DS 4400

Machine Learning and Data Mining I
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Outline

- Ensemble models
  - Reduction in error and variance
- Bagging
  - Random forest
  - Variable importance
- Boosting
  - AdaBoost
  - Properties of boosting
  - Bagging vs Boosting

Ensemble Learning

Consider a set of classifiers h_1, ..., h_L

Idea: construct a classifier $H(\mathbf{x})$ that combines the individual decisions of h_1, ..., h_L

- e.g., could have the member classifiers vote, or
- e.g., could use different members for different regions of the instance space

Successful ensembles require **diversity**

- Classifiers should make different mistakes
- Can have different types of base learners

Reduce error

- Suppose there are 25 base classifiers
- Each classifier has error rate, $\varepsilon = 0.35$
- Assume independence among classifiers
- Probability that the ensemble classifier makes a wrong prediction:

$$\sum_{i=13}^{25} \binom{25}{i} \varepsilon^{\mathrm{i}} (1-\varepsilon)^{25-i} = 0.06$$

Reduce Variance

- Averaging reduces variance:

$$Var(\bar{X}) = \frac{Var(X)}{N}$$

(when predictions are **independent**)

Average models to reduce model variance

One problem:

only one training set

where do multiple models come from?

How to Achieve Diversity

- Avoid overfitting
  - Vary the training data
- Features are noisy
  - Vary the set of features

Two main ensemble learning methods

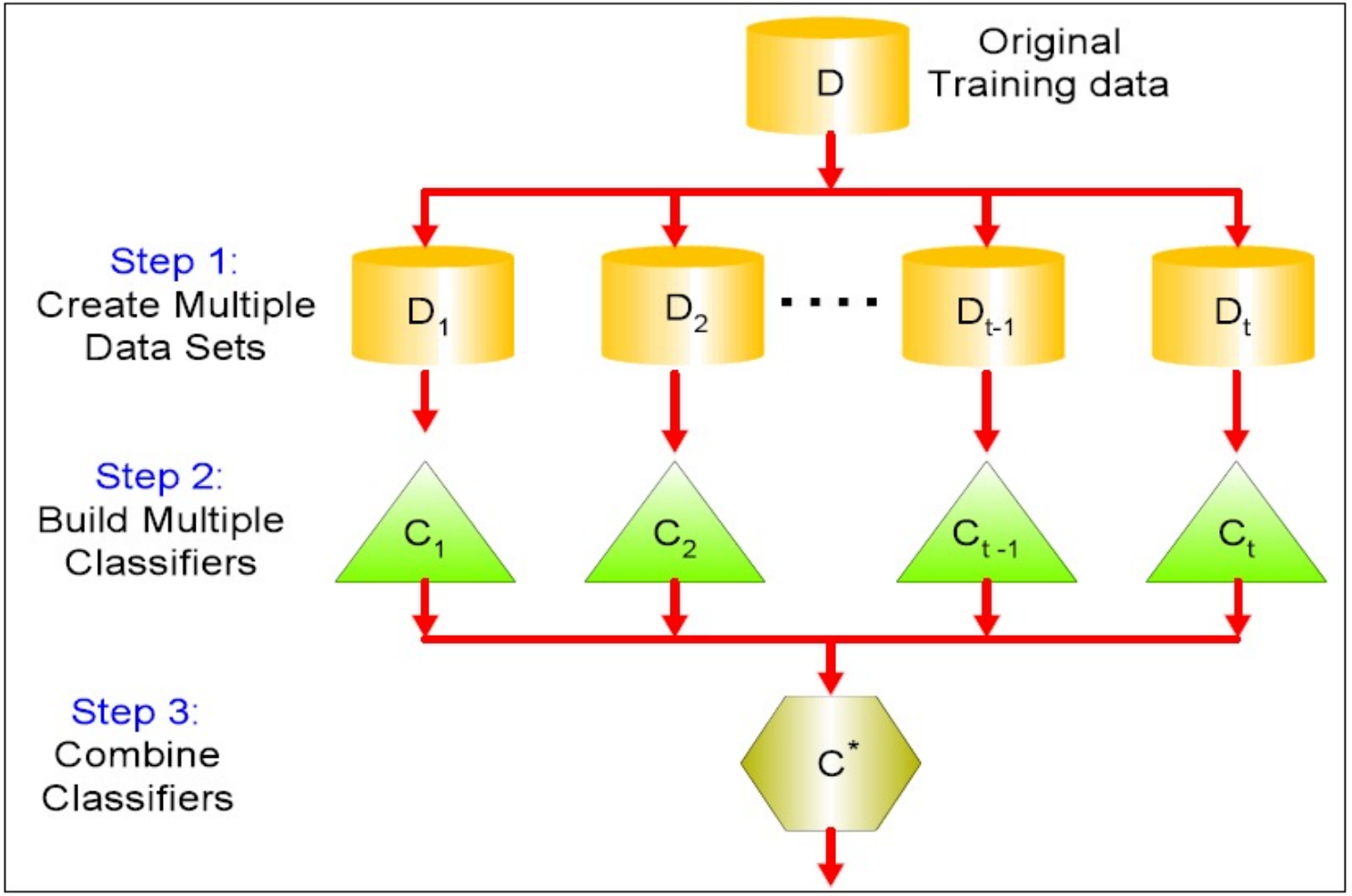
- Bagging (e.g., Random Forests)
- Boosting (e.g., AdaBoost)

