SF2930 Regression Analysis

Alexandre Chotard

Tree-based regression and classification

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Overview

Regression trees

Pruning

Bagging, random forests

Today

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Pruning

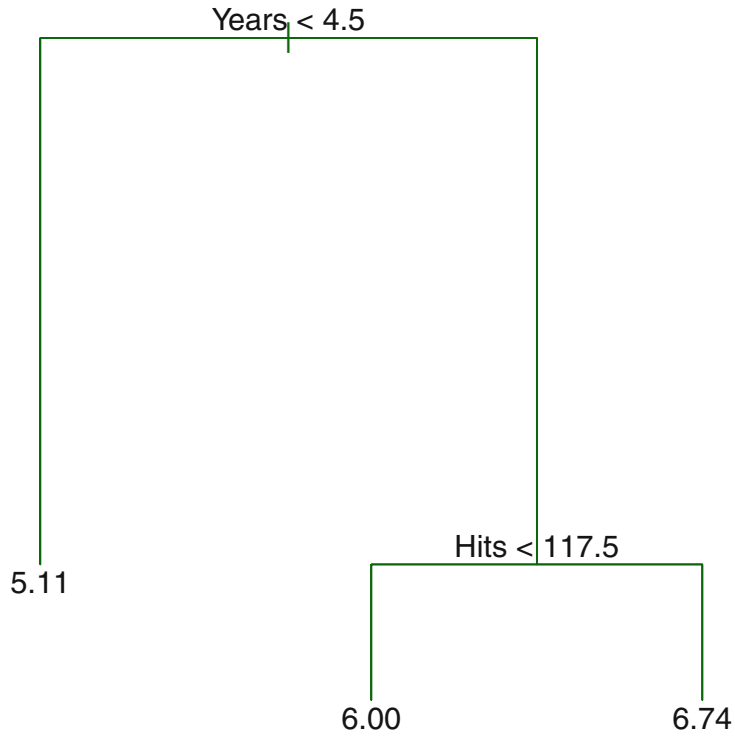
Bagging, random forests

Setup

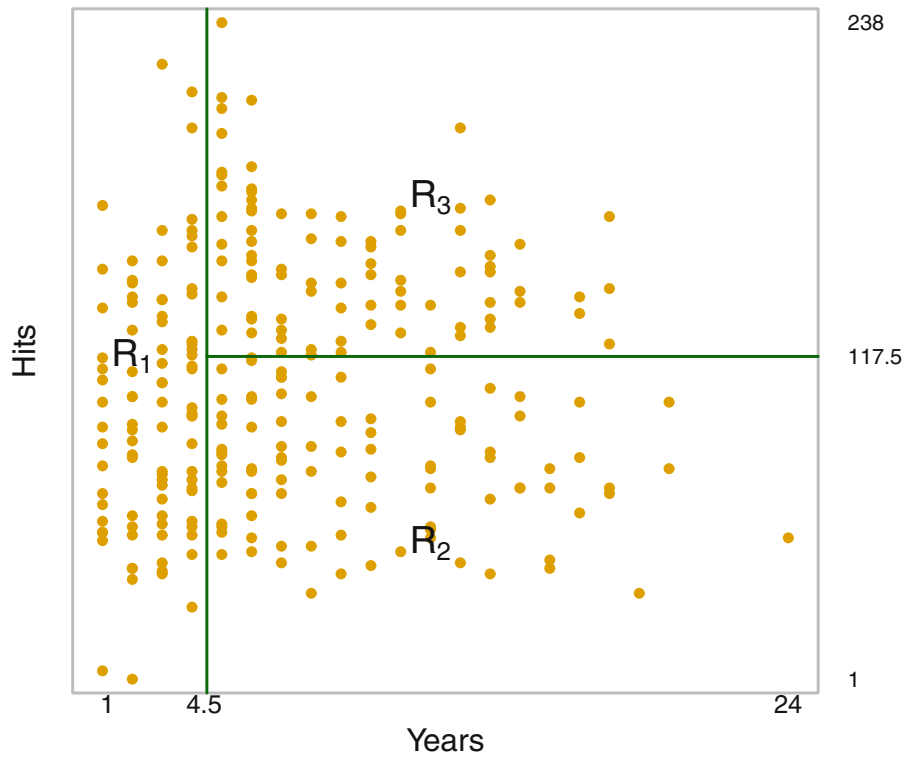
- Let Y be a real-valued random variable. Given $\boldsymbol{x} \in \mathbb{X} \subset \mathbb{R}^d$, we want to predict the value of Y.
- To understand how different values of $\boldsymbol{x}$ influence Y, we have $N \in \mathbb{N}^*$ examples $(\boldsymbol{x}_i, y_i)_{i \in [1..N]}$.
- The variable Y can have discrete or continuous values, corresponding respectively to classification and regression problems.
- We consider here binary decision trees. A decision tree partitions $\mathbb{X}$ into simple regions $(R_j)_{j \in [1..J]}$. For $\boldsymbol{x} = (x^1, \ldots, x^d) \in \mathbb{R}^d$ and j such that $\boldsymbol{x} \in R_j$, the value predicted by the tree is
  - the most represented class y among $\{x_i \in R_j\}$ in classification problems,
  - the average of $\{y_i | \boldsymbol{x}_i \in R_j, i \in [1..N]\}$ in regression problems.

