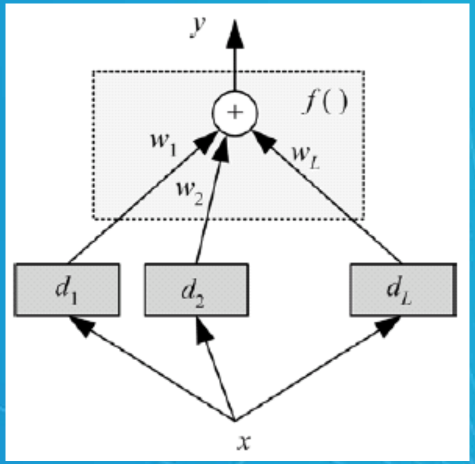
Carnegie Mellon University
School of Computer Science

10701: Introduction to Machine Learning

Ensemble methods:
Boosting from Weak Learners



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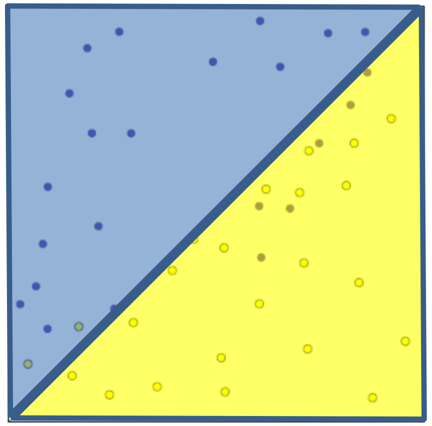
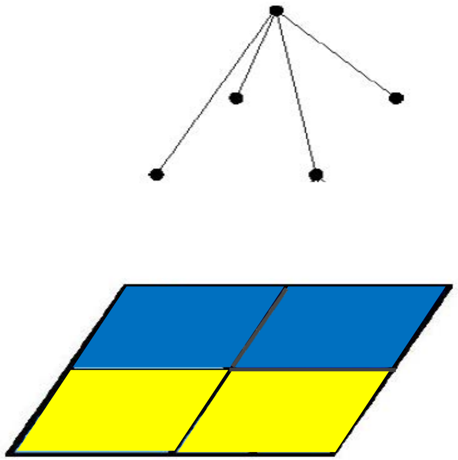
Lecture 12, October 14, 2020

Reading: see class homepage

Weak Learners: Fighting the bias-variance tradeoff

- Simple (a.k.a. weak) learners e.g., naïve Bayes, logistic regression, decision stumps (or shallow decisi





Are good ☺ - Low variance, don't usually overfit

Are bad ☹ - High bias, can't solve hard learning problems

- Can we make weak learners always good???
  - No!!! But often yes…

Why boost weak learners?

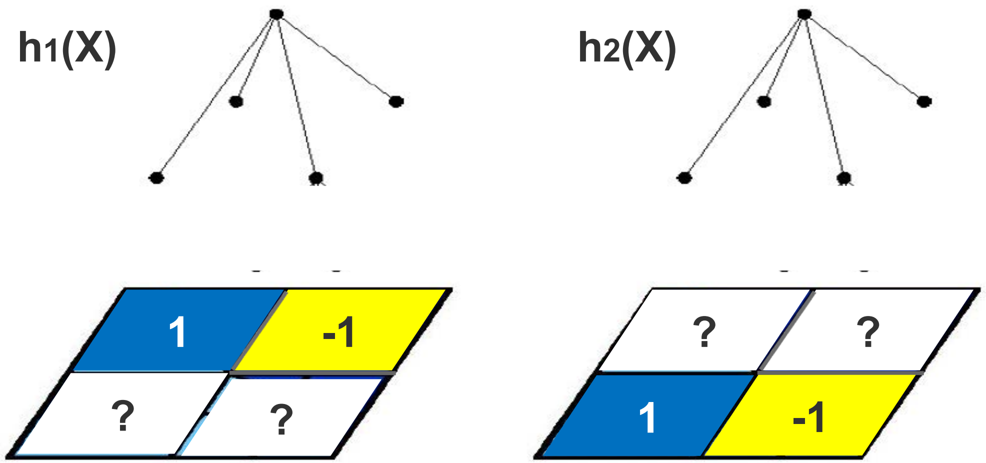
Goal: Automatically categorize type of call requested
(Collect, Calling card, Person-to-person, etc.)

