Lecture 6: Decision Tree, Random Forest, and Boosting

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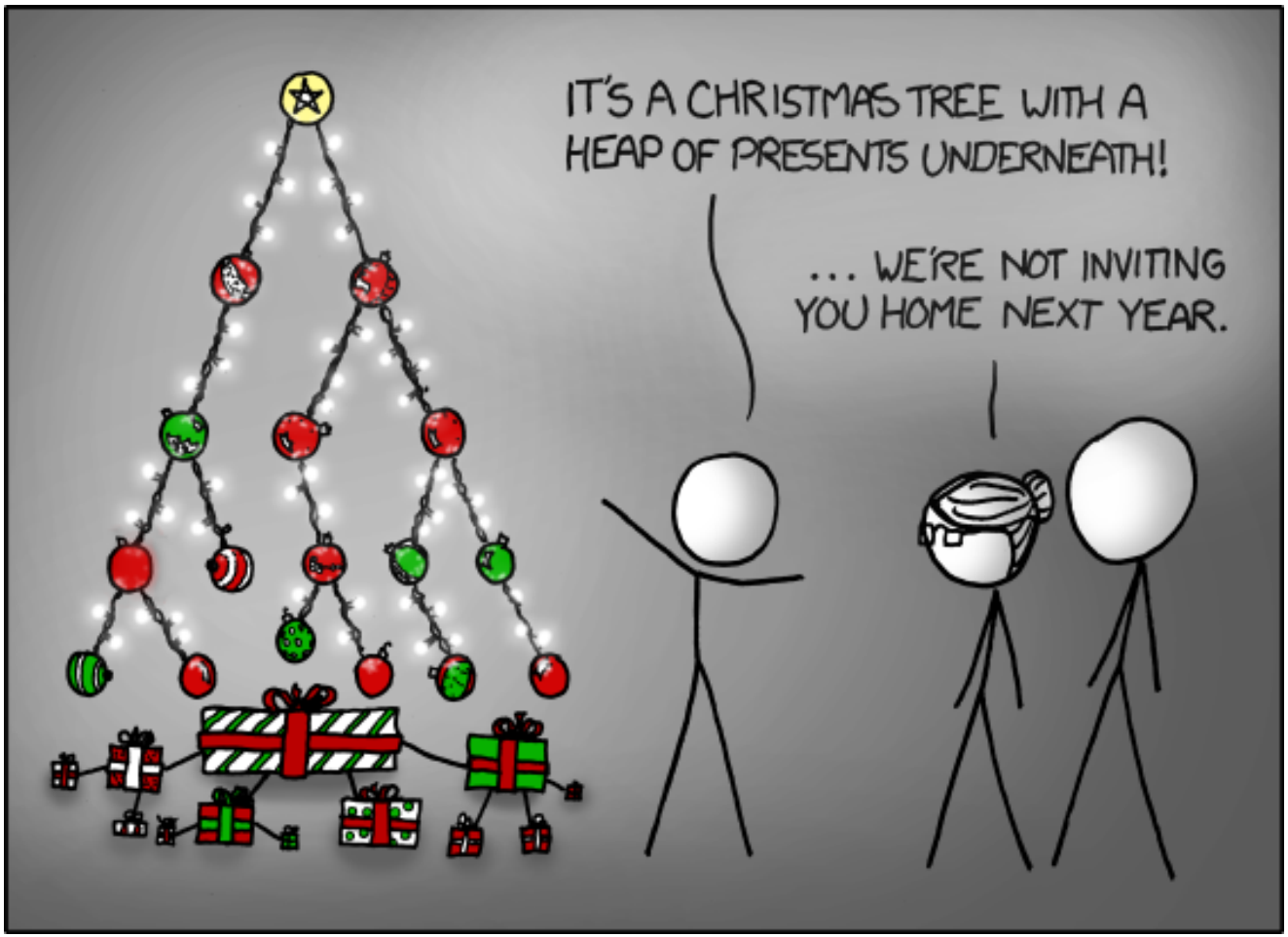
Tree?


IT'S A CHRISTMAS TREE WITH A HEAP OF PRESENTS UNDERNEATH!
... WE'RE NOT INVITING YOU HOME NEXT YEAR.

Decision Trees

Decision Trees

- Decision trees have a long history in machine learning
  - The first popular algorithm dates back to 1979
- Very popular in many real world problems
- Intuitive to understand
- Easy to build

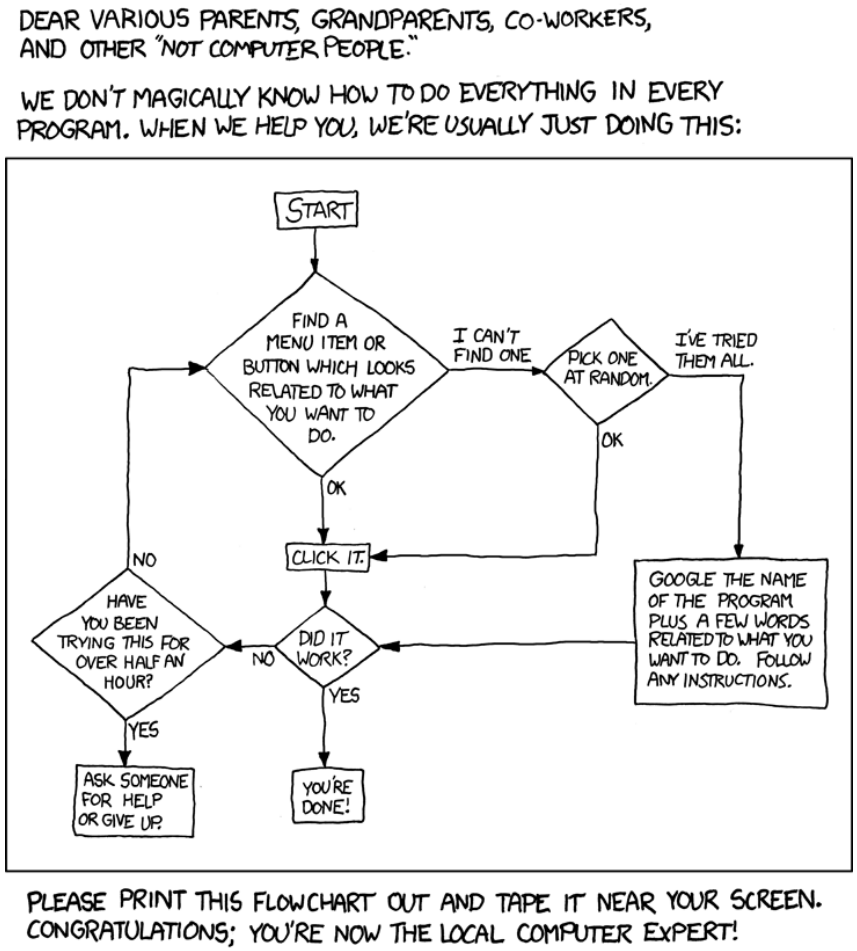
History

- EPAM- Elementary Perceiver and Memorizer
  - 1961: Cognitive simulation model of human concept learning
- 1966: CLS-Early algorithm for decision tree construction
- 1979: ID3 based on information theory
- 1993: C4.5 improved over ID3
- Also has history in statistics as CART (Classification and regression tree)

