DS 5220

Supervised Machine Learning and Learning Theory

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Logistics

- Projects
  - Feedback in Gradescope
  - Team document in Piazza
  - Start working on project!
  - Milestone on Monday, Nov 18
  - 3 pages on progress
- Holiday on Monday, November 11
- Last assignment on ensembles, neural networks released late next week
- Final exam will be 2 hours on Wed 12/04

Summary Decision Trees

- Representation: decision trees
- Bias: prefer small decision trees
- Search algorithm: greedy
- Heuristic function: information gain or information content or others
- Overfitting / pruning

Strengths

- Fast to evaluate
- Interpretable
- Generate rules
- Supports categorical and numerical data

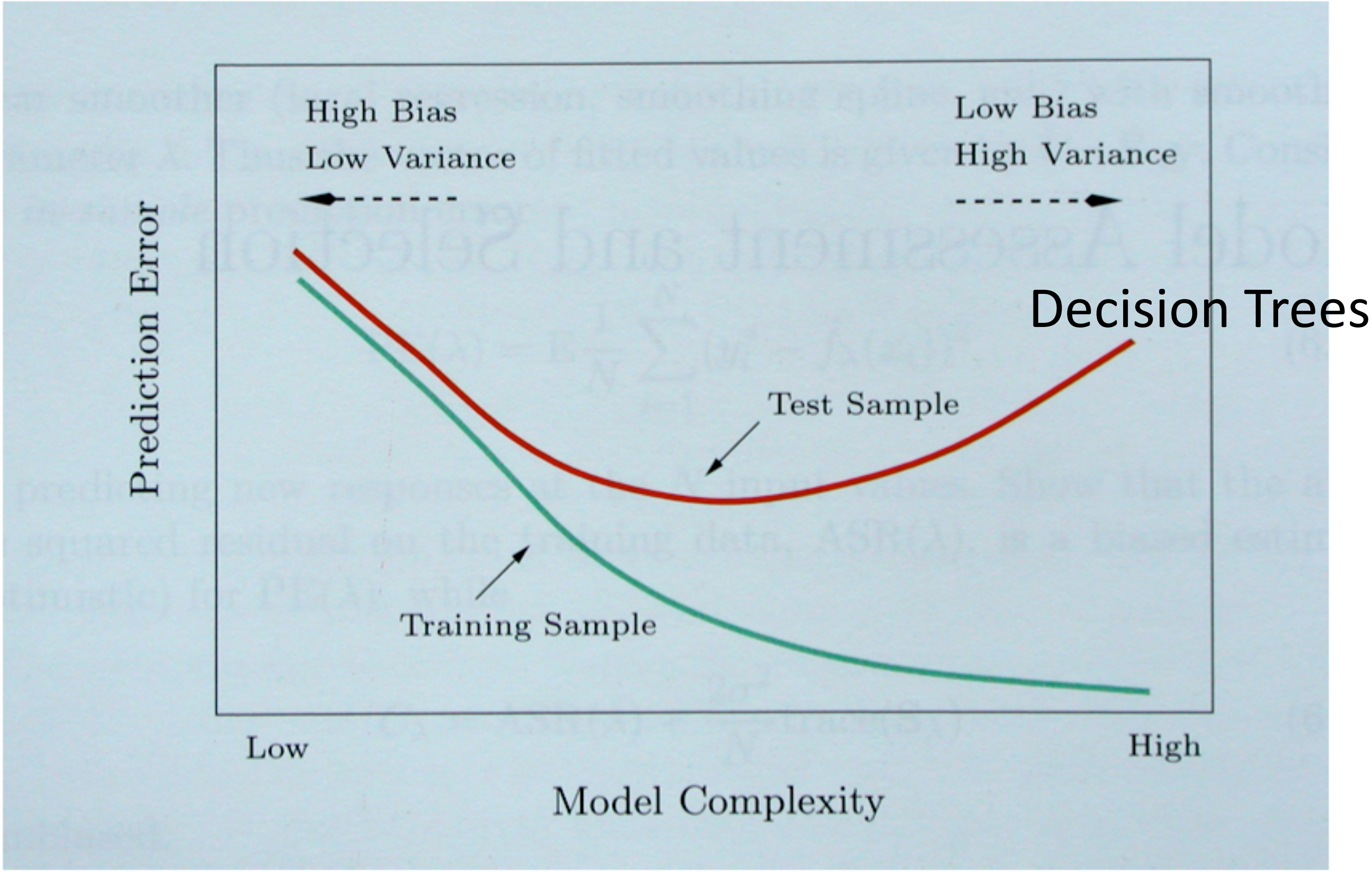
Weaknesses

- Overfitting
- Splitting method might not be optimal
- Accuracy is not always high
- Batch learning

Outline

- Ensemble learning
  - Combine multiple classifiers to reduce model variance and improve accuracy
- Bagging
  - Bootstrap samples
  - Random Forests
- Boosting
  - AdaBoost

Bias/Variance Tradeoff



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

How to reduce variance of single decision tree?

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

Build Ensemble Classifiers

- Basic idea
  - Build different “experts”, and let them vote
- Advantages
  - Improve predictive performance
  - Easy to implement
  - No too much parameter tuning
- Disadvantages
  - The combined classifier is not transparent and interpretable
  - Not a compact representation

Practical Applications

Goal: predict how a user will rate a movie

- Based on the user's ratings for other movies
- and other peoples' ratings
- with no other information about the movies

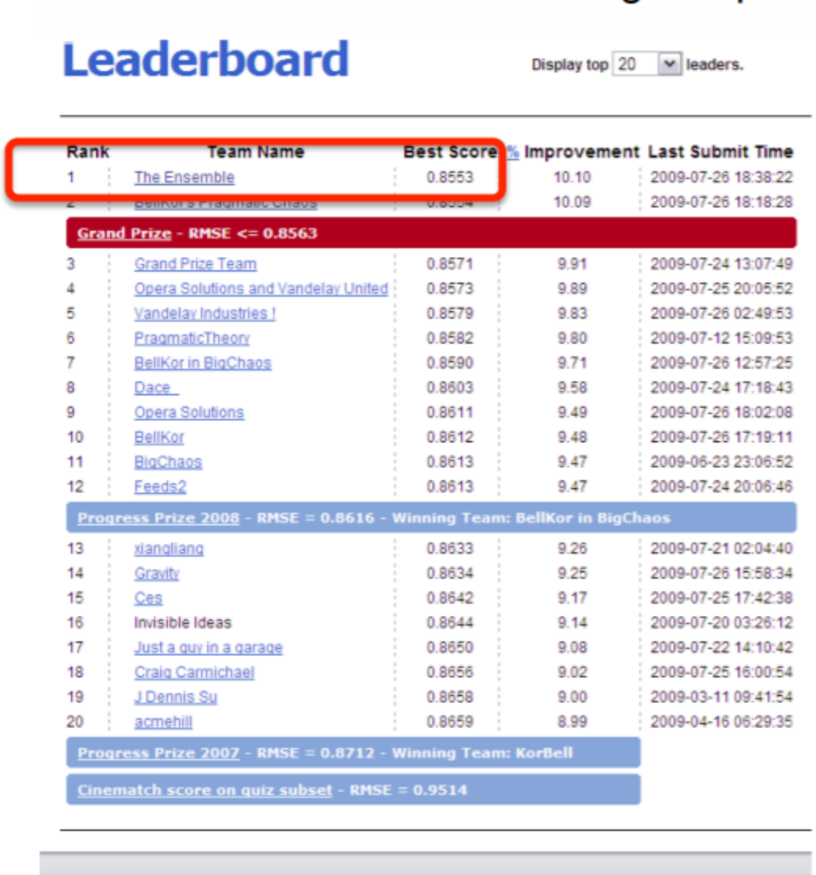
This application is called "collaborative filtering"