- yes I'd like to place a collect call long distance please (Collect)
- operator I need to make a call but I need to bill it to my office (ThirdNumber)
- yes I'd like to place a call on my master card please (CallingCard)

- Easy to find "rules of thumb" that are "often" correct.
  E.g. If 'card' occurs in utterance, then predict 'calling card'
- Hard to find single highly accurate prediction rule.

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!



$H: X \rightarrow Y\ (-1,1)$

$H(X) = h_1(X)+h_2(X)$

$H(X) = \text{sign}(\sum_t \alpha_t h_t(X))$

weights

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 h_t to learn about different parts of the input space?
  - weigh the votes of different classifiers? α_t

Bagging

- Recall decision trees (lecture 3)
  - Pros: interpretable, can handle discrete and continuous features, robust to outliers, low bias, etc.
  - Cons: high variance
- Trees are perfect candidates for ensembles
  - Consider averaging many (nearly) unbiased tree estimators
  - Bias remains similar, but variance is reduced
- This is called **bagging** (bootstrap aggregating) (Breiman, 1996)
  - Train many trees on bootstrapped data, then take average

$$f(x) = \frac{1}{B}\sum_{b=1}^{B} f_b(x)$$

  - Bootstrap: statistical term for “roll n-face dice n times”

Random Forest

- Reduce correlation between trees, by introducing randomness

1. For b = 1, …, B,
   1. Draw a bootstrap dataset Z^*
   2. Learn a tree $f_b(\cdot)$ on Z^*, in particular select m features randomly out of p features as candidates before splitting
2. Output:
   - Regression: $f(x) = \frac{1}{B}\sum_{b=1}^{B} f_b(x)$
   - Classification: majority vote

- Typically take $m \leq \sqrt{p}$

Boosting [Schapire'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: $\boxed{H(X) = \text{sign}(\sum \alpha_t h_t(X))}$

- Practically useful, and theoretically interesting
- Important issues:
  - what is the criterion that we are optimizing? (measure of loss)
  - we would like to estimate each new component classifier in the same manner (modularity)

AdaBoost

- At the kth iteration we find (any) classifier $h(\mathbf{x};\, \theta_k^*)$ for which the weighted classification error:

$$\varepsilon_k = \sum_{i=1}^{n} W_i^{k-1} I(y_i \neq h(\mathbf{x}_i;\theta_k^*)) \Big/ \sum_{i=1}^{n} W_i^{k-1}$$

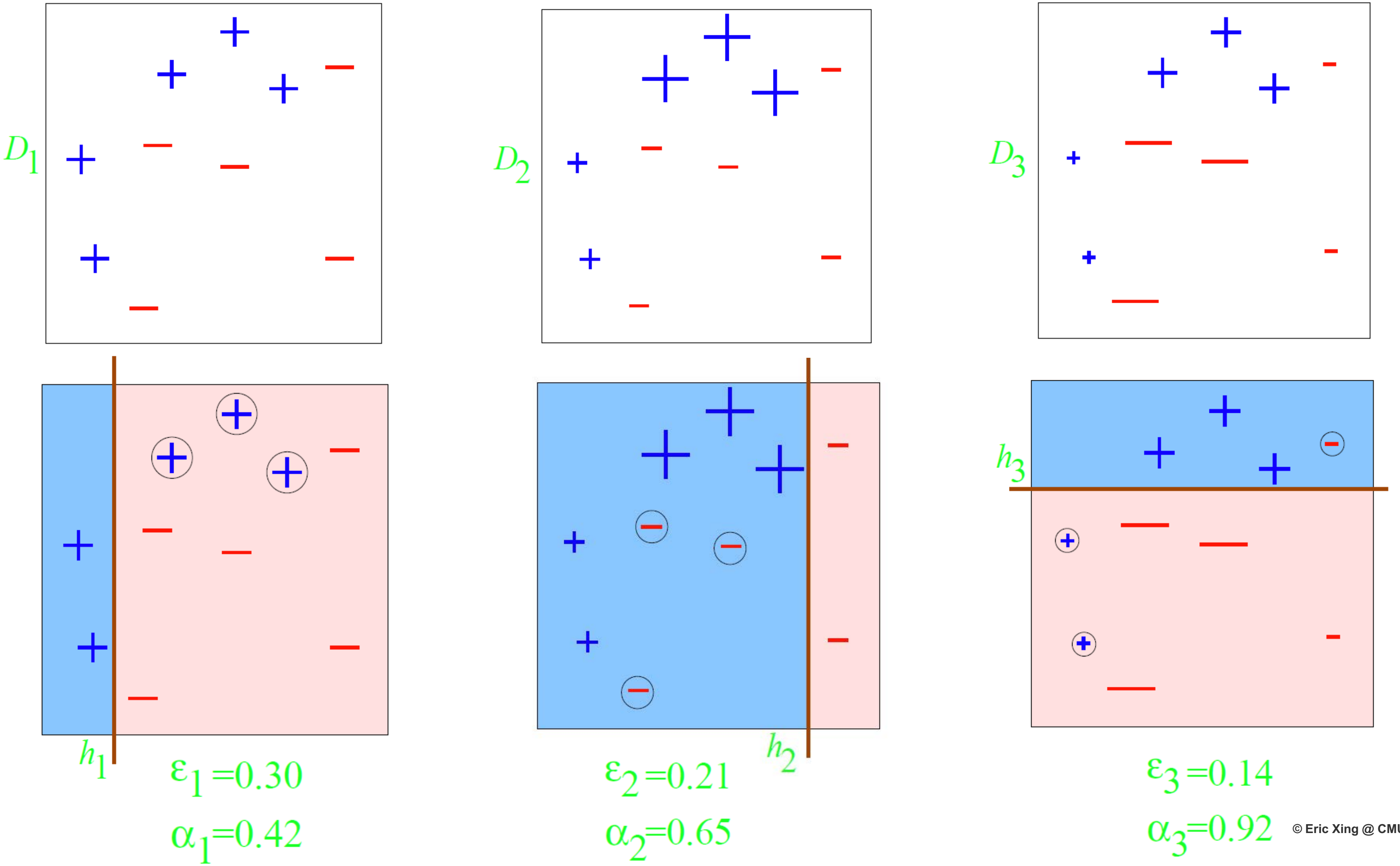
  is better than chance.
  - This is meant to be "easy" --- weak classifier
- Determine how many “votes” to assign to the new component classifier:

