CSE 417T Introduction to Machine Learning

Lecture 14

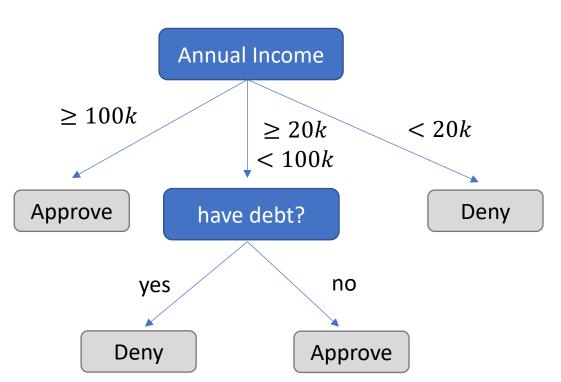
Instructor: Chien-Ju (CJ) Ho

Logistics

- Homework 3: due yesterday (Wednesday)
 - If you still have late days, the final due is tomorrow
 - Track your own late-day usages
 - Assignments over-using late days won't be graded
- Exam 1: October 27 (Thursday)
 - Topics: LFD Chapters 1 to 5
 - Timed exam (75 min) during lecture time
 - Location TBD
 - Closed-book exam with 2 letter-size cheat sheets allowed (4 pages in total)
 - No format limitations (it can be typed, written, or a combination)
- October 25 (Tuesday) will be a review session
 - Practice questions are posted on Piazza (will be discussed during the review session)

Recap

Decision Tree <u>Hypothesis</u>



Pros

- Easy to interpret (interpretability is getting attention and is important in some domains)
- Can handle multi-type data (Numerical, categorical. ...)
- Easy to implement (Bunch of if-else rules)

Cons

- Generally speaking, bad generalization
- VC dimension is infinity
- High variance (small change of data leads to very different hypothesis)
- Easily overfit
- Why we care?
 - One of the classical model
 - Building block for other models (e.g., random forest)

Credit Card Approval Example

ID3: Using Information Gain as Selection Criteria

- Information gain of choosing feature A to split
 - $Gain(D,A) = H(D) \sum_{i} \frac{|D_{i}|}{|D|} H(D_{i})$ [The amount of decrease in entropy]
- ID3: Choose the split that maximize Gain(D, A)

Notations: H(D): Entropy of D |D| is the number of points in D

DecisionTreeLearn(D)

Create a root node r

If termination conditions are met

return a single node tree with leaf prediction based on

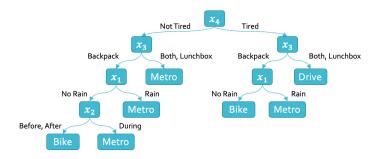
Else: Greedily find a feature A to split according to split criteria For each possible value v_i of A

Let D_i be the dataset containing data with value v_i for feature ACreate a subtree DecisionTreeLearn(D_i) that being the child of root r

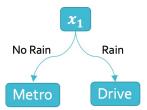
- ID3 termination conditions
 - If all labels are the same
 - If all features are the same
 - If dataset is empty
- ID3 leaf predictions
 - Most common labels (majority voting)
- ID3 split criteria
 - Information gain

Ensemble Learning

- Goal: Utilize a set of weak learners to obtain a strong learner.
- One common way to construct weak learners is via decision trees
 - Fully grown decision trees
 - High variance
 - Low bias



- Decision stump (One-depth decision trees, split on only one attribute)
 - Low variance
 - High bias



Ensemble Learning

Goal: Utilize a set of weak learners to obtain a strong learner.

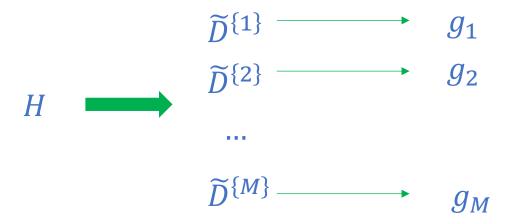
- Format of ensemble learning
 - Construct many diverse weak learners
 - Aggregate the weak learners

Bagging

- Construct diverse weak learners
 - (Simultaneously) bootstrap datasets
 - Train weak learners on them
- Aggregate the weak learners
 - Uniform aggregation

Bagging - Bootstrapped Aggregating

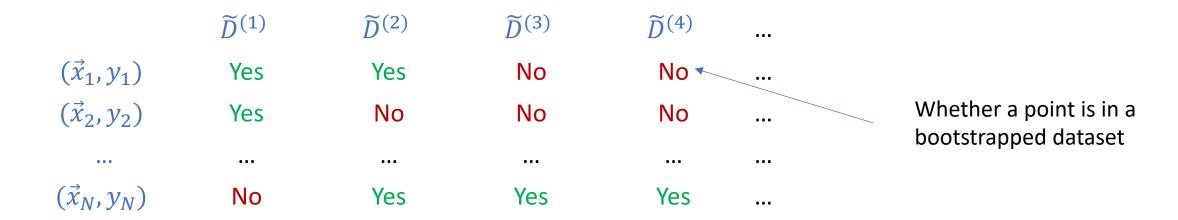
- Bootstrap M datasets $\{\widetilde{D}^{\{m\}}\}$ (Sample with replacement from D)
- Learn a hypothesis from each of them