Bagging

- Leo Breiman (1994)
- Take repeated bootstrap samples from training set *D*
- *Bootstrap sampling*: Given set *D* containing *N* training examples, create *D*' by drawing *N* examples at random with replacement from *D*.

- Bagging:
  - Create *k* bootstrap samples D_1 ... D_k.
  - Train distinct classifier on each D_i.
  - Classify new instance by majority vote / average.

General Idea



Majority Votes

Example of Bagging

- Sampling with replacement

Training Data

Data ID

Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

- Sample each training point with probability 1/N
- Out-Of-Bag (OOB) observation: point not in sample

Example of Bagging

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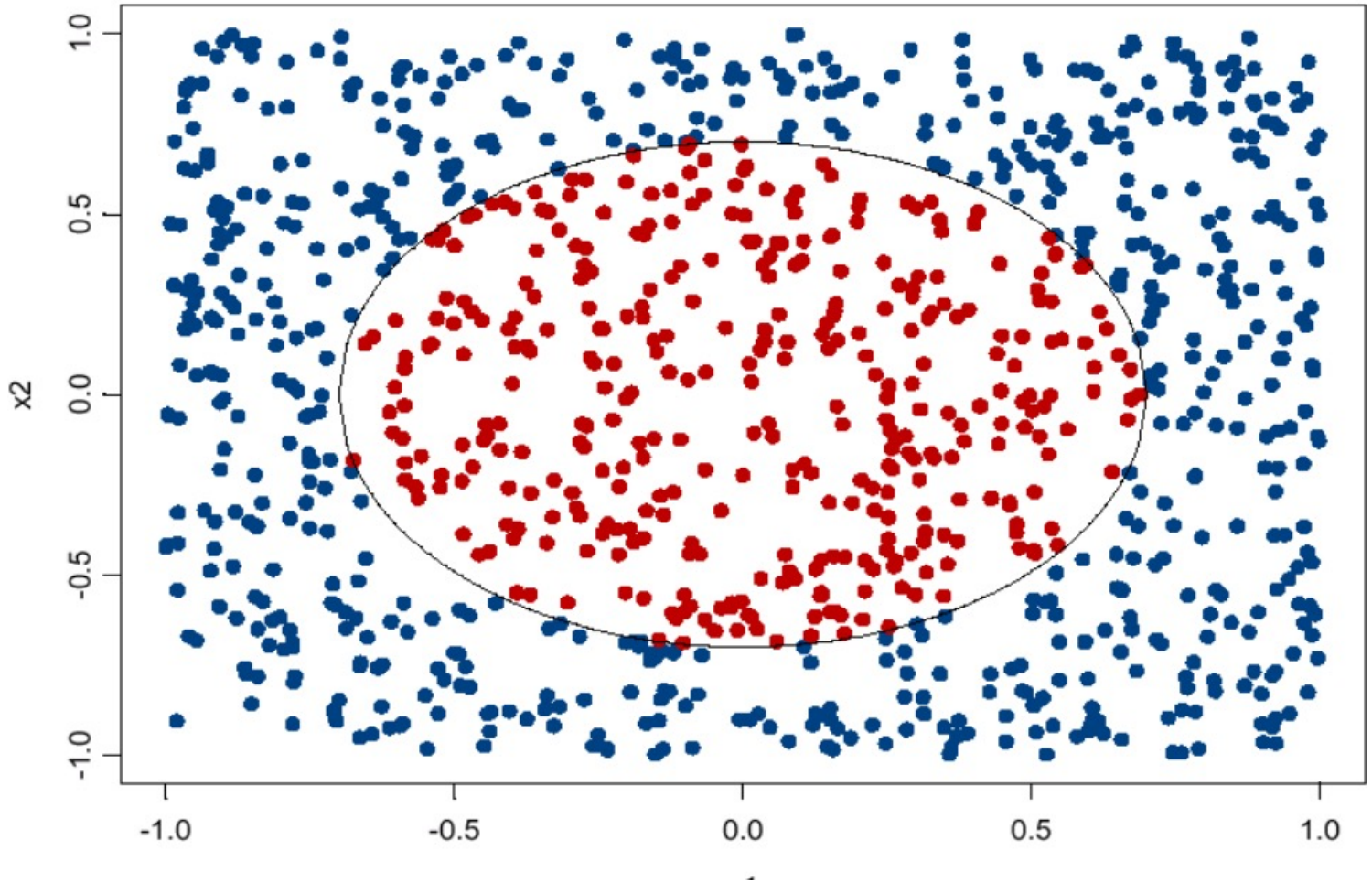
- Sample each training point with probability 1/n
- Out-Of-Bag (OOB) observation: point not in sample
  - For each point: prob $(1-1/n)^n$
  - About 1/3 of data
  - OOB error: error on OOB samples
- OOB average error
  - Compute across all models in Ensemble
  - Use instead of Cross-Validation error

