Decision Trees, cont.

Boosting

Machine Learning – 10701/15781
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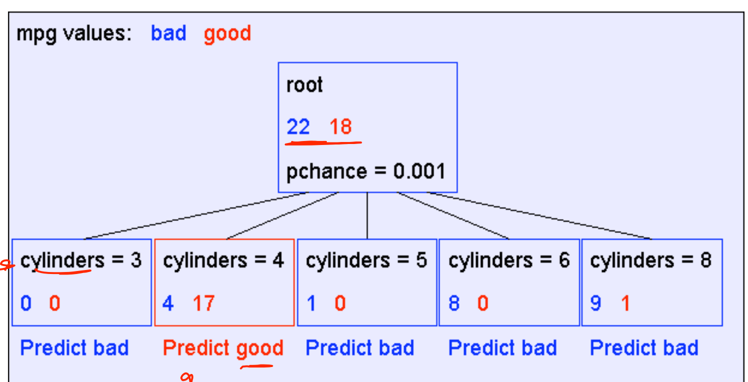
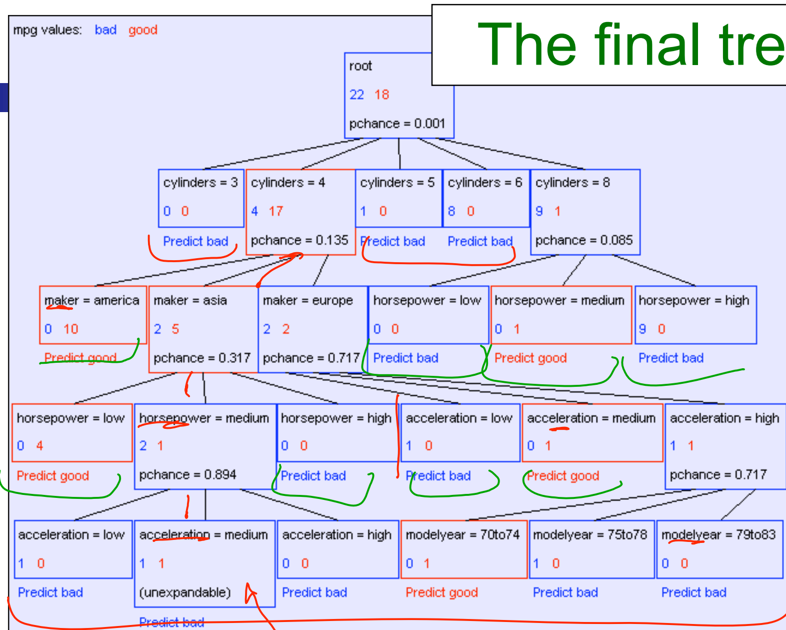
October 1st, 2007

A Decision Stump



9
17 74

The final tree



no more distinctions

Basic Decision Tree Building Summarized

BuildTree(*DataSet*,*Output*)

- If all output values are the same in *DataSet*, return a leaf node that says "predict this unique output"
- If all input values are the same, return a leaf node that says "predict the majority output"
- Else find attribute *X* with highest Info Gain
- Suppose *X* has n_X distinct values (i.e. X has arity n_X).
  - Create and return a non-leaf node with n_X children.
  - The *i*'th child should be built by calling

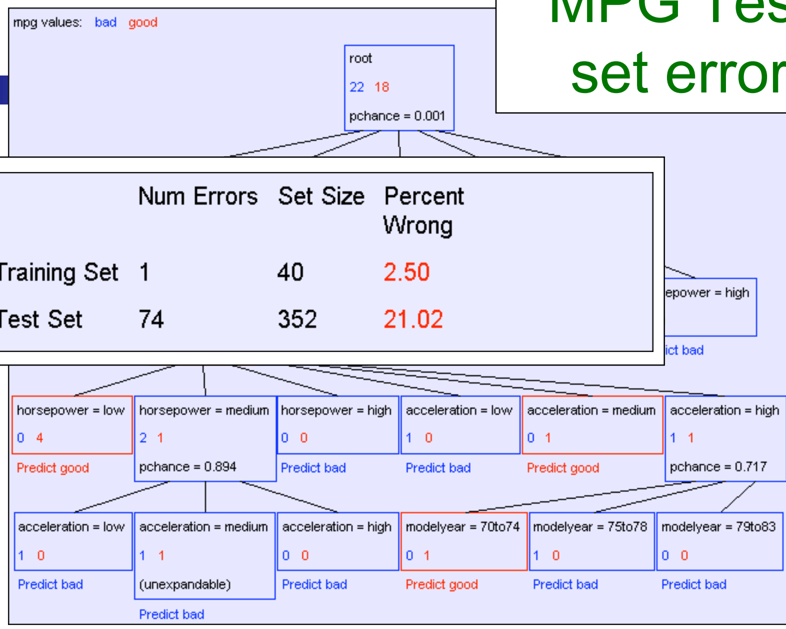
    BuildTree(DS_i,*Output*)