Motivation

- How do people make decisions?
  - Consider a variety of factors
  - Follow a logical path of checks
- Should I eat at this restaurant?
  - If there is no wait
    - Yes
  - If there is short wait and I am hungry
    - Yes
  - Else
    - No

Decision Flowchart

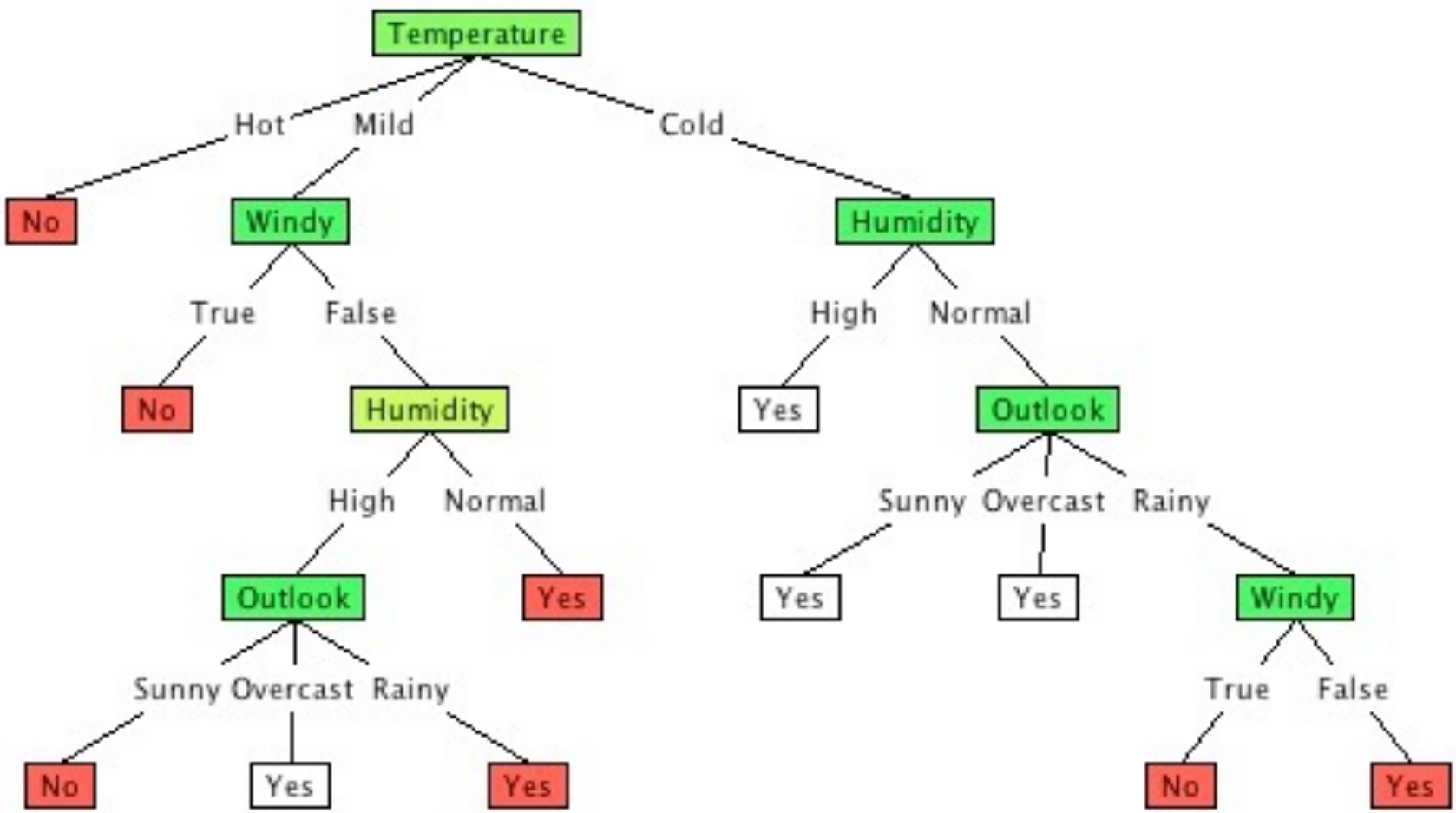


Example: Should We Play Tennis?

Play Tennis	Outlook	Temperature	Humidity	Windy
No	Sunny	Hot	High	No
No	Sunny	Hot	High	Yes
Yes	Overcast	Hot	High	No
Yes	Rainy	Mild	High	No
Yes	Rainy	Cold	Normal	No

- If temperature is not hot
  - Play
- If outlook is overcast
  - Play tennis
- Otherwise
  - Don't play tennis

Decision Tree



Structure

A decision tree consists of

- Nodes
  - Tests for variables
- Branches
  - Results of tests
- Leaves
  - Classification

Function Class

- What functions can decision trees model?
  - Non-linear: very powerful function class
  - A decision tree can encode any Boolean function
  - Proof
    - Given a truth table for a function
    - Construct a path in the tree for each row of the table
    - Given a row as input, follow that path to the desired leaf (output)
- Problem: exponentially large trees!

Smaller Trees

- Can we produce smaller decision trees for functions?
  - Yes (Possible)
  - Key decision factors
  - Counter examples
    - Parity function: Return 1 on even inputs, 0 on odd inputs
    - Majority function: Return 1 if more than half of inputs are 1
- Bias-Variance Tradeoff
  - Bias: Representation Power of Decision Trees
  - Variance: require a sample size exponential in depth

Fitting Decision Trees

What Makes a Good Tree?