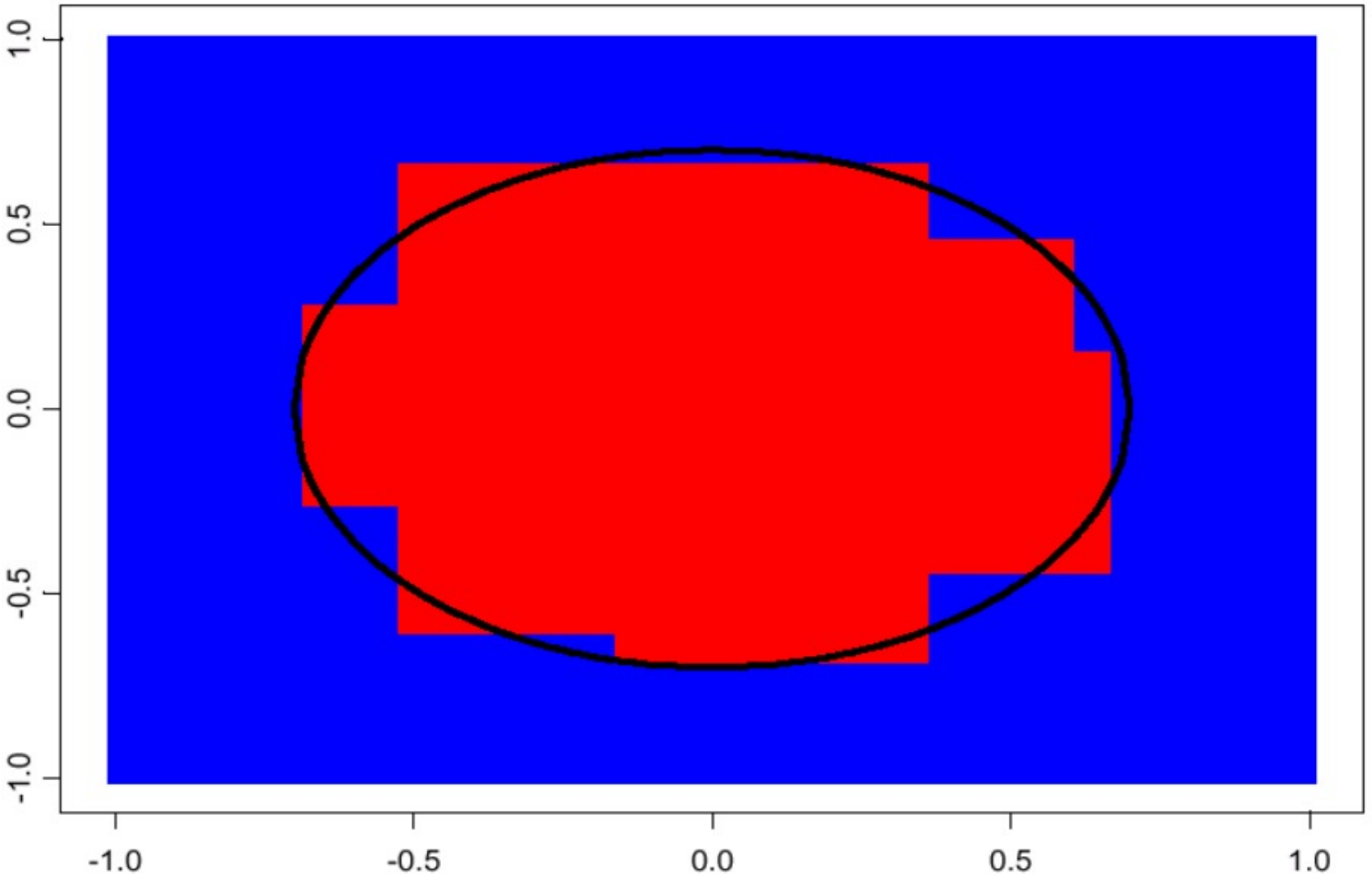
Bagging

- Can be applied to multiple classification models
- Very successful for decision trees
  - Decision trees have high variance
  - Don’t prune the individual trees, but grow trees to full extent
  - Precision accuracy of decision trees improved substantially
- OOB average error used instead of Cross Validation