    Where DS_i built consists of all those records in DataSet for which X = *i*th distinct value of X.

recurse on children

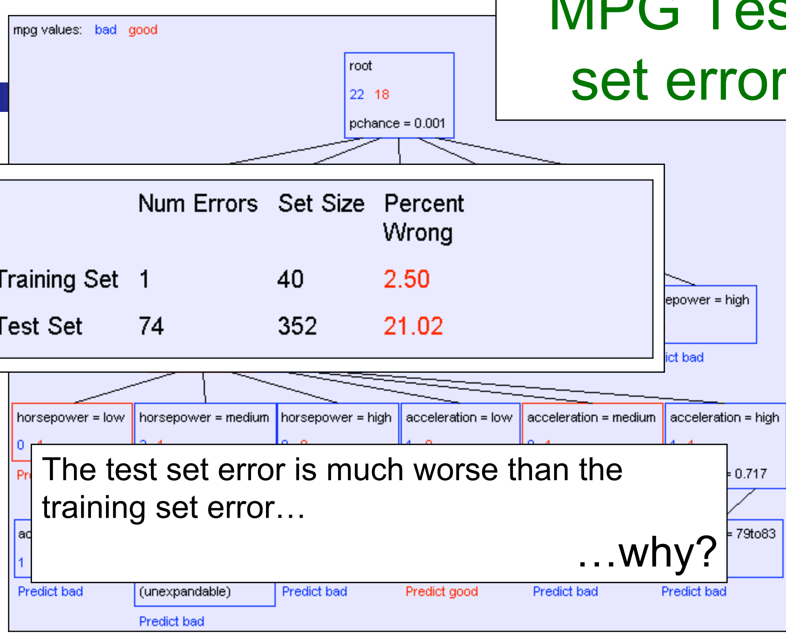
pick part of dataset consistent with children

MPG Test set error



	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

MPG Test set error



	Num Errors	Set Size	Percent Wrong
Training Set	1	40	2.50
Test Set	74	352	21.02

The test set error is much worse than the training set error…

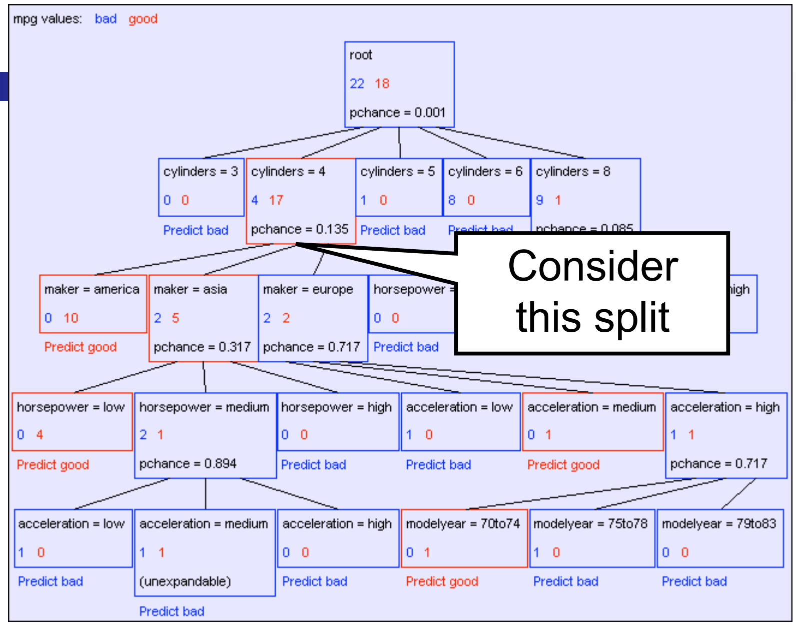
…why?