Netflix Prize: \$1M to the first team to do 10% better then Netflix' system (2007-2009)

Winner: BellKor's Pragmatic Chaos – an ensemble of more than 800 rating systems

Netflix Prize

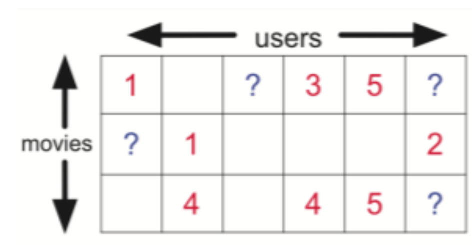
Machine learning competition with a $1 million prize



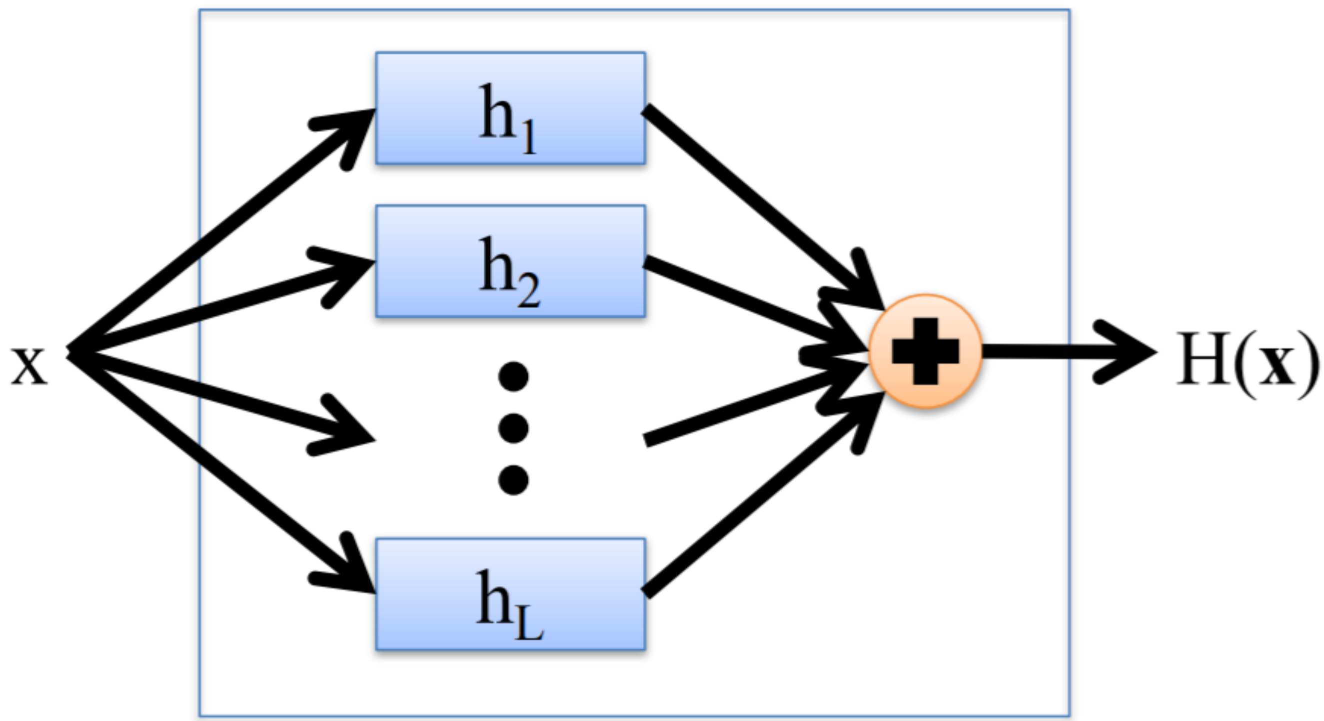
Leaderboard

Display top 20 leaders.

Rank	Team Name	Best Score	% Improvement	Last Submit Time
1	The Ensemble	0.8553	10.10	2009-07-26 18:38:22
2	[illegible]	[illegible]	10.09	2009-07-26 18:18:28
Grand Prize - RMSE <= 0.8563				
3	Grand Prize Team	0.8571	9.91	2009-07-24 13:07:49
4	Opera Solutions and Vandelay United	0.8573	9.89	2009-07-25 20:05:52
5	Vandelay Industries !	0.8579	9.83	2009-07-26 02:49:53
6	PragmaticTheory	0.8582	9.80	2009-07-12 15:09:53
7	BellKor in BigChaos	0.8590	9.71	2009-07-26 12:57:25
8	Dace_	0.8603	9.58	2009-07-24 17:18:43
9	Opera Solutions	0.8611	9.49	2009-07-26 18:02:08
10	BellKor	0.8612	9.48	2009-07-26 17:19:11
11	BigChaos	0.8613	9.47	2009-06-23 23:06:52
12	Feeds2	0.8613	9.47	2009-07-24 20:06:46
Progress Prize 2008 - RMSE = 0.8616 - Winning Team: BellKor in BigChaos				
13	xiangliang	0.8633	9.26	2009-07-21 02:04:40
14	Gravity	0.8634	9.25	2009-07-26 15:58:34
15	Ces	0.8642	9.17	2009-07-25 17:42:38
16	Invisible Ideas	0.8644	9.14	2009-07-20 03:26:12
17	Just a guy in a garage	0.8650	9.08	2009-07-22 14:10:42
18	Craig Carmichael	0.8656	9.02	2009-07-25 16:00:54
19	J Dennis Su	0.8658	9.00	2009-03-11 09:41:54
20	acmehill	0.8659	8.99	2009-04-16 06:29:35
Progress Prize 2007 - RMSE = 0.8712 - Winning Team: KorBell				
Cinematch score on quiz subset - RMSE = 0.9514				