• Aggregate the learned hypothesis (assume we are doing classification)

$$G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})\right)$$

Out-Of-Bag (OOB) Error



- G_n^- : the aggregation of hypothesis that \vec{x}_n is OOB of
 - $G_1^- = \operatorname{aggregate}(g_3, g_4, \dots)$
 - $G_2^- = aggregate(g_2, g_3, g_4, ...)$
 - $G_N^- = \operatorname{aggregate}(g_1, \dots)$

Aggregate:

Majority voting for classification Average for regression

- OOB Error
 - $E_{OOB}(G) = \frac{1}{N} \sum_{n=1}^{N} \text{error}(G_n^-(\vec{x}_n), y_n)$

Error:

Binary error for classification Squared error for regression

Out-Of-Bag (OOB) Error

$$E_{OOB}(G) = \frac{1}{N} \sum_{n=1}^{N} \operatorname{error}(G_n^-(\vec{x}_n), y_n)$$

- Bagging provided an intrinsic mechanism for us to perform validation
- Practical issues (you might face this in HW4)
 - What if some \vec{x}_n appears in all bootstrapped datasets?
 - The probability of this happening is small when the number of bags M is large
 - Let S be the set of points that is out of bag for at least one bootstrapped dataset

•
$$E_{OOB}(G) = \frac{1}{|S|} \sum_{(\vec{x}_n, y_n) \in S} \operatorname{error}(G_n^-(\vec{x}_n), y_n)$$

Random Forest

- Construct many random trees
 - Bootstrapping datasets and learn a max-depth tree for each of them
 - Other randomizations (not required in HW4)
 - When choosing split features, choose from a random subset (instead of all features)
 - Randomly project features (similar to non-linear transformation) for each tree
- Aggregate the random trees
 - Classification: Majority vote $\bar{g}(\vec{x}) = sign\left(\frac{1}{M}\sum_{m=1}^{M}g_m(\vec{x})\right)$
 - Regression: Average $\bar{g}(\vec{x}) = \frac{1}{M} \sum_{m=1}^{M} g_m(\vec{x})$

Today's Lecture

The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook. Let me know if you spot errors.

Boosting

Ensemble Learning

Goal: Utilize a set of weak learners to obtain a strong learner.

- Format of ensemble learning
 - Construct many diverse weak learners
 - Aggregate the weak learners

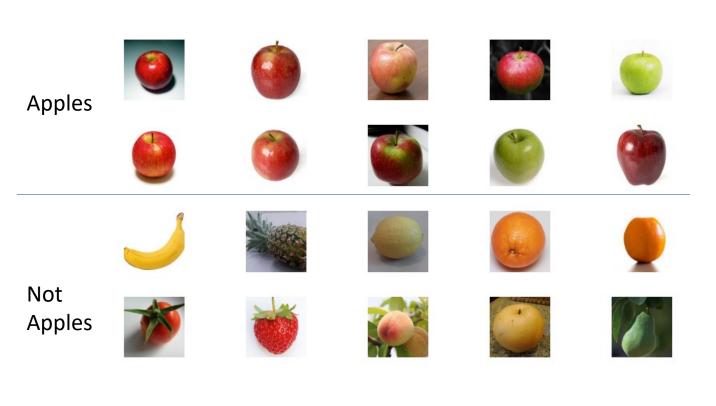
Bagging:

- Construct diverse weak learners
 - (Simultaneously) bootstrapping datasets
 - Train weak learners on them
- Aggregate the weak learners
 - Uniform aggregation

Boosting

- Construct diverse weak learners
 - Adaptively generating datasets
 - Train weak learners on them
- Aggregate the weak learners
 - Weighted aggregation

• Example: Teach a class of kids to identify apples from data



Alice: Apples are circular

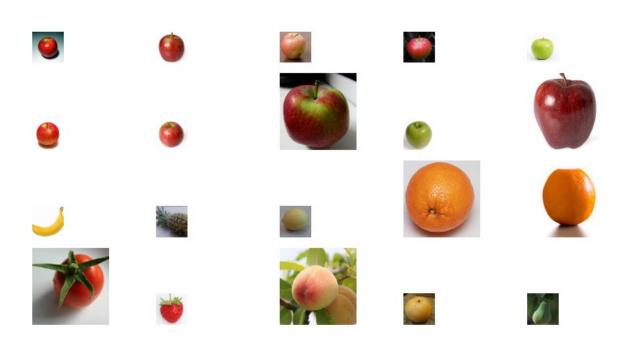
• Teacher:

Circular is a good feature, but using this feature might make some mistakes

Let me highlight the mistakes.