- Small tree:
  - Occam's razor: Simpler is better
  - Avoids over-fitting
- A decision tree may be human readable, but not use human logic!
- How do we build small trees that accurately capture data?
- Learning an optimal decision tree is computationally intractable

Greedy Algorithm

- We can get good trees by simple greedy algorithms
- Adjustments are usually to fix greedy selection problems
- Recursive:
  - Select the "best" variable, and generate child nodes: One for each possible value;
  - Partition samples using the possible values, and assign these subsets of samples to the child nodes;
  - Repeat for each child node until all samples associated with a node that are either all positive or all negative.

Variable Selection

- The best variable for partition
  - The most informative variable
  - Select the variable that is most informative about the labels
  - Classification error?
- Example:

$$\mathbb{P}(Y = 1|X_1 = 1) = 0.75 \quad \text{v.s.} \quad \mathbb{P}(Y = 1|X_2 = 1) = 0.55$$

Which to choose?

Information Theory

- The quantification of information
- Founded by Claude Shannon
- Simple concepts:
  - Entropy: $H(X) = -\sum_x \mathbb{P}(X = x) \log \mathbb{P}(X = x)$
  - Conditional Entropy: $H(Y|X) = \sum_x \mathbb{P}(X = x) H(Y|X = x)$
  - Information Gain: $\mathrm{IG(Y|X)} = \mathrm{H(Y)} - \mathrm{H(Y|X)}$
- Select the variable with the highest information gain

Example: Should We Play Tennis?

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No	Sunny	Hot	High	No
No	Sunny	Hot	High	Yes
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Yes	Rainy	Mild	High	No
Yes	Rainy	Cold	Normal	No

$$H(\text{Tennis}) = -3/5 \log_2 3/5 - 2/5 \log_2 2/5 = 0.97$$
$$H(\text{Tennis}|\text{Out.} = \text{Sunny}) = -2/2 \log_2 2/2 - 0/2 \log_2 0/2 = 0$$
$$H(\text{Tennis}|\text{Out.} = \text{Overcast}) = -0/1 \log_2 0/1 - 1/1 \log_2 1/1 = 0$$
$$H(\text{Tennis}|\text{Out.} = \text{Rainy}) = -0/2 \log_2 0/2 - 2/2 \log_2 2/2 = 0$$
$$H(\text{Tennis}|\text{Out.}) = 2/5 \times 0 + 1/5 \times 0 + 2/5 \times 0 = 0$$

Example: Should We Play Tennis?

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Yes	Rainy	Cold	Normal	No

- $\mathrm{IG}(\mathrm{Tennis}|\mathrm{Out.}) = 0.97 - 0 = 0.97$
- If we knew the Outlook we'd be able to predict Tennis!
- Outlook is the variable to pick for our decision tree

When to Stop Training?

- All data have same label
  - Return that label
- No examples
  - Return majority label of all data
- No further splits possible
  - Return majority label of passed data
- If max IG $= 0$?

Example: No Information Gain?

Y	X_1	X_2
0	0	0
1	0	1
1	1	0
0	1	1

- Both features give 0 IG
- Once we divide the data, perfect classification!
- We need a little exploration sometimes (Unstable Equilibrium)

Decision Tree with Continuous Features

- Decision Stump
  - Threshold for binary classification:

$$\text{Check } X_j \geq \delta_j \text{ or } X_j < \delta_j.$$

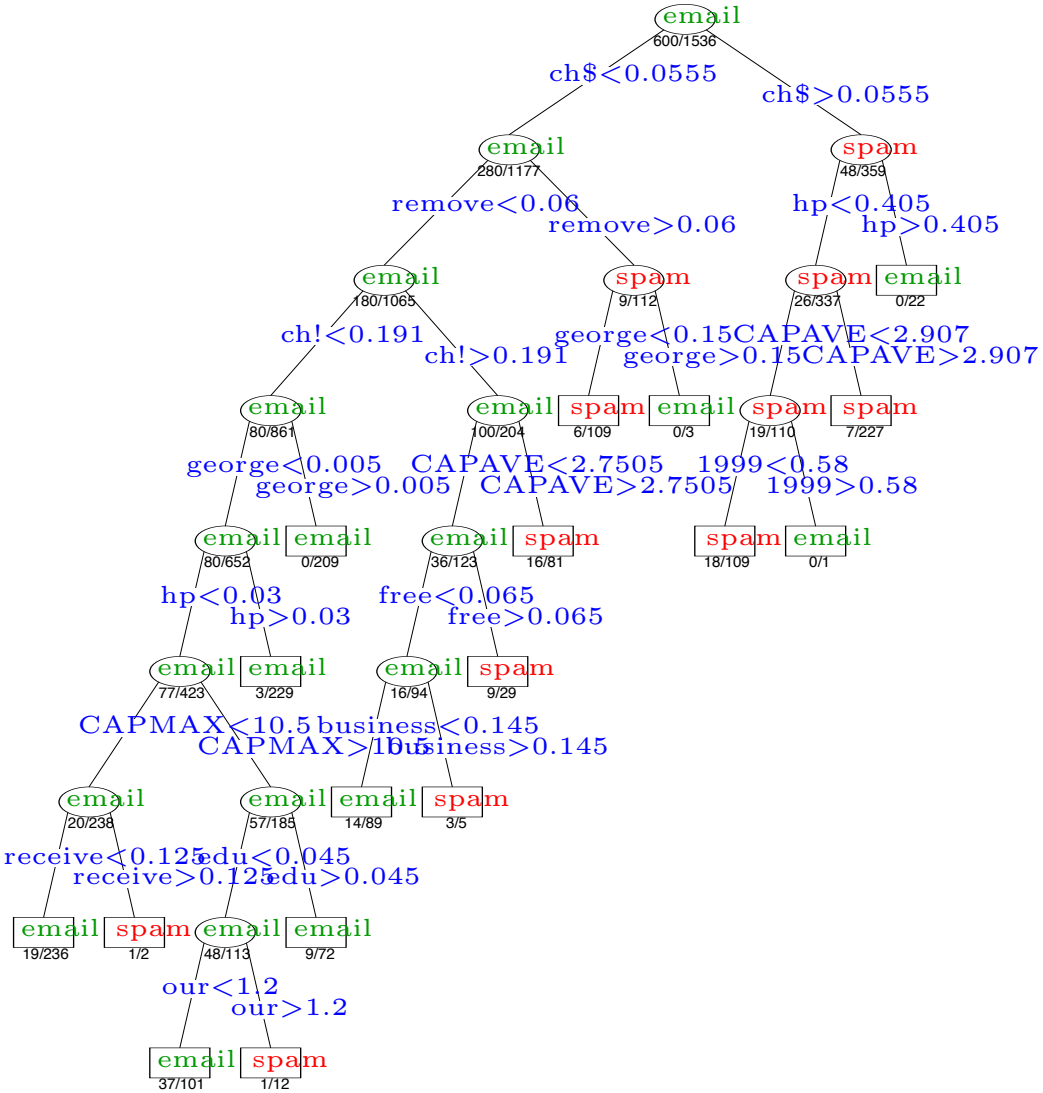
- More than two classes:
  - Threshold for three classes:

$$\text{Check } X_j \geq \delta_j,\ \gamma_j \geq X_j < \delta_j \text{ or } \gamma_j < X_j.$$

