

Lecture 13

Decision Trees and Random Forest

EL-GY 6143/CS-GY 6923: INTRODUCTION TO MACHINE LEARNING
PROF. PEI LIU



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End of Semester Logistics

- ❑ Final exam on Tuesday May 10 6:00PM-8:30PM
 - Assigned seats for in-person exam
 - Same format as midterm
- ❑ We will grade all the homework by the end of next week.
 - If there are any problems, talk with Mustafa during office hours on May 16 (Monday), 17(Tuesday).
 - Last homework (this lecture) will not be graded since solution will be posted before the exam.
- ❑ Final project (optional) due by May 17, 23:59PM
 - Submission via Gradescope
 - Submit a quad chart, a brief report and .ipynd (both pdf and executable)
 - <https://github.com/pliugithub/MachineLearning/blob/master/projects/submission.md>
 - More details on the requirements for projects can be found on Github
 - <https://github.com/pliugithub/MachineLearning/blob/master/sequence.md>



Outline

- ❑ Decision tree as constrained space partition
- ❑ Regression tree design
- ❑ Decision tree pruning
- ❑ Classification tree design
- ❑ Bagging
- ❑ Random Forest
- ❑ Feature ranking from random forest



Decision tree as constrained space partitioning

- Each region is regressed/classified to the same value
- The partition can be specified sequentially by splitting the range of one feature at a time.
- The splitting rule can be described by a tree.
 - Each leaf node = One region
 - Size of tree $|T|$ = number of leaf nodes
- The partition is constrained: only rectangles in the 2D case.
 - The top left partition cannot be realized by a decision tree.

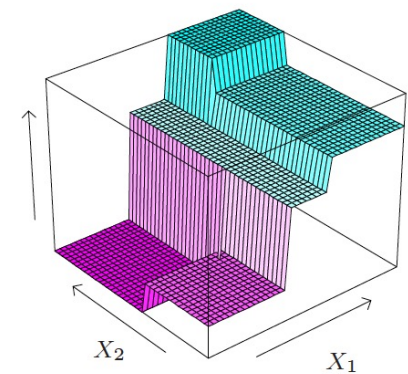
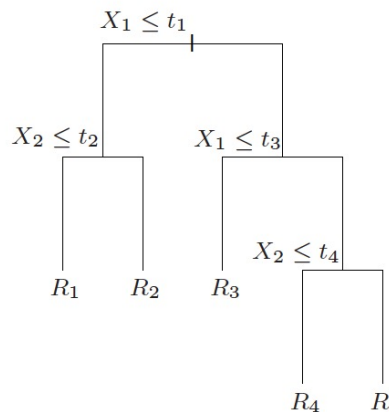
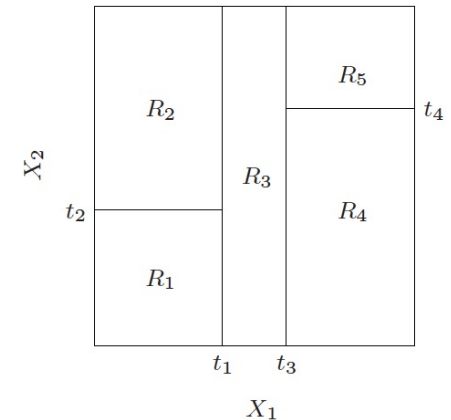
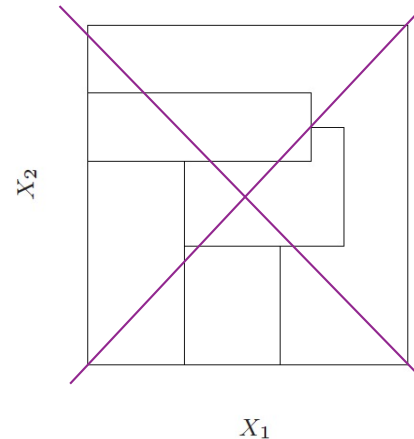


Fig. 9.2 in ESL

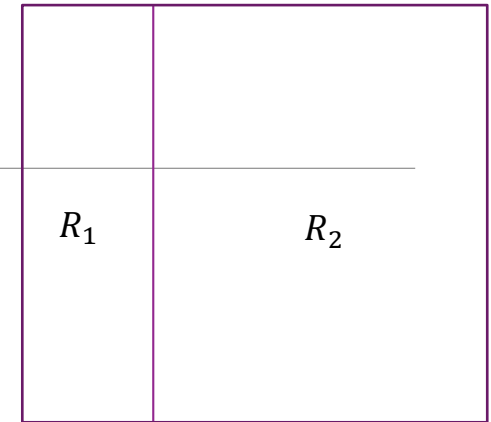


How to build a decision tree? (Regression Case)

