CSCI4622 Machine Learning 2020 Spring

# Ensemble method

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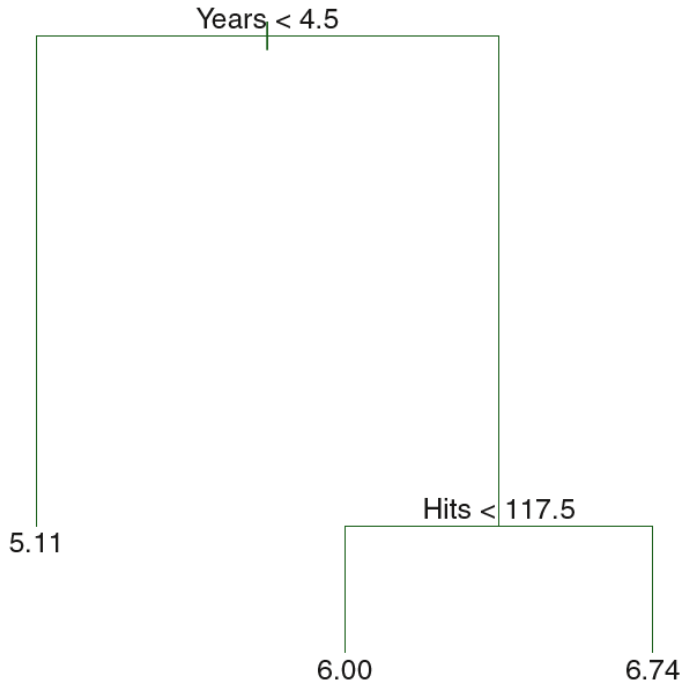
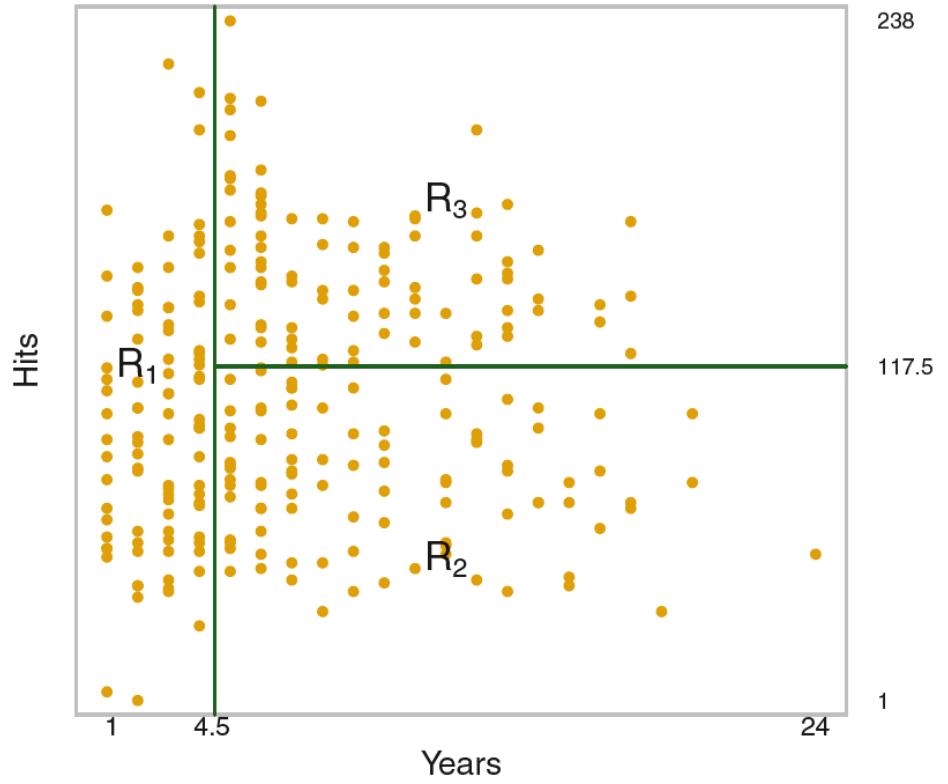
*Slide contents adopted from ISLR material