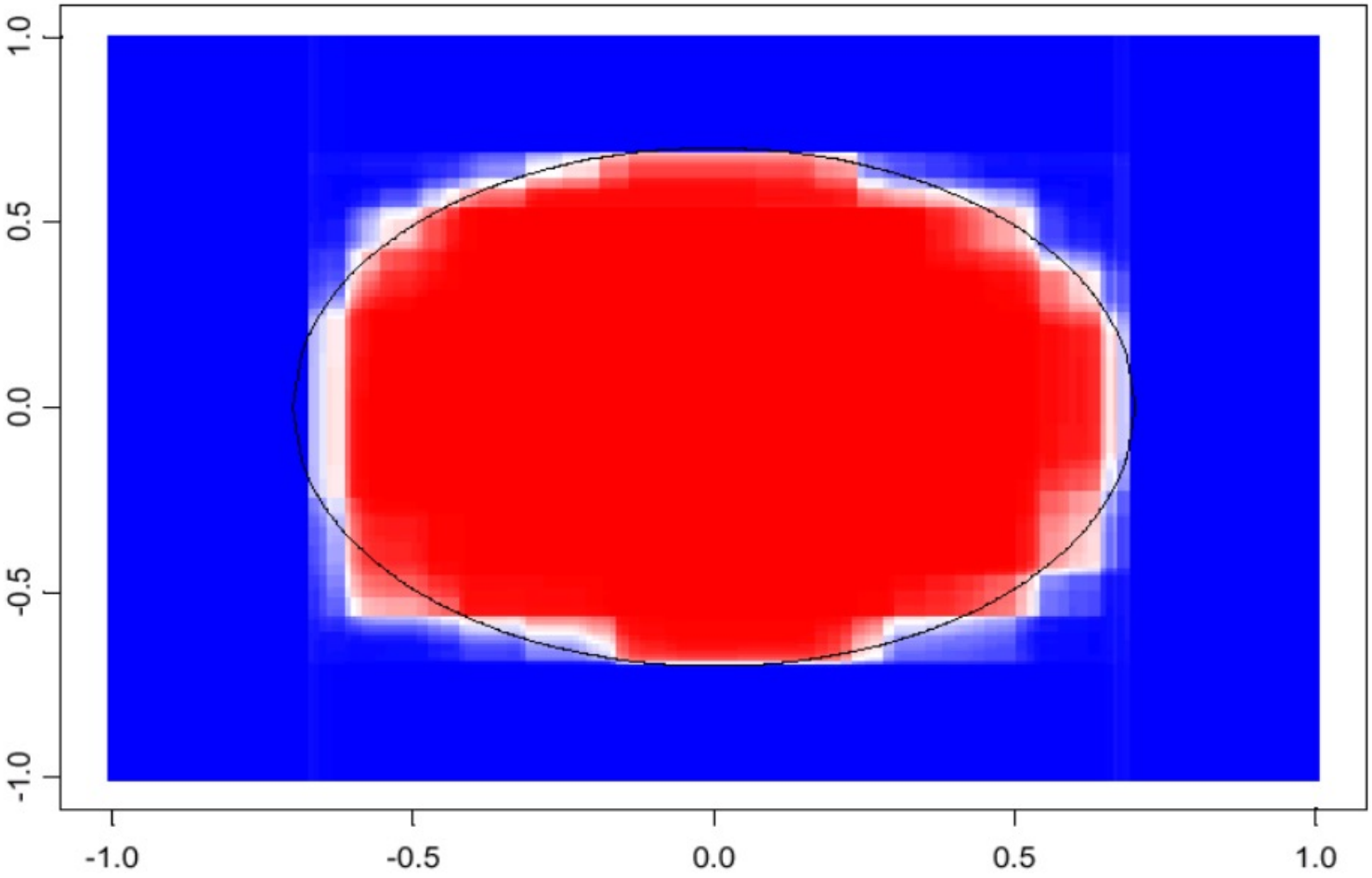
Example Distribution



Decision Tree Decision Boundary



100 Bagged Trees



shades of blue/red indicate strength of vote for particular classification

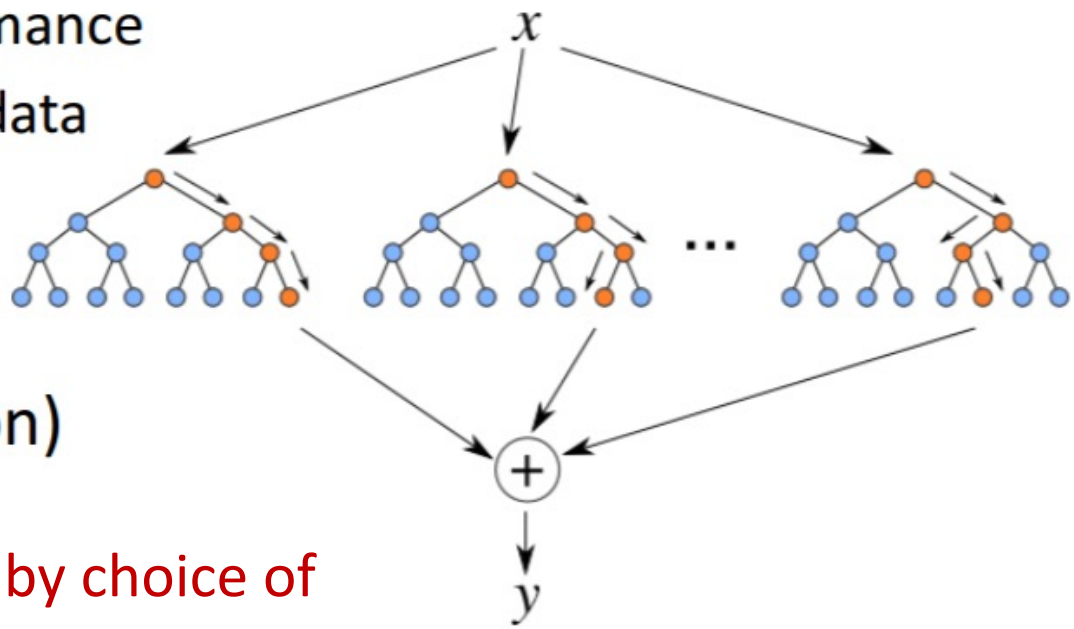
Random Forests

- Ensemble method specifically designed for decision tree classifiers

- Introduce two sources of randomness: "Bagging" and "Random input vectors"
  - Bagging method: each tree is grown using a bootstrap sample of training data
  - Random vector method: At each node, best split is chosen from a random sample of *m* attributes instead of all attributes

Random Forests

- Construct decision trees on bootstrap replicas
  - Restrict the node decisions to a small subset of features picked randomly for each node
- Do not prune the trees
  - Estimate tree performance on out-of-bootstrap data
- Average the output of all trees (or choose mode decision)



Trees are de-correlated by choice of random subset of features

Random Forest Algorithm

1. For $b = 1$ to B:

   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.

   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.

      i. Select m variables at random from the p variables.

      ii. Pick the best variable/split-point among the m.

      iii. Split the node into two daughter nodes.