Decision trees & Learning Bias

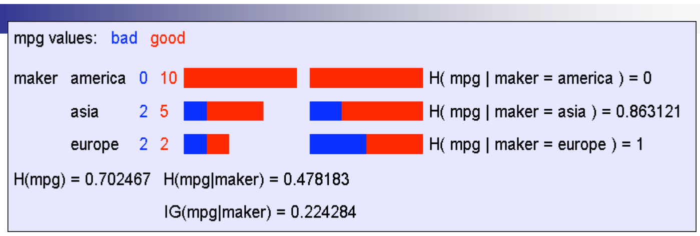
mpg	cylinders	displacement	horsepower	weight	acceleration	modelyear	maker
good	4	low	low	low	high	75to78	asia
bad	6	medium	medium	medium	medium	70to74	america
bad	4	medium	medium	medium	low	75to78	europe
bad	8	high	high	high	low	70to74	america
bad	6	medium	medium	medium	medium	70to74	america
bad	4	low	medium	low	medium	70to74	asia
bad	4	low	medium	low	low	70to74	asia
bad	8	high	high	high	low	75to78	america
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
bad	8	high	high	high	low	70to74	america
good	8	high	medium	high	high	79to83	america
bad	8	high	high	high	low	75to78	america
good	4	low	low	low	low	79to83	america
bad	6	medium	medium	medium	high	75to78	america
good	4	medium	low	low	low	79to83	america
good	4	low	low	medium	high	79to83	america
bad	8	high	high	high	low	70to74	america
good	4	low	medium	low	medium	75to78	europe
bad	5	medium	medium	medium	medium	75to78	europe

Decision trees will overfit

- Standard decision trees are have no learning biased
  - Training set error is always zero!
    - (If there is no label noise)
  - Lots of variance
  - Will definitely overfit!!!
  - Must bias towards simpler trees
- Many strategies for picking simpler trees:
  - Fixed depth
  - Fixed number of leaves
  - Or something smarter…

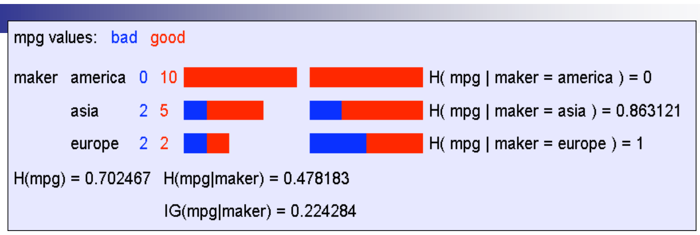


A chi-square test



- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

A chi-square test



- Suppose that mpg was completely uncorrelated with maker.
- What is the chance we'd have seen data of at least this apparent level of association anyway?

By using a particular kind of chi-square test, the answer is 7.2%

(Such simple hypothesis tests are very easy to compute, unfortunately, not enough time to cover in the lecture,
but in your homework, you'll have fun! :))

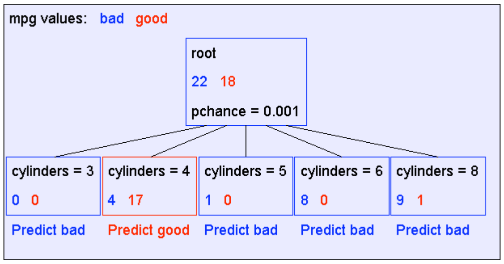
Using Chi-squared to avoid overfitting

- Build the full decision tree as before
- But when you can grow it no more, start to prune:
  - Beginning at the bottom of the tree, delete splits in which p_{chance} > *MaxPchance*
  - Continue working you way up until there are no more prunable nodes

MaxPchance is a magic parameter you must specify to the decision tree, indicating your willingness to risk fitting noise

Pruning example

- With MaxPchance = 0.1, you will see the following MPG decision tree:

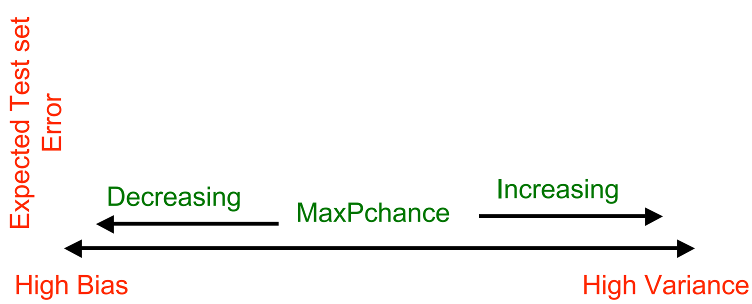


Note the improved test set accuracy compared with the unpruned tree

	Num Errors	Set Size	Percent Wrong
Training Set	5	40	12.50
Test Set	56	352	15.91

MaxPchance

- Technical note MaxPchance is a regularization parameter that helps us bias towards simpler models



We'll learn to choose the value of these magic parameters soon!