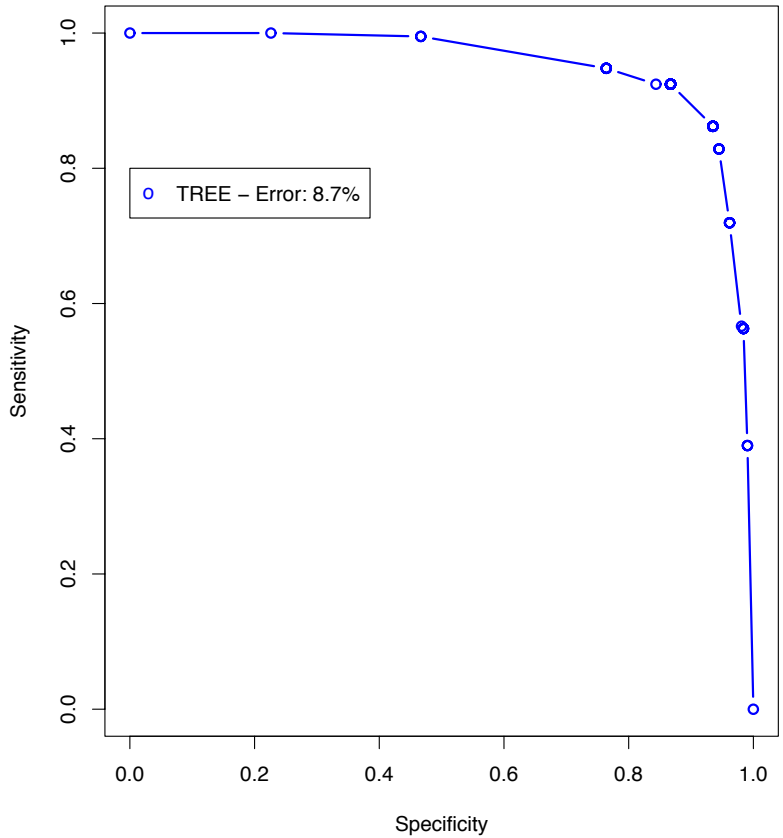
- Decompose one node to two modes:

$$\text{First node: Check } X_j \geq \delta_j \text{ or } X_j < \delta_j,$$
$$\text{Second node: If } X_j < \delta_j,\ \text{check } \gamma_j \geq X_j \text{ or } \gamma_j < X_j.$$

Decision Tree for Spam Classification

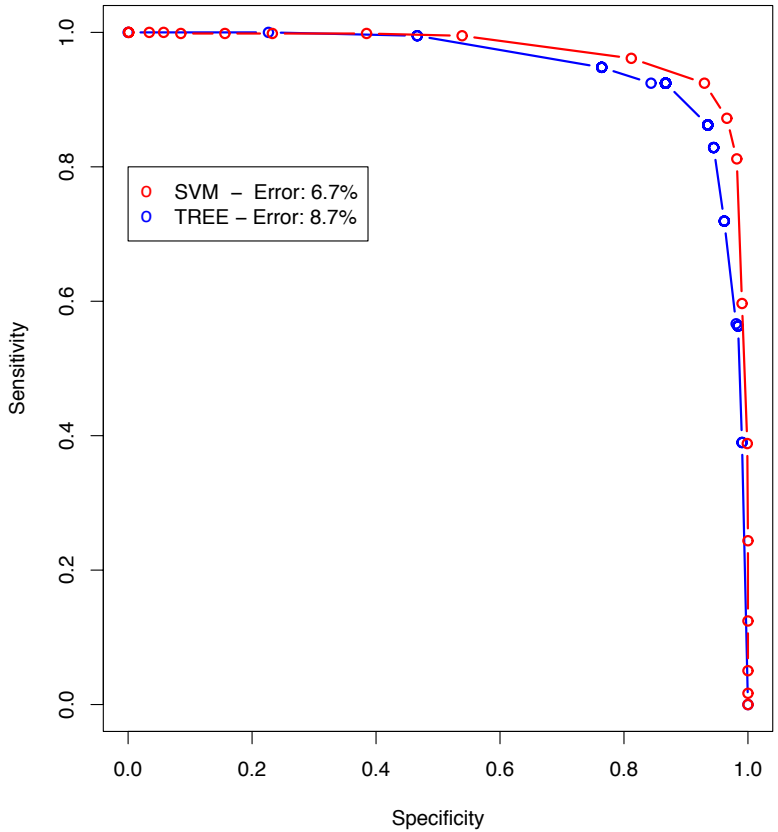


Decision Tree for Spam Classification



- Sensitivity: proportion of true spam identified
- Specificity: proportion of true email identified.

