# CSCE 970 Lecture 6: System Evaluation and Combining Classifiers

Stephen D. Scott
(Adapted partially from Tom Mitchell's slides)

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## Introduction

- Once features generated/selected and classifier built, need to assess its performance on new data
- Assume all data drawn according to some prob. distribution $\mathcal{D}$ and try to estimate classifier's prediction error on new data drawn according to $\mathcal{D}$
- If error estimate unacceptable, need to select/gen. new features and/or build new classifier
  - Change features used
  - Change size/structure of neural network
  - Change assumptions in Bayesian classifier
  - Choose new learning method, e.g. decision tree



## Introduction
(cont'd)

- Can't use error on training set to estimate ability to generalize, because it's too optimistic
- So use sepearate testing set to estimate error
- Can use statistical hypothesis testing techniques to:
  - Give confidence intervals for error estimate
  - Contrast performance of two classifiers (see if the difference in their error estimates is statistically significant)
- Sometimes need to train and test with a small data set
- Will also look at improving a classifier's performance



## Outline

- Sample error vs. true error
- Confidence intervals for observed hypothesis error
- Estimators
- Binomial distribution, Normal distribution, Central Limit Theorem
- Paired $t$ tests
- Comparing learning methods
- Combining classifiers to improve performance: Weighted Majority, Bagging, Boosting

## Two Definitions of Error

- Denote the learned classifier by the hypothesis $h$ and the target function (that labels examples) by $f$
- The true error of hypothesis $h$ with respect to target function $f$ and distribution $\mathcal{D}$ is the probability that $h$ will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

- The sample error of $h$ with respect to target function $f$ and data sample $S$ is the proportion of examples $h$ misclassifies

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq h(x))$$

  Where $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

- How well does $error_S(h)$ estimate $error_{\mathcal{D}}(h)$?



## Problems Estimating Error

- Bias: If $S$ is training set, $error_S(h)$ is optimistically biased

$$bias \equiv E[error_S(h)] - error_{\mathcal{D}}(h)$$

  For unbiased estimate, $h$ and $S$ must be chosen independently

- Variance: Even with unbiased $S$, $error_S(h)$ may still *vary* from $error_{\mathcal{D}}(h)$



## Estimators

Experiment:

1. Choose sample $S$ of size $n$ according to distribution $\mathcal{D}$
2. Measure $error_S(h)$

$error_S(h)$ is a random variable (i.e., result of an experiment)

$error_S(h)$ is an unbiased estimator for $error_{\mathcal{D}}(h)$

Given observed $error_S(h)$, what can we conclude about $error_{\mathcal{D}}(h)$?



## Confidence Intervals

If

- $S$ contains $n$ examples, drawn independently of $h$ and each other
- $n \geq 30$

Then

- With approximately 95% probability, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

E.g. hypothesis $h$ misclassifies 12 of the 40 examples in test set $S$:

$$error_S(h) = \frac{12}{40} = 0.30$$

Then with approx. 95% confidence, $error_{\mathcal{D}}(h) \in [0.158, 0.442]$

## Confidence Intervals
(cont'd)

If

- $S$ contains $n$ examples, drawn independently of $h$ and each other
- $n \geq 30$

Then

- With approximately $N\%$ probability, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

where

| $N\%$: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z_N$: | 0.67 | 1.00 | 1.28 | 1.64 | 1.96 | 2.33 | 2.58 |

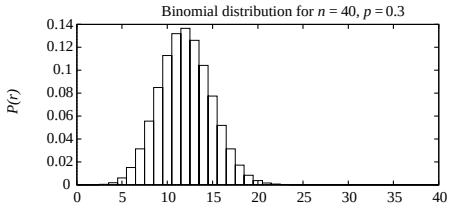
Why?



