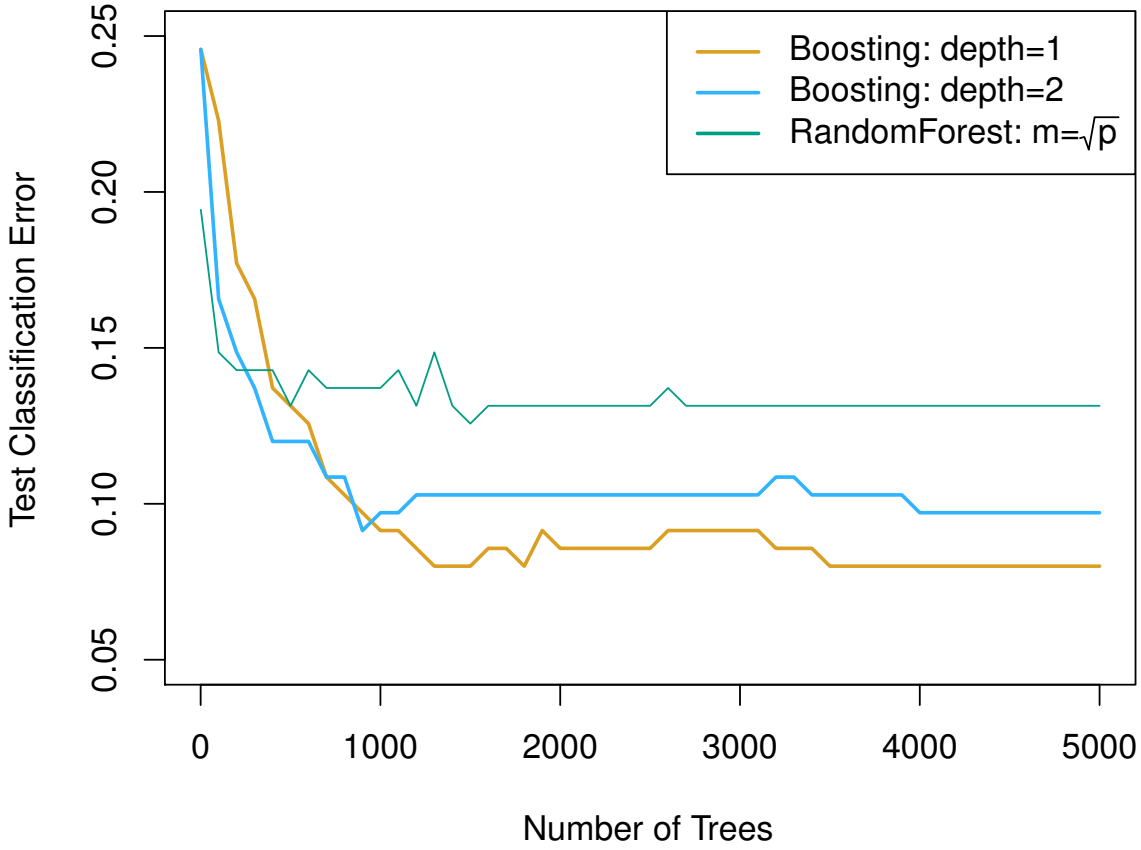
   $$r_i \leftarrow r_i - \lambda \hat{f}_k(x_i), \quad i = 1, \ldots, n.$$

3. Output boosted model

   $$\hat{f}(x) = \sum_{k=1}^{N_b} \lambda \hat{f}_k(x).$$

Tree-Based Methods

Gene expression example revisited



Boosting and random forests for gene expression example: test error against # trees using $\lambda = 0.01$ for boosted models. Depth-1 trees slightly outperform depth-2 trees, both outperform random forest, but difference is within standard error. Single tree has error rate 24%.