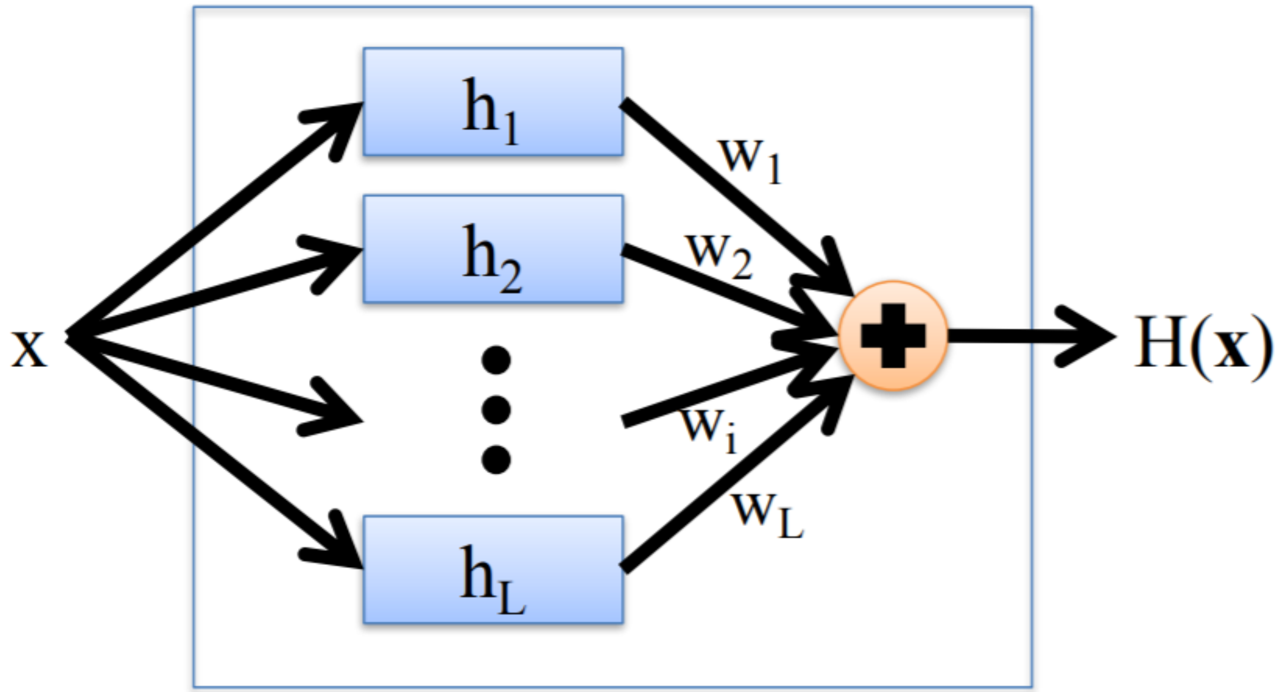


Combining Classifiers: Averaging



- Final hypothesis is a simple vote of the members

Combining Classifiers: Weighted Averaging



- Coefficients of individual members are trained using a validation set

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:

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

(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

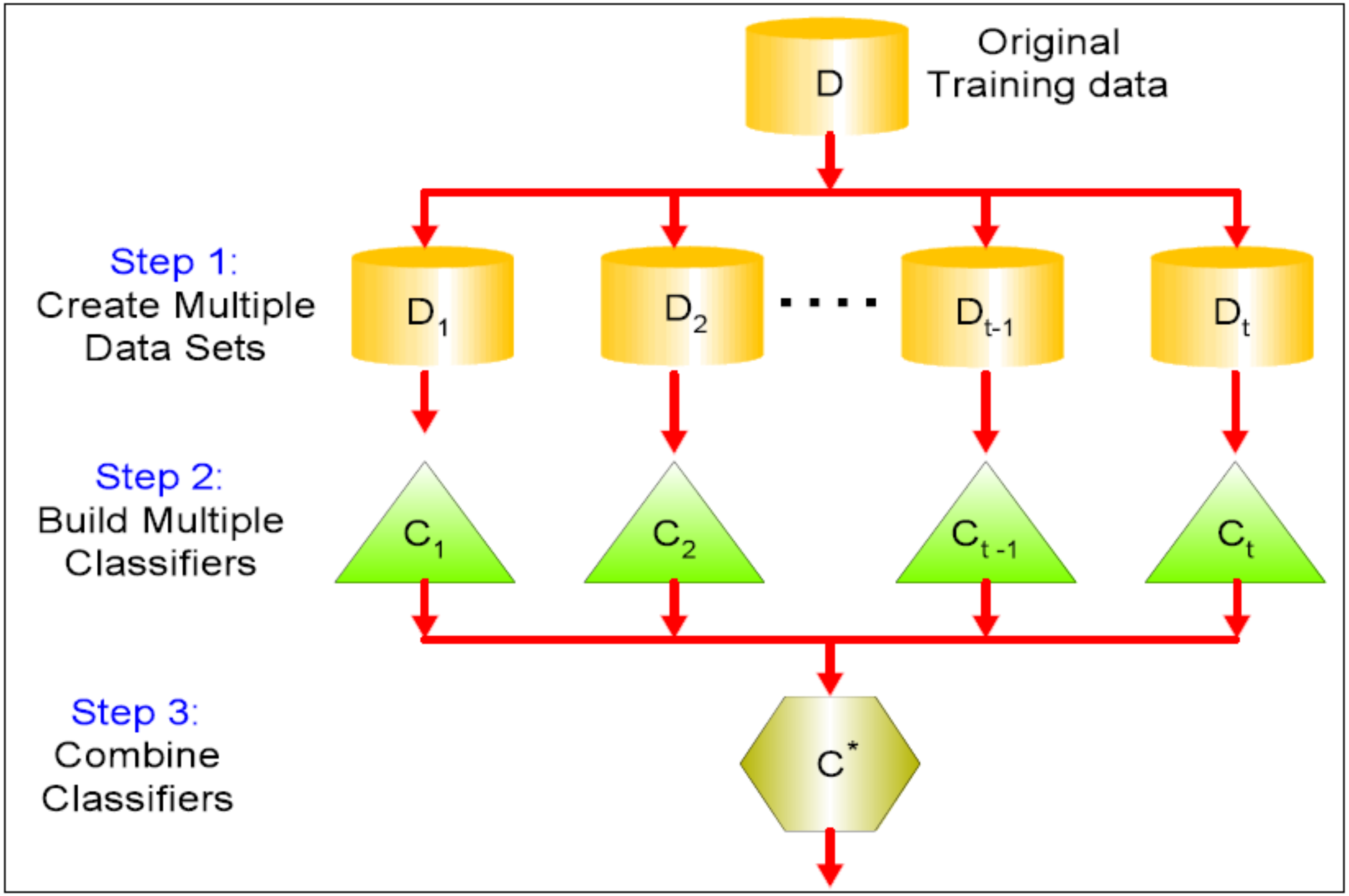
- Bagging (e.g., Random Forests)
- Boosting (e.g., AdaBoost)

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 $D_1 \ldots D_k$.
  - 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

