CSE 417T
Introduction to Machine Learning

Lecture 16
Instructor: Chien-Ju (CJ) Ho

Logistics

- Homework 4 is due April 19 (Monday)
  - Please start it early
  - The deadline is intentionally delayed to accommodate wellness day
  - Keep track of your own late days
    - Gradescope doesn't allow separate deadlines
    - Your submissions won't be graded if you exceed the late-day limit
- Homework 5 will overlap with Homework 4
  - Plan to announce it in the week of Apr 13

Logistics: E-Chapters of LFD

- The textbook offers a set of e-chapters
  - Chap 6: Similarity-Based Methods
  - Chap 7: Neural Networks
  - Chap 8: Support Vector Machines
  - Chap 9: Learning Aides

- How to access e-chapters
  - http://book.caltech.edu/bookforum/forumdisplay.php?f=148

    - User Name: **bookreaders**
    - Password: *Enter the first word on page 27 of the book.*

Exam 1 Questions Discussion

I plan to finish grading this week and return the exam.

Recap

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

Bagging and Random Forest

- Construct many random trees
  - Bootstrapping datasets (sample with replacement from D)
  - 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 $\bar{g}(\vec{x}) = \frac{1}{M}\sum_{m=1}^{M} g_m(\vec{x})$

Outline of a Boosting Algorithm

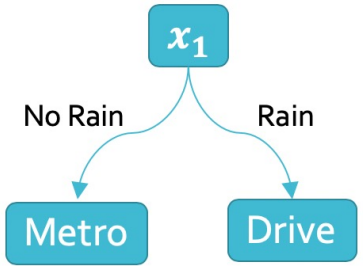
- Initialize D_1 (usually the same as the initial dataset D)
- For $t = 1$ to T
  - Learn g_t from D_t
  - Reweight the distribution and obtain D_{t+1} based on g_t and D_t
- Output weighted-aggregate$(g_1, \dots, g_T)$
  - Classification: $G(\vec{x}) = \bar{g}(\vec{x}) = sign\left(\frac{1}{T}\sum_{t=1}^{T}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

Questions

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

AdaBoost Algorithm

How to learn g_t from D_t
- Decision stump



How to reweight D_{t+1}
- Make $E_{in}^{(D_{t+1})}(g_t) = 0.5$
- So g_t and g_{t+1} are "diverse"

How to weighted aggregation
- More weights on better g_t
- Lower ϵ_t: proxy for better g_t

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

Theoretical Properties of AdaBoost

- See Freund & Schapire's Tutorial 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

Lecture Notes Today

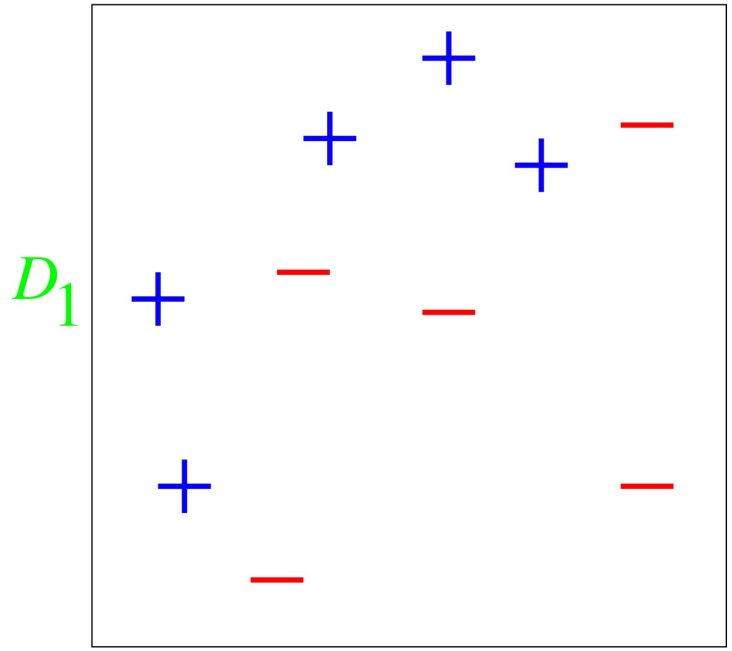
The notes are not intended to be comprehensive. They should be accompanied by lectures and/or textbook.

Let me know if you spot errors.