Real-Valued inputs

- What should we do if some of the inputs are real-valued?

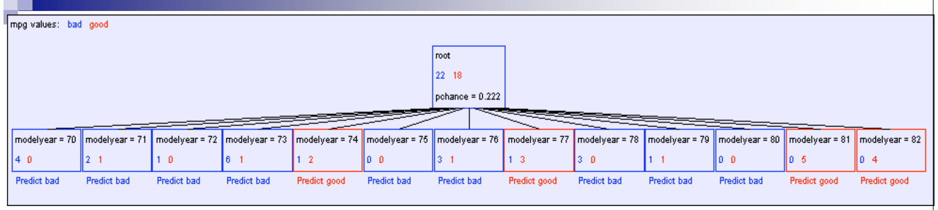
mpg	cylinders	displacemen	horsepower	weight	acceleration	modelyear	maker
good	4	97	75	2265	18.2	77	asia
bad	6	199	90	2648	15	70	america
bad	4	121	110	2600	12.8	77	europe
bad	8	350	175	4100	13	73	america
bad	6	198	95	3102	16.5	74	america
bad	4	108	94	2379	16.5	73	asia
bad	4	113	95	2228	14	71	asia
bad	8	302	139	3570	12.8	78	america
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
:	:	:	:	:	:	:	:
good	4	120	79	2625	18.6	82	america
bad	8	455	225	4425	10	70	america
good	4	107	86	2464	15.5	76	europe
bad	5	131	103	2830	15.9	78	europe

Infinite number of possible split values!!!

Finite dataset, only finite number of relevant splits!

Idea One: Branch on each possible real value

"One branch for each numeric value" idea:



Hopeless: with such high branching factor will shatter the dataset and overfit

Threshold splits

- Binary tree, split on attribute X
  - One branch: X < t
  - Other branch: $X \geq t$

Choosing threshold split

- Binary tree, split on attribute X
  - One branch: X < t
  - Other branch: $X \geq t$
- Search through possible values of *t*
  - Seems hard!!!
- But only finite number of *t*'s are important
  - Sort data according to X into $\{x_1,\ldots,x_m\}$
  - Consider split points of the form $x_i + (x_{i+1} - x_i)/2$

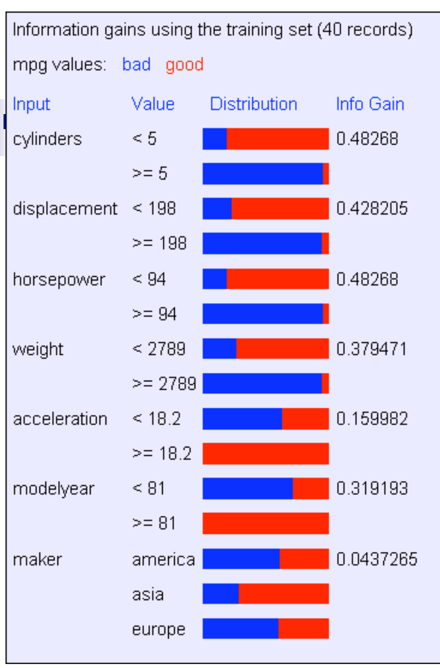
A better idea: thresholded splits

- Suppose X is real valued
- Define *IG(Y|X:t)* as *H(Y) - H(Y|X:t)*
- Define *H(Y|X:t)* =

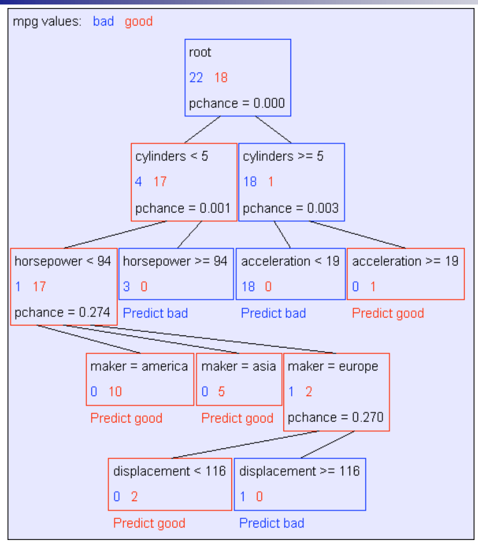
  $H(Y|X < t)\, P(X < t) + H(Y|X >= t)\, P(X >= t)$