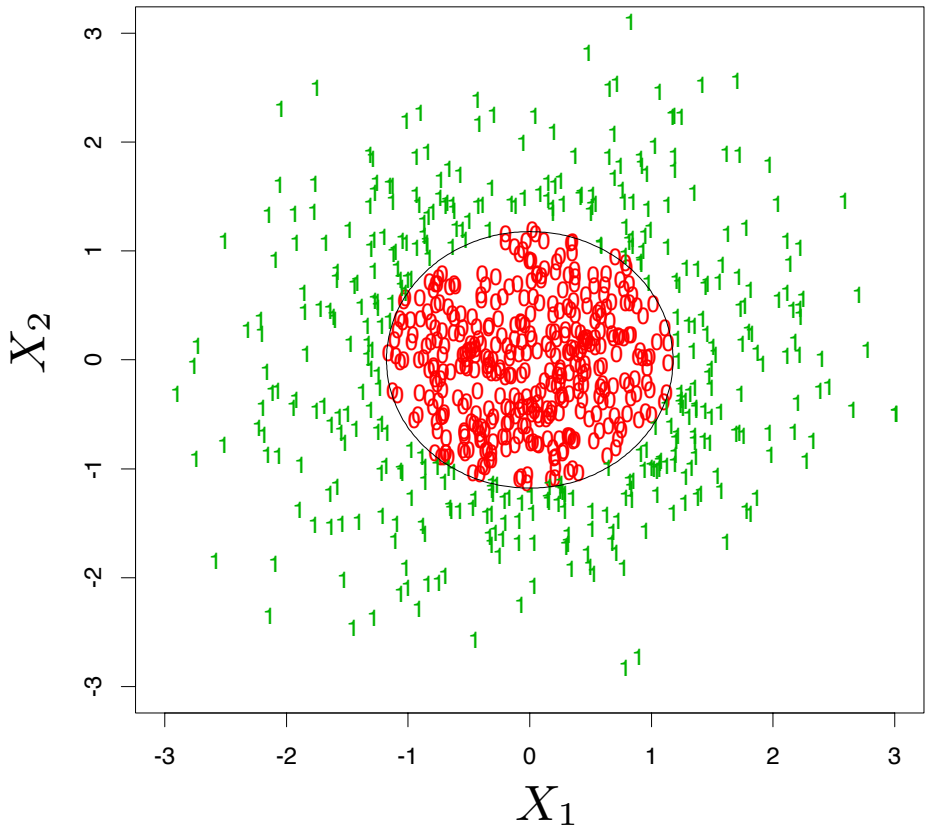
Decision Tree v.s. SVM



- SVM outperforms Decision Tree.
- AUC: Area Under Curve.

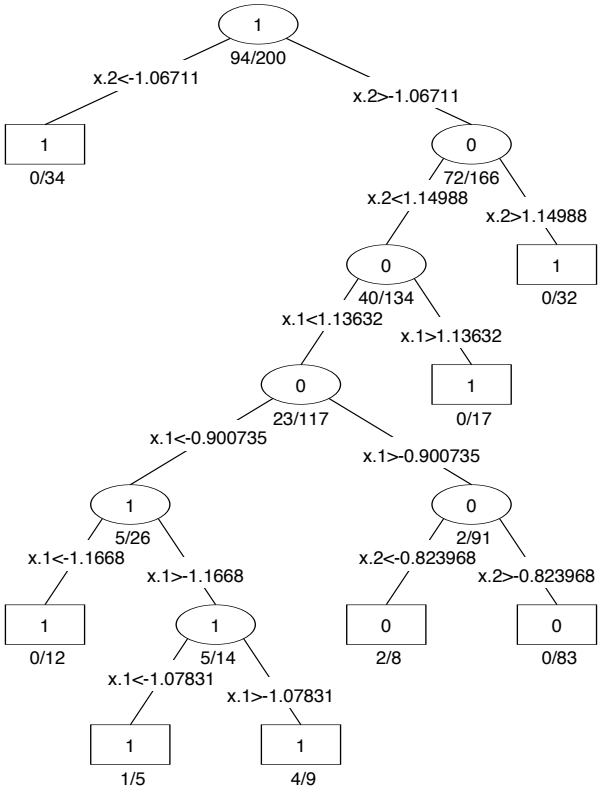
Bagging and Random Forest

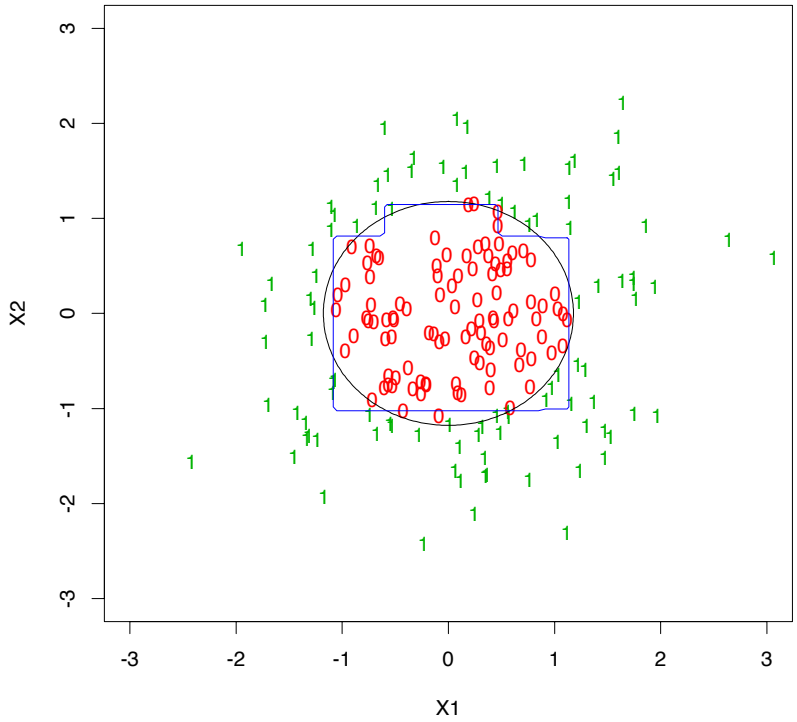
Toy Example



- Nonlinear separable data.
- Optimal decision boundary: $X_1^2 + X_2^2 = 1$.

Toy Example: Decision Tree





- Sample size: 200
- 7 branching nodes; 6 layers.
- Classification error: 7.3% when $d = 2$; $> 30\%$ when $d = 10$.

Model Averaging

Decision trees can be simple, but often produce noisy (bushy) or weak (stunted) classifiers.

- Bagging (Breiman, 1996): Fit many large trees to bootstrap-resampled versions of the training data, and classify by majority vote.
- Boosting (Freund & Shapire, 1996): Fit many large or small trees to reweighted versions of the training data. Classify by weighted majority vote.
- Random Forests (Breiman 1999): Fancier version of bagging.

In general Boosting>Random Forests>Bagging>Single Tree.

Bagging/Bootstrap Aggregation

Motivation: Average a given procedure over many samples to reduce the variance.

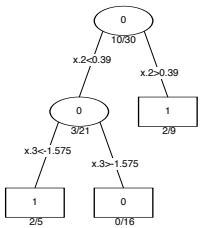
- Given a classifier $C(S, x)$, based on our training data S, producing a predicted class label at input point x.
- To bag C, we draw bootstrap samples $S_1, ..., S_B$ each of size N with replacement from the training data. Then

$$\widehat{C}_{\text{Bag}} = \text{Mojarity Vote}\{C(S_b, x)\}_{b=1}^{B}.$$

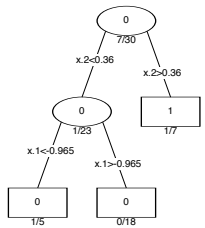
- Bagging can dramatically reduce the variance of unstable procedures (like trees), leading to improved prediction.
- All simple structures in a tree are lost.