Setup

- Each node n of the tree is associated to a subset R_n of $\mathbb{X}$, which is further split into two regions through a test comparing x^i for some $i \in [1..d]$ with a value $c \in \mathbb{R}$. Then for l and r left and right children of n,
  - $R_l := \{\boldsymbol{x} \in R_n | x^i < c\}$
  - $R_r := \{\boldsymbol{x} \in R_n | x^i \geq c\}$

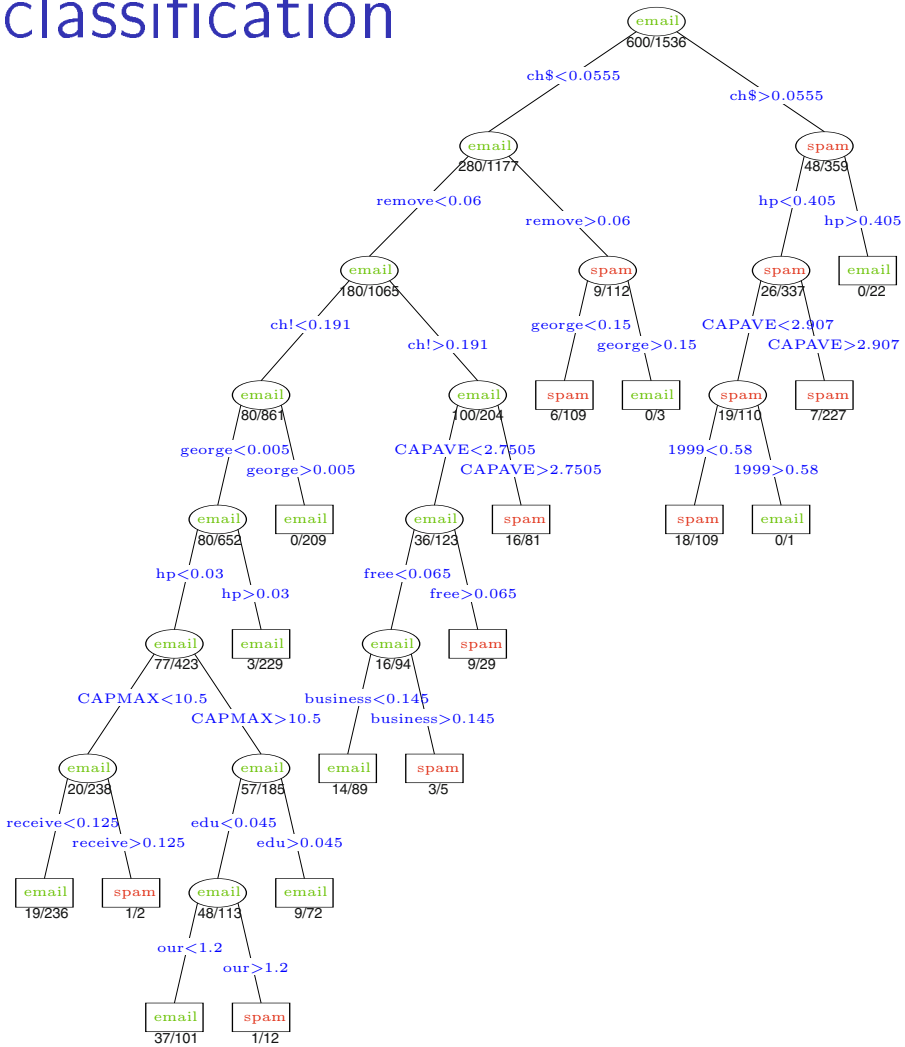


Figur: A regression tree for predicting the log salary (in 1,000\$) of a baseball player, based on the number of years played and the number of hits made in the previous year.