## $error_S(h)$ is a Random Variable

Repeatedly run the experiment, each with different randomly drawn $S$ (each of size $n$)

Probability of observing $r$ misclassified examples:



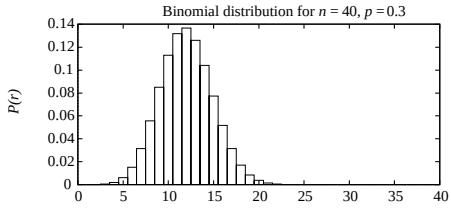

$$P(r) = \binom{n}{r} error_{\mathcal{D}}(h)^r (1 - error_{\mathcal{D}}(h))^{n-r}$$

I.e. let $error_{\mathcal{D}}(h)$ be probability of heads in biased coin, the $P(r)$ = prob. of getting $r$ heads out of $n$ flips

What kind of distribution is this?



## Binomial Probability Distribution




$$P(r) = \binom{n}{r} p^r (1-p)^{n-r} = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

Probability $P(r)$ of $r$ heads in $n$ coin flips, if $p =$ Pr($heads$)

- Expected, or mean value of $X$, $E[X]$, is

$$E[X] \equiv \sum_{i=0}^{n} iP(i) = np$$

- Variance of $X$ is

$$Var(X) \equiv E[(X - E[X])^2] = np(1-p)$$

- Standard deviation of $X$, $\sigma_X$, is

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$$



## Approximate Binomial Dist. with Normal

$error_S(h) = r/n$ is binomially distributed, with

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$ (i.e. unbiased est.)
- standard deviation $\sigma_{error_S(h)}$

$$\sigma_{error_S(h)} = \sqrt{\frac{error_{\mathcal{D}}(h)(1 - error_{\mathcal{D}}(h))}{n}}$$

(i.e. increasing $n$ decreases variance)

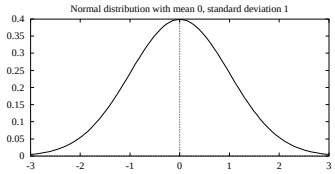
Want to compute confidence interval = interval centered at $error_{\mathcal{D}}(h)$ containing $N\%$ of the weight under the distribution (difficult for binomial)

Approximate binomial by normal (Gaussian) dist:

- mean $\mu_{error_S(h)} = error_{\mathcal{D}}(h)$
- standard deviation $\sigma_{error_S(h)}$

$$\sigma_{error_S(h)} \approx \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

## Normal Probability Distribution




$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right)$$

- Defined completely by $\mu$ and $\sigma$
- The probability that $X$ will fall into the interval $(a, b)$ is given by

$$\int_a^b p(x)dx$$

- Expected, or mean value of $X$, $E[X]$, is

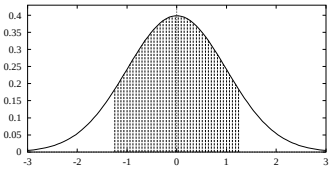
$$E[X] = \mu$$

- Variance of $X$ is $Var(X) = \sigma^2$
- Standard deviation of $X$, $\sigma_X$, is

$$\sigma_X = \sigma$$



## Normal Probability Distribution
(cont'd)

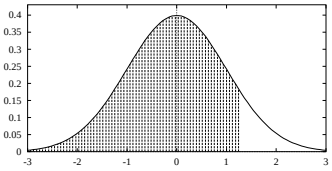


80% of area (probability) lies in $\mu \pm 1.28\sigma$

$N$% of area (probability) lies in $\mu \pm z_N \sigma$

| $N$%: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z_N$: | 0.67 | 1.00 | 1.28 | 1.64 | 1.96 | 2.33 | 2.58 |

Can also have one-sided bounds:



$N$% of area lies $< \mu + z'_N \sigma$ or $> \mu - z'_N \sigma$, where $z'_N = z_{100-(100-N)/2}$

| $N$%: | 50% | 68% | 80% | 90% | 95% | 98% | 99% |
|---|---|---|---|---|---|---|---|
| $z'_N$: | 0.0 | 0.47 | 0.84 | 1.28 | 1.64 | 2.05 | 2.33 |



## Confidence Intervals Revisited

If

- $S$ contains $n$ examples, drawn independently of $h$ and each other
- $n \geq 30$

Then

- With approximately 95% probability, $error_S(h)$ lies in interval

$$error_{\mathcal{D}}(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

Equivalently, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_{\mathcal{D}}(h)(1-error_{\mathcal{D}}(h))}{n}}$$

which is approximately

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1-error_S(h))}{n}}$$

(One-sided bounds yield upper or lower error bounds)



## Central Limit Theorem

How can we justify approximation?