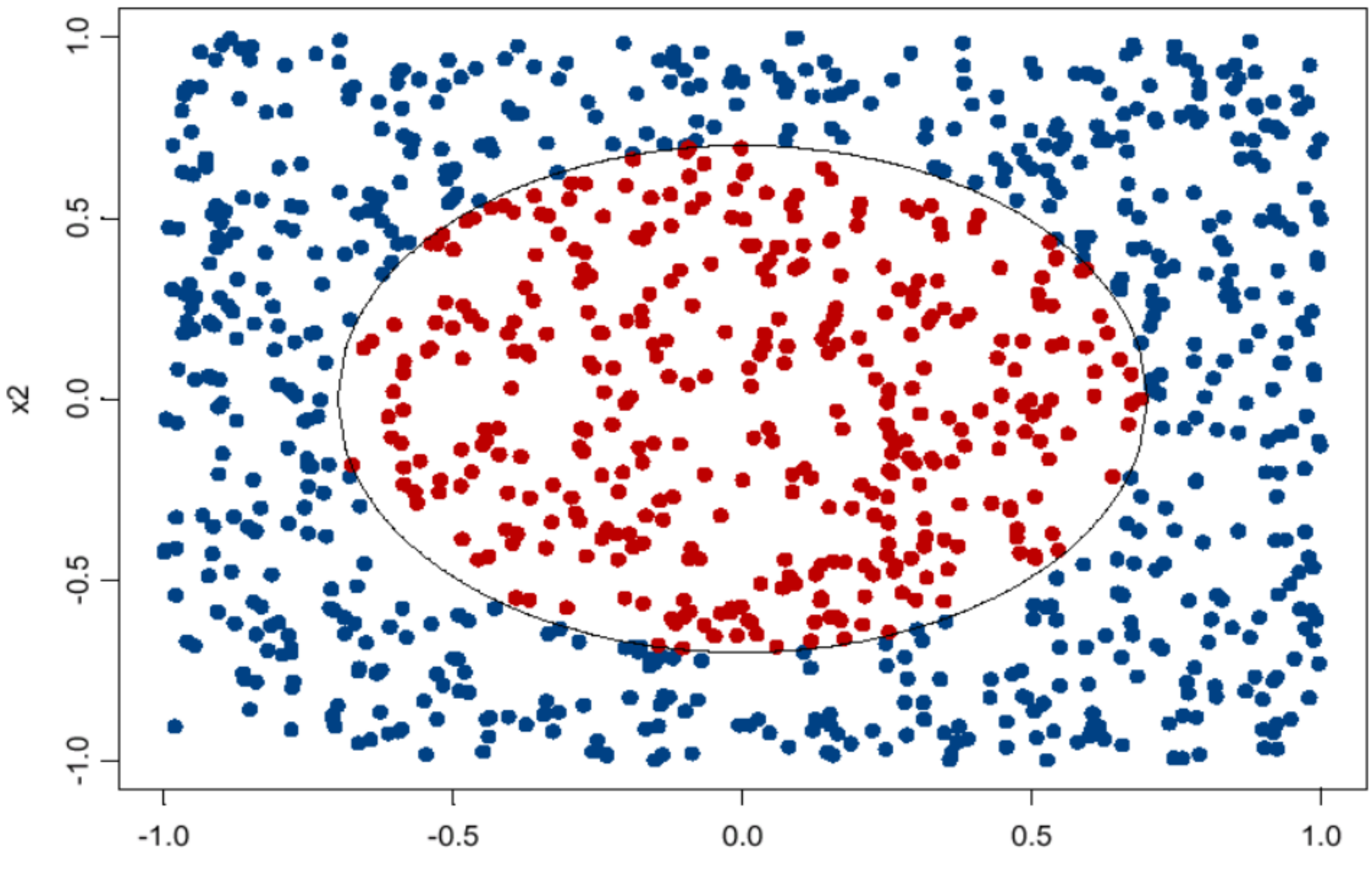
Original Data	1	2	3	4	5	6	7	8	9	10
Bagging (Round 1)	7	8	10	8	2	5	10	10	5	9
Bagging (Round 2)	1	4	9	1	2	3	2	7	3	2
Bagging (Round 3)	1	8	5	10	5	5	9	6	3	7

