Fundamentals of AI/ML

Ensemble Learning

Ashley Gao

William & Mary

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Ensemble Learning

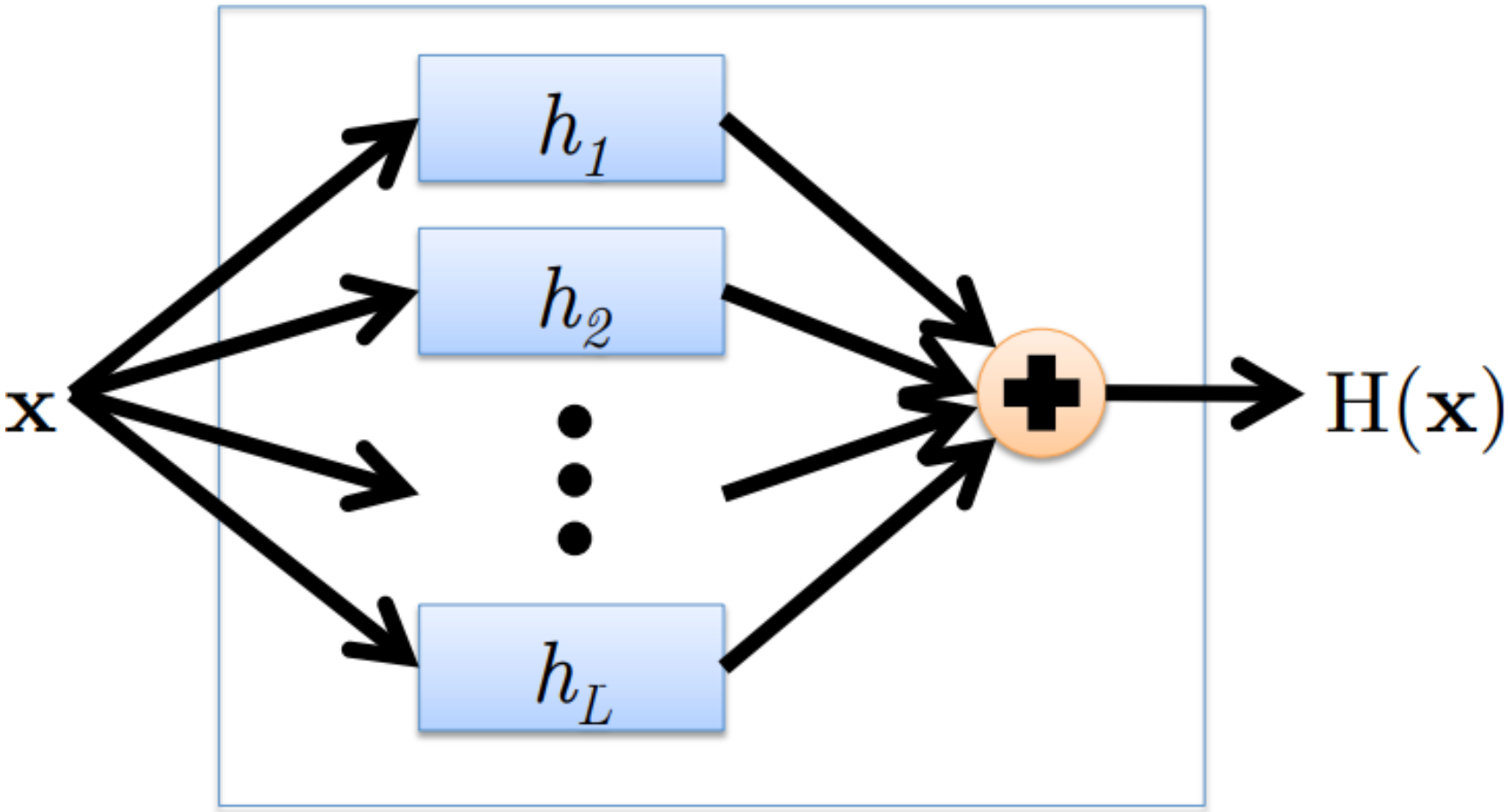
- Consider a set of classifiers $h_1, ..., h_L$
- Idea: construct a classifier $H(\boldsymbol{x})$ that combines the individual decisions of $h_1, ..., h_L$
  - e.g. could have the member classifiers vote
  - e.g. could use different members for different regions of the instance space
  - works well if the members each have low error rates
- Successful ensembles require diversity
  - Classifiers should make different mistakes
  - Can have different types of base learners

Practical Application: Netflix Prize

- Goal: predict how a user will rate a movie
  - Based on the user's ratings for other movies
  - and other people's ratings
  - with no other information about the movies
- This application is called "collaborative filtering"
- Netflix Prize: $1M to the first team to do 10% better than the Netflix' system (2007-2009)
- Winner: Bellkor's Pragmatic Chaos
  - An ensemble of more than 800 rating systems