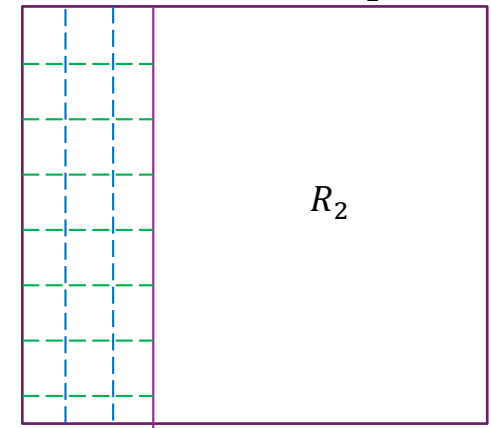
- Goal: minimize RSS

$$L = \sum_{m=1}^{|T|} \sum_{x_n \in R_m} (y_n - \bar{y}_m)^2$$

- Greedy algorithm:
- Start with a single region (entire space) and iterate:
- For each region R_m , select a feature x_j , and a splitting threshold s , such that splitting R_k with the criterion $x_j < s$ produces the largest decrease in RSS in R_m
 - Exhaustive search: for each x_j , try all possible s in the current range of x_j in R_m
- Stop splitting a region if it contains $\leq N_{min}$ samples



All possible splits of R_1 :



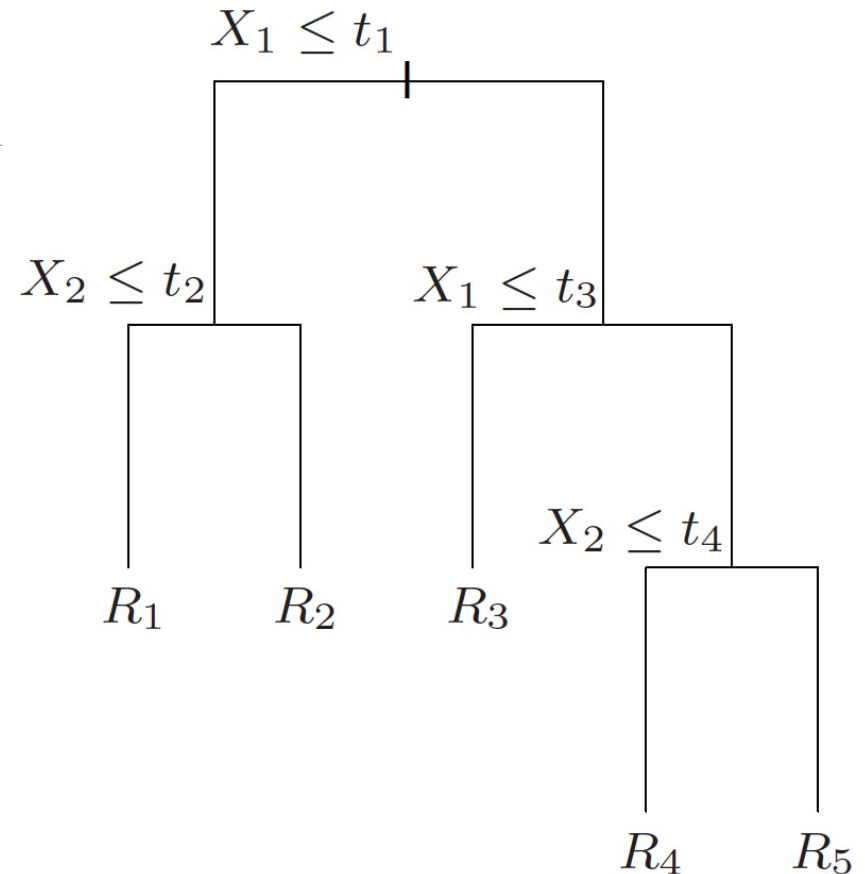
Overfitting

- ❑ Decision tree is very prone to overfitting
- ❑ Can exactly represent any function defined by the training set by having as many regions (or leaf nodes) as needed (Fully grown tree)
- ❑ How to control overfitting?
 - Find optimal subtree (with a certain constraint on the minimum number of samples in the leaf nodes or maximum depth) by cross validation: too many possibilities
 - Stop growing once RSS stop decreasing by a threshold with any new cut:
 - Not good because we use greedy search. It is possible to find a good cut after a bad one.
 - Better idea: grow a full tree first, then prune the tree.