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

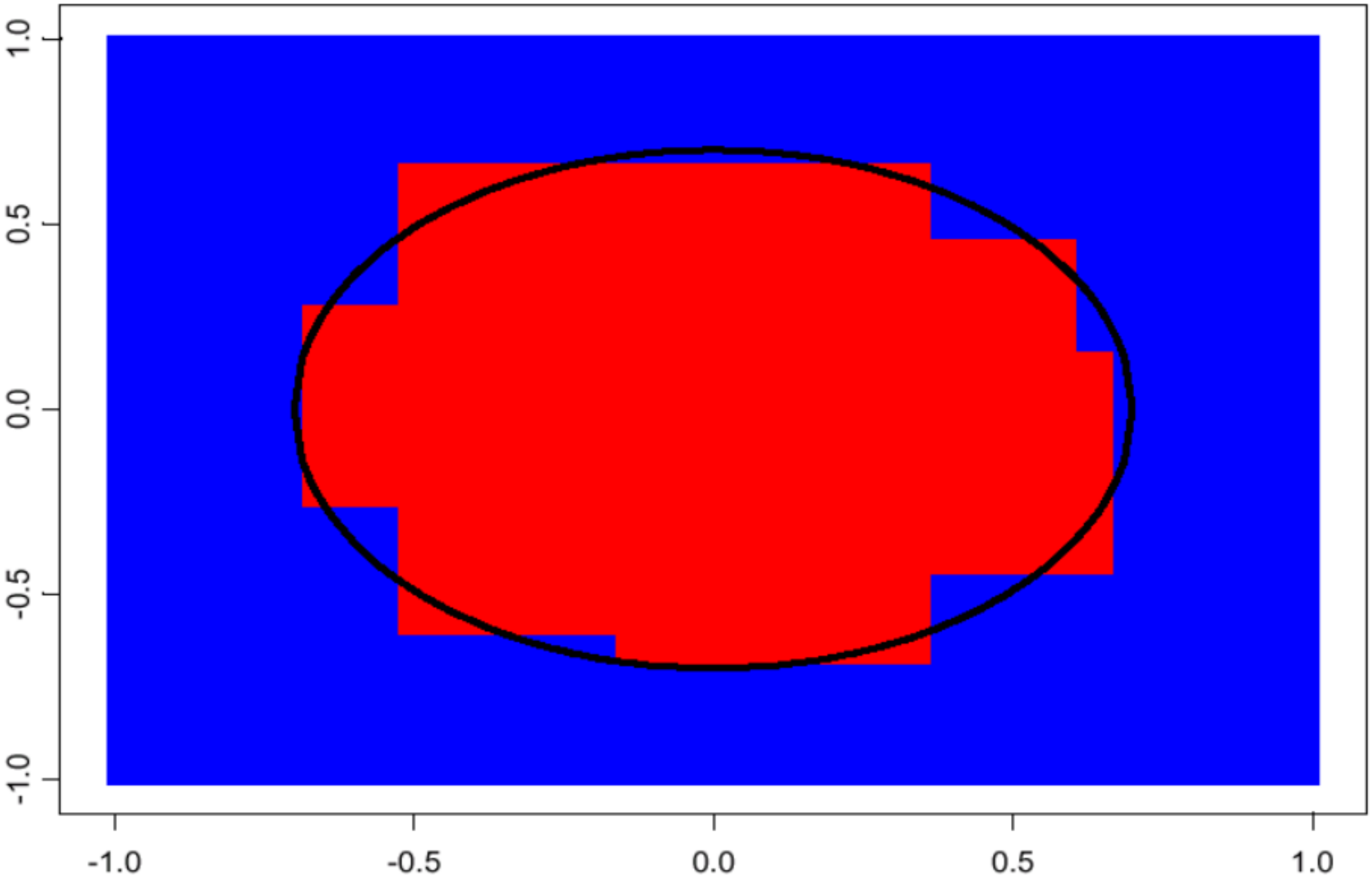
Bagging

- 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

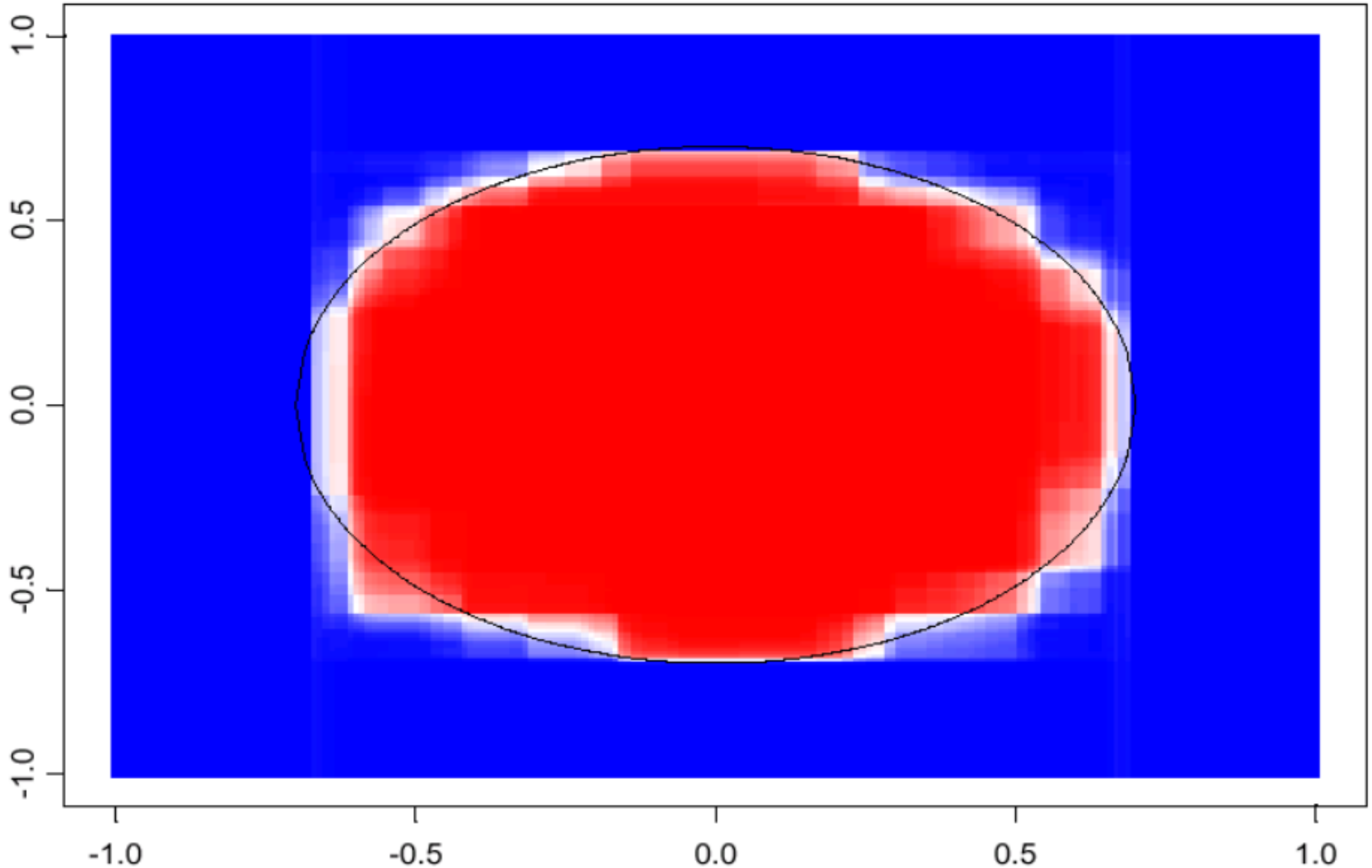
Example Distribution



Decision Tree Decision Boundary



100 Bagged Trees



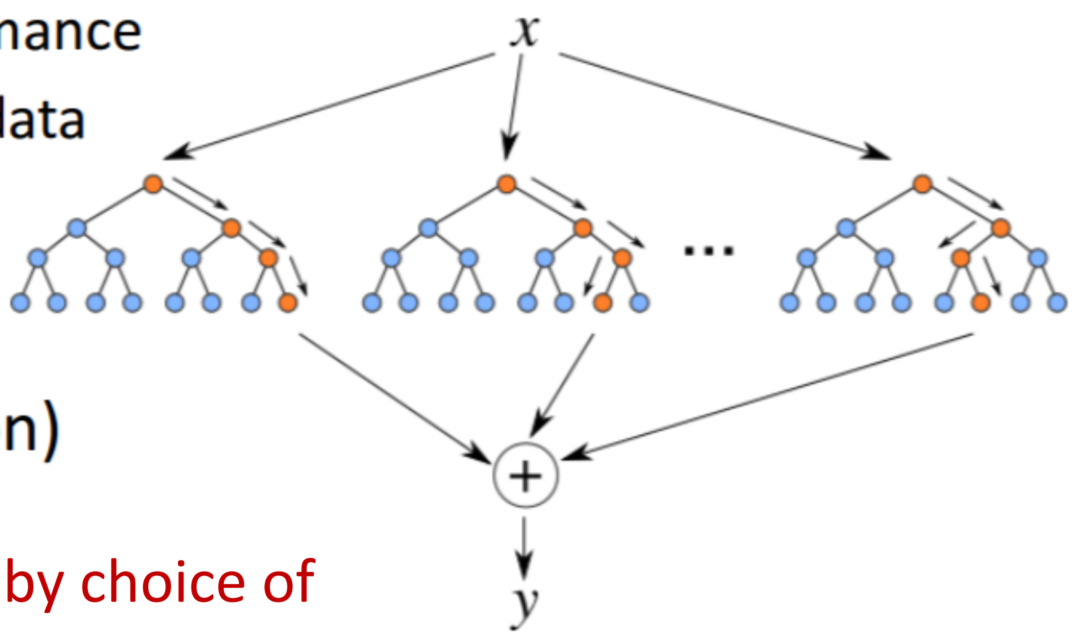
shades of blue/red indicate strength of vote for particular classification

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 $\{T_b\}_1^B$.