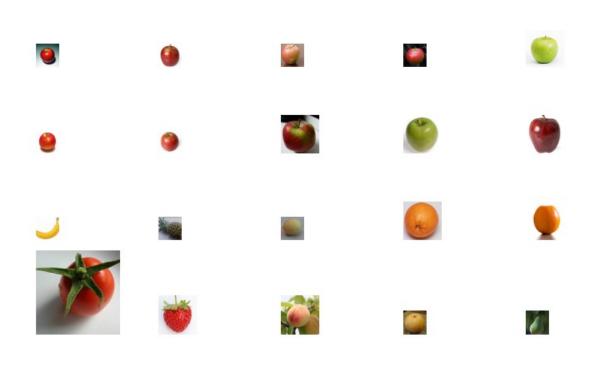
- Make correct images smaller
- Make incorrect images larger

• Example: Teach a class of kids to identify apples from data



- Alice: Apples are circular
- Bob: Apples are red

• Example: Teach a class of kids to identify apples from data



- Alice: Apples are circular
- Bob: Apples are red
- Charlie: Apples could be green

• Example: Teach a class of kids to identify apples from data



- Alice: Apples are circular
- Bob: Apples are red
- Charlie: Apples could be green
- David: Apples have stems at the top
- Class: Apples are somewhat circular, somewhat red, possibly green, and may have stems at the top

• Example: Teach a class of kids to identify apples from data

Key steps of this process:

- Learn a simple hypothesis for each dataset
- Iteratively update the dataset to focus on what we got wrong (i.e., create diversity)
- Aggregate the learned simple hypothesis

- Alice: Apples are circular
- Bob: Apples are red
- Charlie: Apples could be green
- David: Apples have stems at the top
- Class: Apples are somewhat circular, somewhat red, possibly green, and may have stems at the top

Outline of a Boosting Algorithm

- Initialize D_1 (usually the same as the initial dataset D)
- For t = 1 to T
 - Learn g_t from D_t
 - Reweight the distribution and obtain D_{t+1} based on g_t and D_t
- Output weighted-aggregate($g_1, ..., g_T$)
 - Classification: $G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{T}\sum_{t=1}^{M} \alpha_t g_t(\vec{x})\right)$

Questions

How to learn g_t from D_t How to reweight the distribution and obtain D_{t+1} How to perform weighted aggregation

Discussion on Re-weighted D_t (What does re-weighting mean?)

- Original Dataset $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}$
- Notation of D_t
 - $D_t(n)$ is the weight/probability of data point (\vec{x}_n, y_n) in D_t
 - $\sum_{n=1}^{N} D_t(n) = 1$
- What is $E_{in}(h)$ on D_t ? (Expressed as $E_{in}^{(D_t)}(h)$)
 - Re-sample dataset (noisier)
 - Re-sample the dataset from D according to distribution D_t
 - Calculate E_{in} on the re-sampled dataset as usual
 - Calculate weighted error
 - $E_{in}^{(D_t)}(h) = \sum_{n=1}^{N} D_t(n) \operatorname{error}(h(\vec{x}_n), y_n)$

When $D_t(n) = 1/N$. This reduces to standard definition of E_{in} .

AdaBoost – Adaptive Boosting

How to learn g_t from D_t How to reweight the distribution and obtain D_{t+1} How to perform weighted aggregation

[AdaBoost focuses on classification problem]

Boosting Background

- A theoretical question asked by Kearns and Valiant
 - Whether a "weak" learning algorithm which performs just slightly better than random guessing in the PAC model can be "boosted" into an arbitrarily accurate "strong" learning algorithm
- AdaBoost
 - The first adaptive boosting algorithm that
 - has nice theoretical guarantees
 - successfully deployed in real-world applications

What Does AdaBoost Do?

Outline of a Boosting Algorithm

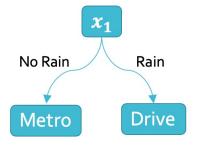
Initialize D_1 (usually the same as the initial dataset D)

```
For t=1 to T
Learn g_t from D_t
Reweight the distribution and obtain D_{t+1} based on g_t and D_t
Output weighted-aggregate(g_1, \ldots, g_T)
Classification: G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{T}\sum_{t=1}^{M} \alpha_t g_t(\vec{x})\right)
```

- Will discuss the following for AdaBoost
 - 1. How to learn g_t from D_t
 - 2. How to reweight the distribution and obtain D_{t+1}
 - 3. How to perform weighted aggregation

1. Learn a Weak Learner g_t from D_t

- AdaBoost uses simple weak learners
 - low variance, high bias
 - Decision stump (one-level decision tree) is one good option