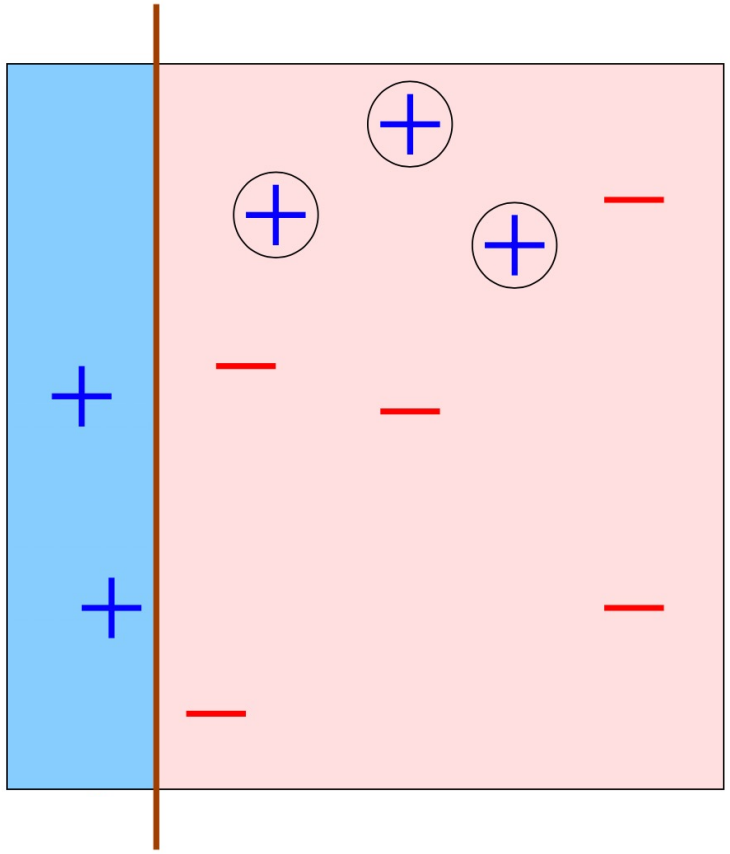
AdaBoost in Action

AdaBoost in Action

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



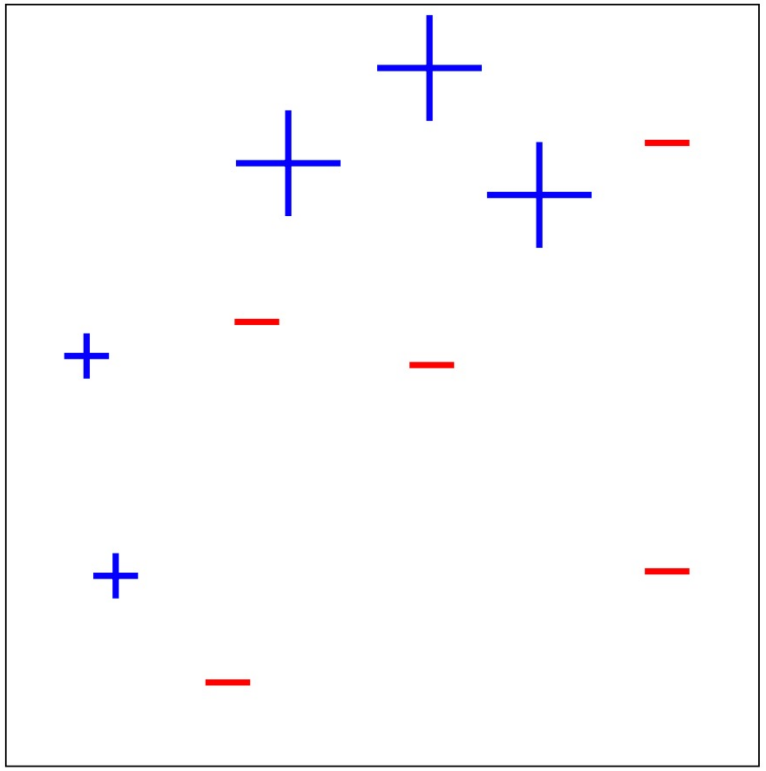
Round 1



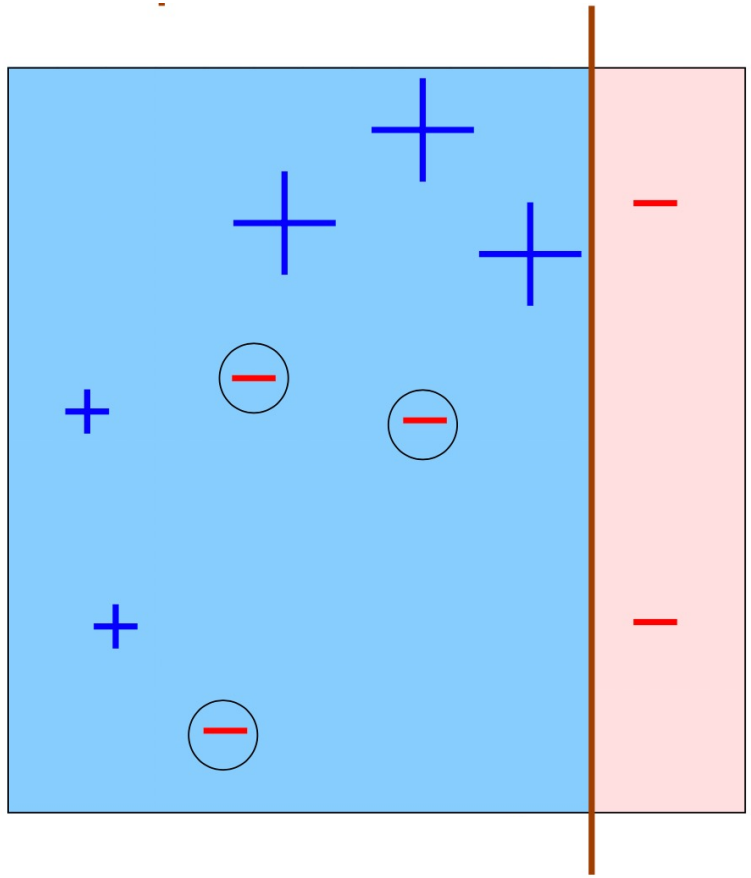
$\varepsilon_1 = 0.30$

$\alpha_1 = 0.42$

D_2



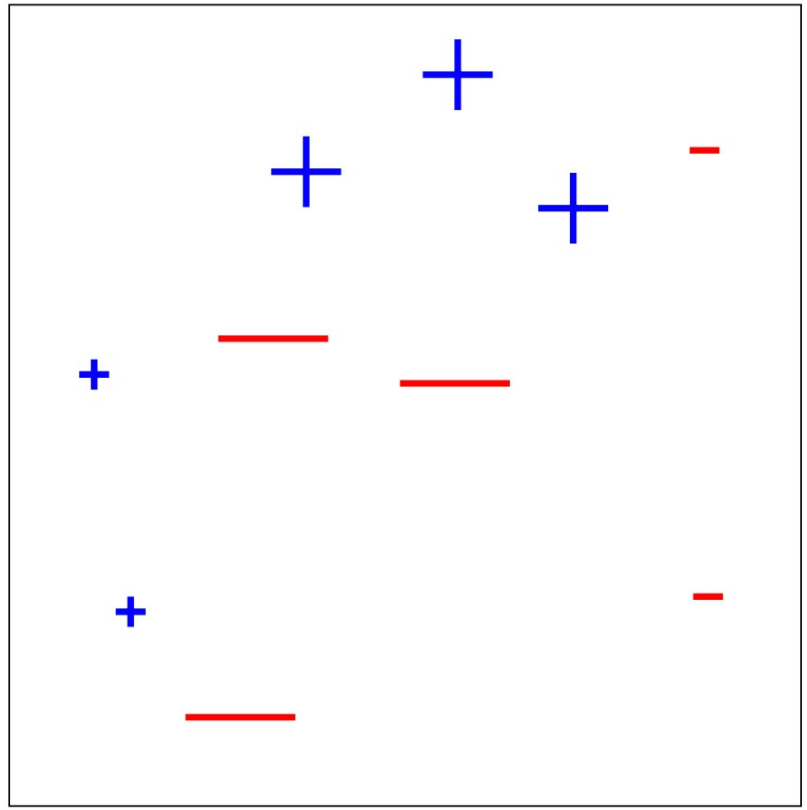
Round 2