Consider a set of independent, identically distributed random variables $Y_1 \ldots Y_n$, all governed by an arbitrary probability distribution with mean $\mu$ and finite variance $\sigma^2$. Define the sample mean,

$$\bar{Y} \equiv \frac{1}{n}\sum_{i=1}^{n} Y_i$$

Note that $\bar{Y}$ is itself a random variable, i.e. the result of an experiment (e.g. $error_S(h) = r/n$)

Central Limit Theorem: As $n \to \infty$, the distribution governing $\bar{Y}$ approaches a Normal distribution, with mean $\mu$ and variance $\sigma^2/n$

Thus the distribution of $error_S(h)$ is approximately normal for large $n$, and its expected value is $error_{\mathcal{D}}(h)$

(Rule of thumb: $n \geq 30$ when estimator's distribution is binomial, might need to be larger for other distributions)

## Calculating Confidence Intervals

1. Pick parameter $p$ to estimate
   - $error_{\mathcal{D}}(h)$
2. Choose an estimator
   - $error_S(h)$
3. Determine probability distribution that governs estimator
   - $error_S(h)$ governed by binomial distribution, approximated by normal when $n \geq 30$
4. Find interval $(L, U)$ such that $N$% of probability mass falls in the interval
   - Could have $L = -\infty$ or $U = \infty$
   - Use table of $z_N$ or $z'_N$ values



## Difference Between Hypotheses

Test $h_1$ on sample $S_1$, test $h_2$ on $S_2$

1. Pick parameter to estimate
   $$d \equiv error_{\mathcal{D}}(h_1) - error_{\mathcal{D}}(h_2)$$
2. Choose an estimator
   $$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$
   (unbiased)
3. Determine probability distribution that governs estimator (difference between two normals is also normal, variances add)

$$\sigma_{\hat{d}} \approx \sqrt{\frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}}$$

4. Find interval $(L, U)$ such that $N$% of prob. mass falls in the interval: $\hat{d} \pm Z_n \sigma_{\hat{d}}$

(Can also use $S = S_1 \cup S_2$ to test $h_1$ and $h_2$, but not as accurate)



## Paired $t$ test to compare $h_A$,$h_B$

1. Partition data into $k$ disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For $i$ from 1 to $k$, do
   $$\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$$
3. Return the value $\bar{\delta}$, where
   $$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

$N$% confidence interval estimate for $d$:

$$\bar{\delta} \pm t_{N,k-1} \; s_{\bar{\delta}}$$

$$s_{\bar{\delta}} \equiv \sqrt{\frac{1}{k(k-1)} \sum_{i=1}^{k} \left(\delta_i - \bar{\delta}\right)^2}$$

$t$ plays role of $z$, $s$ plays role of $\sigma$

$t$ test gives more accurate results since std. deviation approximated and test sets not independent



## Comparing Learning Algorithms $L_A$ and $L_B$

What we'd like to estimate:

$$E_{S \subset \mathcal{D}}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

where $L(S)$ is the hypothesis output by learner $L$ using training set $S$

I.e., the expected difference in true error between hypotheses output by learners $L_A$ and $L_B$, when trained using randomly selected training sets $S$ drawn according to distribution $\mathcal{D}$

But, given limited data $D_0$, what is a good estimator?

- Could partition $D_0$ into training set $S_0$ and training set $T_0$, and measure
  $$error_{T_0}(L_A(S_0)) - error_{T_0}(L_B(S_0))$$
- Even better, repeat this many times and average the results (next slide)

## Comparing learning algorithms $L_A$ and $L_B$ (cont'd)

1. Partition data $D_0$ into $k$ disjoint test sets $T_1, T_2, \ldots, T_k$ of equal size, where this size is at least 30.
2. For $i$ from 1 to $k$, do

   (use $T_i$ for the test set, and the remaining data for training set $S_i$)