  - *IG(Y|X:t)* is the information gain for predicting Y if all you know is whether X is greater than or less than *t*
- Then define $IG^*(Y|X) = max_t\, IG(Y|X:t)$
- For each real-valued attribute, use *IG*(Y|X)* for assessing its suitability as a split
- Note, may split on an attribute multiple times, with different thresholds

Example with MPG



Example tree using reals



What you need to know about decision trees

- Decision trees are one of the most popular data mining tools
  - Easy to understand
  - Easy to implement
  - Easy to use
  - Computationally cheap (to solve heuristically)
- Information gain to select attributes (ID3, C4.5,…)
- Presented for classification, can be used for regression and density estimation too
- Decision trees will overfit!!!
  - Zero bias classifier → Lots of variance
  - Must use tricks to find “simple trees”, e.g.,
    - Fixed depth/Early stopping
    - Pruning
    - Hypothesis testing

Acknowledgements

- Some of the material in the decision trees presentation is courtesy of Andrew Moore, from his excellent collection of ML tutorials:
  - http://www.cs.cmu.edu/~awm/tutorials

Announcements

- Homework 1 due Wednesday beginning of class
  - started early, started early, started early, started early, started early, started early, started early, started early
- Exam dates set:
  - Midterm: Thursday, Oct. 25th, 5-6:30pm, MM A14
  - Final: Tuesday, Dec. 11, 05:30PM-08:30PM

Fighting the bias-variance tradeoff

- **Simple (a.k.a. weak) learners are good**
  - e.g., naïve Bayes, logistic regression, decision stumps (or shallow decision trees)
  - Low variance, don't usually overfit
- **Simple (a.k.a. weak) learners are bad**
  - High bias, can't solve hard learning problems
- Can we make weak learners always good???
  - **No!!!**
  - **But often yes…**

Voting (Ensemble Methods)

- Instead of learning a single (weak) classifier, learn **many weak classifiers** that are **good at different parts of the input space**
- **Output class:** (Weighted) vote of each classifier
  - Classifiers that are most "sure" will vote with more conviction
  - Classifiers will be most "sure" about a particular part of the space
  - On average, do better than single classifier!
- **But how do you ???**
  - force classifiers to learn about different parts of the input space?
  - weigh the votes of different classifiers?

Boosting [Schapire, 1989]

- 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 hypothesis – h_t
  - A strength for this hypothesis – α_t
- Final classifier:
- **Practically useful**
- **Theoretically interesting**

Learning from weighted data

- **Sometimes not all data points are equal**
  - Some data points are more equal than others
- **Consider a weighted dataset**
  - D(i) – weight of *i* th training example $(\mathbf{x}^i, y^i)$
  - Interpretations:
    - *i* th training example counts as D(i) examples
    - If I were to "resample" data, I would get more samples of "heavier" data points
- **Now, in all calculations, whenever used, *i* th training example counts as D(i) "examples"**
  - e.g., MLE for Naïve Bayes, redefine *Count(Y=y)* to be weighted count

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train base learner using distribution D_t.
- Get base classifier $h_t : X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

$$D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

where Z_t is a normalization factor

$$Z_t = \sum_{i=1}^{m} D_t(i) \exp(-\alpha_t y_i h_t(x_i))$$

Output the final classifier:

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

Figure 1: The boosting algorithm AdaBoost.

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For $t = 1, \ldots, T$:

- Train base learner using distribution D_t.
- Get base classifier $h_t : X \to \mathbb{R}$.
- Choose $\alpha_t \in \mathbb{R}$.
- Update:

$$\boxed{\alpha_t = \frac{1}{2} \ln\left(\frac{1 - \epsilon_t}{\epsilon_t}\right)}$$

$$D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

$$\boxed{\epsilon_t = P_{i \sim D_i}[\mathbf{x}^i \neq y^i]}$$

$$\boxed{\epsilon_t = \frac{1}{\sum_{i=1}^{n} D_t(i)} \sum_{i=1}^{m} D_t(i) \delta(h_t(x_i) \neq y_i)}$$

What α_t to choose for hypothesis h_t?