# Decision Tree

Split Rule:  Minimize the metric (MSE, entropy, etc) of the boxes



# Decision Tree Split Criteria

**Regression Tree**

MSE

$$H(X_m) = \frac{1}{N_m} \sum_{i \in N_m} (y_i - \bar{y}_m)^2$$

MAE

$$H(X_m) = \frac{1}{N_m} \sum_{i \in N_m} |y_i - \bar{y}_m|$$

**Classification Tree**

Gini

$$H(X_m) = \sum_k p_{mk}(1 - p_{mk})$$

Entropy

$$H(X_m) = -\sum_k p_{mk} \log(p_{mk})$$

Information Gain

$$IG = E_{parent} - \frac{N_L}{N} E_L - \frac{N_R}{N} E_R$$

# Improving Trees

Problems with a single Decision Tree

- Overfitting
- Trees are weak learner

# Hyperparameter search

## Grid Search Tip

- Give a range of values for each hyperparameter
- Measure a training time for one, then estimate how long for the loop
- Adjust number of values, range, or hyperparameters to include

**max_depth**

**min_samples_split**

**min_samples_leaf**

**max_features**

**min_impurity_decrease**

# Decision Tree – Pruning

## Minimal Cost-Complexity Pruning

$$R_\alpha(T) = R(T) + \alpha|T|$$

α : complexity parameter

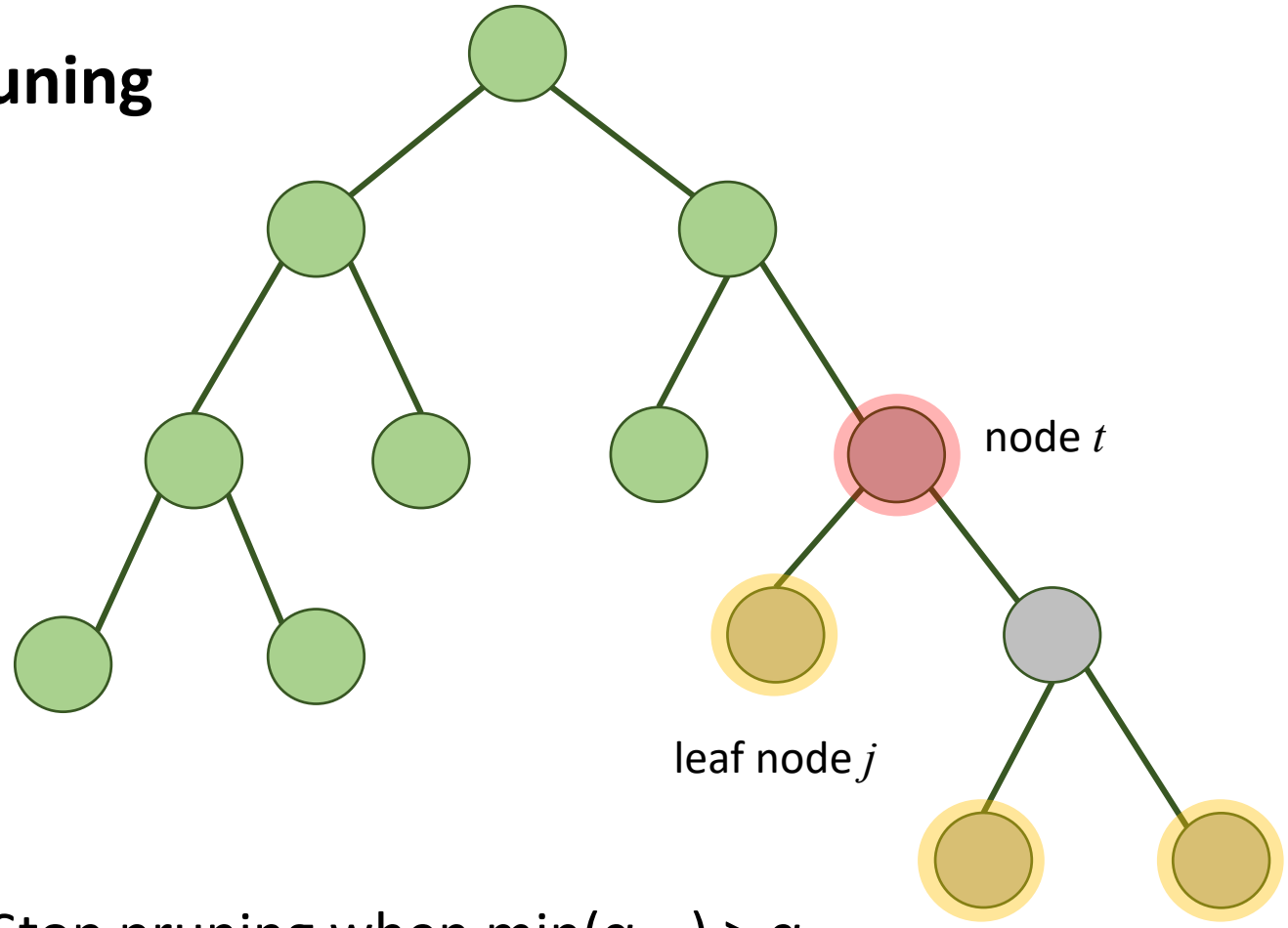
|T|: number of leaf nodes of the subtree