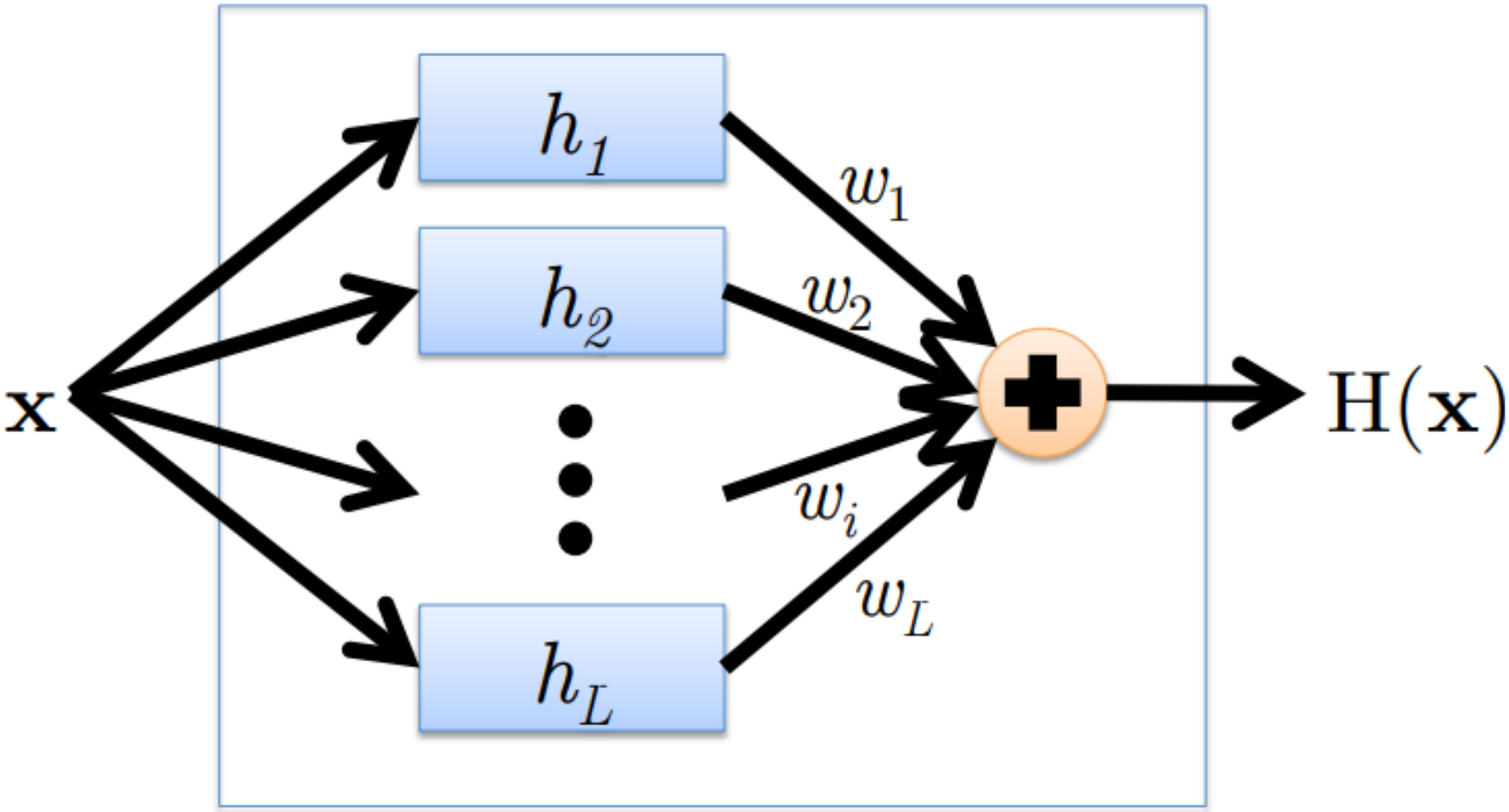
Combining Classifiers: Averaging

- Final hypothesis is a simple vote of the members



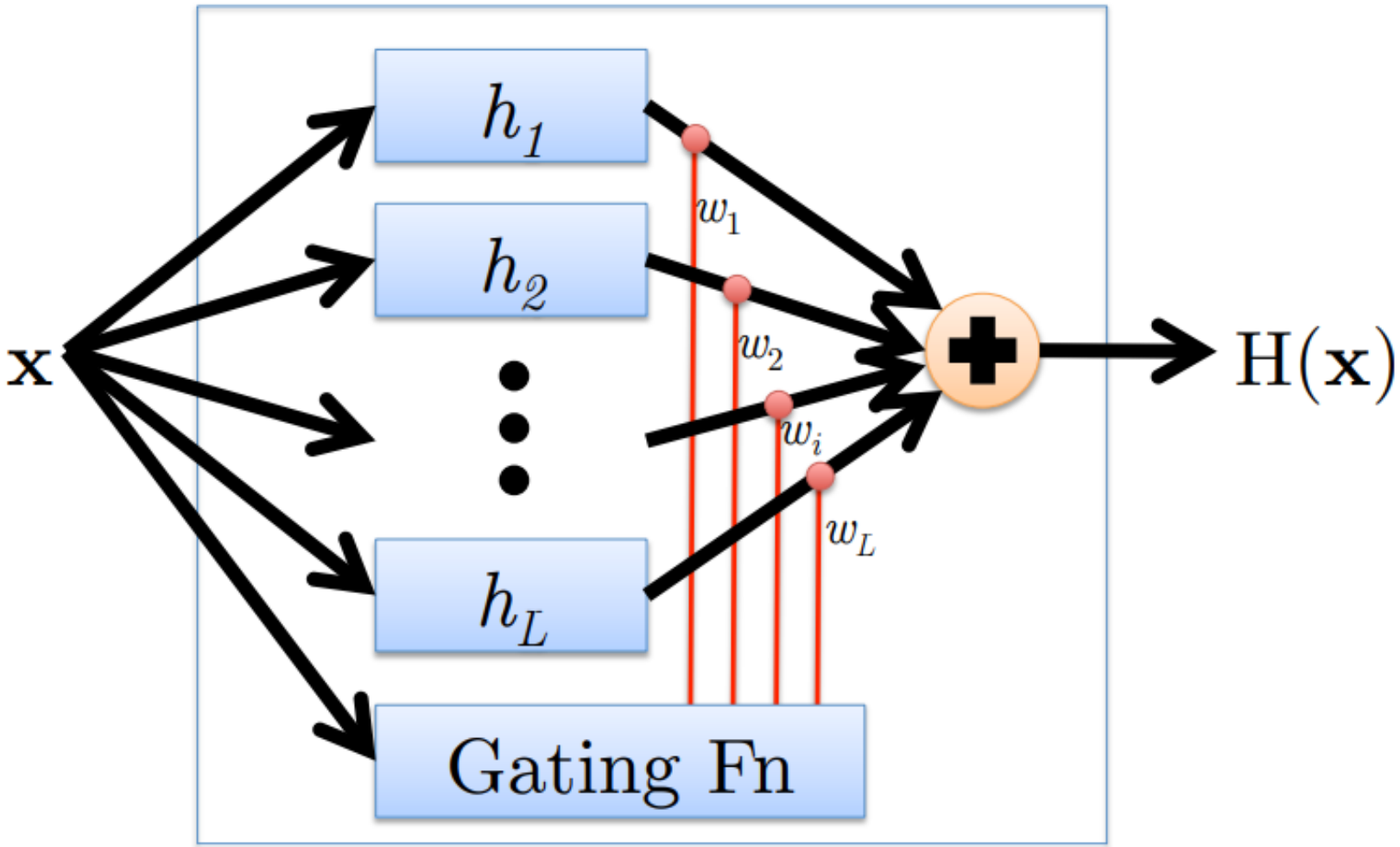
Combining Classifiers: Weighted Averaging