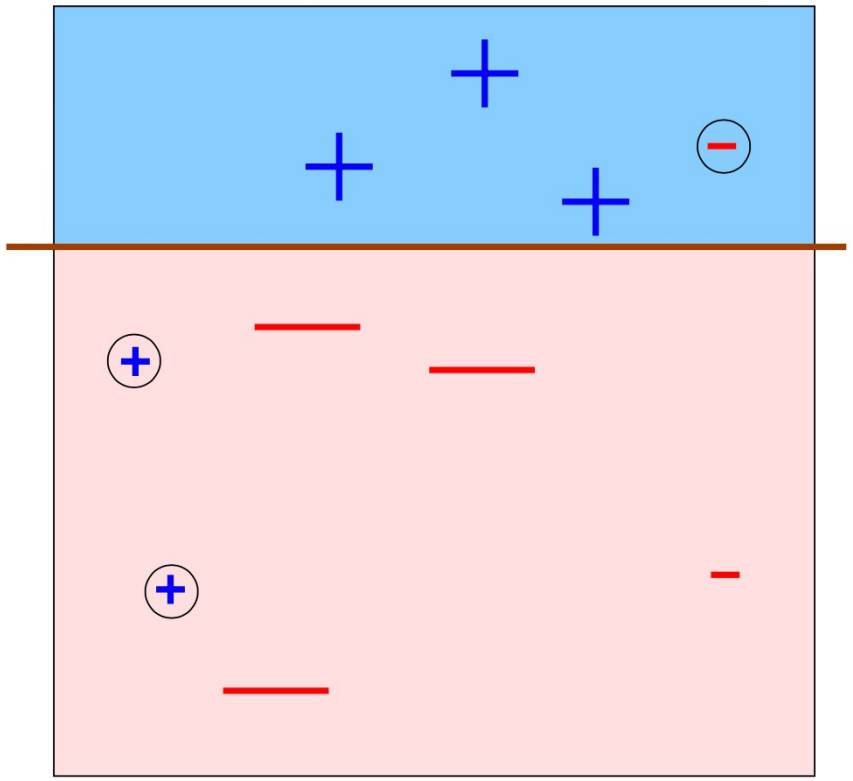
$\varepsilon_2 = 0.21$

$\alpha_2 = 0.65$

D_3

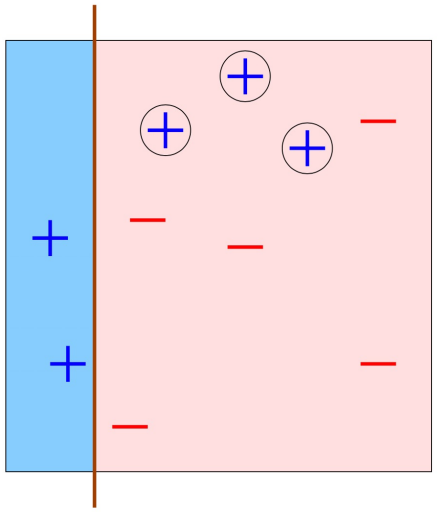


Round 3



$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$



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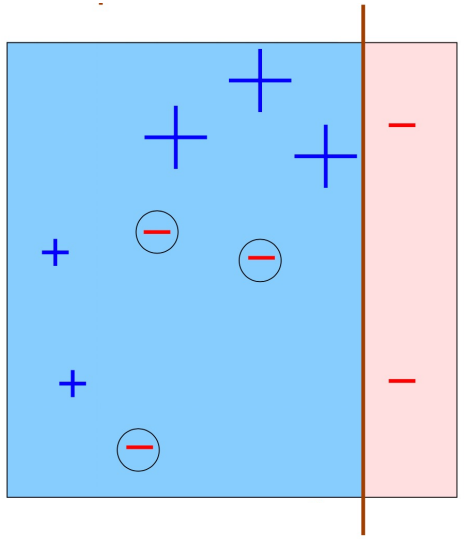
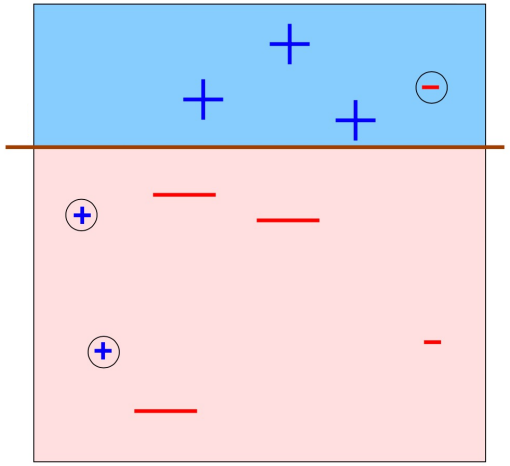
$\alpha_1 = 0.42$