Impurity at the node $t$

$$R(T_t) < R(t)$$

Sum of the impurities at the leaf nodes of the subtree $T_t$

$$\alpha_{eff}(t) = \frac{R(t) - R(T_t)}{|T| - 1}$$




Stop pruning when $\min(\alpha_{eff}) > \alpha_{ccp}$

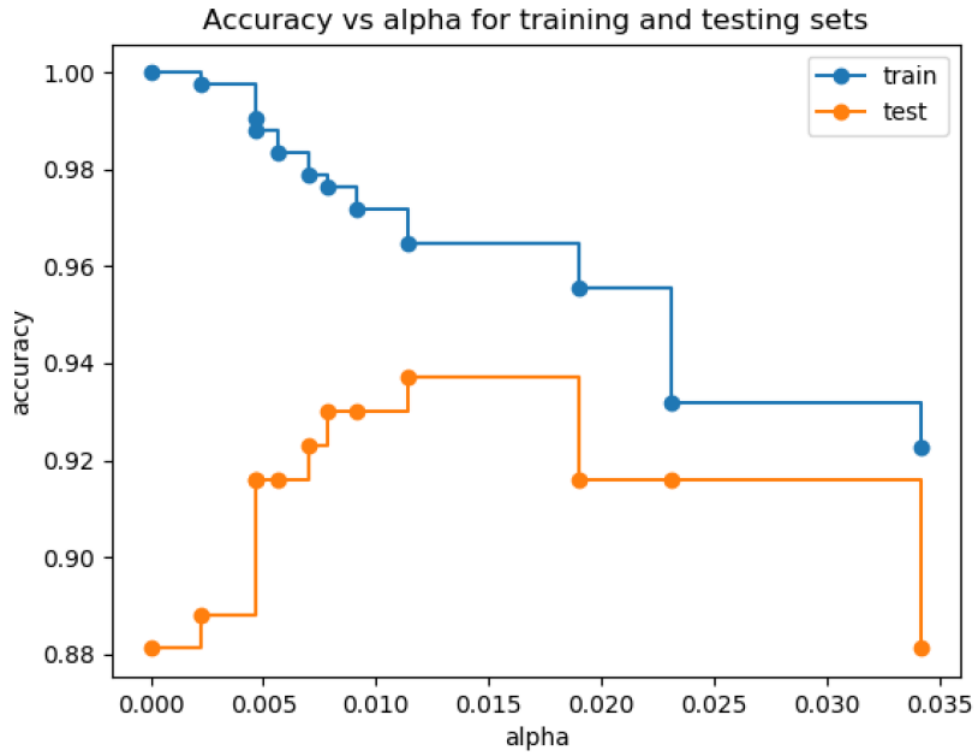
$\alpha_{ccp}$ : cost complexity parameter, "ccp_alpha"

# Decision Tree – Pruning

The cost complexity parameter(`ccp_alpha`) is a hyperparameter

How do we determine the right cost complexity parameter?

-> Use validation dataset (or cross-validation)



# Ensemble method

What is an Ensemble?