- Coefficients of individual members are tuned using a validation set



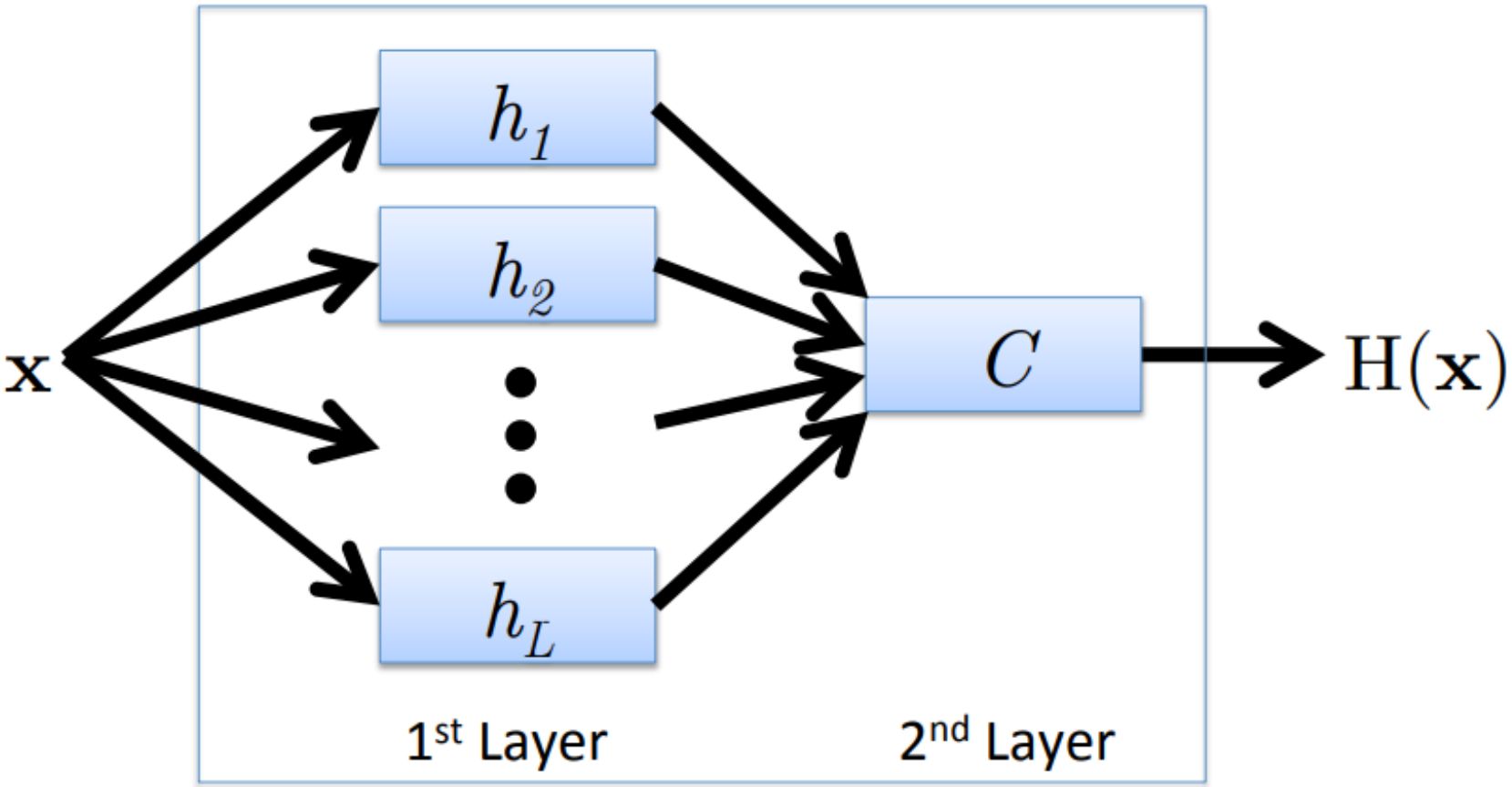
Combining Classifiers: Gating

- Coefficients of individual members depend on the input
- Train gating function via the validation set



Combining Classifiers: Stacking

- Predictions of the first layer used as input to the second laer
- Train the second layer on the validation set



How to Achieve Diversity

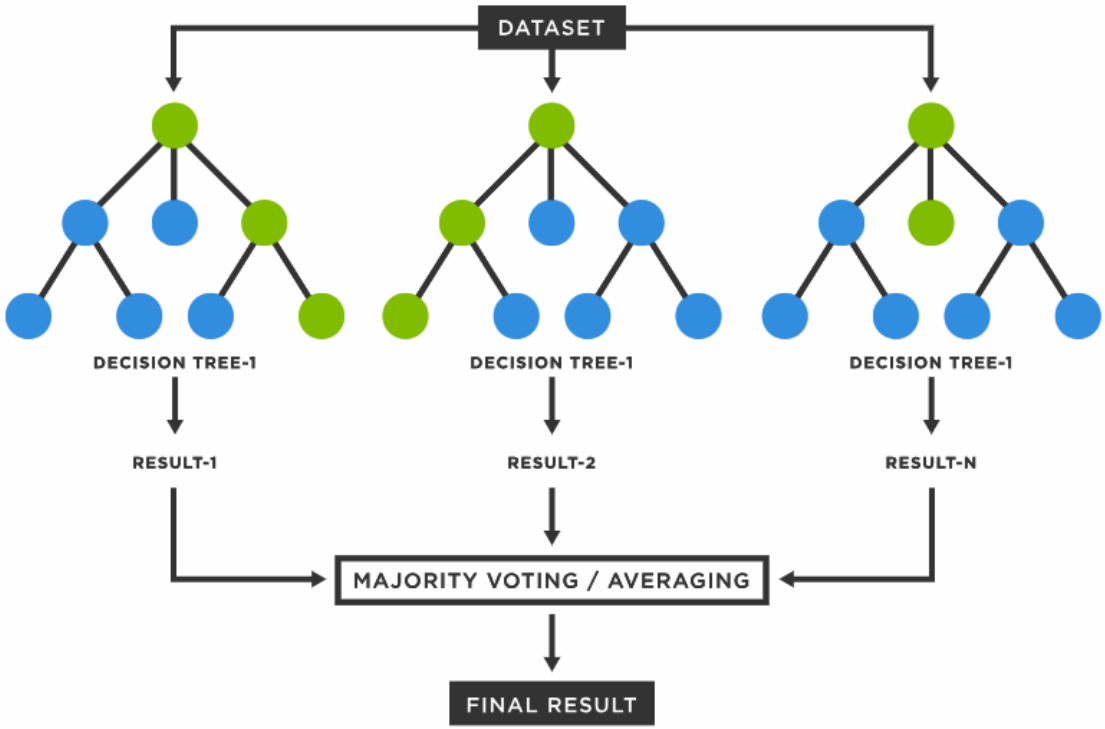
Cause of the Mistake	Diversification Strategy
Pattern was difficult	Hopeless
Overfitting	Vary the training sets
Some features are noisy	Vary the set of input features

Manipulating the Training Data

- Bootstrap replication
  - Given n training examples, construct a new training set by sampling n instances with replacement
  - Exclude about 30% of the training instances
- Bagging
  - Create bootstrap replicates of the training set
  - Train a classifier (e.g. a decision tree) for each replicate
  - Estimate classifier performance using out-of-bootstrap data
  - Average output of all classifiers
- Boosting
  - (in just a minute ...)