$\varepsilon_2 = 0.21$

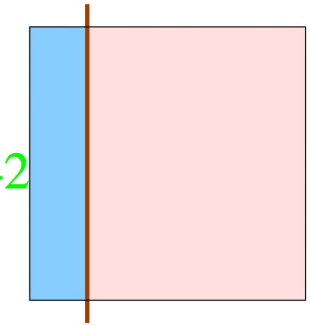
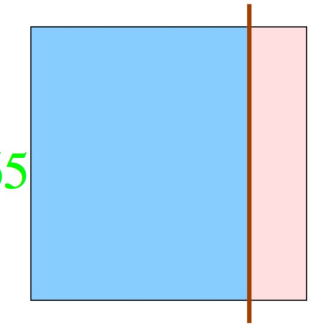
$\alpha_2 = 0.65$

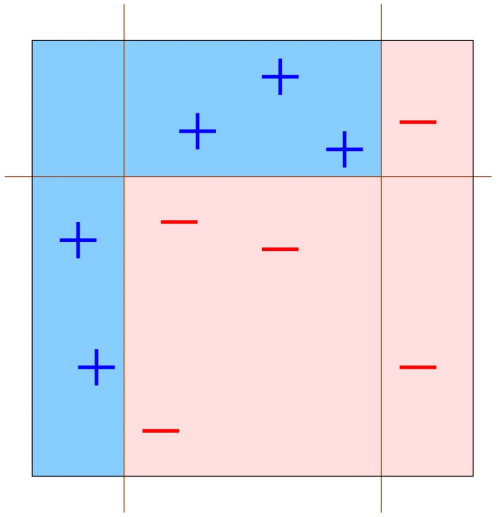


$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

H_{final}

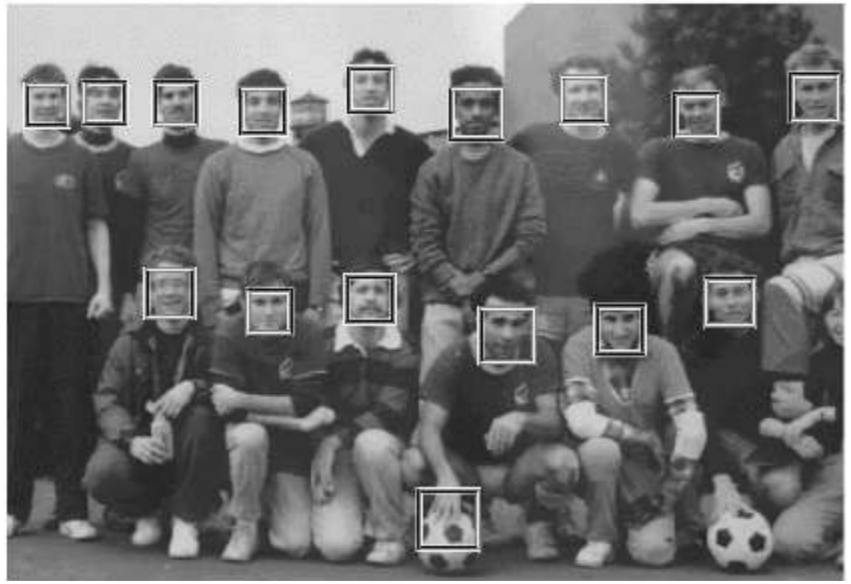
$= \text{sign}\Big(0.42$  $+ 0.65$  $+ 0.92$  $\Big)$