Figur: The three-region partition provided by the regression tree in the previous figure.

Example: spam classification



Figur: Tree for spam classification. Split variables are shown in blue. `CAPMAX` and `CAPAVE` = maximal and average length of the longest uninterrupted sequences of capital letters, respectively.

Questions

- How do we construct such trees?
- How large should a tree be?
- What are the pros and cons of tree-based methods?

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Regression trees vs. linear regression

- We generally want to approximate a relation $Y = f(\boldsymbol{x}) + \varepsilon$.
- Linear regression involves linear functions

$$f(\boldsymbol{x}) = \beta_0 + \sum_{j=1}^{p} \beta_j \boldsymbol{x}_j.$$

- We will instead consider

$$f(\boldsymbol{x}) = \sum_{j=1}^{J} m_j \mathbb{1}_{R_j}(\boldsymbol{x}),$$

for a partition $\{R_j\}_{j \in [1..J]}$ of $\mathbb{X}$.

Building a regression tree: cost function

- We will construct the tree by minimizing

$$\text{RSS}(m_1, \ldots, m_J, R_1, \ldots, R_J) = \sum_{i=1}^{N} (y_i - f(\boldsymbol{x}_i))^2$$

$$= \sum_{j=1}^{J} \sum_{i:\boldsymbol{x}_i \in R_j} (y_i - f(\boldsymbol{x}_i))^2 = \sum_{j=1}^{J} \sum_{i:\boldsymbol{x}_i \in R_j} (y_i - m_j)^2.$$

- For each j, the m_j minimizing the sum of squares $\sum_{i:\boldsymbol{x}_i \in R_j} (y_i - m_j)^2$ is always

$$m_j = \bar{y}_{R_j} = \text{average over all } y_i \text{ such that } \boldsymbol{x}_i \in R_j.$$

- To find the minimizing R_j is however computationally infeasible in general.

Building a regression tree: top-down minimization

- Thus, in order to find regions $\{R_j\}_{j=1}^{J}$ minimizing

$$\sum_{j=1}^{J} \underbrace{\sum_{i:\boldsymbol{x}_i \in R_j} (y_i - \bar{y}_{R_j})^2}_{Q_{R_j}}$$

  we proceed with a *top-down*, *greedy* approach.

- In the first step, when splitting $\mathbb{X}$ into

$$R_1(k,s) = \{\boldsymbol{x} \in \mathbb{X} : x^k < s\} \quad \text{and} \quad R_2(k,s) = \{\boldsymbol{x} \in \mathbb{X} : x^k \geq s\},$$

  we minimize

$$Q_{R_1(k,s)} + Q_{R_2(k,s)}$$

  w.r.t. k and s.

Building a regression tree: top-down minimization (cont.)

- For a given k, the optimal s is quite easily found by scanning though the data.
- Repeating for all $k \in [1..d]$ yields an optimal pair (k, s).
- Having found the best split, we partition the data into the two resulting regions and repeat the splitting process on each of these. And so forth.
- We stop growing the tree when some stopping criterion is reached, e.g., when no region contains more than five training data.

Bias versus variance

- The tree size is a tuning parameter governing the model's complexity.
- A too large tree leads to *overfitting* (high variance on test sets), while a too small tree leads to high bias.
- The optimal tree size should be determined adaptively from the data.
- One possibility is to split a node only if the split implies an RSS reduction exceeding a certain threshold; this is however treacherous in top-down minimization, as an apparently meaningless split may imply a good split later on.