Weakest link pruning

- Starting with the initial full tree T_0 , merge two adjacent leaf nodes (daughter nodes) to a single leaf node (mother). Select which nodes to merge by minimizing error increase. This produces a tree with one less region (or node)
- Repeat to merge another two nodes, until the minimum size tree is reached (e.g. a stump with 2 nodes)
- Generate a sequence of trees
 $T_0, T_1, T_2, T_3, \dots$
- Which one to choose?



Cost complexity pruning

- Minimize a complexity regularized loss, over all possible trees T_0, T_1, T_2, \dots

$$L(T, \alpha) = \sum_{m=1}^{|T|} \sum_{x_n \in R_m} (y_n - \bar{y}_m)^2 + \alpha |T|$$

- $\alpha=0$: Full tree, $\alpha = \infty$: minimum sized tree

Number of
leaf nodes
(regions)

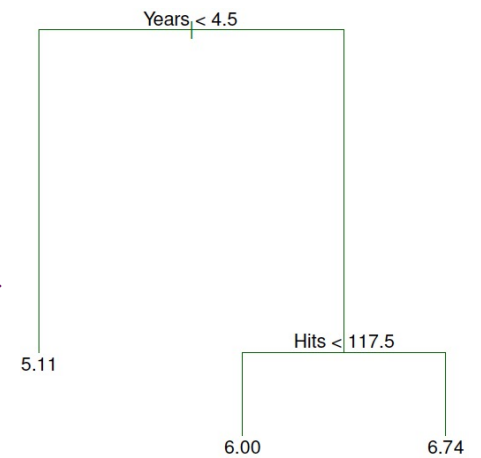
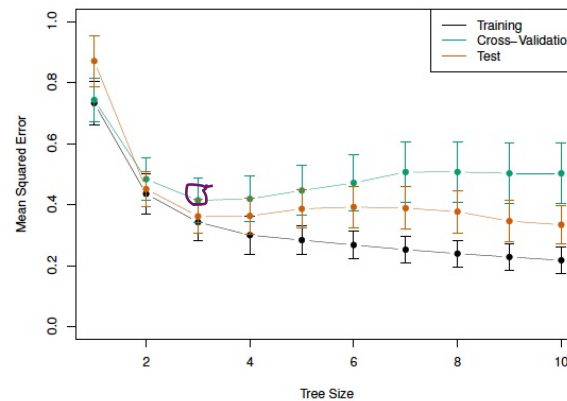
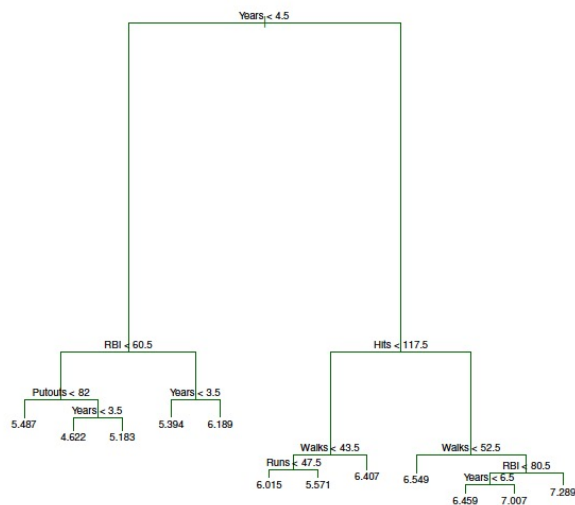
- How to choose α ? Cross validation!

- For each α
 - For each validation fold:
 - build a sequence of trees using the training set, and finding the RSS on the testing set for each candidate tree. Find a tree that minimizes $L(T, \alpha)$
 - Find average $L(T, \alpha)$ over all validation folds

- When dataset is very large, can just pick one tree that has minimal RSS for the testset.



Example: Predicting baseball player salaries



From <http://web.stanford.edu/class/stats202/notes/Tree/Regression-trees.html>



Feature importance

- ❑ For each feature, find all splits where this feature was used as the split variable and add up the loss reduction at all such splits
- ❑ The sum reflects the importance of this feature!