Manipulating the Features

- Random Forest
  - Construct decision trees on bootstrap replicas
    - Restrict the node decisions to a small subset of features picked randomly for each node
  - Do not prune the rees
    - Estimate tree performance on out-of-bootstrap data
  - Average the output of all trees



Boosting

AdaBoost

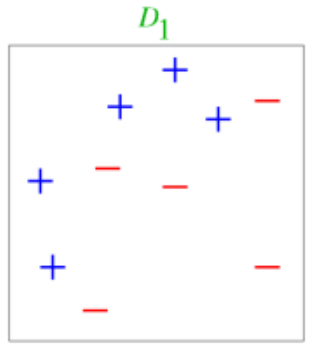
- Developed by Freund & Schapire in 1997
- A meta-learning algorithm with great theoretical and empirical performance
- Turns a base learner (e.g. “weak hypothesis”) into a high performance classifier
- Create an ensemble of weak hypotheses by repeatedly emphasizing mispredicted instances

Weak Learners and Classifiers

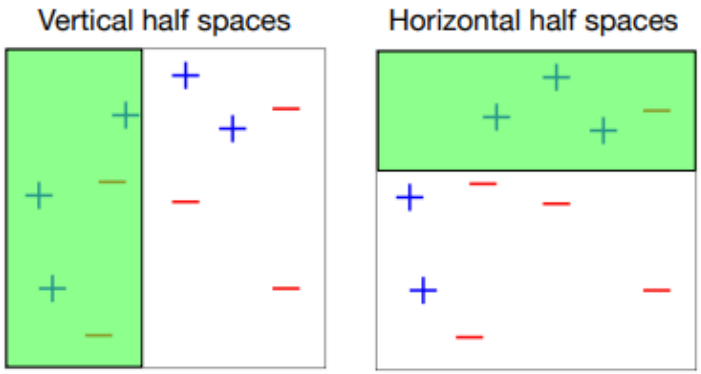
- (Informal) A weak learner is a learning algorithm that outputs a hypothesis (e.g. a classifier) that performs slightly better than chance.
  - e.g. it predicts the correct label with probability 0.51 in binary label case
- We are interested in weak learners that are computationally efficient
  - Decision tree
  - Even simpler - decision stumps: Decision trees with a single split

Weak Classifiers

- Suppose these are the data

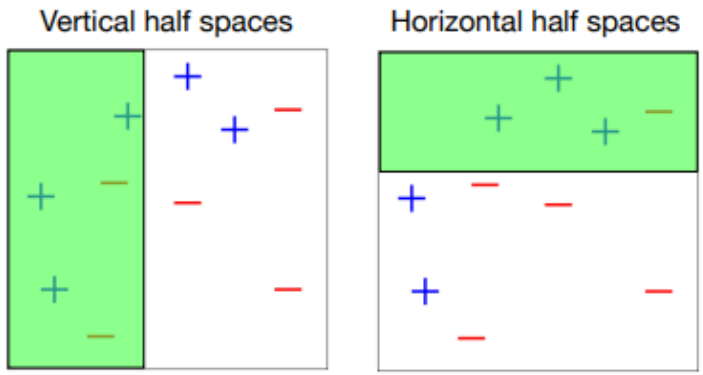


- These weak classifiers, which are decision stumps, consist of the set of horizontal and vertical half-spaces.



Weak Classifiers

- A single weak classifier is not capable of making the training error small
- But if we can guarantee that it performs slightly better than chance
- Using it with AdaBoost gives us a universal function approximator



- Now let's see how AdaBoost combines a set of weak classifiers in order to make a better ensemble of classifiers...

AdaBoost

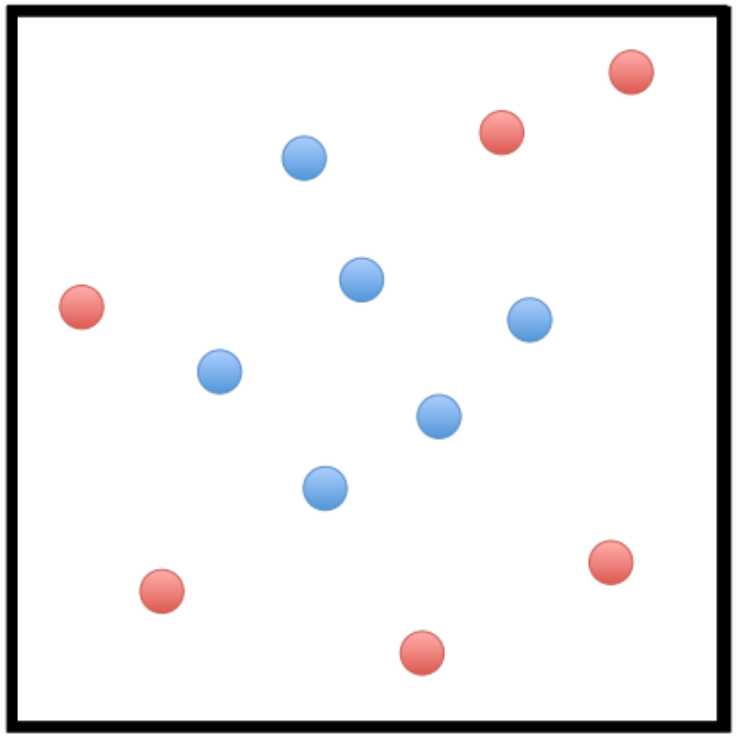
- The size of a point or instance represents the instance's weight

1: Initialize a vector of n uniform weights $\mathbf{w}_1$
2: **for** $t = 1, \ldots, T$
3: Train model h_t on X, y with weights $\mathbf{w}_t$
4: Compute the weighted training error of h_t
5: Choose $\beta_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right)$
6: Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right)$$

7: Normalize $\mathbf{w}_{t+1}$ to be a distribution
8: **end for**
9: **Return** the hypothesis

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



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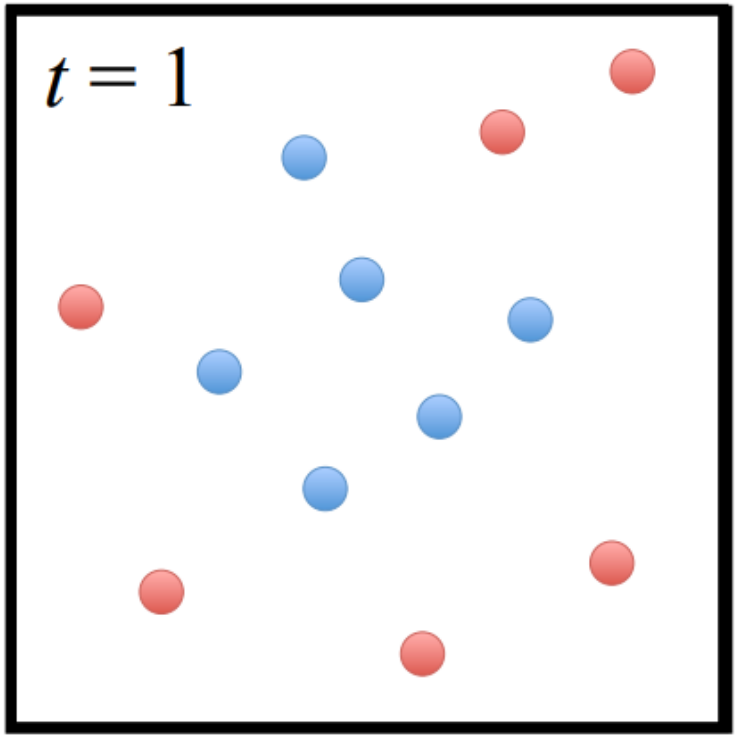