- How to learn g_t from D_t
 - Find the decision stump that
 - Minimizes $E_{in}^{(D_t)}$ (recall the definition on this weighted in-sample error earlier)
 - Approximately: Maximize (weighted) information gain (you can call decision tree library directly)

2. How to Reweight D_{t+1} (based on g_t and D_t)

- We want to make g_{t+1} (learned from D_{t+1}) to be diverse from g_t
 - Increase the weights of points that g_t makes wrong predictions
 - Decrease the weights of points that g_t makes correct predictions
- Define a parameter $\gamma > 1$
 - If g_t makes wrong predictions on $\vec{\chi}_n$
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \cdot \gamma$ (increase the weight)
 - If g_t makes correct predictions on \vec{x}_n
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) / \gamma$ (decrease the weight)

 Z_t : normalization constant We need to ensure $\sum_{n=1}^{N} D_{t+1}(n) = 1$

- Goal:

 - Choose γ such that $E_{in}^{(D_{t+1})}(g_t)=0.5$ Since g_{t+1} minimizes $E_{in}^{(D_{t+1})}=>g_t$ and g_{t+1} are diverse

Choose
$$\gamma$$
 such that $E_{in}^{(D_{t+1})}(g_t)=0.5$

Math derivations in the next few slides

- Define $\epsilon_t = E_{in}^{(D_t)}(g_t) = \sum_{n=1}^N D_t(n) \mathbb{I}[g_t(\vec{x}_n) \neq y_n]$
 - Weighted in-sample error of g_t on D_t
 - $\epsilon_t < 0.5$ (requirement of weak learners)
- Goal: Want to make $E_{in}^{(D_{t+1})}(g_t) = 0.5$

We consider the case weak learners are better than random guessing: $\epsilon_t < 0.5$

$$E_{in}^{(D_t)}(h) = \sum_{n=1}^{N} D_t(n) \operatorname{error}(h(\vec{x}_n), y_n)$$

- If g_t makes wrong predictions on \vec{x}_n
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \cdot \gamma$ (increase the weight)
- $| \cdot |$ If g_t makes correct predictions on \vec{x}_n
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) / \gamma$ (decrease the weight)

• Define
$$\epsilon_t = E_{in}^{(D_t)}(g_t) = \sum_{n=1}^{N} D_t(n) \mathbb{I}[g_t(\vec{x}_n) \neq y_n]$$

- Weighted in-sample error of g_t on D_t
- $\epsilon_t < 0.5$ (requirement of weak learners)

We consider the case weak learners are better than random guessing: $\epsilon_t < 0.5$

• Goal: Want to make $E_{in}^{(D_{t+1})}(g_t) = 0.5$

$$E_{in}^{(D_{t+1})}(g_t) = \sum_{n=1}^{N} D_{t+1}(n) \mathbb{I}[g_t(\vec{x}_n) \neq y_n]$$

$$= \sum_{n=1}^{N} \frac{1}{Z_t} D_t(n) \gamma \mathbb{I}[g_t(\vec{x}_n) \neq y_n]$$

$$= \frac{\gamma}{Z_t} \sum_{n=1}^{N} D_t(n) \mathbb{I}[g_t(\vec{x}_n) \neq y_n] = \frac{\gamma}{Z_t} \epsilon_t$$

$$E_{in}^{(D_t)}(h) = \sum_{n=1}^{N} D_t(n) \operatorname{error}(h(\vec{x}_n), y_n)$$

- If g_t makes wrong predictions on \vec{x}_n
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \cdot \gamma$ (increase the weight)
- If g_t makes correct predictions on \vec{x}_n
 - $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) / \gamma$ (decrease the weight)

• Remember Z_t is the normalization constant

$$\begin{split} Z_t &= \sum_{n=1}^N D_t(n) \gamma \, \mathbb{I}[g_t(\vec{x}_n) \neq y_n] + \sum_{n=1}^N D_t(n) \frac{1}{\gamma} \, \mathbb{I}[g_t(\vec{x}_n) = y_n] \\ &= \gamma \epsilon_t + \frac{1}{\gamma} \left(1 - \epsilon_t \right) \end{split}$$

• Want to make $E_{in}^{(D_{t+1})}(g_t) = 0.5$

•
$$E_{in}^{(D_{t+1})}(g_t) = \frac{\gamma}{Z_t} \epsilon_t$$

•
$$Z_t = \gamma \epsilon_t + \frac{1}{\gamma} (1 - \epsilon_t)$$

• Want to make $E_{in}^{(D_{t+1})}(g_t) = 0.5$

•
$$E_{in}^{(D_{t+1})}(g_t) = \frac{\gamma}{Z_t} \epsilon_t$$

•
$$Z_t = \gamma \epsilon_t + \frac{1}{\gamma} (1 - \epsilon_t)$$

•
$$\frac{\gamma \epsilon_t}{\gamma \epsilon_t + (1 - \epsilon_t)/\gamma} = 0.5 \implies \frac{1 - \epsilon_t}{\gamma} = \gamma \epsilon_t \implies \gamma = \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}}$$