Toy Example: Bagging Trees

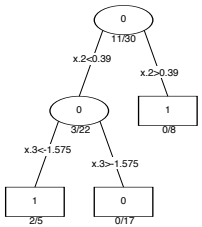
Original Tree



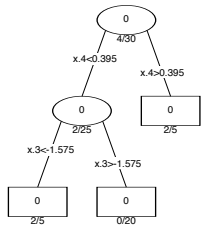
Bootstrap Tree 1



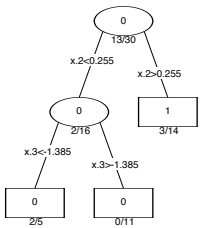
Bootstrap Tree 2



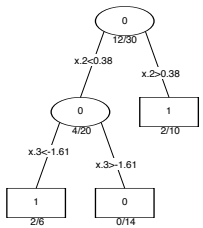
Bootstrap Tree 3



Bootstrap Tree 4

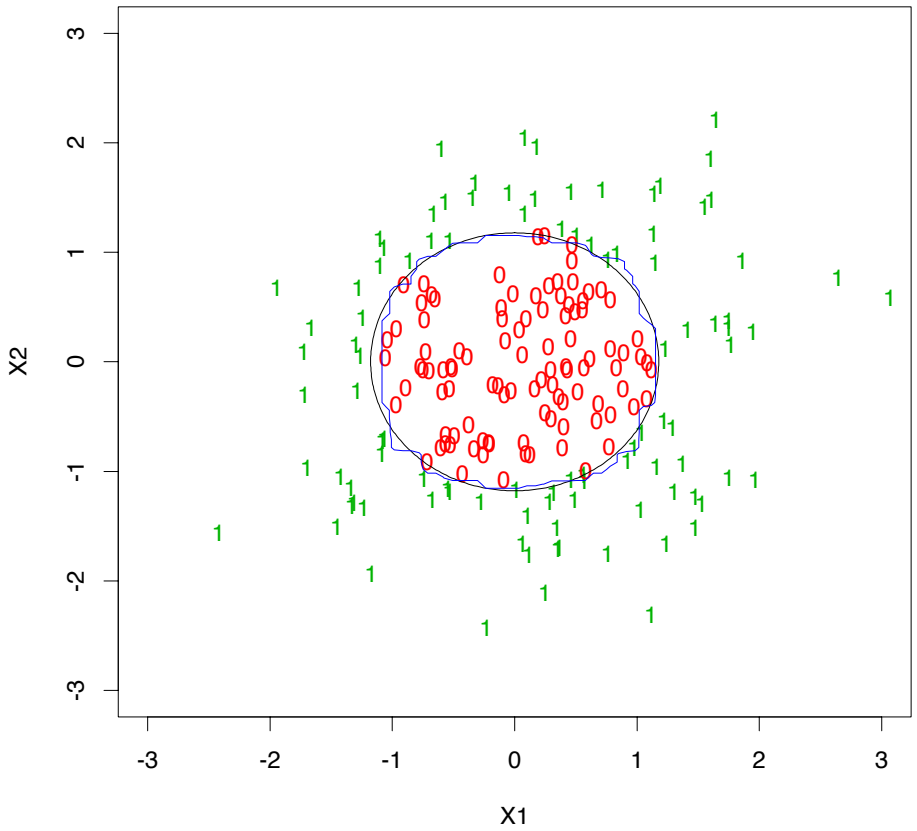


Bootstrap Tree 5



- 2 branching nodes; 2 layers.
- 5 dependent trees.

Toy Example: Bagging Trees



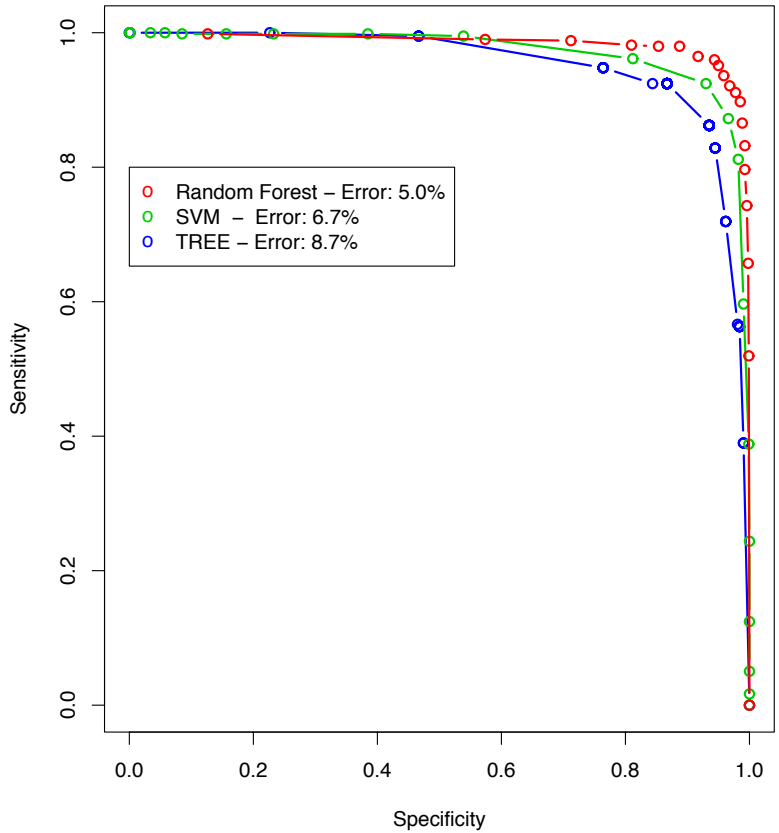
- A smoother decision boundary.
- Classification error: 3.2% (Single deeper tree 7.3%).