   - $S_i \leftarrow \{D_0 - T_i\}$
   - $h_A \leftarrow L_A(S_i)$
   - $h_B \leftarrow L_B(S_i)$
   - $\delta_i \leftarrow error_{T_i}(h_A) - error_{T_i}(h_B)$
3. Return the value $\bar{\delta}$, where

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$



## Comparing learning algorithms $L_A$ and $L_B$ (cont'd)

- Notice we'd like to use the paired $t$ test on $\bar{\delta}$ to obtain a confidence interval
- Not really correct, because the training sets in this algorithm are not independent (they overlap!)
- More correct to view algorithm as producing an estimate of

$$E_{S \subset D_0}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

instead of

$$E_{S \subset \mathcal{D}}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

- But even this approximation is better than no comparison



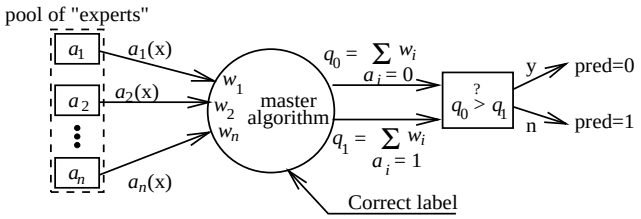
## Combining Classifiers

- Sometimes a single classifier (e.g. neural network, decision tree) won't perform well, but a weighted combination of them will
- Each classifier (or expert) in the pool has its own weight
- When asked to predict the label for a new example, each expert makes its own prediction, and then the master algorithm combines them using the weights for its own prediction (i.e. the "official" one)
- If the classifiers themselves cannot learn (e.g. heuristics) then the best we can do is to learn a good set of weights
- If we are using a learning algorithm (e.g. NN, dec. tree), then we can rerun the algorithm on different subsamples of the training set and set the classifiers' weights during training



## Weighted Majority Algorithm (WM)

[Mitchell, Sec. 7.5.4]



## Weighted Majority Algorithm (WM) (cont'd)

$a_i$ is $i$th pred. algorithm in pool $A$ of algs; each alg is arbitrary function from $X$ to $\{0,1\}$ or $\{-1,1\}$

$w_i$ is weight the master alg associates with $a_i$

$\beta \in [0,1)$ is parameter

- $\forall\, i$ set $w_i \leftarrow 1$
- For each training example (or trial) $\langle x, c(x)\rangle$
  - Set $q_0 \leftarrow q_1 \leftarrow 0$
  - For each algorithm $a_i$
    - If $a_i(x) = 0$ then $q_0 \leftarrow q_0 + w_i$ else $q_1 \leftarrow q_1 + w_i$
    - If $q_1 > q_0$ then predict 1 for $c(x)$, else predict 0 (case for $q_1 = q_0$ is arbitrary)
    - For each $a_i \in A$
      - If $a_i(x) \neq c(x)$ then $w_i \leftarrow \beta\, w_i$

Setting $\beta = 0$ yields Halving algorithm over $A$



## Weighted Majority
Mistake Bound (On-Line Model)

- Let $a_{opt} \in A$ be expert that makes fewest mistakes on arb. sequence $S$ of exs; let $k =$ its number of mistakes
- Let $\beta = 1/2$ and $W_t = \sum_{i=1}^{n} w_{i,t}$ = sum of wts at trial $t$ ($W_0 = n$)
- On trial $t$ such that WM makes a mistake, the total weight reduced is

$$W_t^{mis} = \sum_{a_i(x_t) \neq c(x_t)} w_i \geq W_t/2$$

so

$$W_{t+1} = \left(W_t - W_t^{mis}\right) + W_t^{mis}/2 = W_t - W_t^{mis}/2 \leq 3W_t/4$$