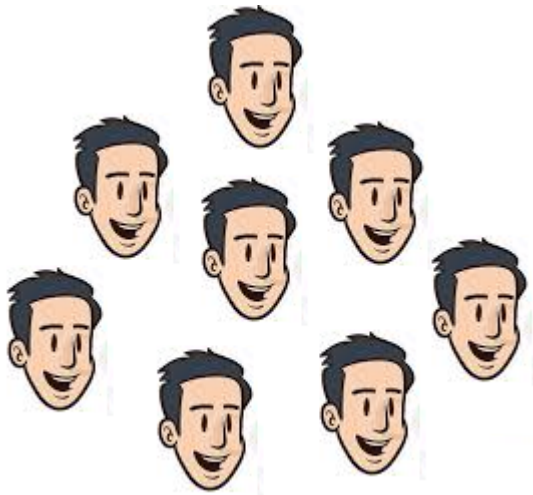
# Ensemble method

What is an Ensemble?

- An individual model might be a weak-learner,
- Averaging models can predict better

# Ensemble method

Diversity matters



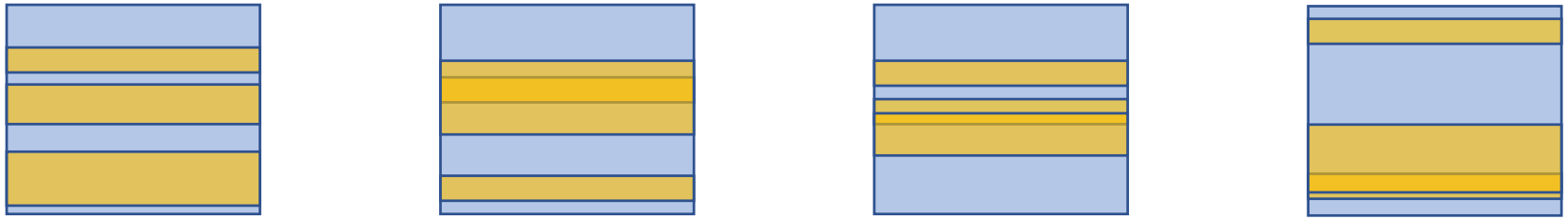
# Ensemble method

How do we diversify our models?

- Idea1: Models trained on different data subset

# Bagging

# Bagging (Bootstrap-Aggregation)



STEP1: Randomly sample a subset of training data with replacement (Bootstrap)

STEP2: Grow a tree (without pruning) on the subset of data

STEP3: Ensemble the result (regression : average, classification : vote)

Out of Bag error (OOB) : test the grown tree on the rest of data, then average

# Random Forest

# Random Forest

Bagging : random sampling of data

+

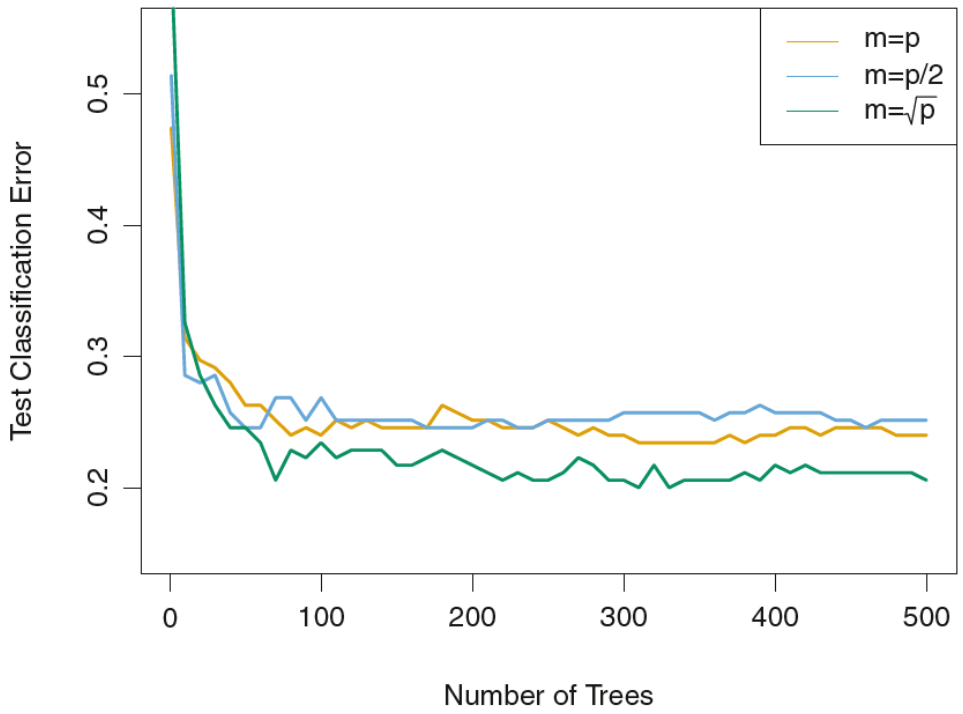
Decorrelation : random sampling of features