Random Forest

Bagging features and samples simultaneously:

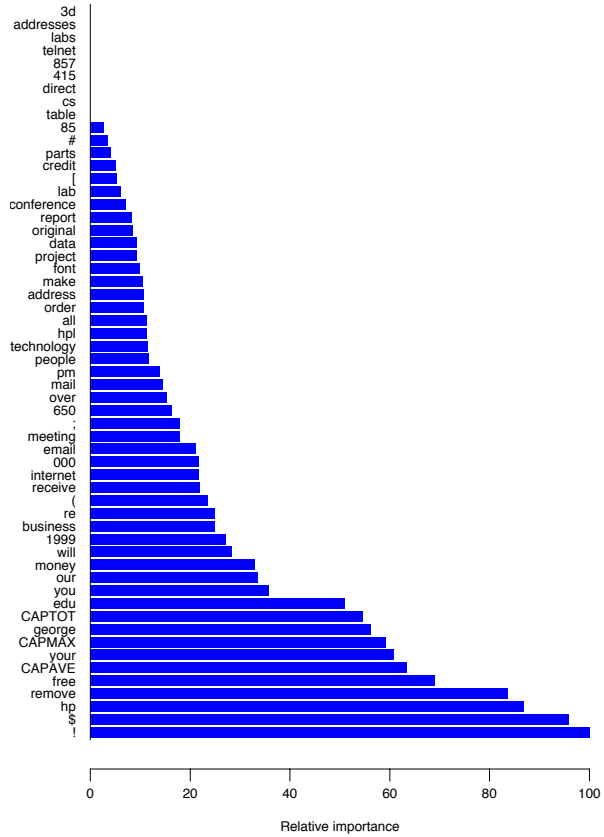
- At each tree split, a random sample of m features is drawn, and only those m features are considered for splitting. Typically $m = \sqrt{d}$ or $\log_2 d$, where d is the number of features
- For each tree grown on a bootstrap sample, the error rate for observations left out of the bootstrap sample is monitored. This is called the "out-of-bag" error rate.
- random forests tries to improve on bagging by "de-correlating" the trees. Each tree has the same expectation.

Random Forest for Spam Classification



- RF outperforms SVM.
- 500 Trees.

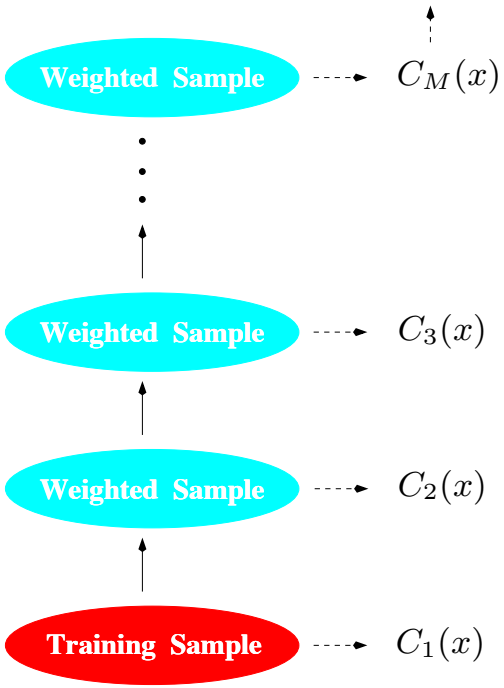
Random Forest: Variable Importance Scores



- The bootstrap roughly covers $1/3$ samples for each time.
- Do permutations over variables to check how important they are.

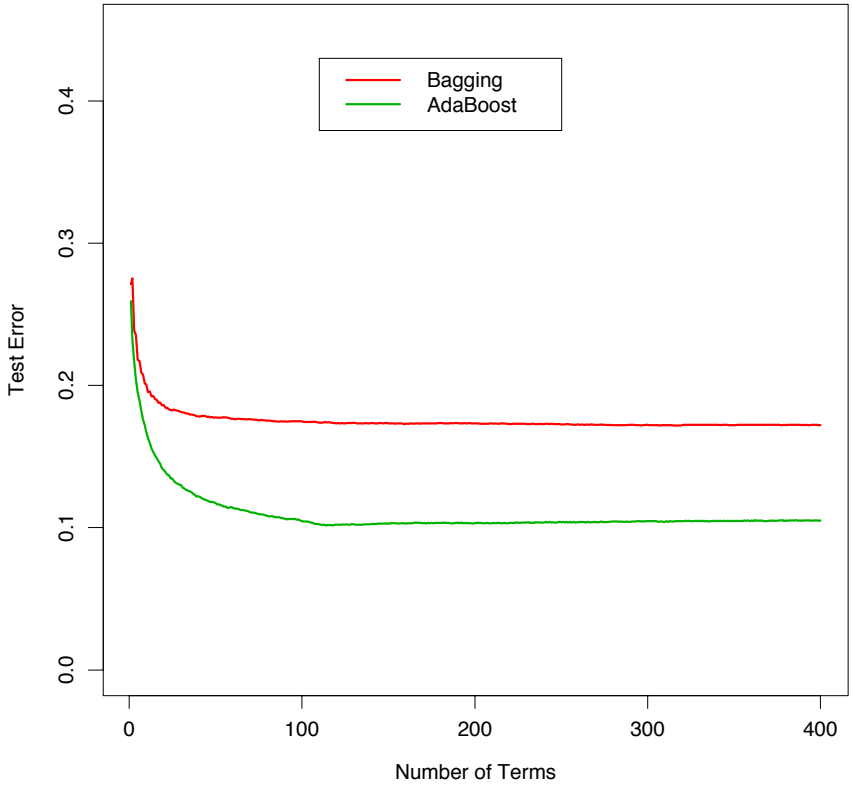
Boosting

Boosting



- Average many trees, each grown to re-weighted versions of the training data (Iterative).
- Final Classifier is weighted average of classifiers:

Adaboost v.s. Bagging



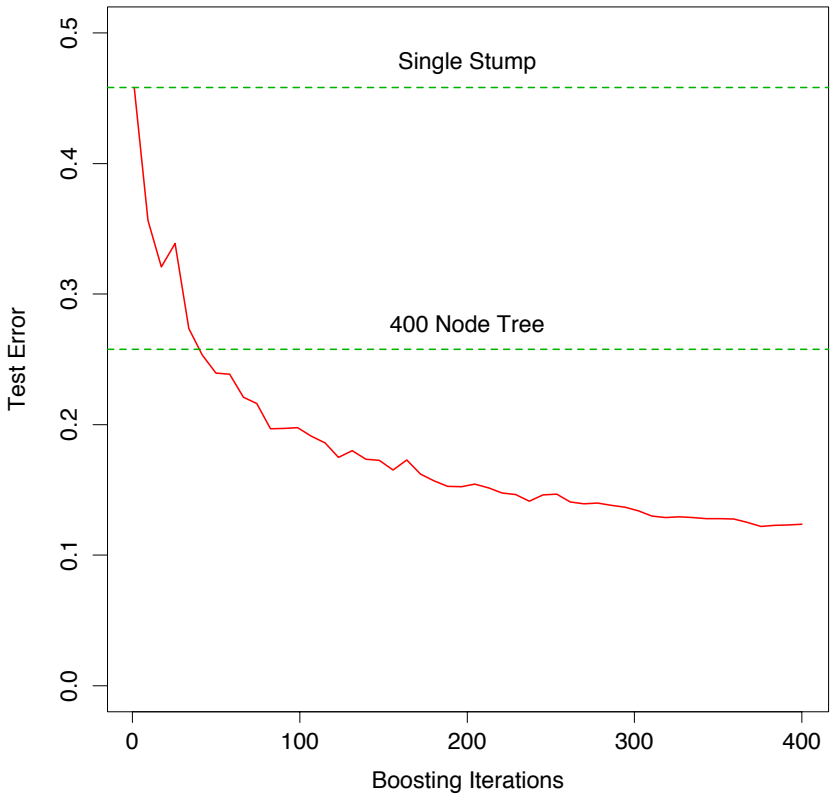
- Each classifier for bagging is a tree with a single node (decision stump).
- 2000 samples from Spheres in $\mathbb{R}^{10}$.