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Cost complexity pruning

- Grow a large tree T_0 while storing the different Q_{R_j} associated with each split.
- We define a subtree $T \subseteq T_0$ obtained by *pruning* T_0 in a *bottom-up* fashion.
- Let $|T|$ denote the number of leaves $R_m(T)$ in T.
- Define, for some $\alpha \geq 0$, the cost function

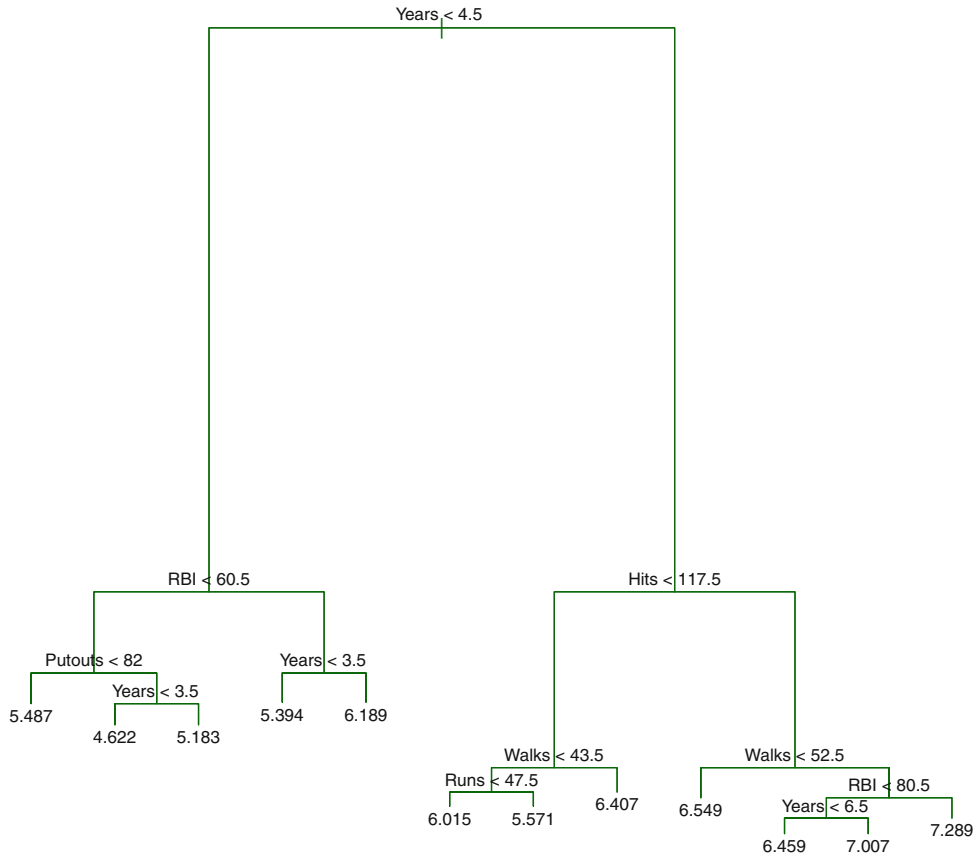
$$C_\alpha(T) = \sum_{m=1}^{|T|} Q_{R_m(T)} + \alpha|T|,$$

  where the $Q_{R_m(T)}$ are available from the first step.
- The idea is to find a subtree T_α minimizing $C_\alpha(T)$.

Cost complexity pruning (cont.)