- After seeing all of $S$, $w_{opt,|S|} = (1/2)^k$ and $W_{|S|} \leq n(3/4)^M$ where $M =$ total number of mistakes, yielding

$$\left(\frac{1}{2}\right)^k \leq n\left(\frac{3}{4}\right)^M,$$

so

$$\boxed{M \leq \frac{k + \log_2 n}{-\log_2(3/4)} \leq 2.41\,(k + \log_2 n)}$$



## Weighted Majority
Mistake Bound (cont'd)

- Thus for any arbitrary sequence of examples, WM guaranteed to not perform much worse than best expert in pool plus log of number of experts
  - Implicitly agnostic
- Other results:
  - Bounds hold for general values of $\beta \in [0,1)$
  - Better bounds hold for more sophisticated algorithms, but only better by a constant factor (worst-case lower bound: $\Omega(k + \log n)$)
  - Get bounds for real-valued labels and predictions
  - Can track shifting concept, i.e. where best expert can suddenly change in $S$; key: don't let any weight get too low relative to other weights, i.e. don't overcommit



## Bagging Classifiers
[Breiman, ML Journal, '96]

Bagging = Bootstrap aggregating

Bootstrap sampling: given a set $D$ containing $m$ training examples:

- Create $D_i$ by drawing $m$ examples at random with replacement from $D$
- Expect $D_i$ to omit $\approx 37\%$ of examples from $D$

Bagging:

- Create $k$ bootstrap samples $D_1, \ldots, D_k$
- Train a classifier on each $D_i$
- Classify new instance $x \in X$ by majority vote of learned classifiers (equal weights)

## Bagging Experiment
[Breiman, ML Journal, '96]

Given sample $S$ of labeled data, Breiman did the following 100 times and reported avg:

1. Divide $S$ randomly into test set $T$ (10%) and training set $D$ (90%)
2. Learn decision tree from $D$ and let $e_S$ be its error rate on $T$
3. Do 50 times: Create bootstrap set $D_i$, learn decision tree and let $e_B$ be the error of a majority vote of the trees on $T$

Results

| Data Set | $\bar{e}_S$ | $\bar{e}_B$ | Decrease |
|---|---|---|---|
| waveform | 29.0 | 19.4 | 33% |
| heart | 10.0 | 5.3 | 47% |
| breast cancer | 6.0 | 4.2 | 30% |
| ionosphere | 11.2 | 8.6 | 23% |
| diabetes | 23.4 | 18.8 | 20% |
| glass | 32.0 | 24.9 | 27% |
| soybean | 14.5 | 10.6 | 27% |



## Bagging Experiment
(cont'd)

Same experiment, but using a nearest neighbor classifier, where prediction of new feature vector $\mathbf{x}$'s label is that of $\mathbf{x}$'s nearest neighbor in training set, where distance is e.g. Euclidean distance

Results

| Data Set | $\bar{e}_S$ | $\bar{e}_B$ | Decrease |
|---|---|---|---|
| waveform | 26.1 | 26.1 | 0% |
| heart | 6.3 | 6.3 | 0% |
| breast cancer | 4.9 | 4.9 | 0% |
| ionosphere | 35.7 | 35.7 | 0% |
| diabetes | 16.4 | 16.4 | 0% |
| glass | 16.4 | 16.4 | 0% |

What happened?



## When Does Bagging Help?

When learner is unstable, i.e. if small change in training set causes large change in hypothesis produced

- Decision trees, neural networks
- Not nearest neighbor

Experimentally, bagging can help substantially for unstable learners; can somewhat degrade results for stable learners



## Boosting Classifiers
[Freund & Schapire, ICML '96; many more]

Similar to bagging, but don't always sample uniformly; instead adjust resampling distribution over $D$ to focus attention on previously misclassified examples

Final classifier weights learned classifiers, but not uniform; instead weight of classifier $h_t$ depends on its performance on data it was trained on

Repeat for $t = 1, \ldots, T$:

1. Run learning algorithm on examples randomly drawn from training set $D$ according to distribution $\mathcal{D}_t$ ($\mathcal{D}_1$ = uniform)
2. Output of learner is hypothesis $h_t : X \to \{-1, +1\}$
3. Compute expected error of $h_t$ on examples drawn according to $\mathcal{D}_t$ (can compute exactly)
4. Create $\mathcal{D}_{t+1}$ from $\mathcal{D}_t$ by increasing weight of examples that $h_t$ mispredicts