$$\alpha_k = 0.5 \log\left((1-\varepsilon_k)/\varepsilon_k\right)$$

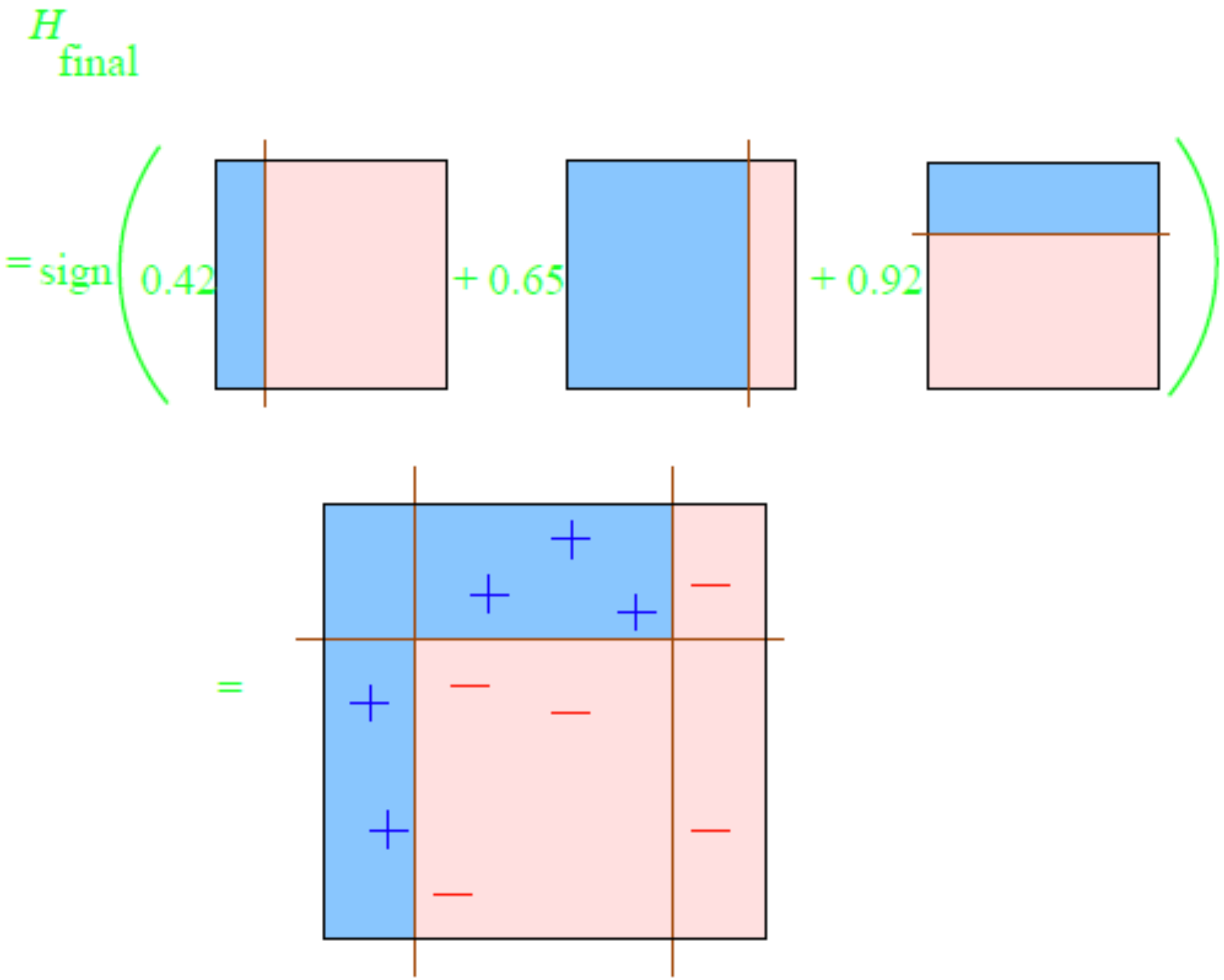
  - stronger classifier gets more votes
- Update the weights on the training examples:

$$W_i^k = W_i^{k-1} \exp\left\{-y_i a_k h(\mathbf{x}_i;\theta_k)\right\}$$

Boosting Example (Decision Stumps)



Boosting Example (Decision Stumps)



- What is the criterion that we are optimizing? (measure of loss)

Measurement of error

- Loss function:

$$\lambda(y, h(\mathbf{x})) \qquad\qquad \left(\text{e.g.}\ I(y \neq h(\mathbf{x}))\right)$$

- Generalization error:

$$L(h) = E\left[\lambda(y, h(\mathbf{x}))\right]$$

- Objective: find *h* with minimum *generalization* error

- Main boosting idea: minimize the *empirical* error:

$$\hat{L}(h) = \frac{1}{N}\sum_{i=1}^{N} \lambda(y_i, h(\mathbf{x}_i))$$

Exponential Loss

- Empirical loss:

$$\hat{L}(h) = \frac{1}{N}\sum_{i=1}^{N} \lambda(y_i, \hat{h}_m(\mathbf{x}_i))$$

- Another possible measure of empirical loss is

$$\hat{L}(h) = \sum_{i=1}^{n} \exp\left\{-y_i \hat{h}_m(\mathbf{x}_i)\right\}$$

Exponential Loss

- One possible measure of empirical loss is

$$\hat{L}(h) = \sum_{i=1}^{n} \exp\left\{- y_i \hat{h}_m(\mathbf{x}_i)\right\}$$

$$= \sum_{i=1}^{n} \exp\left\{- y_i \hat{h}_{m-1}(\mathbf{x}_i) - y_i a_m h(\mathbf{x}_i; \theta_m)\right\}$$

$$= \sum_{i=1}^{n} \exp\left\{- y_i \hat{h}_{m-1}(\mathbf{x}_i)\right\} \exp\left\{- y_i a_m h(\mathbf{x}_i; \theta_m)\right\}$$

$$= \sum_{i=1}^{n} W_i^{m-1} \exp\left\{- y_i a_m h(\mathbf{x}_i; \theta_m)\right\}$$

Recall that:

$$\hat{h}_m(\mathbf{x}) = \alpha_1 h(\mathbf{x}; \theta_1) + \ldots + \alpha_m h(\mathbf{x}; \theta_m)$$

$$W_i^{m-1} = \exp\left\{- y_i \hat{h}_{m-1}(\mathbf{x}_i)\right\}$$

- The combined classifier based on m – 1 iterations defines a weighted loss criterion for the next simple classifier to add
- each training sample is weighted by its "classifiability" (or difficulty) seen by the classifier we have built so far

Linearization of loss function

- We can simplify a bit the estimation criterion for the new component classifiers (assuming α is small)

$$\exp\{-y_i a_m h(\mathbf{x}_i;\theta_m)\} \approx 1 - y_i a_m h(\mathbf{x}_i;\theta_m)$$