2. Output the ensemble of trees $\{T_b\}_1^B$.

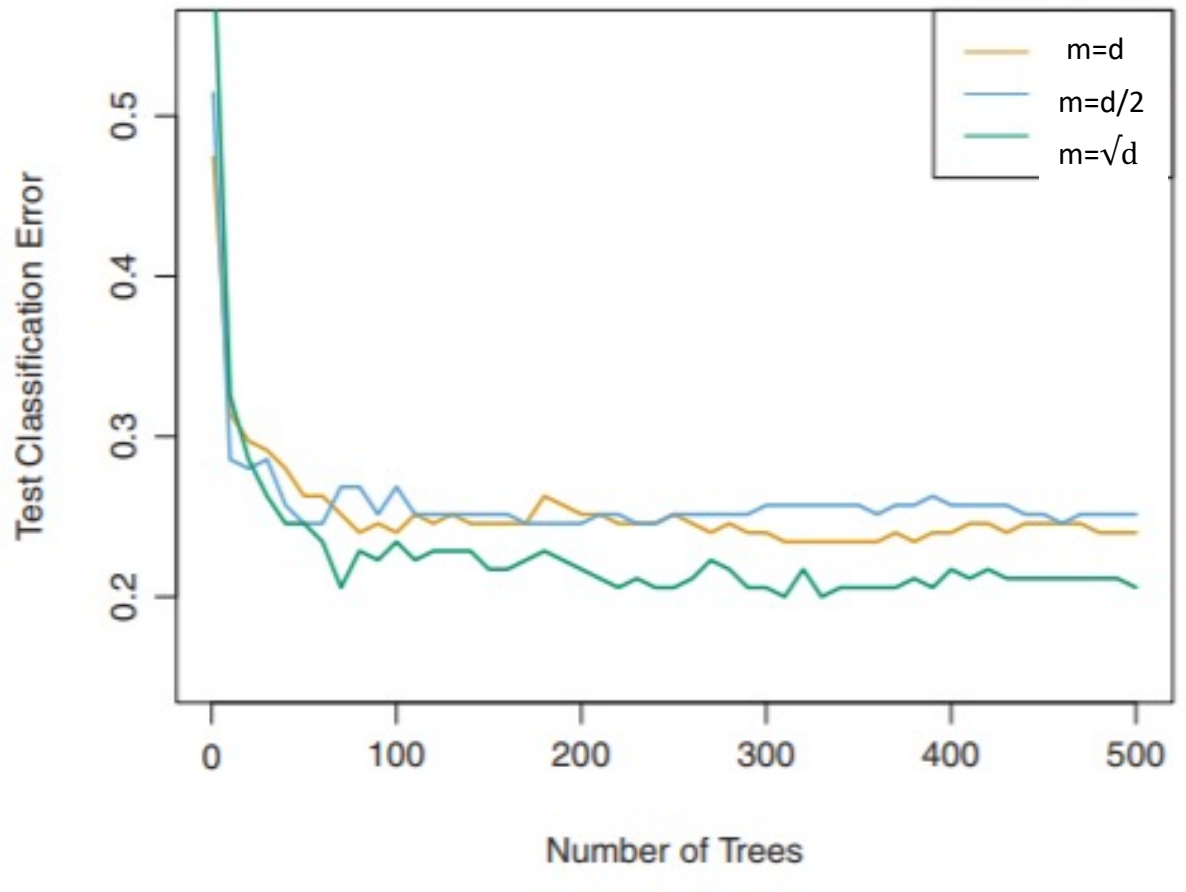
To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

If m=p, this is equivalent to Bagging with Decision Trees as base learner

Effect of Number of Predictors



- d = total number of predictors; m = predictors chosen in each split
- Random Forests uses $m = \sqrt{d}$

Variable Importance

- Ensemble of trees looses somewhat interpretability of decision trees
- Which variables contribute mostly to prediction?
- Random Forests computes a Variable Importance metric per feature
  - For each tree in the ensemble, consider the split by the particular feature
  - How much information gain / Gini index decreases after the split
  - Average over all trees