$=$ 

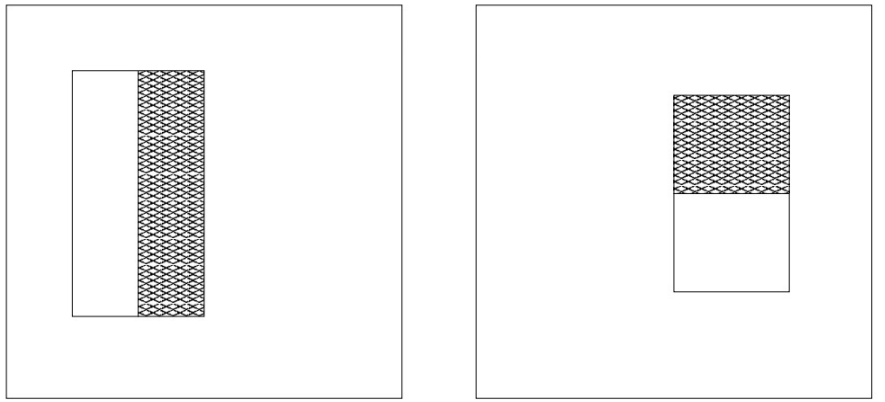
Practical Success of AdaBoost

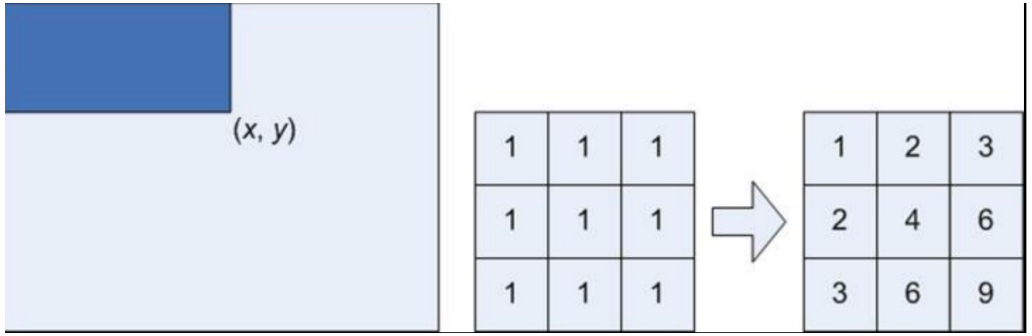
Viola-Jones Face Detection (2001)

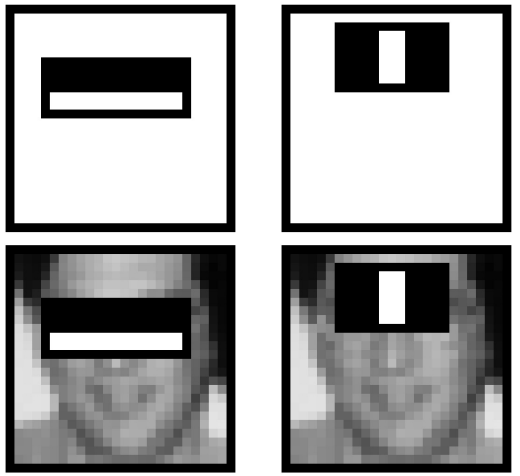
- First real-time object detection framework
- Paul Viola and Michael Jones. Rapid object detection using a boosted cascade of simple features. CVPR 2001.



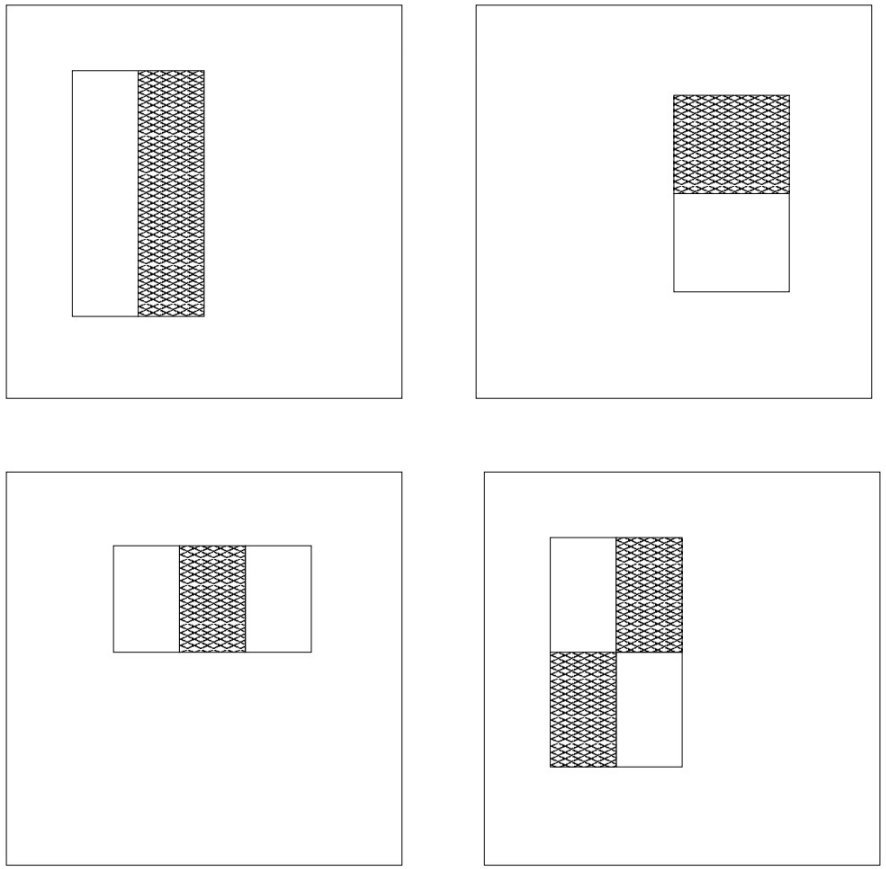
Weak Learners (Haar wavelet features)