- Now our empirical loss criterion reduces to

$$\sum_{i=1}^{n} \exp\left\{-y_i \hat{h}_m(\mathbf{x}_i)\right\}$$

$$\approx \sum_{i=1}^{n} W_i^{m-1}(1 - y_i a_m h(\mathbf{x}_i;\theta_m))$$

$$W_i^{m-1} = \exp\left\{-y_i \hat{h}_{m-1}(\mathbf{x}_i)\right\}$$

$$= \sum_{i=1}^{n} W_i^{m-1} - a_m \sum_{i=1}^{n} W_i^{m-1} y_i h(\mathbf{x}_i;\theta_m)$$

- We could choose a new component classifier to optimize this weighted agreement

A possible algorithm

- At stage m we find θ^* that maximize (or at least give a sufficiently high) weighted agreement:

$$\sum_{i=1}^{n} W_i^{m-1} y_i h(\mathbf{x}_i; \theta_m^*)$$

  - each sample is weighted by its "difficulty" under the previously combined $m-1$ classifiers,
  - more "difficult" samples received heavier attention as they dominates the total loss
- Then we go back and find the "votes" $\alpha_m{}^*$ associated with the new classifier by minimizing the original weighted (exponential) loss

$$\hat{L}(h) = \sum_{i=1}^{n} W_i^{m-1} \exp\{-y_i a_m h(\mathbf{x}_i; \theta_m)\}$$

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

The AdaBoost algorithm

$$W_i^{m-1} = \exp\left\{-y_i \hat{h}_{m-1}(\mathbf{x}_i)\right\}$$

- At the kth iteration we find (any) classifier $h(\mathbf{x};\ \theta_k^*)$ for which the weighted classification error:

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The AdaBoost algorithm cont'd

- The final classifier after m boosting iterations is given by the sign of

$$\hat{h}(\mathbf{x}) = \frac{\alpha_1 h(\mathbf{x};\theta_1) + \ldots + \alpha_m h(\mathbf{x};\theta_m)}{\alpha_1 + \ldots + \alpha_m}$$

  - the votes here are normalized for convenience

Boosting

- We have basically derived a Boosting algorithm that sequentially adds new component classifiers, each trained on reweighted training examples
  - each component classifier is presented with a slightly different problem

- AdaBoost preliminaries:
  - we work with *normalized weights* W_i on the training examples, initially uniform ($W_i = 1/n$)
  - the weight reflect the "*degree of difficulty*" of each datum on the latest classifier

AdaBoost: summary

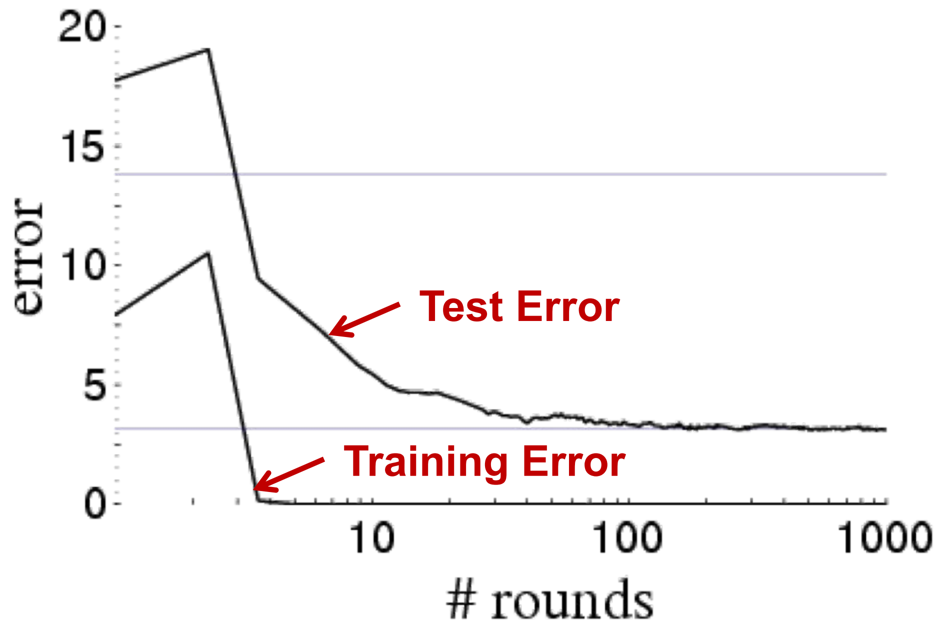
- Input:
  - N examples $S_N = \{(x_1,y_1),\ldots, (x_N,y_N)\}$
  - a weak base learner $h = h(x,\theta)$
- Initialize: equal example weights $w_i = 1/N$ for all $i = 1..N$
- Iterate for $t = 1\ldots T$:
  1. train base learner according to weighted example set (w_t,x) and obtain hypothesis $h_t = h(x,\theta_t)$
  2. compute hypothesis error ε_t
  3. compute hypothesis weight α_t
  4. update example weights for next iteration w_{t+1}
- Output: final hypothesis as a linear combination of h_t