• The rule for reweighting

• If
$$g_t(\vec{x}_n) \neq y_n$$
, then $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)$

• If
$$g_t(\vec{x}_n) = y_n$$
, then $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}}\right)^{-1}$

Both $g_t(\vec{x}_n)$ and y_n are either +1 or -1 If $g_t(\vec{x}_n) \neq y_n$, $g_t(\vec{x}_n)y_n = -1$ If $g_t(\vec{x}_n) = y_n$, $g_t(\vec{x}_n)y_n = 1$ • Want to make $E_{in}^{(D_{t+1})}(g_t) = 0.5$

•
$$E_{in}^{(D_{t+1})}(g_t) = \frac{\gamma}{Z_t} \epsilon_t$$

•
$$Z_t = \gamma \epsilon_t + \frac{1}{\gamma} (1 - \epsilon_t)$$

•
$$\frac{\gamma \epsilon_t}{\gamma \epsilon_t + (1 - \epsilon_t)/\gamma} = 0.5 \implies \frac{1 - \epsilon_t}{\gamma} = \gamma \epsilon_t \implies \gamma = \sqrt{\frac{1 - \epsilon_t}{\epsilon_t}}$$

• The rule for reweighting

• If
$$g_t(\vec{x}_n) \neq y_n$$
, then $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)^{-g_t(x_n)y_n}$

• If
$$g_t(\vec{x}_n) = y_n$$
, then $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)^{-1} = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)^{-g_t(\vec{x}_n)y_n}$

• Reweight rule:
$$D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)^{-g_t(\vec{x}_n)y_n}$$

2. How to Reweight D_{t+1} : Summary

• Reweight rule:

•
$$D_{t+1}(n) = \frac{1}{Z_t} D_t(n) \left(\sqrt{\frac{1-\epsilon_t}{\epsilon_t}} \right)^{-g_t(\vec{x}_n)y_n}$$

- A bit more manipulations (the reason will be clear later)
 - Define $\alpha_t = \frac{1}{2} \ln \left(\frac{1 \epsilon_t}{\epsilon_t} \right)$
 - $e^{\alpha_t} = \sqrt{\frac{1-\epsilon_t}{\epsilon_t}}$
- Final reweight rule: $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) e^{-\alpha_t g_t(\vec{x}_n) y_n}$

3. How to Aggregate Weak Learners

• Intuition:

- We want to put more weights on better weak learners
- $\epsilon_t = E_{in}^{(D_t)}(g_t)$ is a proxy on how well g_t performs (smaller ϵ_t => better g_t)
- Recall that $\alpha_t = \frac{1}{2} \ln \left(\frac{1 \epsilon_t}{\epsilon_t} \right)$
 - Better g_t , smaller ϵ_t , higher α_t
 - When $\epsilon_t = 0.5$, $\alpha_t = 0$ (random guessing leads to 0 weights)
 - When $\epsilon_t = 0$, $\alpha_t = \infty$ (if a feature perfectly classifies the data, use it as our final hypothesis)

Aggregation rule

•
$$G(\vec{x}) = sign(\sum_{t=1}^{T} \alpha_t g_t(\vec{x}))$$

AdaBoost Algorithm

- Given $D = \{(\vec{x}_1, y_1), ..., (\vec{x}_N, y_N)\}$
- Initialize $D_1(n) = 1/N$ for all n = 1, ..., N
- For t = 1, ..., T
 - Learn g_t from D_t (using decision stumps)
 - Calculate $\epsilon_t = E_{in}^{(D_t)}(g_t)$
 - Set $\alpha_t = \frac{1}{2} \ln \left(\frac{1 \epsilon_t}{\epsilon_t} \right)$
 - Update $D_{t+1}(n) = \frac{1}{Z_t} D_t(n) e^{-\alpha_t y_n g_t(\vec{x}_n)}$
- Output $G(\vec{x}) = sign(\sum_{t=1}^{T} \alpha_t g_t(\vec{x}))$