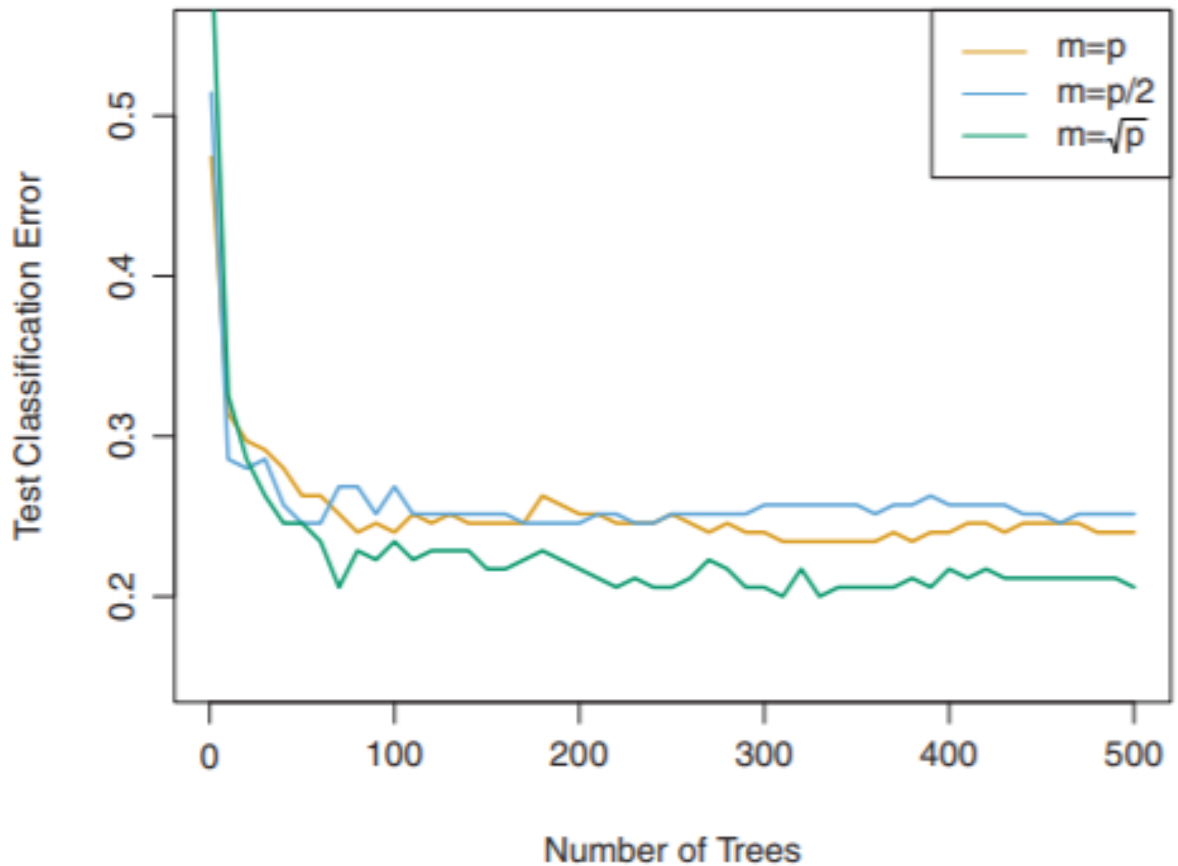
To make a prediction at a new point x:

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

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

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

Effect of Number of Predictors



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

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 impurity metric decreases after the split
  - Average over all trees

Variable Importance Plots

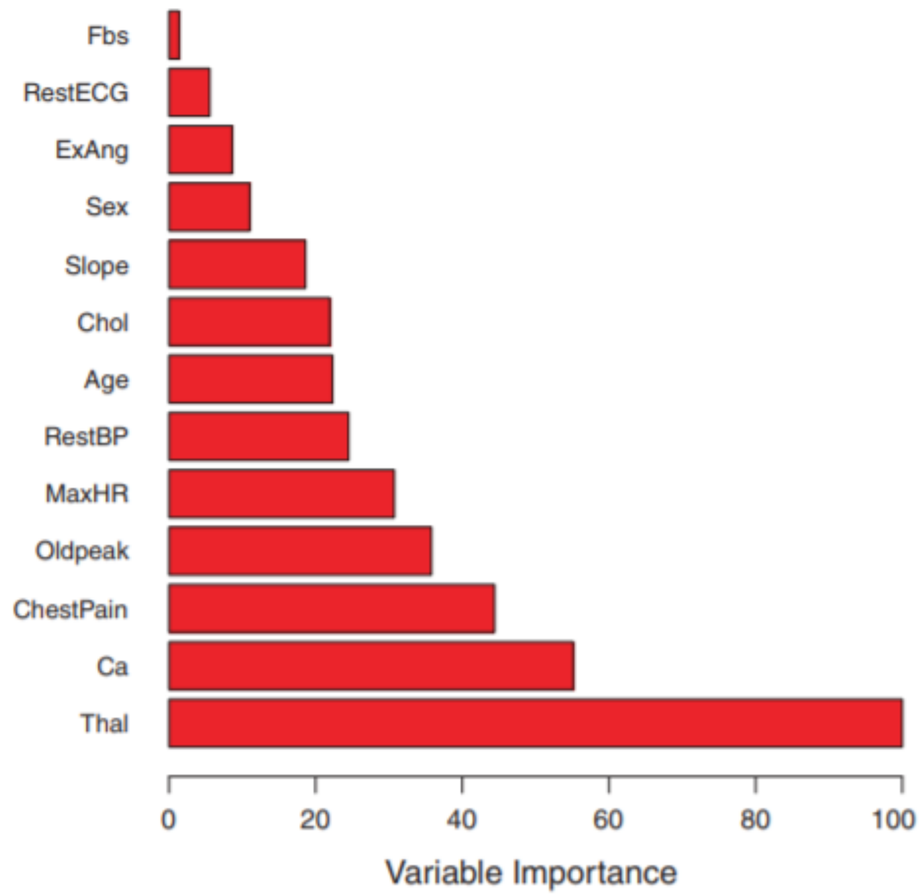


FIGURE 8.9. *A variable importance plot for the* `Heart` *data. Variable importance is computed using the mean decrease in Gini index, and expressed relative to the maximum.*

Lab

```
>
> library(randomForest)
> rf.carseats=randomForest(High~.-Sales,Carseats,subset=train,importance=TRUE)
> rf.carseats

Call:
 randomForest(formula = High ~ . - Sales, data = Carseats, importance = TRUE,      subset = train)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 3

        OOB estimate of  error rate: 18.5%
Confusion matrix:
     No Yes class.error
No  104  14   0.1186441
Yes  23  59   0.2804878
```