Base Learners

- Weak learners used in practice:
  - Decision stumps (axis parallel splits)
  - Decision trees (e.g. C4.5 by Quinlan 1996)
  - Multi-layer neural networks
  - Radial basis function networks

- Can base learners operate on weighted examples?
  - In many cases they can be modified to accept weights along with the examples
  - In general, we can sample the examples (with replacement) according to the distribution defined by the weights

Boosting results – Digit recognition [Schapire, 1989]



- Boosting often, **but not always**
  - Robust to overfitting
  - Test set error decreases even after training error is zero

Generalization Error Bounds

[Freund & Schapire'95]

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

	bias	variance	
tradeoff	large	small	T small
	small	large	T large

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

Generalization Error Bounds

[Freund & Schapire'95]

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

With high probability

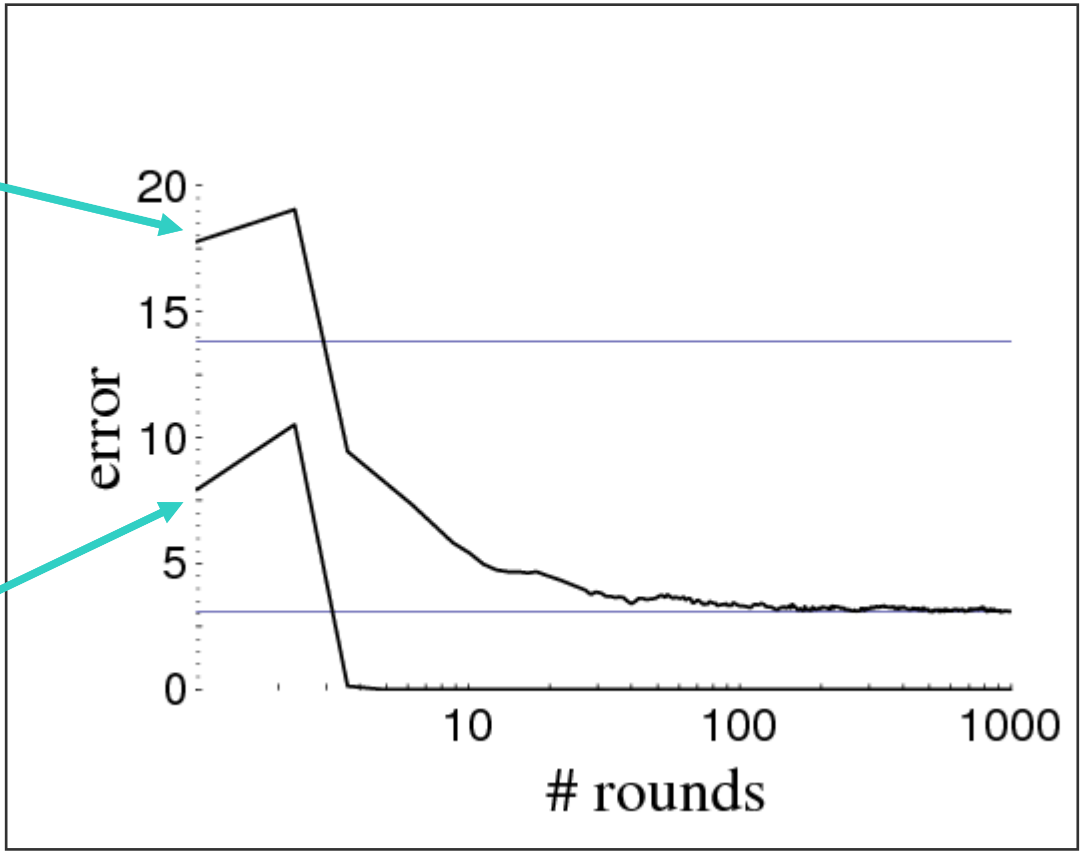
Boosting can overfit if T is large

Boosting often, Contradicts experimental results
- Robust to overfitting
- Test set error decreases even after training error is zero

Need better analysis tools – margin based bounds

Experiments

Test error



Training error

The Boosting Approach to Machine Learning, by Robert E. Schapire

Training Margins

- When a vote is taken, the more predictors agreeing, the more confident you are in your prediction.