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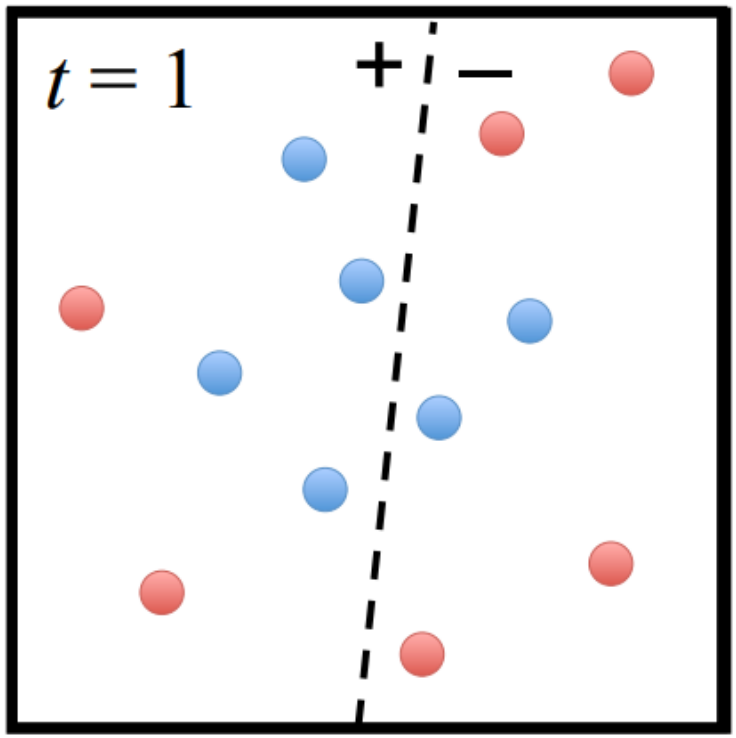

AdaBoost

- β_t measures the importance of h_t
- if $\epsilon_t \leq 0.5$ then $\beta_t \geq 0$ (can trivially gurantee)

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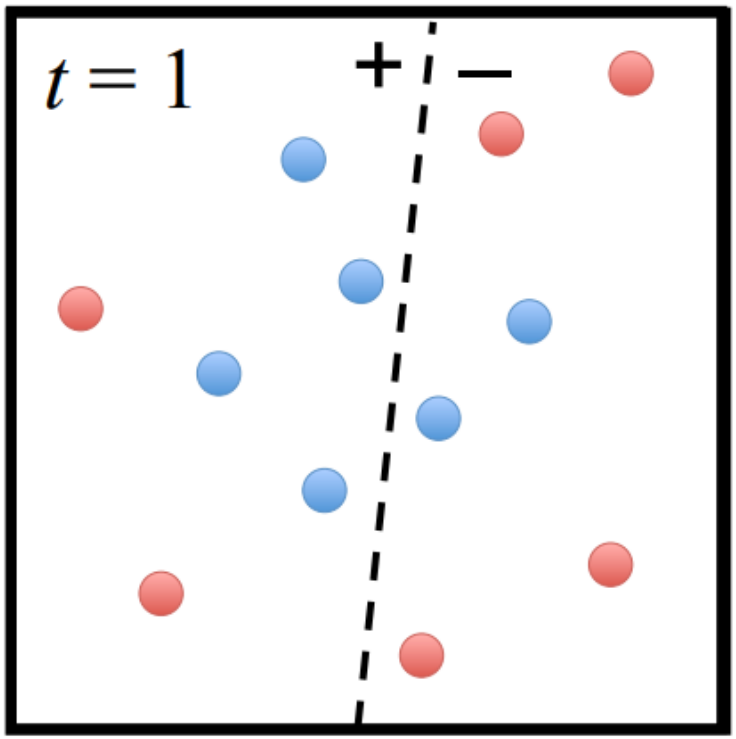

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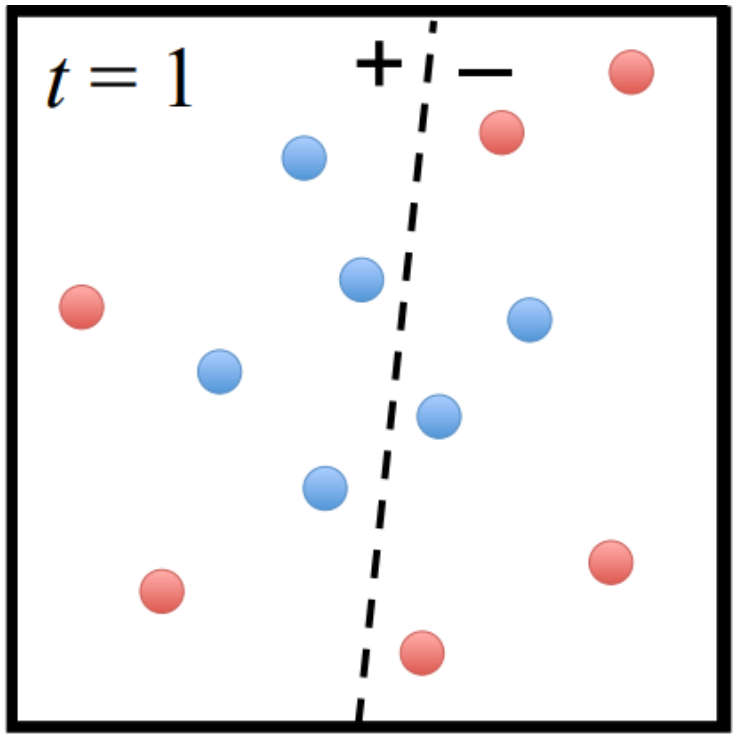

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- Note: resized points in the illustration are not necessarily to scale with β_t