II

Random Forest

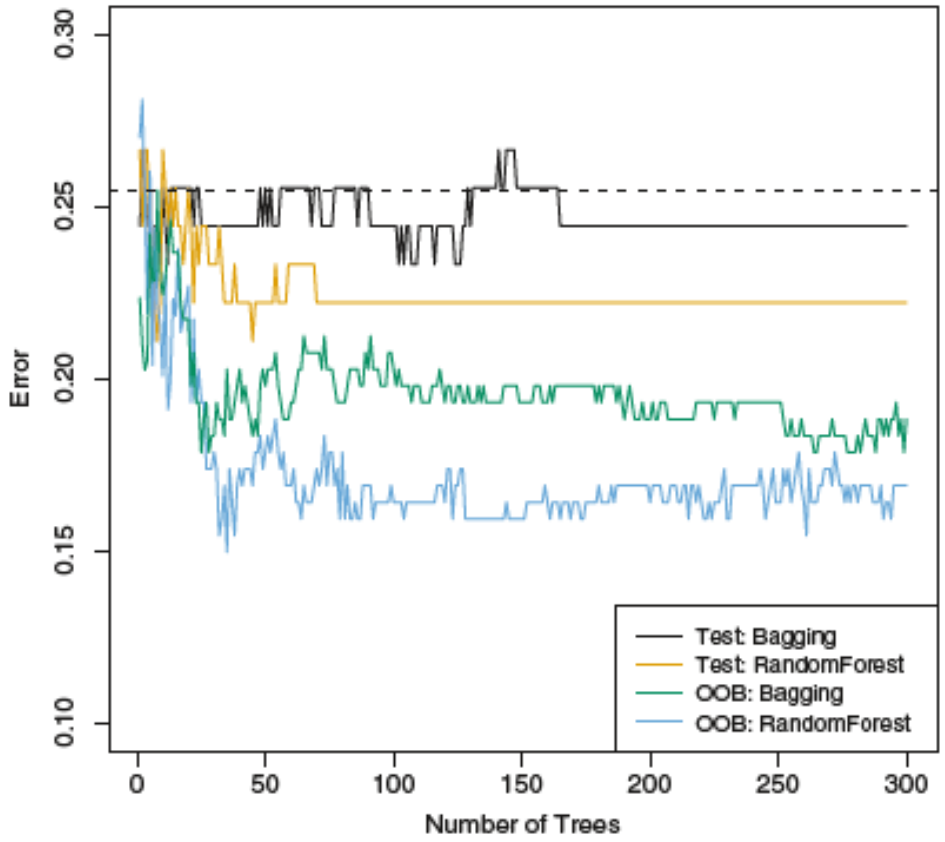
How do we sample features?

-> Rule of thumb : $\sqrt{n}$

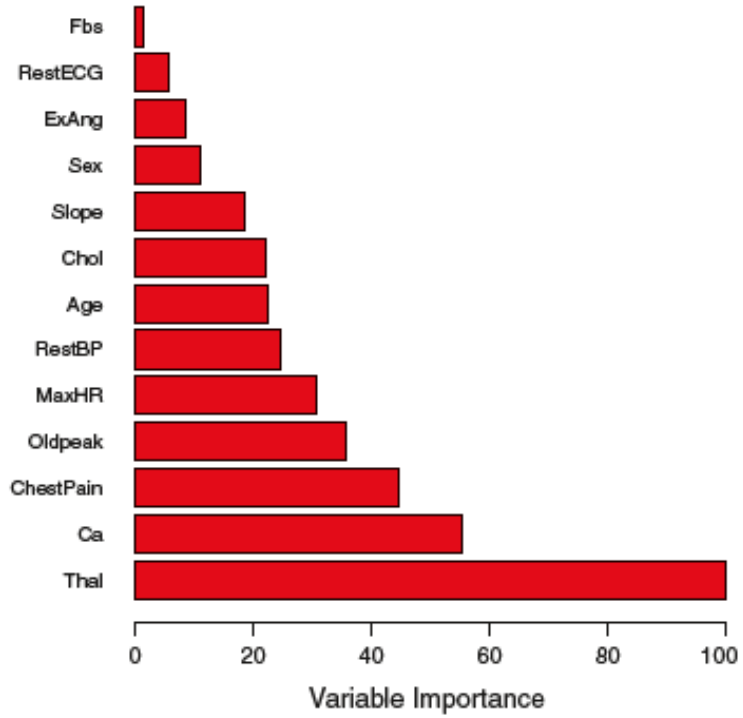


# Power of an ensemble of trees

**Increased performance**




**Built-in feature importance**



# Ensemble method

Is diversity always good?