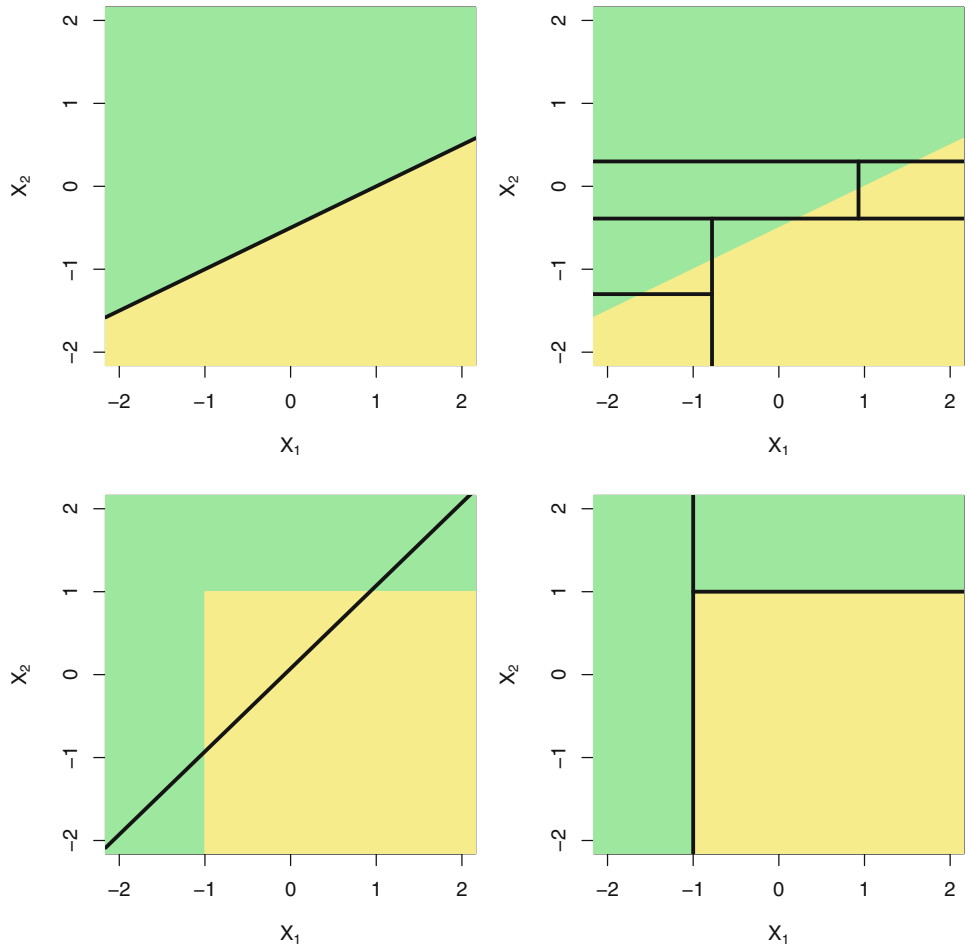
- Large values of α leads to smaller trees.
- For $\alpha = 0$, the solution is T_0.
- To find T_α, we create a sequence of subtrees by removing successively leaves whose elimination leads to the smallest increase of $\sum_{m=1}^{|T|} Q_{R_m(T)}$.
- To find the optimal α, apply K-fold cross validation.

Example: baseball player salaries (cont.)



Figur: Unpruned tree for the log salary (in 1,000\$) of a baseball player.

Trees vs. linear models



Figur: True decision boundary is indicated by the shaded regions. Linear boundary vs. decision tree (boxes).

Node impurity

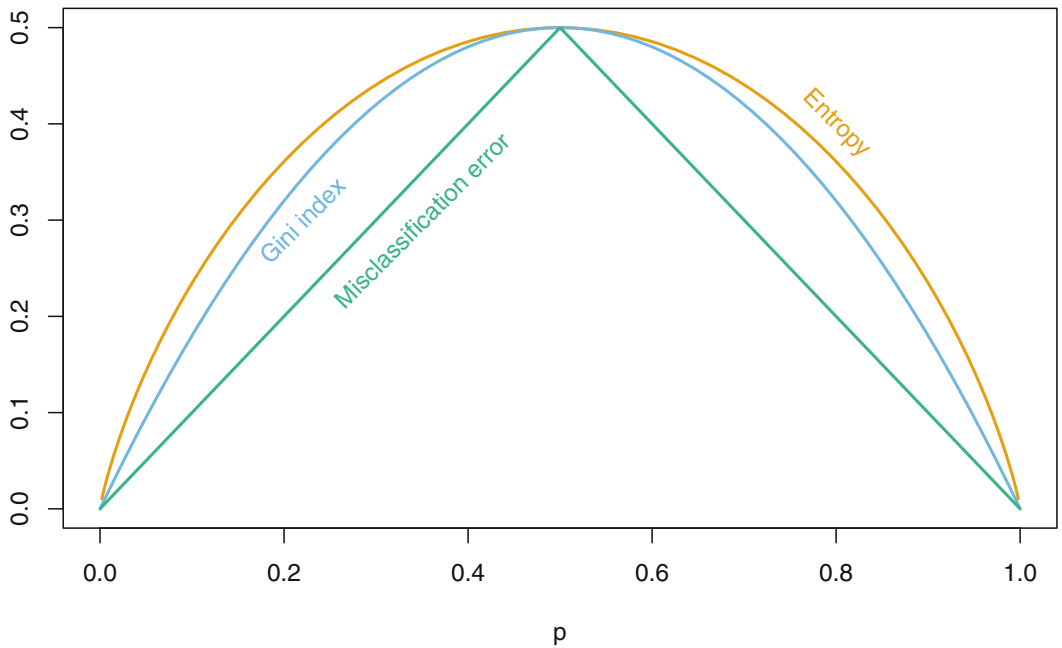
- The task of growing a classification tree is very similar to that of growing a regression tree. The only difference is that the RSS is not meaningful any longer.
- We thus need to find alternative measures $Q_m(T)$ of *node impurity*. For this purpose, define