Variable Importance Plots

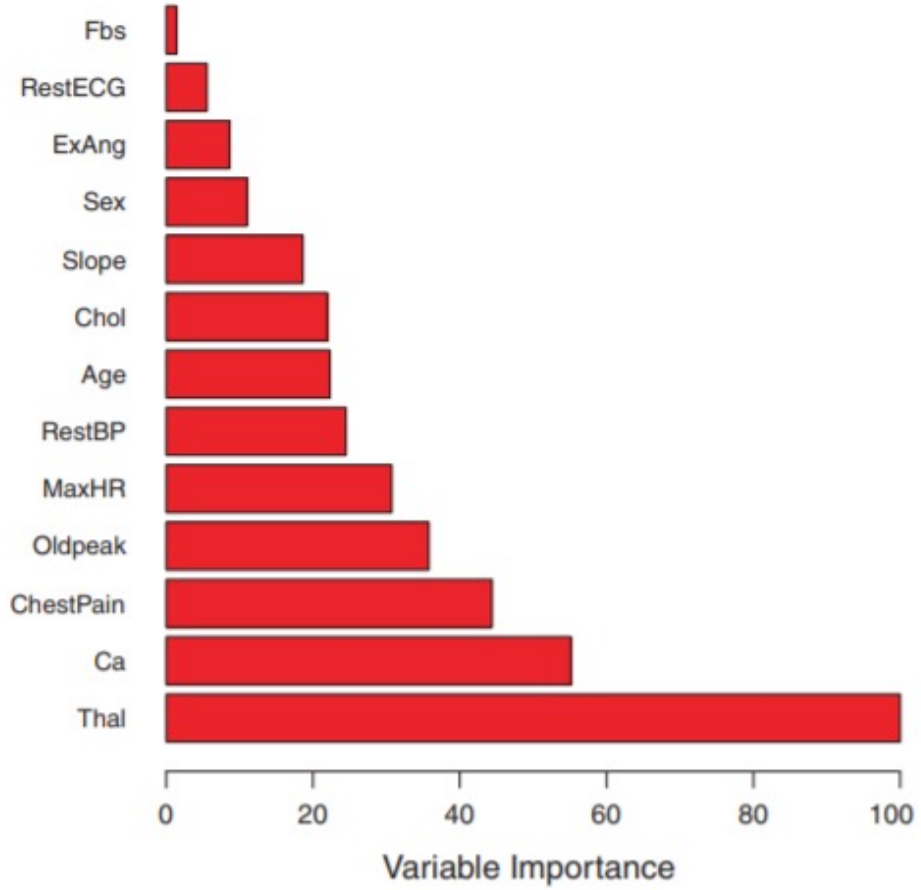


FIGURE 8.9. *A variable importance plot for the* `Heart` *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

Variable Importance

- Ensembles of trees loose in interpretability
  - Variable importance helps with determining important features
- Can be used for feature selection
  - Train Random Forest model
  - Compute variable importance
  - Select top k features by highest important
  - Train other models with the k features

How to Achieve Diversity

- Avoid overfitting
  - Vary the training data
- Features are noisy
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Two main ensemble learning methods

- Bagging (e.g., Random Forests)
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AdaBoost

- A meta-learning algorithm with great theoretical and empirical performance
- Turns a base learner (i.e., a "weak hypothesis") into a high performance classifier
- Creates an ensemble of weak hypotheses by repeatedly emphasizing mispredicted instances

Adaptive Boosting
Freund and Schapire 1997

Overview of AdaBoost

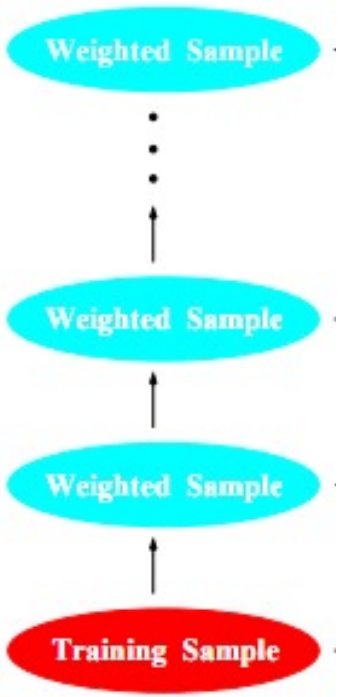
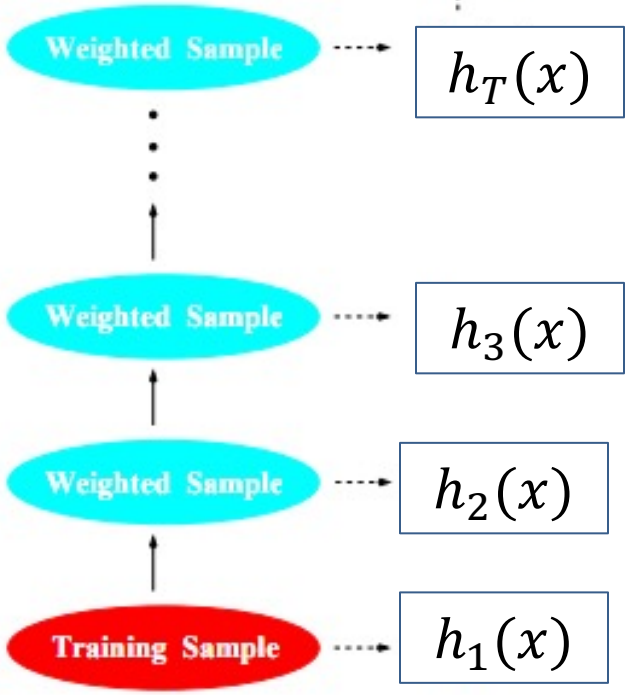


FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

Overview of AdaBoost

Sequential training process

$$G(x) = sign(\sum_{t=1}^{T} \beta_t h_t(x))$$



Better classifiers will get higher weights

- Mis-classified examples get higher weights
- Correct examples get lower weights