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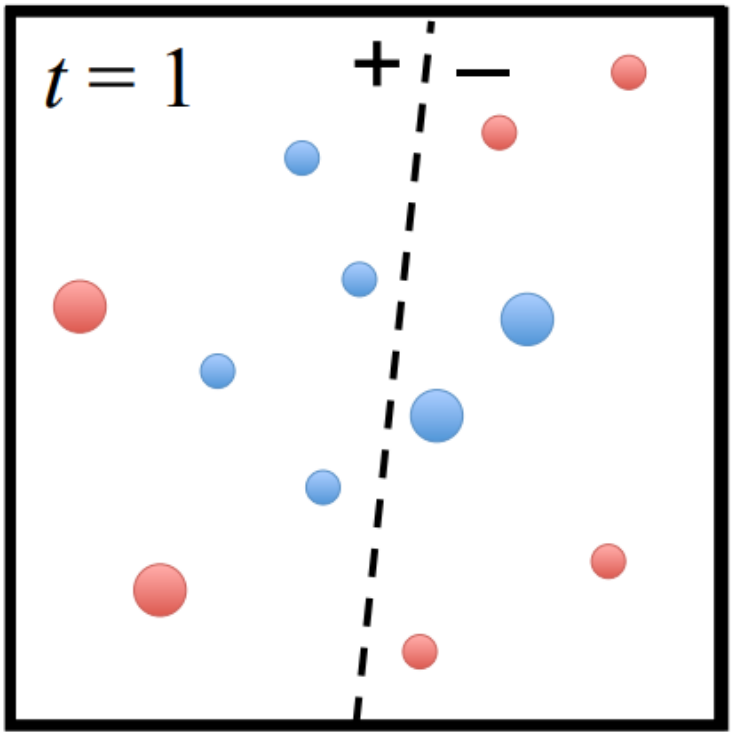

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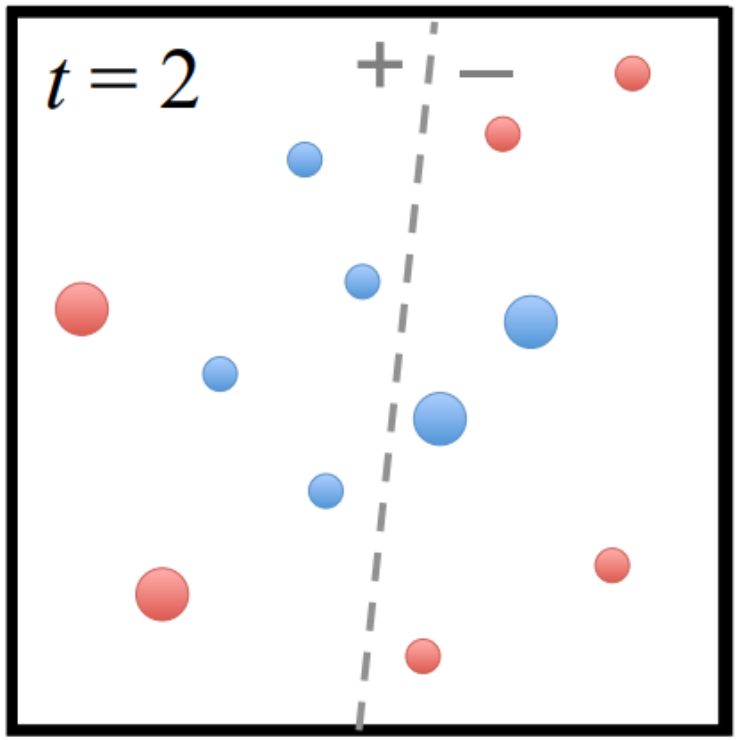

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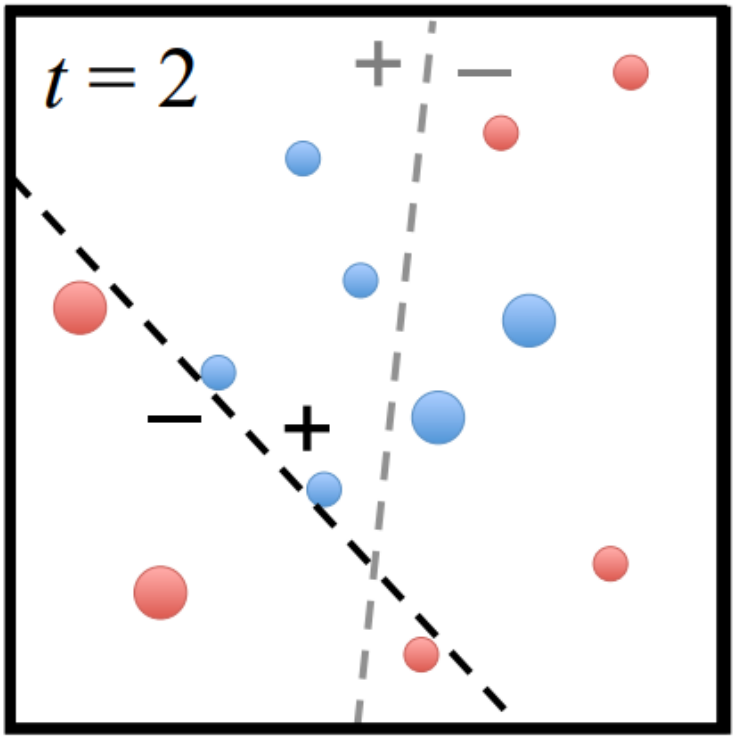

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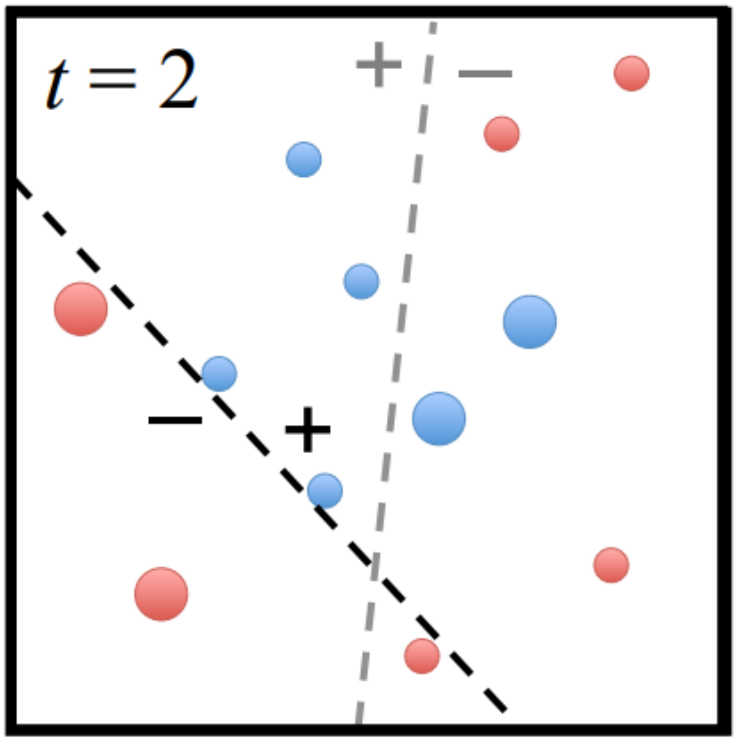