$$\hat{p}_{j,k} = \frac{1}{|R_j|} \sum_{i:\boldsymbol{x}_i \in R_j} \mathbb{1}_{\{y_i = k\}} \quad \text{and} \quad k(j) = \arg\max_k \hat{p}_{j,k}$$

and let, e.g.,

$$Q_m(T) = \begin{cases} 1 - \hat{p}_{j,k(j)} & \textit{misclassification error}, \\ \sum_{k=1}^{K} \hat{p}_{j,k}(1 - \hat{p}_{j,k}) & \textit{Gini index}, \\ -\sum_{k=1}^{K} \hat{p}_{j,k} \log \hat{p}_{j,k} & \textit{cross-entropy}. \end{cases}$$

Node impurity measures



Figur: Node impurity measures for two-class classification, as a function of the proportion p in class 2. (Cross-entropy has been scaled.)

Pros and cons with tree-based methods

- Pros:
  - Easy to explain,
  - able to handle categorical or numerical data,
  - scales well with N
- Cons:
  - Do not, in their most basic form, have the same level of predictive accuracy as some other regression and classification approaches,
  - can be very non-robust (i.e., small changes in the data leads to completely different trees).
  - highly sensitive to data-representation: ill-suited to many problems
- The predictive accuracy can however be drastically improved using ideas as *bagging* and *random forests* discussed in the following.

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Prelude: the bootstrap

- Given an i.i.d. sample $\{\boldsymbol{x}_i\}_{i=1}^N$ from a probability density p, the *bootstrap algorithm* is based on the approximation

$$\hat{p}(\boldsymbol{x}) = \frac{1}{N}\sum_{i=1}^{N}\delta_{\boldsymbol{x}_i}(\boldsymbol{x})$$

  of p.
- Given $\hat{p}$, a new sample set $\{\boldsymbol{x}_i^*\}_{i=1}^N$ with approximately the same distribution as $\{\boldsymbol{x}_i\}_{i=1}^N$ can be formed by sampling from $\hat{p}$, i.e., by drawing repeatedly N times among $\{\boldsymbol{x}_i\}_{i=1}^N$ with replacement.
- In machine learning applications, this can be used for creating artificial replicates of the training set.

Bagging

- In the case of regression, we have approximated the target function using

$$f(\boldsymbol{x}) = \sum_{j=1}^{J} \bar{y}_{R_j} \mathbb{1}_{R_j}(\boldsymbol{x}),$$

  where the partition $\{R_j\}_{j=1}^{N}$ is formed using a decision tree.
- The decision trees discussed above suffer generally from *high variance*, i.e., building the tree using a different training set may lead to a quite different f.
- Better would be to use B independent training sets of similar size, each yielding a tree f_b, and use the model

$$f_{\text{avg}}(\boldsymbol{x}) = \frac{1}{B} \sum_{b=1}^{B} f_b(\boldsymbol{x}).$$

Bagging (cont.)

- We use bootstrap sampling for creating artificially B such training sets, each yielding a tree f_b^*, and use the model

$$f_{\text{bag}}(\boldsymbol{x}) = \frac{1}{B}\sum_{b=1}^{B} f_b^*(\boldsymbol{x}).$$

- The trees f_b^* are grown deep without pruning, implying that each tree has high variance but low bias.
- In the classification case, we can record the class predicted by each of the B trees, and take the *most popular vote*.

Bagging (cont.)

- The number of trees B is not a critical parameter with bagging; using a very large value of B will not lead to overfitting.
- The reason is that the probability of making an error *converges* as $B \to \infty$.
- The probability of making an error depends also on the expected correlation between errors of different trees $f_b(\boldsymbol{x})$ and $f_{b'}(\boldsymbol{x})$ when $(\boldsymbol{x}, Y)$ varies.