Adaboost

1. Initialize the observation weights $w_i = 1/N,\ i = 1, 2, \ldots, N$.
2. For $m = 1$ to M repeat steps (a)–(d):
   (a) Fit a classifier $C_m(x)$ to the training data using weights w_i.
   (b) Compute weighted error of newest tree
   $$\text{err}_m = \frac{\sum_{i=1}^{N} w_i I(y_i \neq C_m(x_i))}{\sum_{i=1}^{N} w_i}.$$
   (c) Compute $\alpha_m = \log[(1 - \text{err}_m)/\text{err}_m]$.
   (d) Update weights for $i = 1, \ldots, N$:
   $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq C_m(x_i))]$
   and renormalize to w_i to sum to 1.
3. Output $C(x) = \text{sign}\left[\sum_{m=1}^{M} \alpha_m C_m(x)\right]$.

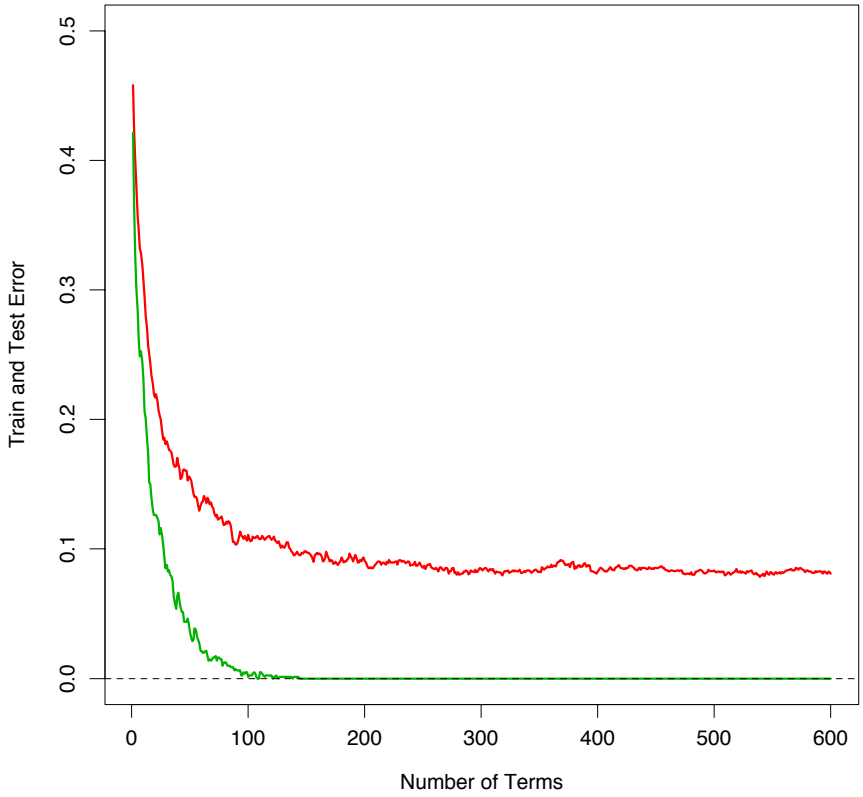
- w_i's are the weights of the samples.
- err_m is the weighted training error.

Adaboost



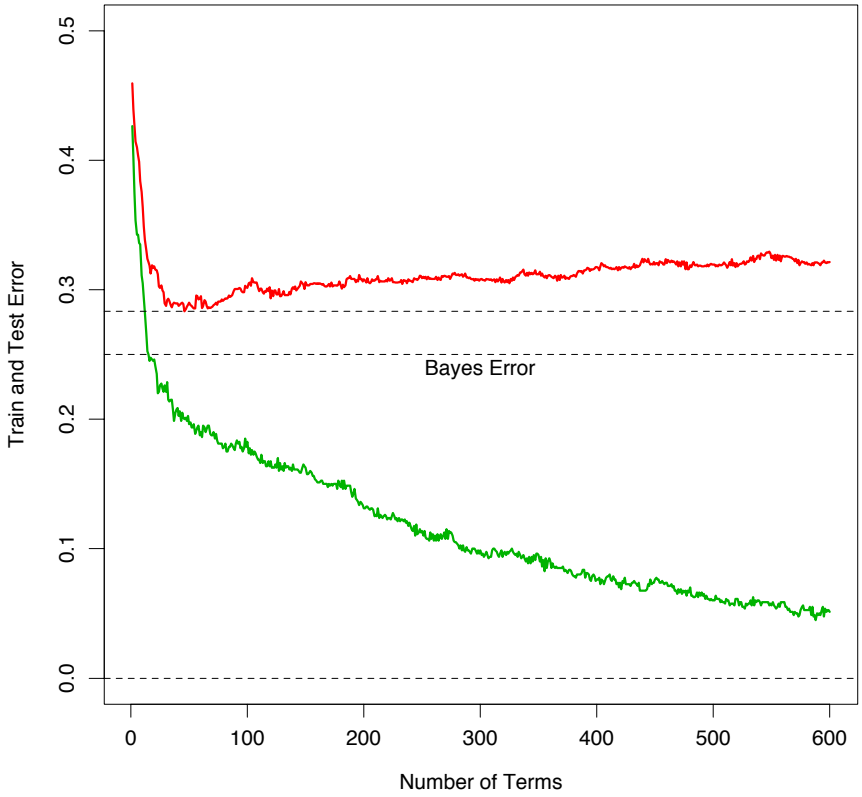
- The ensemble of classifiers is much more efficient than the simple combination of classifiers.

Overfitting of Adaboost



- More iterations continue to improve test error in many examples.
- The Adaboost is often observed to be robust to overfitting.

Overfitting of Adaboost



- Optimal Bayes classification error: 25%.
- The test error does increase, but quite slowly.