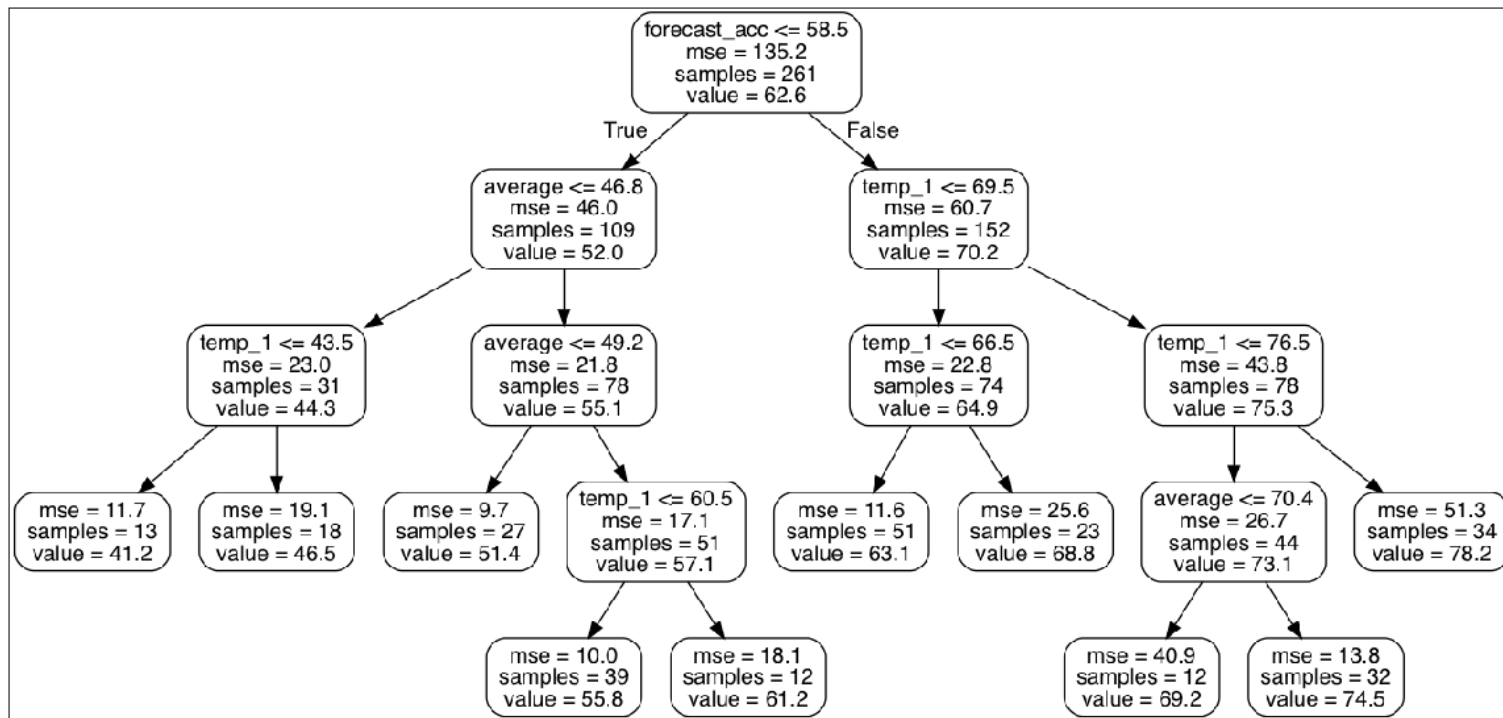
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Demo: weather prediction using decision tree



What about classification?

- ❑ The predicted class for each region = the majority class of training samples in the region
- ❑ How to design the tree?
 - Can use the same greedy algorithm
 - Split each region (by picking a feature and a threshold) to minimize a loss
 - What loss functions to use?



Classification loss

❑ Misclassification rate

$$L = \sum_{m=1}^{|T|} \sum_{x_n \in R_m} 1(y_n \neq \bar{y}_m) \quad , \bar{y}_m = \text{majority class of } R_m$$

❑ Gini index

$$L = \sum_{m=1}^{|T|} q_m \sum_{k=1}^K \hat{p}_{m,k} (1 - \hat{p}_{m,k}), \quad \hat{p}_{m,k} = \text{ratio of samples in } R_m \text{ that is class } k$$

- Expected error rate if we randomly pick an index, with probability $\hat{p}_{m,k}$ and error rate $1 - \hat{p}_{m,k}$

❑ Cross entropy

$$L = - \sum_{m=1}^{|T|} q_m \sum_{k=1}^K \hat{p}_{m,k} \log \hat{p}_{m,k} ,$$

- Smaller entropy means less uniform distribution (the region is more pure!)