Theoretical Properties of AdaBoost

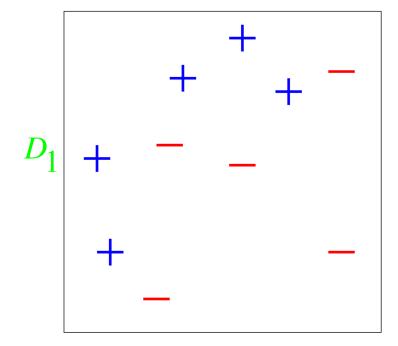
- See <u>Freund & Schapire's Tutorial</u> for more discussion
- The training error of AdaBoost converges fast
 - Let $\gamma_t = \frac{1}{2} \epsilon_t$ (how good each weak learner is better than random guessing)
 - $E_{in} \leq e^{-2\sum_{t=1}^{T} \gamma_t^2}$
- Generalization error
 - VC analysis gives us $E_{out} \leq E_{in} + \tilde{O}\left(\sqrt{\frac{Td_{vc}}{m}}\right)$
 - It seems as T goes large, overfitting could happen
 - Empirically, AdaBoost is relatively robust to overfitting
 - There are some more delicate analysis using the idea of margins to explain why

 d_{vc} is the VC dimension of the weak learner

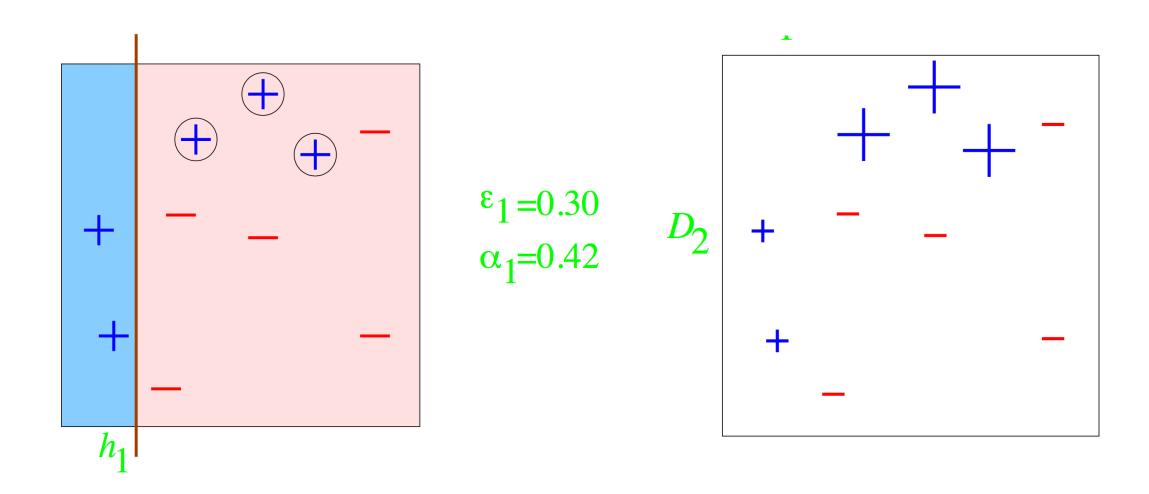
AdaBoost in Action

AdaBoost in Action

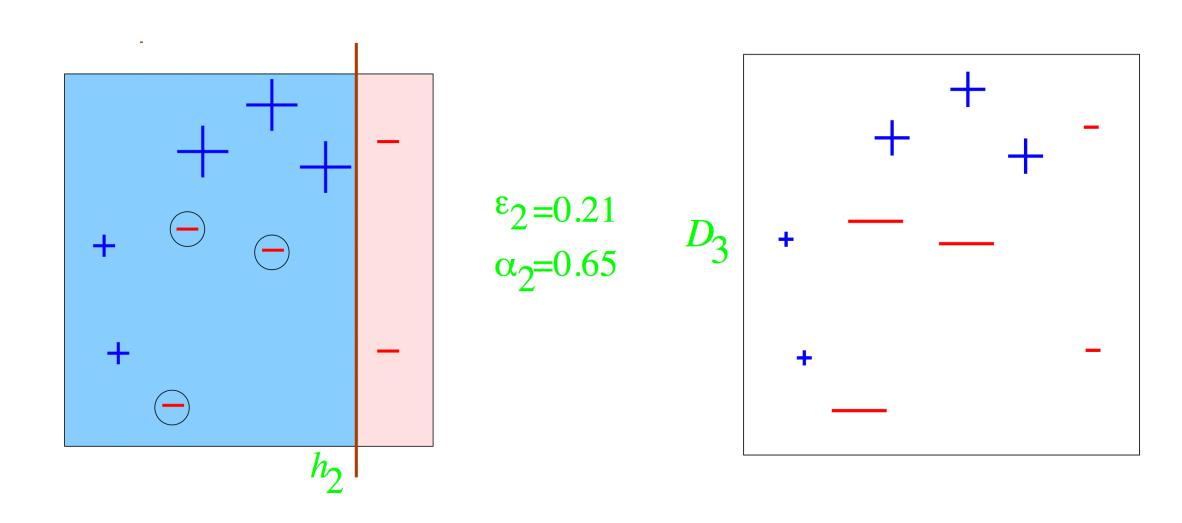
- A toy example (by Yoav Freund Rob Schapire)
- Weak learner: decision stump (one-level decision tree)