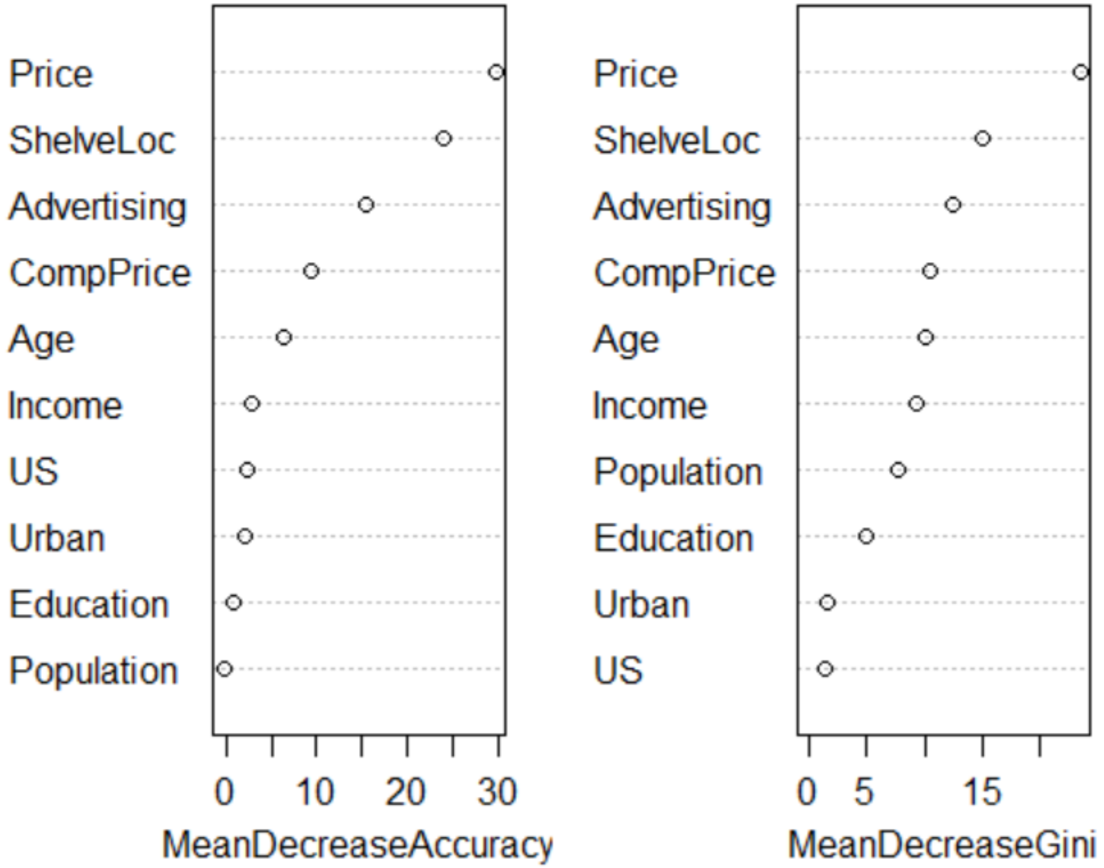
```
>
> rf.pred=predict(rf.carseats,Carseats.test,type="class")
> table(rf.pred,High.test)
       High.test
rf.pred  No Yes
    No  105  25
    Yes  13  57
> mean(rf.pred==High.test)
[1] 0.81
```

Lab

```
> importance(rf.carseats,type=2)
            MeanDecreaseGini
CompPrice          10.444114
Income              9.204883
Advertising        12.367002
Population          7.722053
Price              23.437998
ShelveLoc          15.053694
Age                10.135102
Education           4.879102
Urban               1.585268
US                  1.369725
```

Lab

```
>
> varImpPlot(rf.carseats)
>
```



How to Achieve Diversity

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Two main ensemble learning methods

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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

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

Better classifiers will get higher weights

Uniform weights

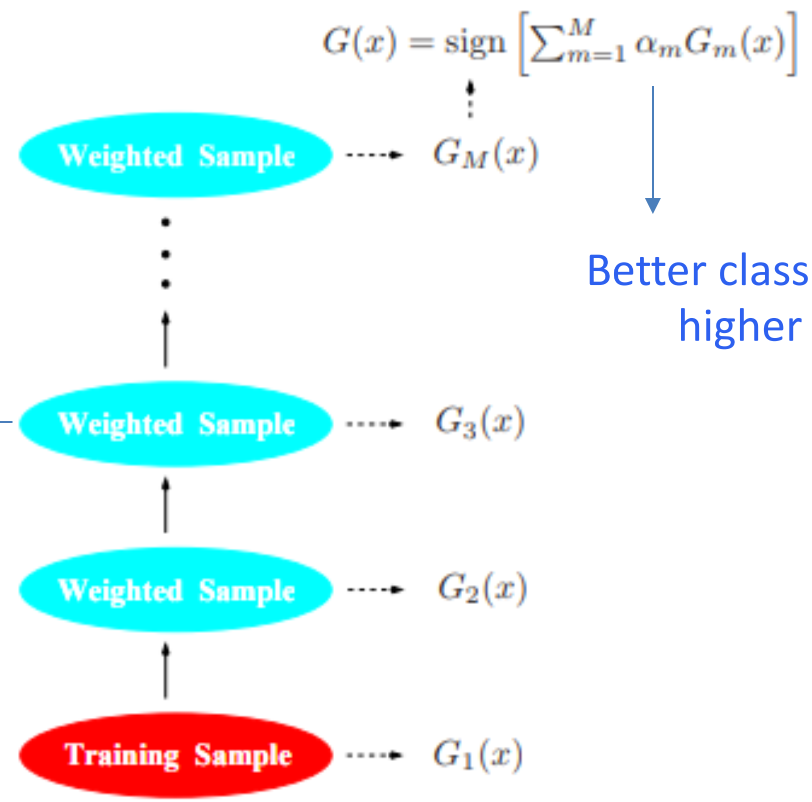


FIGURE 10.1. *Schematic of AdaBoost. Classifiers are trained on weighted versions of the dataset, and then combined to produce a final prediction.*

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 – α_t

- Final classifier: $\boxed{H(X) = \text{sign}(\sum \alpha_t h_t(X))}$

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.

Power of Boosting

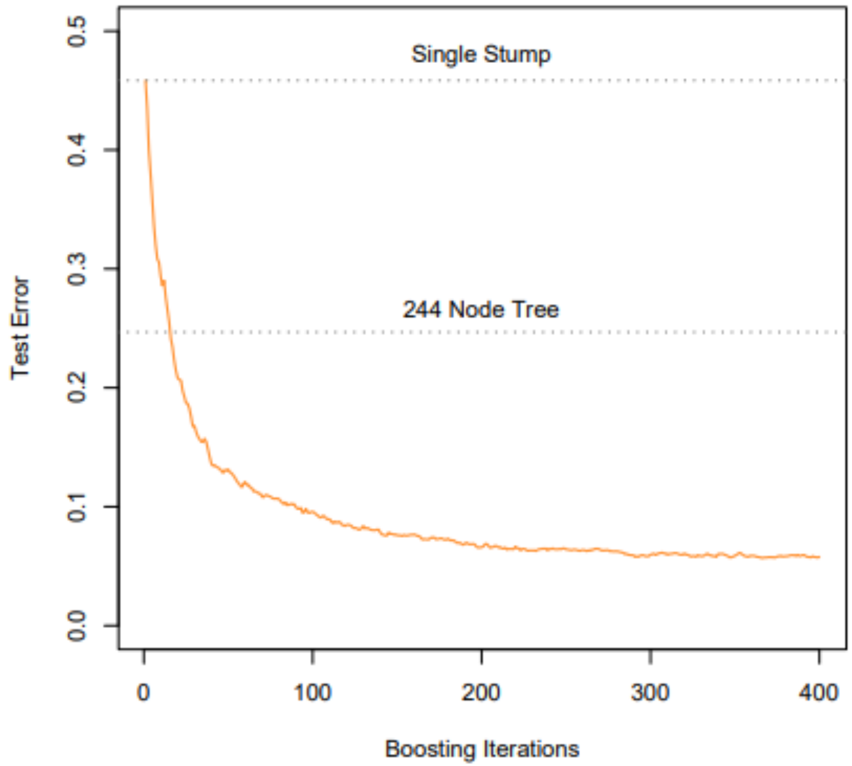


FIGURE 10.2. *Simulated data (10.2): test error rate for boosting with stumps, as a function of the number of iterations. Also shown are the test error rate for a single stump, and a 244-node classification tree.*