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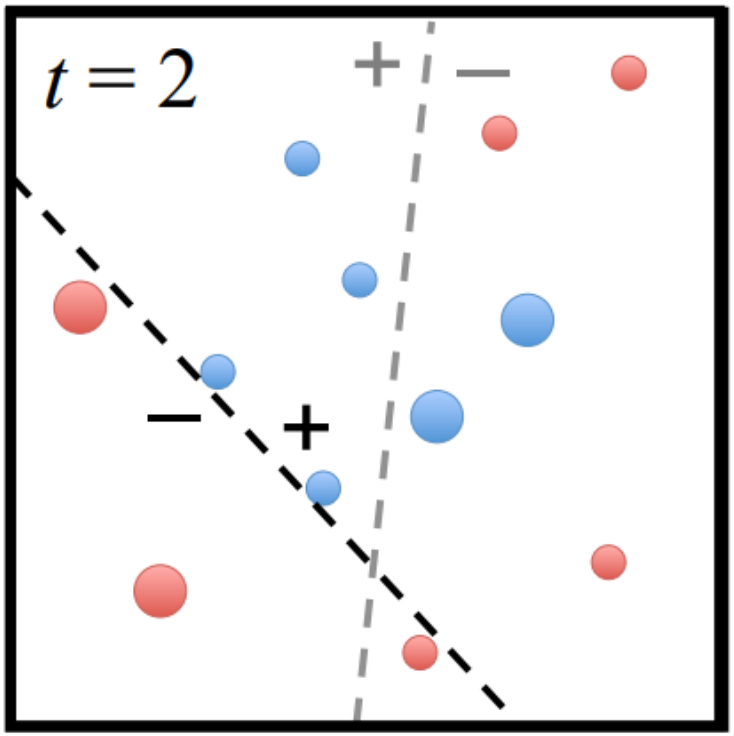

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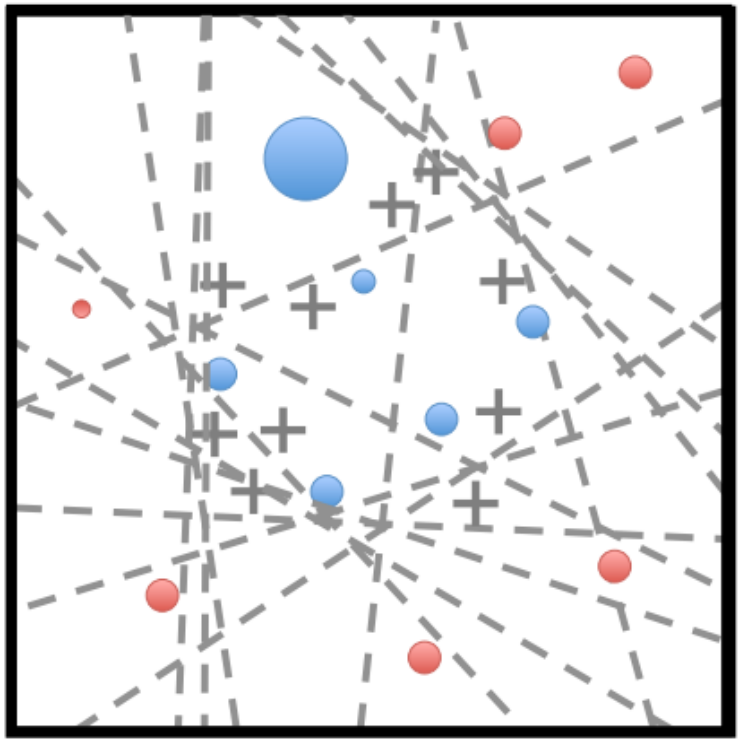

AdaBoost

- Final model is a weighted combination of members
  - Each member weighted by its importance

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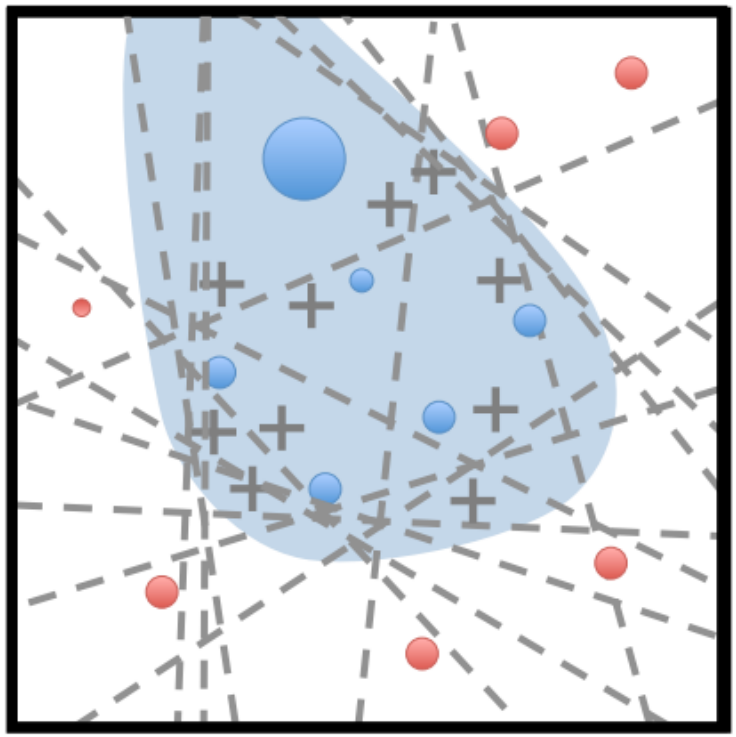

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$\mathbf{w}_t$ is a vector of weights over the instances at iteration t

All points start with equal weight

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We need a way to weight instances differently when learning the model...