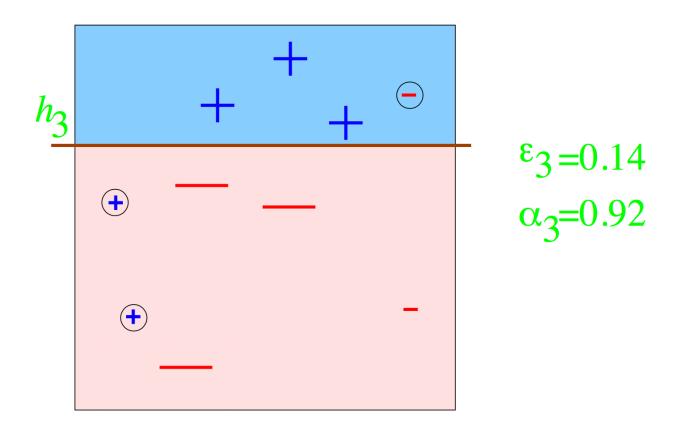
Round 1

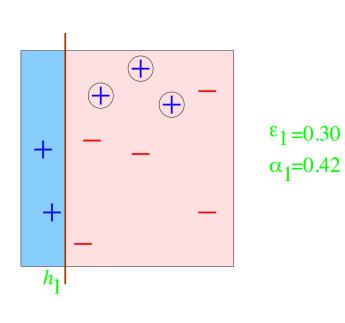


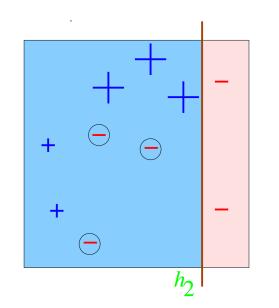
Round 2

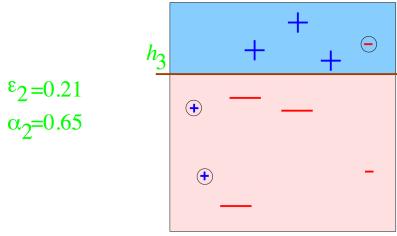


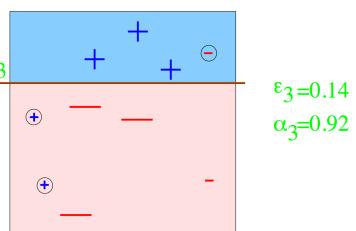
Round 3

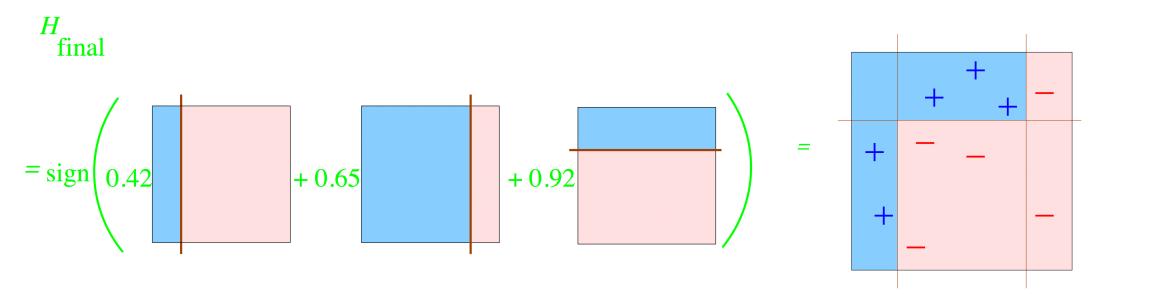








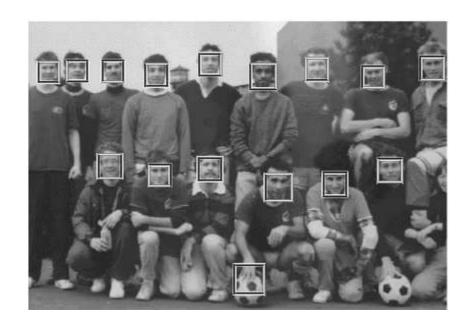




Practical Success of AdaBoost

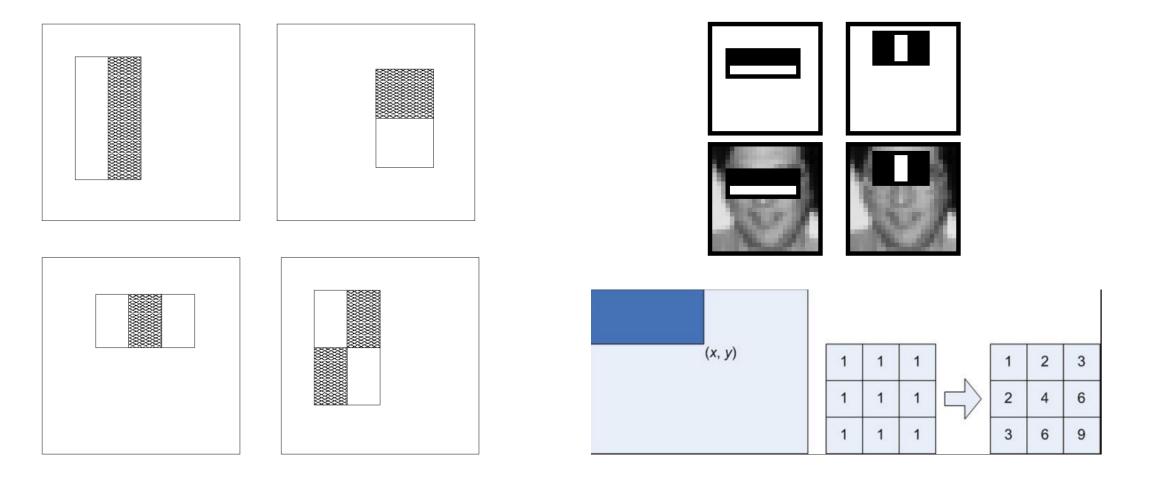
Viola-Jones Face Detection (2001)

- First real-time object detection framework
- Paul Viola and Michael Jones. Rapid object detection using a boosted cascade of simple features. CVPR 2001.

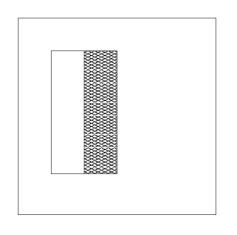


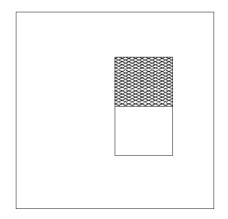


Weak Learners (Haar wavelet features)

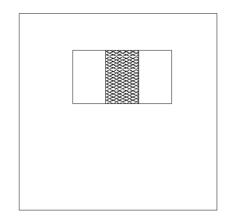


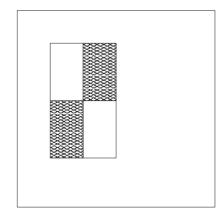
Weak Learners (Haar wavelet features)





- Each hypothesis is very weak.
- There are many possible features.
 - For a 24x24 detection region, more then 160,000 features





- AdaBoost!
 - Training is slow
 - Testing is fast
 - (inherent feature selection)

Brief Discussion on Gradient Boosting

Gradient boosting is safe to skip for Exam 2

Look at the AdaBoost Algorithm Again

```
Given D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_N, y_N)\}
Initialize D_1(n) = 1/N for all n = 1, \dots, N
For t = 1, \dots, T
Learn g_t from D_t (using decision stumps)
Calculate \epsilon_t = E_{in}^{(D_t)}(g_t)