Some theory

- Indeed, in the classification case, let the *margin function* be

$$m(\boldsymbol{x}, y) = \frac{1}{B}\sum_{b=1}^{B} \mathbb{1}_{\{f_b(\boldsymbol{x})=y\}} - \max_{k \neq y} \frac{1}{B}\sum_{b=1}^{B} \mathbb{1}_{\{f_b(\boldsymbol{x})=k\}}$$

- Moreover, define the *generalization error* by

$$\text{PE} = \mathbb{P}(m(\boldsymbol{x}, Y) < 0).$$

- **breiman:2001** (**breiman:2001**) shows that PE *converges* as $B \to \infty$. In addition, the PE can be bounded as

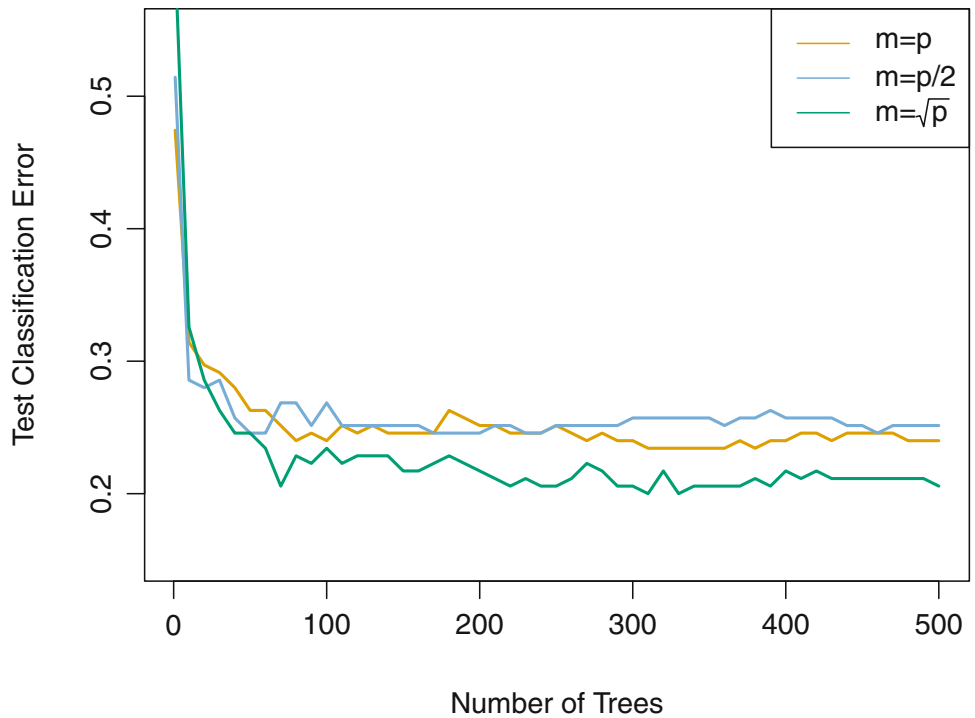
$$\text{PE} \leq (1 - s^2)\rho/s^2,$$

where, roughly, s is the limiting margin function—the *strength*—and ρ describes the expected *correlation* between the trees' errors as $(\boldsymbol{x}, Y)$ varies.

Random park $\Rightarrow$ random forest

- In order to *decorrelate* the trees, it is desirable so build them different.
- Say that there is one strong predictor x^i along with a number of other moderately strong predictors $\Rightarrow$ most or all of the trees will use this strong predictor in the top split $\Rightarrow$ all trees will look quite similar $\Rightarrow$ highly correlated predictions.
- Thus, at each split, consider only splitting of a *randomly chosen subset* of $m \leq d$ predictors.
- Therefore, on average $(d - m)/d$ of the splits will not even consider the strong predictor, and so other predictors will have more of a chance.
- Typically, one uses $m \approx \sqrt{d}$; $m = d$ corresponds to standard bagging.

Example: cancer-type prediction



Figur: Here $p = 500$. The test error as a function of the number of trees. Each colored line corresponds to a different value of m. A single classification tree has an error rate of 45.7%.