Uniform weights

FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

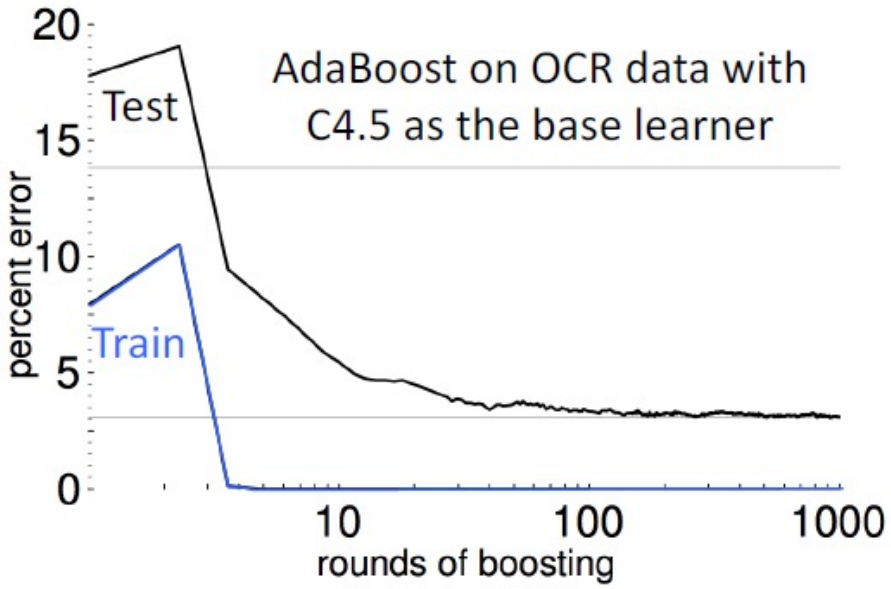
Boosting [Shapire '89]

- **Idea:** given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote
- On each iteration t:
  - weight each training example by how incorrectly it was classified
  - Learn a weak hypothesis – h_t
  - A strength for this hypothesis – β_t
- Final classifier: $G(x) = sign(\sum \beta_t h_t(x))$

Convergence bounds with minimal assumptions on weak learner

If each weak learner h_t is slightly better than random guessing ($\varepsilon_t < 0.5$), then training error of AdaBoost decays exponentially fast in number of rounds T.

Resilience to overfitting



- Empirically, boosting resists overfitting
- Note that it continues to drive down the test error even AFTER the training error reaches zero

Increases confidence in prediction when adding more rounds

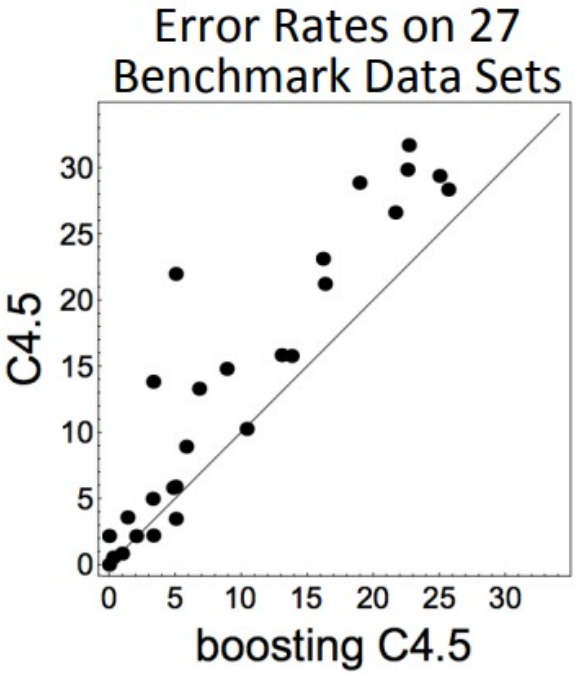
Base Learner Requirements

- AdaBoost works best with "weak" learners
  - Should not be complex
  - Typically high bias classifiers
  - Works even when weak learner has an error rate just slightly under 0.5 (i.e., just slightly better than random)
    - Can prove training error goes to 0 in $O(\log n)$ iterations

- Examples:
  - Decision stumps (1 level decision trees)
  - Depth-limited decision trees
  - Linear classifiers

Boosted Decision Trees

- Boosted decision trees are one of the best "off-the-shelf" classifiers
  - i.e., no parameter tuning
- Limit member hypothesis complexity by limiting tree depth
- Gradient boosting methods are typically used with trees in practice



"AdaBoost with trees is the best off-the-shelf classifier in the world" -Breiman, 1996
(Also, see results by Caruana & Niculescu-Mizil, ICML 2006)

Review

- Ensemble learning are powerful learning methods
  - Better accuracy than standard classifiers
- Bagging uses bootstrapping (with replacement), trains T models, and averages their prediction
  - Random forests vary training data and feature set at each split
- Boosting is an ensemble of T weak learners that emphasizes mis-predicted examples
  - AdaBoost has great theoretical and experimental performance
  - Can be used with linear models or simple decision trees (stumps, fixed-depth decision trees)