- Margin for example:

$$\text{margin}_h(\mathbf{x}_i, y_i) = y_i \left[\frac{\alpha_1 h(\mathbf{x}_i; \theta_1) + \ldots + \alpha_m h(\mathbf{x}_i; \theta_m)}{\alpha_1 + \ldots + \alpha_m} \right]$$

The margin lies in [−1, 1] and is negative for all misclassified examples.

- Successive boosting iterations improve the majority vote or margin for the training examples

A Margin Bound

- For any γ, the generalization error is less than:

$$\Pr\left(\text{margin}_h(\mathbf{x},y) \le \gamma\right) + O\left(\sqrt{\frac{d}{m\gamma^2}}\right)$$

Robert E. Schapire, Yoav Freund, Peter Bartlett and Wee Sun Lee. Boosting the margin: A new explanation for the effectiveness of voting methods. *The Annals of Statistics*, 26(5):1651-1686, 1998.

- It does not depend on T!!!

Summary

- Boosting takes a weak learner and converts it to a strong
- one

- Works by asymptotically minimizing the empirical error

- Effectively maximizes the margin of the combined hypothesis

Supplementary

Some additional points for fun

Boosting and Logistic Regression

- Logistic regression assumes:

$$P(Y=1|X) = \frac{1}{1+\exp(f(x))} \qquad f(x) = w_0 + \sum_j w_j x_j$$

- And tries to maximize data likelihood:

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

- Equivalent to minimizing log loss

$$-\log P(\mathcal{D}|f) = \sum_{i=1}^{m} \ln(1+\exp(-y_i f(x_i)))$$

Boosting and Logistic Regression

Logistic regression equivalent to minimizing log loss

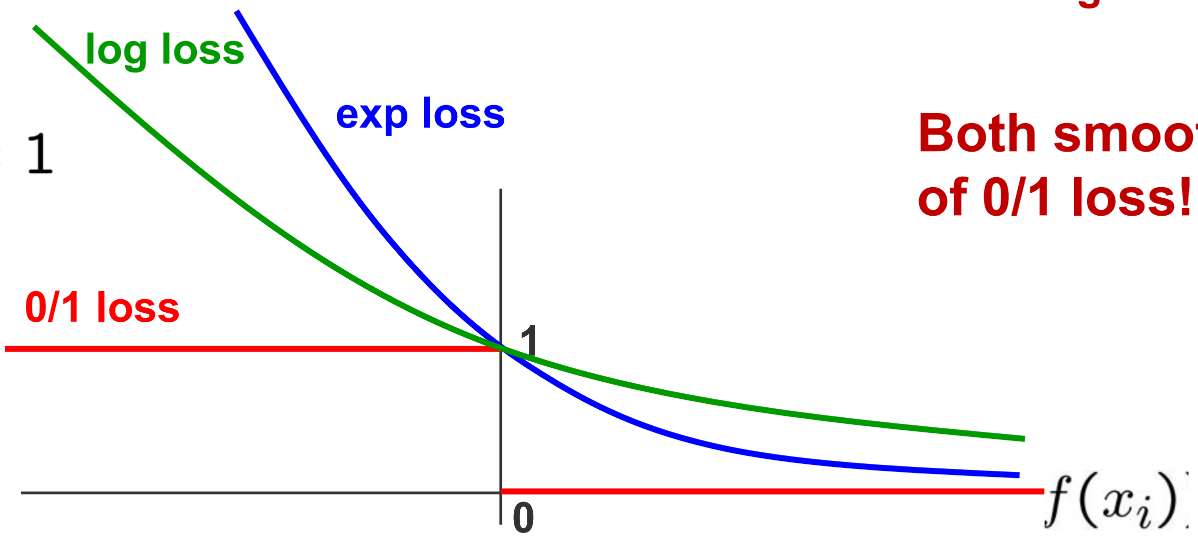
$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i))) \qquad f(x) = w_0 + \sum_j w_j x_j$$

Boosting minimizes similar loss function!!

$$\frac{1}{m}\sum_{i=1}^{m} \exp(-y_i f(x_i)) = \prod_t Z_t \qquad f(x) = \sum_t \alpha_t h_t(x)$$

Weighted average of weak learners

$y_i = 1$



Both smooth approximations of 0/1 loss!