❑ Gini and cross entropy loss lead to more "Pure" regions, with 1 dominate class in each region.



Performance metric and pruning

- ❑ After a tree is designed, the performance is still measured by the misclassification rate or accuracy
- ❑ It is typical to use the Gini index or cross entropy when growing a tree, but use the misclassification rate for pruning a tree



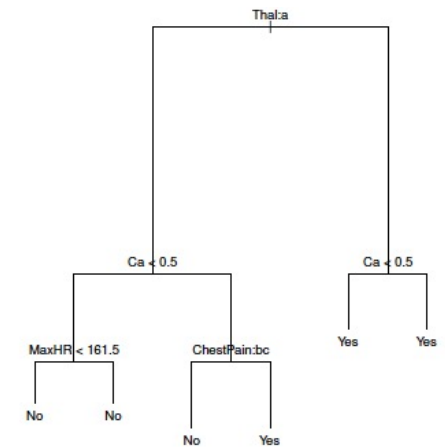
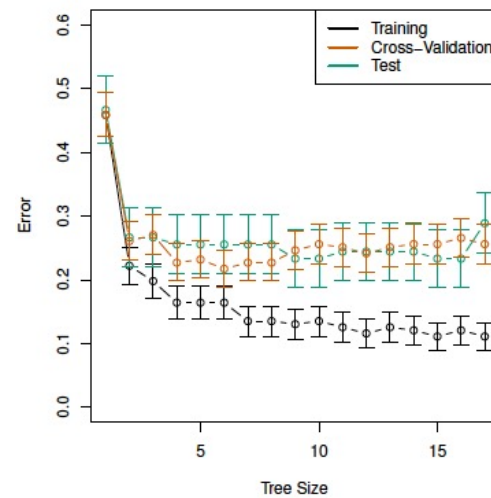
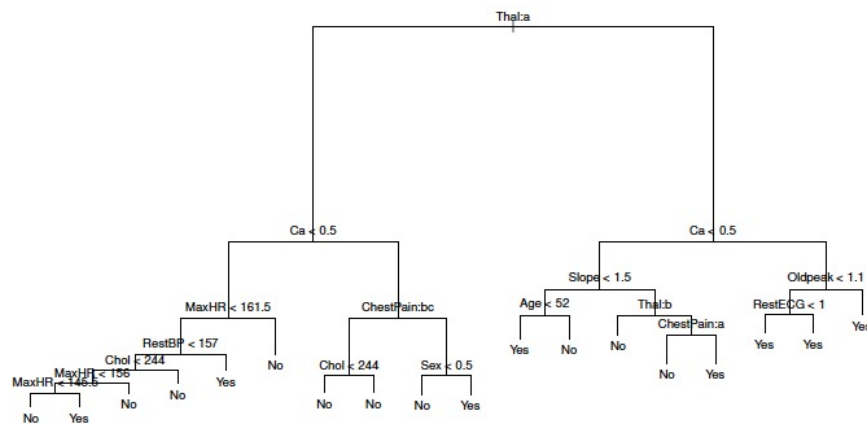
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Example: Classifying heart disease



From <http://web.stanford.edu/class/stats202/notes/Tree/Classification-trees.html>

Advantage of decision tree

- ❑ Easy to interpret: Doctors like them
- ❑ Closer to human decision making
- ❑ Feature importance can be derived during training
- ❑ Can easily handle mixed type of features (numerical and categorical) and missing features in some samples
 - Did not discuss here
- ❑ Problem:
 - To reduce bias, needs to grow the tree deeper
 - Deeper trees tend to overfit the training data (Large variance among different training data)
 - How to overcome ?

Bagging (Bootstrap Aggregating)

- ❑ Idea: Generate multiple trees from different training sets, and apply all models to each test sample and take average (or majority) of the results from all the trees
- ❑ How to generate different training sets giving a dataset?
- ❑ Cross validation: using a subset of data each time for training and the remaining for testing
- ❑ **Bootstrap sampling**: Sampling by **replacement**, each sampling contains the same number of samples as the original dataset, but some samples are replicated, others were not included
- ❑ Bagging: Generate B models from B bootstrap samplings
 - Regression: Average the prediction results from B models
 - Classification: Take the majority class index
- ❑ Apply to other regressors/classifiers as well.