Set \alpha_t = \frac{1}{2} \ln \left( \frac{1 - \epsilon_t}{\epsilon_t} \right)
Update D_{t+1}(n) = \frac{1}{Z_t} D_t(n) e^{-\alpha_t y_n g_t(\vec{x}_n)}
Output G(\vec{x}) = sign(\sum_{t=1}^T \alpha_t g_t(\vec{x}))
```

- The format is similar to gradient descent!
 - If we consider the space of the weak learners (i.e., $g_t(\vec{x})$) as the space of "weights"
 - This observation leads to a general class of boosting algorithms: gradient boosting
 - XGBoost is one implementation of gradient boosting that is popular in practice
 - See CASI 17.4 and the reference in CASI P.350 for more discussion

[Safe to Skip]

Gradient Boosting

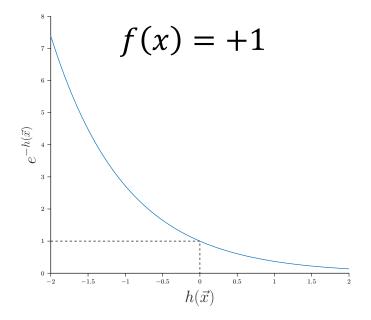
```
Initialize G(\vec{x}) = 0

For t = 1, ..., T

G(\vec{x}) \leftarrow G(\vec{x}) + \alpha_t g_T(\vec{x})

Output sign(G(\vec{x}))
```

- AdaBoost is a special case of Gradient Boosting
 - minimizing the exponential loss ($e_{exp}(h(\vec{x}), y) = e^{-yh(\vec{x})}$)
 - using decision stump as the weak learners



- e_{exp} is a surrogate loss function of the binary classification error we care about
 - Minimizing an alternative error (loss function) is a common trick in ML, especially when the target loss function is hard to optimize.
 - There are some theoretical discussions on when doing this makes sense ("calibration": whether minimizing the surrogate is consistent with minimizing the original loss).

[Safe to Skip]