[Schapire, 1989]

Training error of final classifier is bounded by:

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i) \neq y_i) \leq \frac{1}{m}\sum_{i=1}^{m}\exp(-y_i f(x_i))$$

Where $f(x) = \sum_t \alpha_t h_t(x); H(x) = sign(f(x))$

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What α_t to choose for hypothesis h_t?

[Schapire, 1989]

Training error of final classifier is bounded by:

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i) \neq y_i) \leq \frac{1}{m}\sum_{i=1}^{m}\exp(-y_i f(x_i)) = \prod_t Z_t$$

Where $f(x) = \sum_t \alpha_t h_t(x); H(x) = sign(f(x))$

$$\boxed{Z_t = \sum_{i=1}^{m} D_t(i)\exp(-\alpha_t y_i h_t(x_i))}$$

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What α_t to choose for hypothesis h_t?

[Schapire, 1989]

Training error of final classifier is bounded by:

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i)\neq y_i) \leq \frac{1}{m}\sum_i \exp(-y_i f(x_i)) = \prod_t Z_t$$

Where $f(x) = \sum_t \alpha_t h_t(x);\, H(x) = sign(f(x))$

If we minimize $\prod_t Z_t$, we minimize our training error

We can tighten this bound greedily, by choosing α_t and h_t on each iteration to minimize Z_t.

$$Z_t = \sum_{i=1}^{m} D_t(i)\exp(-\alpha_t y_i h_t(x_i))$$

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What α_t to choose for hypothesis h_t?

[Schapire, 1989]

We can minimize this bound by choosing α_t on each iteration to minimize Z_t.

$$Z_t = \sum_{i=1}^{m} D_t(i)\exp(-\alpha_t y_i h_t(x_i))$$

For boolean target function, this is accomplished by [Freund & Schapire '97]:

$$\boxed{\alpha_t = \frac{1}{2}\ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)}$$

You'll prove this in your homework! ☺

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Strong, weak classifiers

- If each classifier is (at least slightly) better than random
  - $\varepsilon_t < 0.5$
- AdaBoost will achieve zero *training error* (exponentially fast):

$$\frac{1}{m}\sum_{i=1}^{m}\delta(H(x_i)\neq y_i) \leq \prod_t Z_t \leq \exp\left(-2\sum_{t=1}^{T}(1/2-\epsilon_t)^2\right)$$

- Is it hard to achieve better than random training error?

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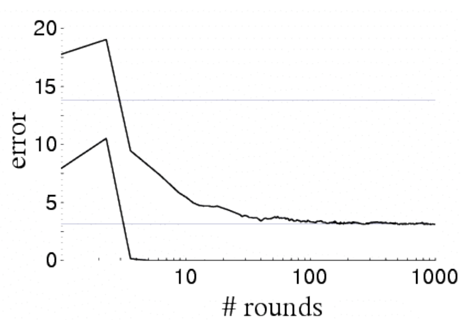
Boosting results – Digit recognition

[Schapire, 1989]



- Boosting often
  - Robust to overfitting
  - Test set error decreases even after training error is zero

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Boosting generalization error bound

[Freund & Schapire, 1996]

$$error_{true}(H) \quad \leq \quad error_{train}(H) + \tilde{O}\left(\sqrt{\frac{Td}{m}}\right)$$

- T – number of boosting rounds
- d – VC dimension of weak learner, measures complexity of classifier
- m – number of training examples

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Boosting generalization error bound

[Freund & Schapire, 1996]

$$error_{true}(H) \quad \leq \quad error_{train}(H) + \tilde{O}\left(\sqrt{\frac{Td}{m}}\right)$$

- **Contradicts**: Boosting often
  - Robust to overfitting
  - Test set error decreases even after training error is zero
- **Need better analysis tools**
  - we'll come back to this later in the semester
- T – number of boosting rounds
- d – VC dimension of weak learner, measures complexity of classifier
- m – number of training examples