Out of bag (OOB) error

❑ Each time we draw a bootstrap sampling, we only use ~63% of the samples

- Probability that a sample is chosen among N samples in each bootstrap sampling

$$1 - \left(1 - \frac{1}{N}\right)^N \sim 1 - e^{-1} = 0.632$$

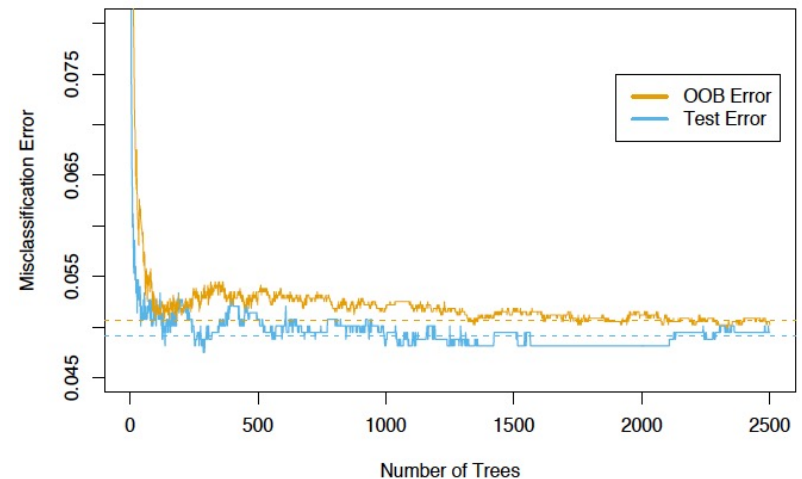
❑ We can use the remaining samples for testing

❑ OOB Error

- For each sample x_n , find the models generated by samplings which do not contain x_n . There are about 0.37B of models. Average predictions by these models for x_n .
- Compute the regression/classification error for x_n
- Average the error over all samples

❑ We can use OOB error as an estimate of the test error.

❑ Does not require design multiple models for multiple folds as in cross validation. OOB can be estimated from one pass of designing multiple trees.



From ESL Fig. 15.4



Why bagging?

- ❑ When a regressor or classifier has tendency to overfit (i.e. sensitive to the training set), bagging reduces the variance of the prediction
 - Reduce the test error
 - Particularly useful for decision trees
- ❑ When the sample number N in a given dataset is large
 - The empirical distribution is similar to the true distribution
 - Each bootstrap sampling is similar to an independent realization of the true distribution
 - Bagging amounts to averaging the fits from many identically distributed datasets



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Problems with bagging?

- ❑ Trees generated by different samplings can be very similar
- ❑ Test error reduces slowly as B increases
 - $f_b(x)$: prediction by tree b for test sample x
 - Assume $f_b(x)$ for all b have the same mean μ and variance σ^2
 - Assume these predictions have pair-wise correlation ρ
 - The variance of the average prediction $f(x) = \frac{1}{B} \sum_b f_b(x)$: (Shown on board)

$$\sigma_B^2 = \rho \sigma^2 + \frac{1}{B} (1 - \rho) \sigma^2$$



Random Forest

- ❑ As with Bagging: fit a different tree for each bootstrap sampling
- ❑ Recall that when growing a tree, at each current node (region), we split the region by choosing a particular feature and a threshold. The feature and the threshold are chosen among all P features to minimize a certain loss.
- ❑ With random forest, randomly choose among a subset of features ($P' < P$) for splitting each node
- ❑ The resulting trees are more different
- ❑ Rule of thumb: $P' = \sqrt{P}$ (but should be tuned using test error or OOB error)



Bagging vs. RF

□ Bagging:

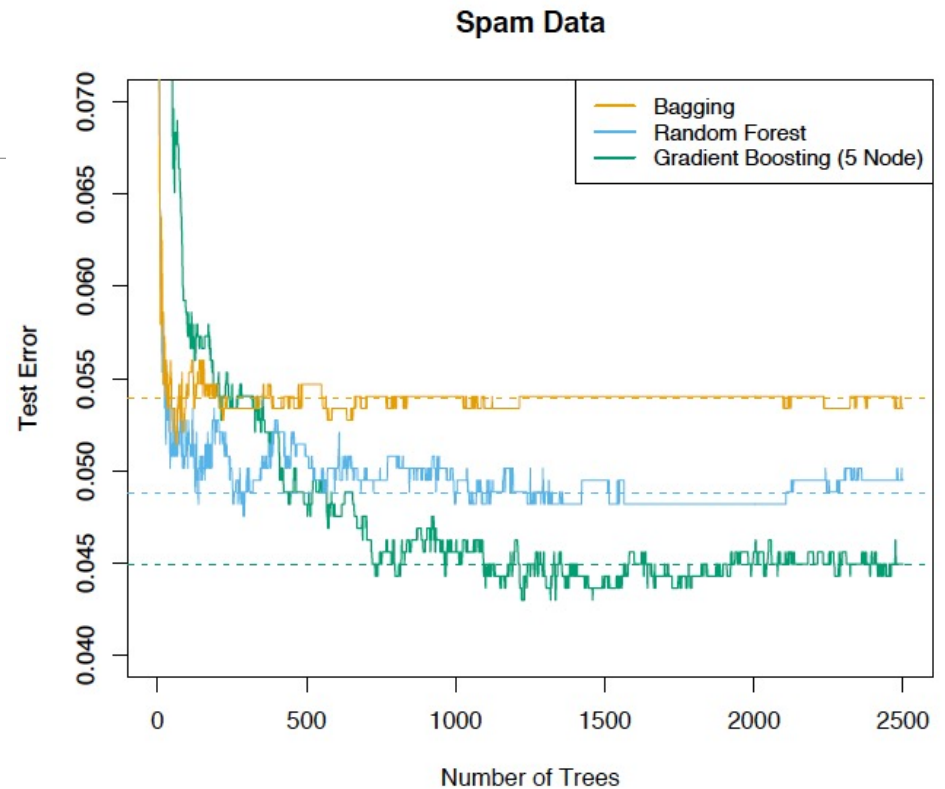
$$\sigma_B^2 = \rho \sigma^2 + \frac{1}{B} (1 - \rho) \sigma^2$$

□ Random forest (assuming $\rho = 0$):

$$\sigma_B^2 = \frac{1}{B} \sigma^2$$

□ Recall:

Test error = bias² + Variance + Noise Variance

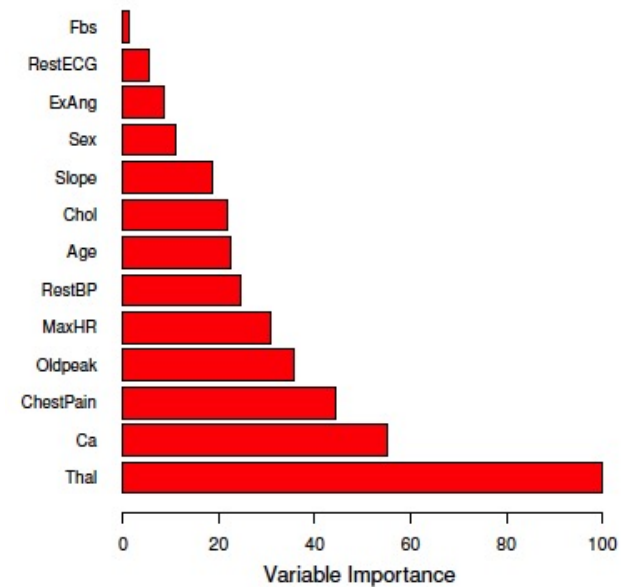


From ESL, Fig. 15.1



Feature importance

- For each feature, add up the loss reduction at splits where this feature was used over all trees.



Demo: Random forest



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Problem with bagging and random forest

- ❑ Resulting model has many trees!
- ❑ Lose interpretability!
- ❑ Related methods (not covered):
 - Boosting
 - Gradient boosting



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What you should know from this lecture

- ❑ How to use/interpret decision tree ?
- ❑ How to train a decision tree ?
 - Loss function for regression
 - Loss function for classification
- ❑ How to reduce overfitting ?
- ❑ What does bagging mean ?
- ❑ How to train and use a random forest ?
- ❑ How to determine feature importance?



References

- [ESL] Hastie, T., & Tibshirani, R. & Friedman, J.(2008). The Elements of Statistical Learning; Data Mining, Inference and Prediction. Sec. 9. (Decision tree), Sec. 15.2 (Random forest)



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