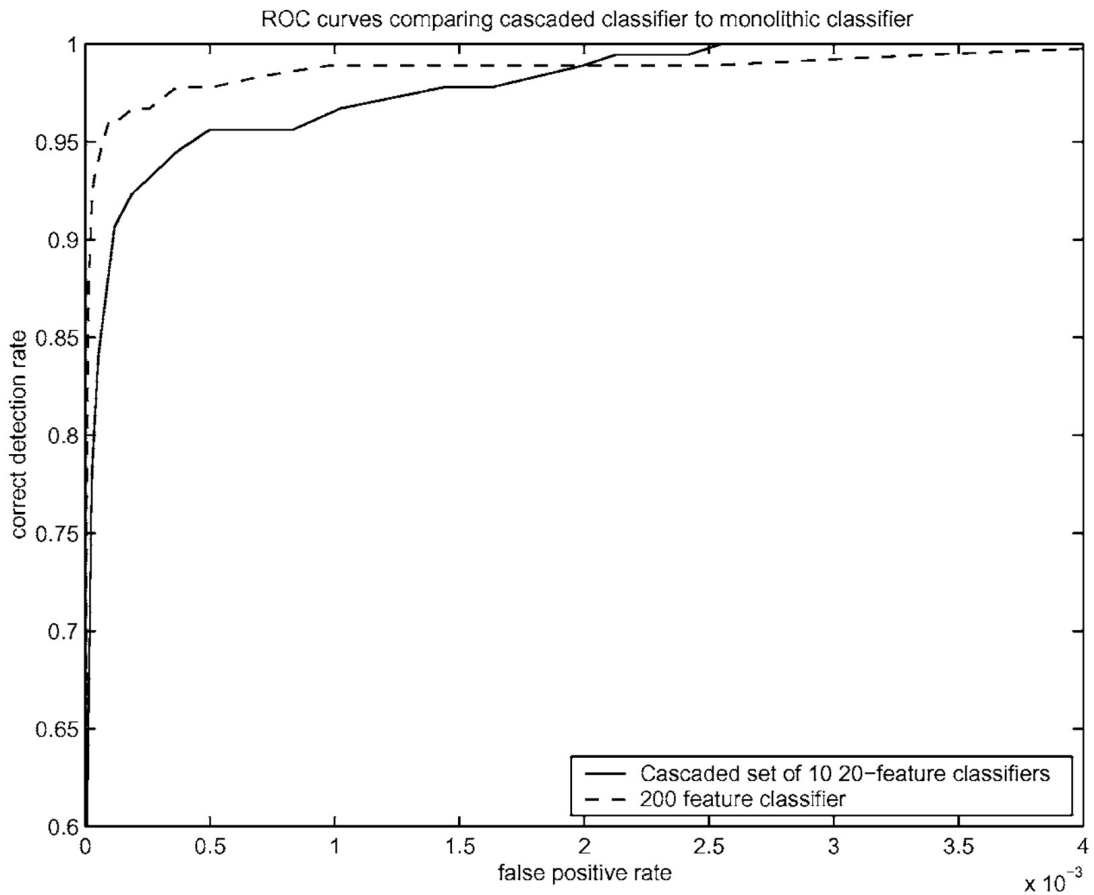
Weak Learners (Haar wavelet features)



- 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)

For 200 features



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

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

For $t = 1, \dots, T$

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

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

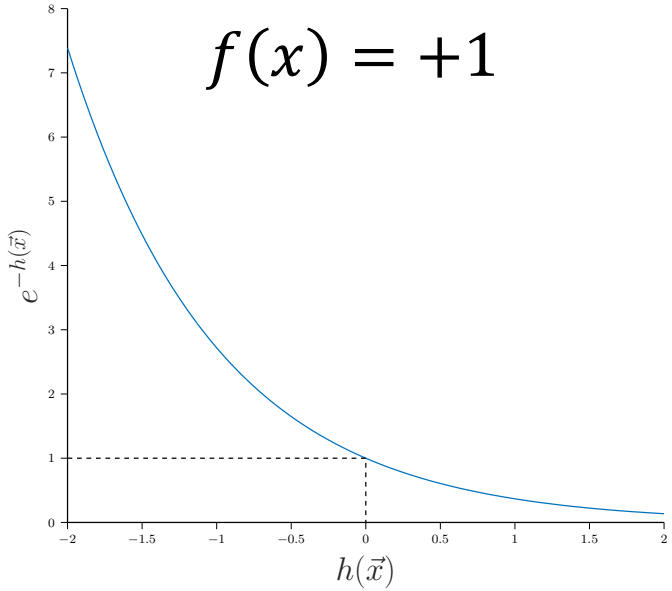
- The format is similar to gradient descent!
  - If we consider the space of the weak learners (i.e., $g_t(\vec{x})$) as the space of "weights"
  - This observation leads to a general class of boosting algorithms: gradient boosting
  - XGBoost is one implementation of gradient boosting that is popular 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 $t = 1, \dots, T$
$G(\vec{x}) \leftarrow G(\vec{x}) + \alpha_t g_T(\vec{x})$
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]