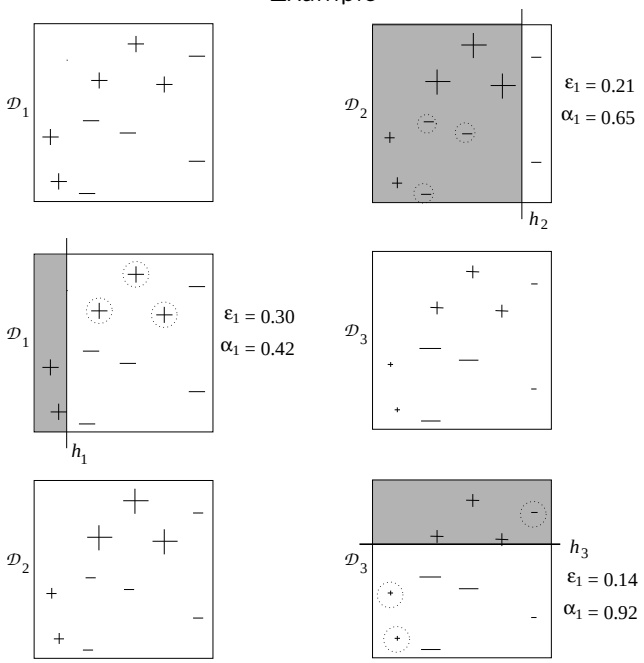
Final classifier is weighted combination of $h_1, \ldots, h_T$, where $h_t$'s weight depends on its error w.r.t. $\mathcal{D}_t$

## Boosting
(cont'd)

- Preliminaries: $D = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$, $y_i \in \{-1, +1\}$, $\mathcal{D}_t(i)$ = weight of $(\mathbf{x}_i, y_i)$ under $\mathcal{D}_t$
- Initialization: $\mathcal{D}_1(i) = 1/m$
- Error Computation: $\epsilon_t = \Pr_{\mathcal{D}_t}[h_t(\mathbf{x}_i) \neq y_i]$
  (easy to do since we know $\mathcal{D}_t$)
- If $\epsilon_t > 1/2$ then halt; else:
- Weighting Factor: $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
  (grows as $\epsilon_t$ decreases)
- Update: $\mathcal{D}_{t+1}(i) = \frac{\mathcal{D}_t(i) \exp\left(-\alpha_t\, y_i\, h_t(\mathbf{x}_i)\right)}{\underbrace{Z_t}_{\text{normalization factor}}}$
  (increase wt. of mispredicted exs, decr. wt of correctly pred.)
- Final Hypothesis: $H(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t\, h_t(\mathbf{x})\right)$
  ($\epsilon_t$ large $\Rightarrow$ flip $h_t$'s prediction strongly)

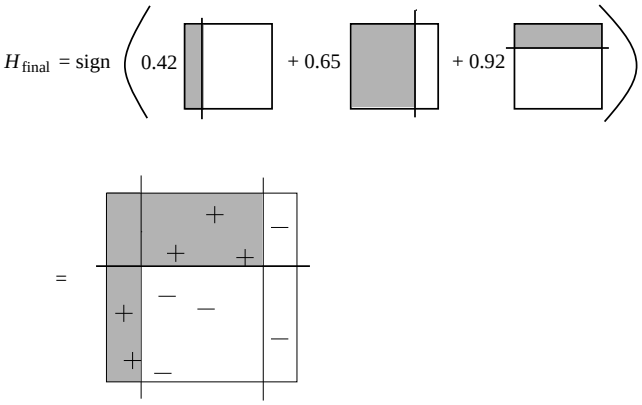


## Boosting
Example






## Boosting
Example (cont'd)






## Boosting
Miscellany

- If each $\epsilon_t < 1/2 - \gamma_t$, error of $H(\cdot)$ on $D$ drops exponentially in $\sum_{t=1}^{T} \gamma_t$
- Can also bound generalization error of $H(\cdot)$ independent of $T$
- Also successful empirically on neural network and decision tree learners
  - Empirically, generalization sometimes improves if training continues after $H(\cdot)$'s error on $D$ drops to 0
  - Contrary to intuition; would expect overfitting
  - Related to increasing the combined classifier's margin (confidence in prediction)
- Can apply to labels that are multi-valued using e.g. error-correcting output codes