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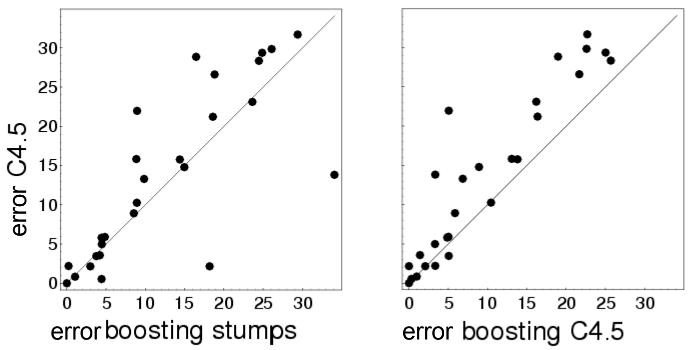
Boosting: Experimental Results

[Freund & Schapire, 1996]

Comparison of C4.5, Boosting C4.5, Boosting decision stumps (depth 1 trees), 27 benchmark datasets



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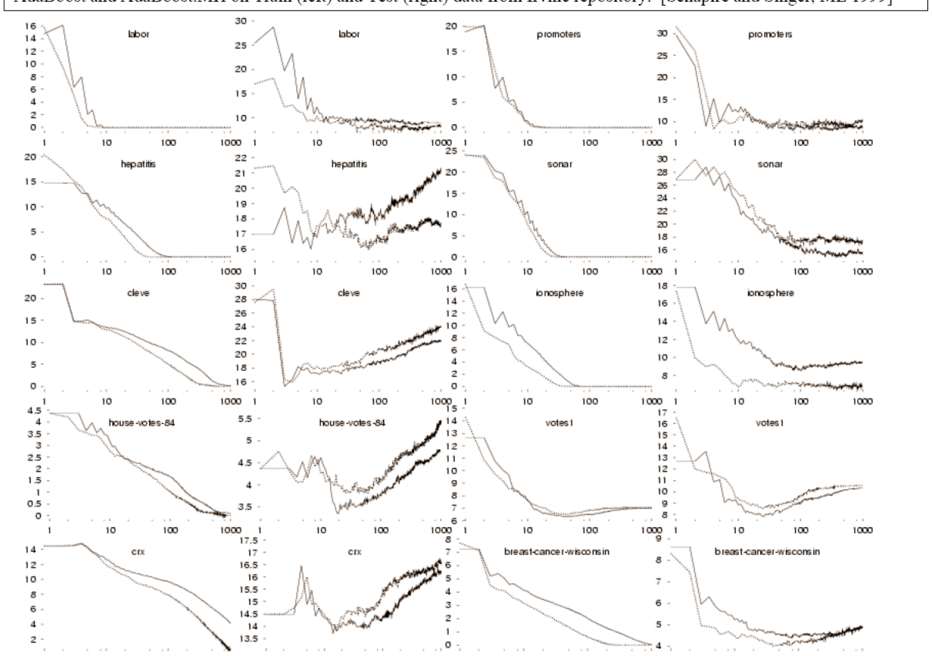
AdaBoost and AdaBoost.MH on Train (left) and Test (right) data from Irvine repository. [Schapire and Singer, ML 1999]



Boosting and Logistic Regression

Logistic regression assumes:

$$P(Y=1|X) = \frac{1}{1+\exp(f(x))}$$

And tries to maximize data likelihood:

$$P(\mathcal{D}|H) = \prod_{i=1}^{m} \frac{1}{1+\exp(-y_i f(x_i))}$$

Equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln(1+\exp(-y_i f(x_i)))$$

Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln(1+\exp(-y_i f(x_i)))$$

Boosting minimizes similar loss function!!

$$\frac{1}{m}\sum_i \exp(-y_i f(x_i)) = \prod_t Z_t$$

Both smooth approximations of 0/1 loss!

Logistic regression and Boosting

Logistic regression:

- Minimize loss fn

$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i)))$$

- Define

$$f(x) = \sum_j w_j x_j$$

where x_j predefined

Boosting:

- Minimize loss fn

$$\sum_{i=1}^{m} \exp(-y_i f(x_i))$$

- Define

$$f(x) = \sum_t \alpha_t h_t(x)$$

where $h_t(x_i)$ defined dynamically to fit data

(not a linear classifier)

- Weights α_j learned incrementally

What you need to know about Boosting

- Combine weak classifiers to obtain very strong classifier
  - Weak classifier – slightly better than random on training data
  - Resulting very strong classifier – can eventually provide zero training error
- AdaBoost algorithm
- Boosting v. Logistic Regression
  - Similar loss functions
  - Single optimization (LR) v. Incrementally improving classification (B)
- Most popular application of Boosting:
  - Boosted decision stumps!
  - Very simple to implement, very effective classifier