Boosting and Logistic Regression

Boosting:

- Minimize exp loss

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

- Define

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

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

(not a linear classifier)

- Weights α_t learned per iteration t incrementally

Logistic regression:

- Minimize log loss

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

- Define

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

where x_j predefined features

(linear classifier)

- Jointly optimize over all weights $w_0, w_1, w_2 \ldots$

Hard & Soft Decision

- Weighted average of weak learners

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

- Hard Decision/Predicted label:

$$H(x) = sign(f(x))$$

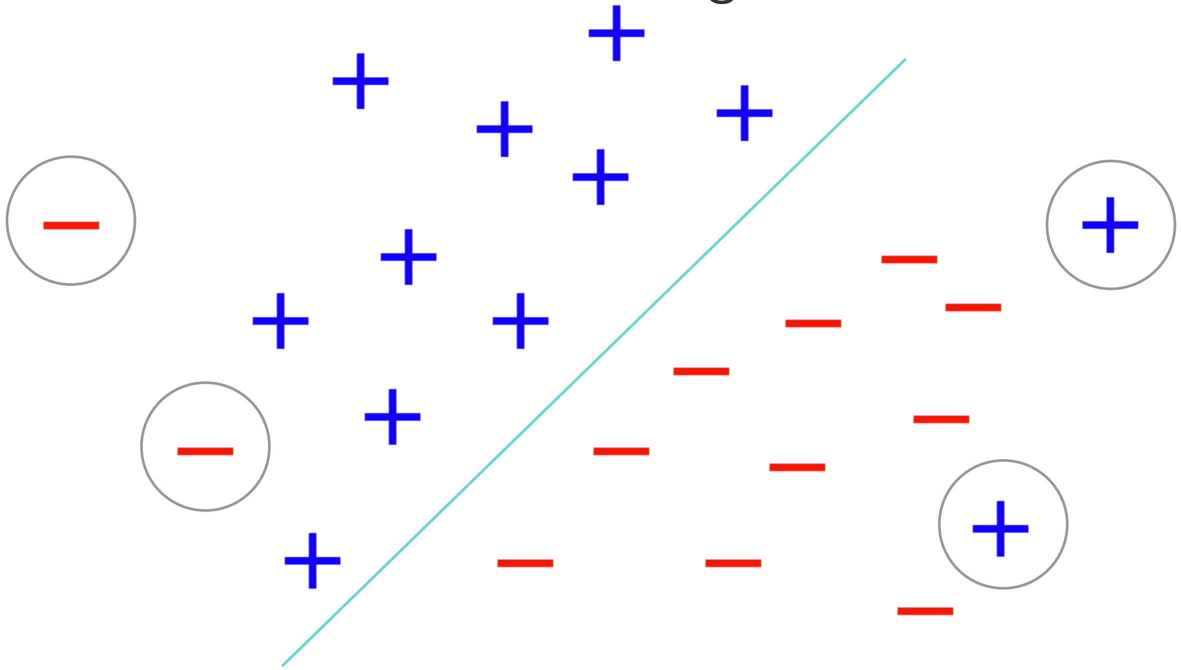
- Soft Decision:
  - (based on analogy with logistic regression)

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

Effect of Outliers

- Good ☺ : Can identify outliers since focuses on examples that are hard to categorize

- Bad ☹ : Too many outliers can degrade classification performance dramatically increase time to convergence



Gradient Boosting

- Goal: Find nonlinear predictor $\hat{h}(x) \in \mathcal{H}$ such that

$$\hat{h} = \arg\min_{h \in \mathcal{H}} \mathcal{L}(h(X), Y)$$

- Gradient boosting generalizes Adaboost (exponential loss) to any smooth loss functions $\mathcal{L}(\cdot, \cdot)$

Square loss (regression)

$$\mathcal{L}(h(X), Y) = \sum_{i=1}^{n} (h(\mathbf{x}_i) - y_i)^2$$

Logistic loss (classification)

$$\mathcal{L}(h(X), Y) = \sum_{i=1}^{n} \ln(1 + e^{-h(\mathbf{x}_i) y_i})$$

Margin loss (ranking)

$$\mathcal{L}(h(X), Y) = \sum_{(i,i'):y_{(i,i')}=1} \max(0, 1 - (h(\mathbf{x}_i) - h(\mathbf{x}_{i'})))^2$$

(prefer item i over j)

Others…

Gradient Boosting Decision Tree

- Let's use decision tree to approximate g_{k-1}
- A J-leaf node decision tree can be viewed as a partition of the input space

$$q : \mathbb{R}^d \to \{1, 2, ..., J\}$$

- and a prediction value (weight) associated with each partition

$$w \in \mathbb{R}^J$$

- Will learn q (tree structure) first, then w