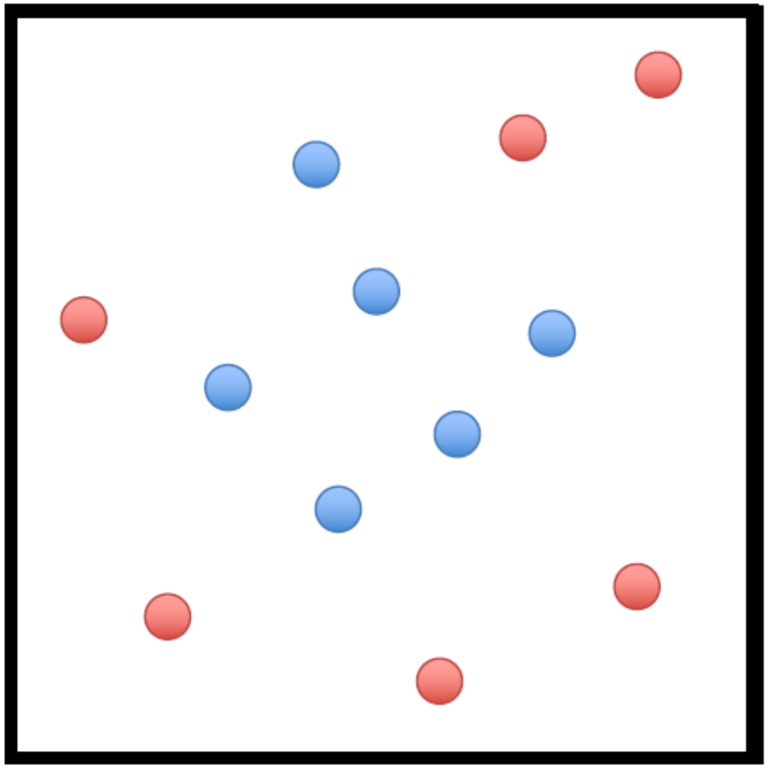
AdaBoost

1: Initialize a vector of n uniform weights $\mathbf{w}_1$
2: **for** $t = 1, \ldots, T$
3: Train model h_t on X, y with weights $\mathbf{w}_t$
4: Compute the weighted training error of h_t
5: Choose $\beta_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right)$
6: Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right)$$

7: Normalize $\mathbf{w}_{t+1}$ to be a distribution
8: **end for**
9: **Return** the hypothesis

$$H(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \beta_t h_t(\mathbf{x}) \right)$$



- Size of point represents the instance's weight

AdaBoost

Initialize a vector of n uniform weights $\mathbf{w}_1$
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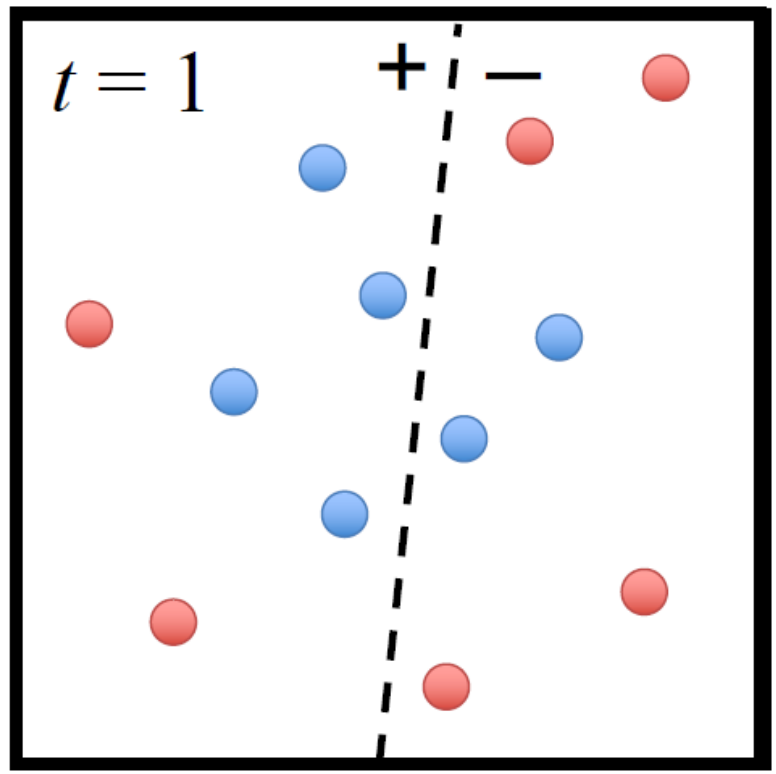

- β_t measures the importance of h_t
- If $\epsilon_t \leq 0.5$, then $\beta_t \geq 0$ (can trivially guarantee)

AdaBoost

Initialize a vector of n uniform weights $\mathbf{w}_1$
for $t = 1, \ldots, T$
    Train model h_t on X, y with weights $\mathbf{w}_t$
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end for
Return the hypothesis
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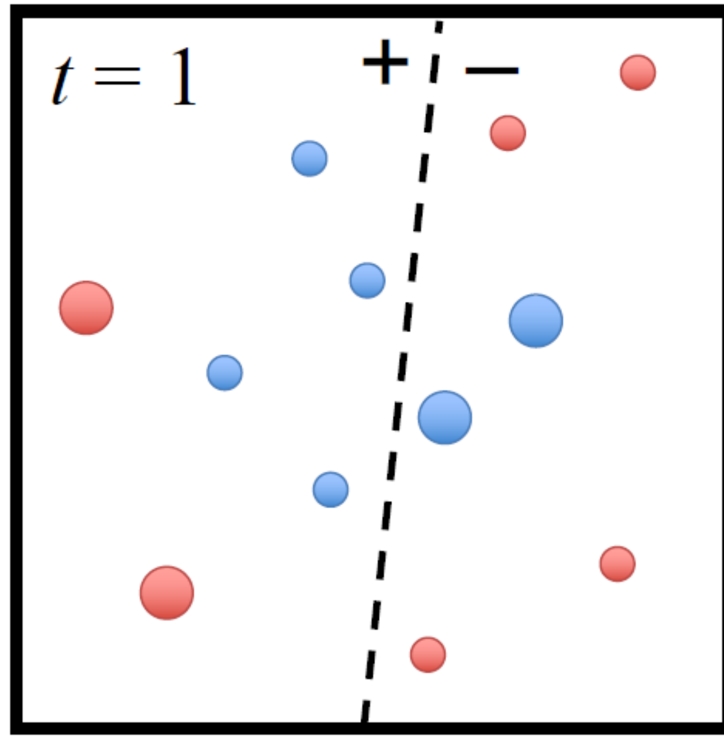

- Weights of correct predictions are multiplied by $e^{-\beta_t} \leq 1$
- Weights of incorrect predictions are multiplied by $e^{\beta_t} \geq 1$

Acknowledgements

- Slides made using resources from:
  - Andrew Ng
  - Eric Eaton
  - David Sontag
  - Andrew Moore
- Thanks!