Similarity-Based Method: Nearest Neighbor

Movie Rating Prediction

- Below is the historical move ratings from users (5 is the highest)

	Movie 1	Movie 2	Movie 3	Movie 4	Movie 5	Movie 6
Alice	5	4	3	1	5	2
Bob	4	5	3	2	5	
Charlie	1	2	4	4	2	3
David	2	3	2	4	4	4
…						

- What do you think Bob's rating will be for Movie 6?
  - Maybe 2, since Bob's taste seems to be similar with Alice's

Movie Recommendation

- Below is the historical move ratings from users (5 is the highest)

	Movie 1	Movie 2	Movie 3	Movie 4	Movie 5	Movie 6
Alice	5	4		1		
Bob	4			2	5	
Charlie	1		4		2	
David		3	2			4
…						

- Which movie will you recommend to Alice, why?
  - Maybe Movie 5, since Bob's taste seems to be similar with Alice's

Nearest Neighbor

- Predict $\vec{x}$ according to its nearest neighbor
  - Given $D = \{(\vec{x}_1, y_1), (\vec{x}_2, y_2), \dots, (\vec{x}_N, y_N)\}$
  - Let $\vec{x}_{[1]}$ be $\vec{x}$'s nearest neighbor in D, i.e., the closest point to $\vec{x}$ in D
  - Similarly, let $\vec{x}_{[i]}$ be the ith closest point to $\vec{x}$ in D
    - With some distance measure $d(\vec{x}, \vec{x}')$
      - $d(\vec{x}, \vec{x}_{[1]}) \leq d(\vec{x}, \vec{x}_{[2]}) \leq \dots \leq d(\vec{x}, \vec{x}_{[N]})$
  - Let $y_{[i]}(\vec{x})$ or $y_{[i]}$ be the label of $\vec{x}_{[i]}$

- Nearest neighbor hypothesis

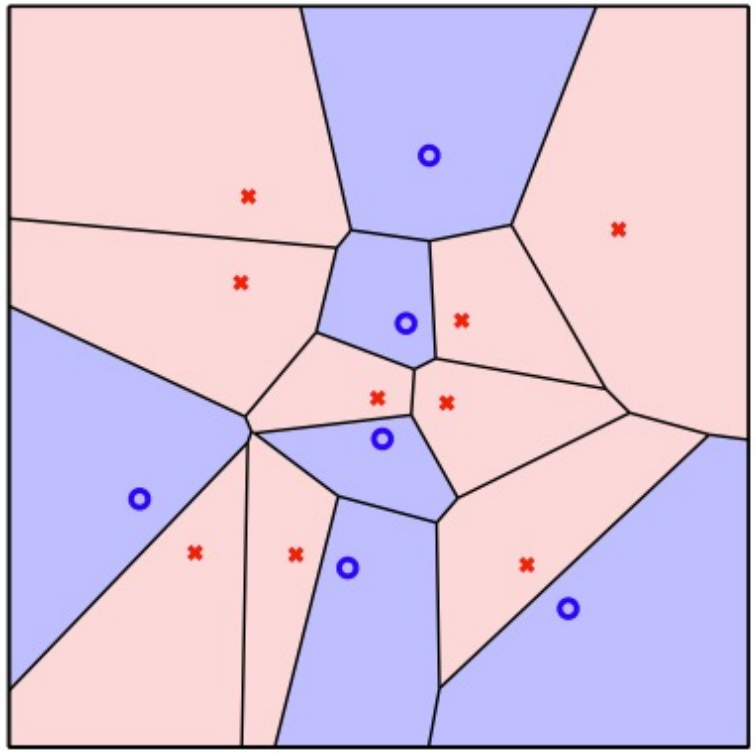
$$g(\vec{x}) = y_{[1]}(\vec{x})$$

Common distance measures:

- Euclidean distance: $d(\vec{x}, \vec{x}') = \|\vec{x} - \vec{x}'\|$
- Cosine similarity: $d(\vec{x}, \vec{x}') = \frac{\vec{x} \cdot \vec{x}'}{\|\vec{x}\| \|\vec{x}'\|}$
- And others…

Nearest Neighbor

Decision boundary of $g(\vec{x})$



- Properties of Nearest Neighbor (NN)
  - No training is needed
  - Good interpretability
  - In-sample error $E_{in} = 0$
  - VC dimension is ∞
- This seems to imply bad learning models from what we talked about so far? Why we care?
- What we really care about is E_{out}
  - VC analysis: $E_{out} \leq E_{in}$ + Generalization error
    - We can infer E_{out} through E_{in} and model complexity
  - NN has nice guarantees outside of VC analysis

Nearest Neighbor is 2-Optimal

- Given mild conditions, for nearest neighbor, when $N \to \infty$, with high probability,

$$E_{out} \leq 2E_{out}^{*}$$

- That is, we can not infer E_{out} from E_{in}, but we know that it cannot be much worse than the best anyone can do.