# Ensemble method

How do we gather models that solve the problem?

- Idea3: Include models that actually contribute
- Idea4: Train each sequentially to improve the error

# Boosting

# Boosting

1. Set $\hat{f}(x) = 0$ and $r_i = y_i$ for all $i$ in the training set.

2. For $b = 1, 2, \ldots, B$, repeat:

   (a) Fit a tree $\hat{f}^b$ with $d$ splits ($d+1$ terminal nodes) to the training data $(X, r)$.

   (b) Update $\hat{f}$ by adding in a shrunken version of the new tree:

   $$\hat{f}(x) \leftarrow \hat{f}(x) + \lambda \hat{f}^b(x).$$

   (c) Update the residuals,

   $$r_i \leftarrow r_i - \lambda \hat{f}^b(x_i).$$

3. Output the boosted model,

$$\hat{f}(x) = \sum_{b=1}^{B} \lambda \hat{f}^b(x).$$

ISLR. *p.323*

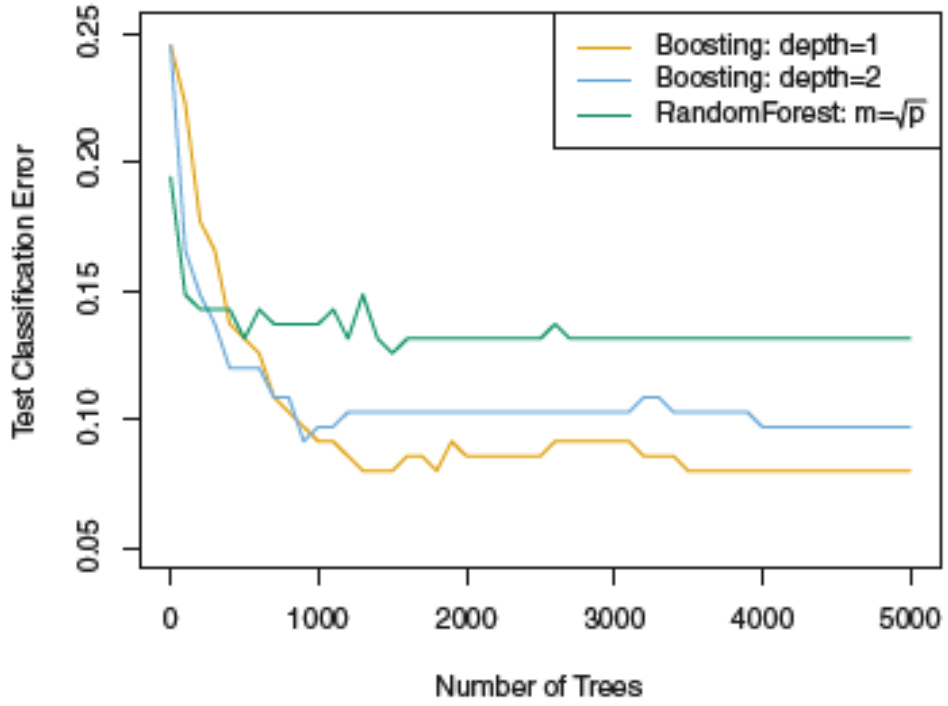
# Boosting- Tuning parameters

- Number of trees B
  If B too large, it can overfit

- Shrinkage parameter (boosting learning rate)
  typical values: 0.01~0.001
  trade-off with B

- Number of splits d in each tree
  as small as d=1~2 enough

# RF vs. Boosting




Both RF and Boosting are tree ensembles

RF randomly subsamples features as well as on bootstrapping on data

RF grows large decorrelated trees to fit y

Boosting fits small trees to the residuals and additively add the small trees

RF cannot overfit while boosting can