Proof Sketch of 2-Optimality $(E_{out} \leq 2E^*_{out})$

- Setup
  - The target function is noisy: $\pi(\vec{x}) = \Pr[y = +1|\vec{x}]$
  - The noisy target π is continuous in $\vec{x}$
    - Similar $\vec{x}$ should have similar label distributions
    - The underlying assumption for nearest neighbor to work

- Let $g^*(\vec{x})$ be the optimal hypothesis
  - $g^*(\vec{x}) = \begin{cases} +1 & \text{if } \pi(\vec{x}) \geq \frac{1}{2} \\ -1 & \text{otherwise} \end{cases}$
  - Pointwise-error $e(g^*(\vec{x}), y) = \min\{\pi(\vec{x}), 1 - \pi(x)\}$

- $E^*_{out} = \mathbb{E}_{\vec{x}}[e(g^*(\vec{x}), y)] = \mathbb{E}_{\vec{x}}[\min\{\pi(\vec{x}), 1 - \pi(x)\}]$

Proof Sketch of 2-Optimality

- $E^*_{out} = \mathbb{E}_{\vec{x}}[e(g^*(\vec{x}), y)] = \mathbb{E}_{\vec{x}}[\min\{\pi(\vec{x}), 1 - \pi(x)\}]$

- Proof sketch:
  - For a new point $(\vec{x}, y)$, let $(\vec{x}_{[1]}, y_{[1]})$ be its nearest neighbor in D
  - Consider the case when $N \to \infty$
    - A new point is "very close" to its nearest neighbor in D
    - $\pi(\vec{x}) \approx \pi(\vec{x}_{[1]})$
  - Error of nearest neighbor hypothesis on a new point is

$$\begin{aligned}\Pr[y \neq y_{[1]}] &= \Pr[y = +1, y_{[1]} = -1] + \Pr[y = -1, y_{[1]} = +1] \\ &= \pi(\vec{x})\left(1 - \pi(\vec{x}_{[1]})\right) + \left(1 - \pi(\vec{x})\right)\pi(\vec{x}_{[1]}) \\ &\approx 2\,\pi(\vec{x})\left(1 - \pi(\vec{x})\right) \\ &\leq 2\min\{\pi(\vec{x}), 1 - \pi(\vec{x})\}\end{aligned}$$

Informal intuitions to summarize the proof:

Assumption for nearest neighbor:

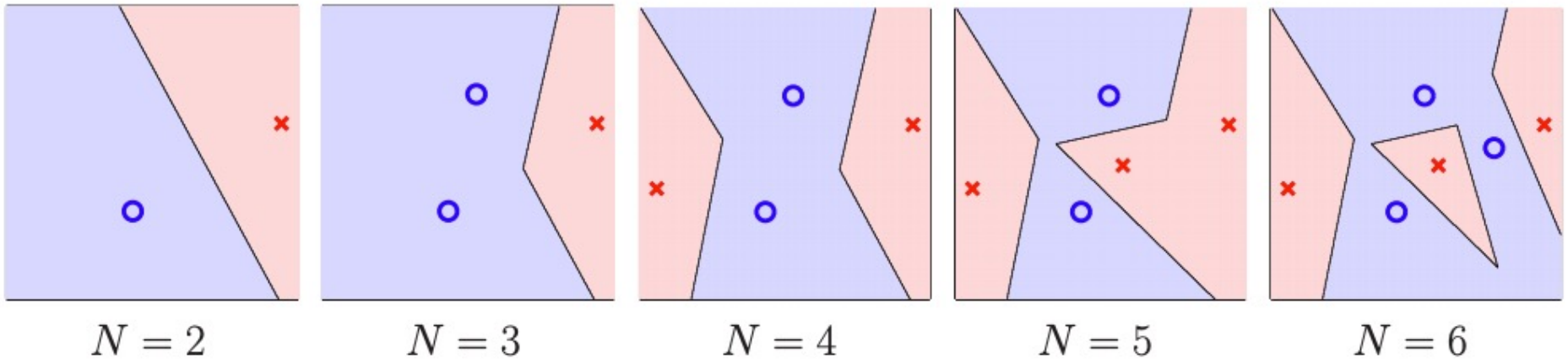
- Target function is continuous
- That is, nearby points have similar label distributions

As N goes large, there are "close enough" points for prediction

Nearest Neighbor is Self-Regularizing

- Intuition of regularization:
  - Use simpler hypothesis if we don't have enough data

- Nearest neighbor hypothesis



The complexity of hypothesis grows with the number of data points

k-Nearest Neighbor

”Stabilize” the Hypothesis

- Instead of ”single” nearest neighbor
  - Making predictions according to k nearest neighbors

- k-nearest neighbor (K-NN)
  - $g(\vec{x}) = sign\left(\sum_{i=1}^{k} y_{[i]}(\vec{x})\right)$
  - (k is often odd for binary classification)