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Training with Weighted Instances

- For algorithms like logistic regression, can simply incorporate weights $\boldsymbol{w}$ into the cost function
  - Essentially, weigh the cost of misclassification differently for each instance

$$\mathcal{J}_{\text{reg}}(\boldsymbol{\theta}) = -\sum_{i=1}^{n} w_i \left[y_1 \log h_{\boldsymbol{\theta}}(\boldsymbol{x}_i) + (1 - y_i) \log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x}_i)) \right] + \lambda ||\boldsymbol{\theta}_{[1:d]}||_2^2 \tag{1}$$

- For algorithms that don't directly support instance weights (e.g. decision trees), use weighted bootstrap sampling
  - Form training set by resampling instances with replacement according to $\boldsymbol{w}$

Bse Learner Requirements

- AdaBoost works with "weak" learners
  - Should not be complex
  - Typically high-bias classifiers
  - Works even when the weak learner has an error rate just slightly under 0.5
    - i.e. just slightly better than random
    - Can prove training error goes to 0 in $O(\log n)$ iterations
- Examples
  - Decision stumps (1 level decision trees)
  - Depth-limited decision trees
  - Linear classifiers

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Error is the sum the weights of all misclassified instances

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9: **Return** the hypothesis

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

AdaBoost

INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$,
the number of iterations T

1: Initialize a vector of n uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$
2: **for** $t = 1, \ldots, T$
3: Train model h_t on X, y with instance weights $\mathbf{w}_t$
4: Compute the weighted training error rate of h_t:

$$\epsilon_t = \sum_{i: y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$$

5: Choose $\beta_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
6: Update all instance weights

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\ldots\right.$$

7: Normalize $\mathbf{w}_{t+1}$ to be a dist

$$w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^n w_{t+1,j}} \quad \forall$$

8: **end for**
9: **Return** the hypothesis

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

- β_t measures the importance of h_t
- If $\epsilon_t \leq 0.5$, then $\beta_t \geq 0$
  - Trivial, otherwise flip h_t's predictions
- β_t grows as error h_t's shrinks

AdaBoost

INPUT: traini
the n

1: Initialize a vecto
2: **for** $t = 1, \ldots, T$
3: Train model
4: Compute the

$$\epsilon_t = \sum_{i:y_i \neq h_t(\mathbf{x}}$$

5: Choose $\beta_t =$ $\frac{1}{2}$ ln $\left(\quad \epsilon_t \right)$

6: Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right) \quad \forall i = 1, \ldots, n$$

7: Normalize $\mathbf{w}_{t+1}$ to be a distribution:

$$w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^{n} w_{t+1,j}} \quad \forall i = 1, \ldots, n$$

8: **end for**
9: **Return** the hypothesis

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

This is the same as:

will be ≤ 1

$$w_{t+1,i} = w_{t,i} \times \begin{cases} e^{-\beta_t} & \text{if } h_t(\mathbf{x}_i) = y_i \\ e^{\beta_t} & \text{if } h_t(\mathbf{x}_i) \neq y_i \end{cases}$$

will be ≥ 1

Essentially this emphasizes misclassified instances.

AdaBoost

INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$,
the number of iterations T

1: Initialize a vector of n uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$
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7: Normalize $\mathbf{w}_{t+1}$ to be a distribution:

$$w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^n w_{t+1,j}} \quad \forall i = 1, \ldots, n$$

8: **end for**
9: **Return** the hypothesis

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

Make $\mathbf{w}_{t+1}$ sum to 1

AdaBoost

INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$,
the number of iterations T

1: Initialize a vector of n uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$
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6: Update all instance weights:

$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right) \quad \forall i = 1, .$$

7: Normalize $\mathbf{w}_{t+1}$ to be a distribution:

$$w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^n w_{t+1,j}} \quad \forall i = 1, \ldots, n$$

8: **end for**
9: **Return** the hypothesis

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

Member classifiers with less error are given more weight in the final ensemble hypothesis

Final prediction is a weighted combination of each member's prediction

Dynamic Behavior of AdaBoost

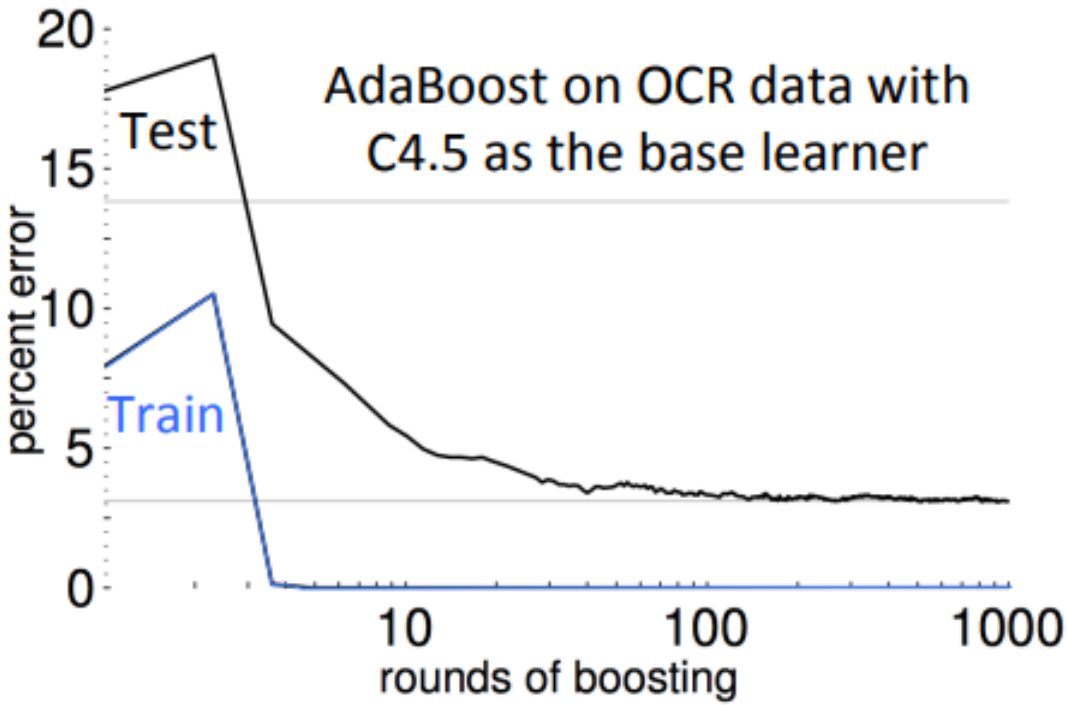
- If a point is repeatedly misclassified
  - Each time, its weight is increased
  - Eventually it will be emphasized enough to generate a hypothesis that correctly predicts it
- Successive member hypotheses focus on the hardest part of the instance space
  - Instances with the highest weight are often outliers

AdaBoost and Overfitting

- The VC (Vapnik-Chervonenkis) theory originally predicted that AdaBoost would always overfit as T grew large
  - Hypothesis keeps growing more complex
- In practice, AdaBoost often did not overfit, contradicting the VC Theory
- Also, AdaBoost does not explicitly regularize the model

Explaining Why AdaBoost Works

- Empirically, boosting resists overfitting
- Note that it continues to drive down the test error even after the training error reaches zero



AdaBoost in Practice

- Strengths:
  - Fast and simple to program
  - No parameters to tune (besides T)
  - No assumption on weak learner
- When boosting can fail:
  - Given insufficient data
  - Overly complex weak hypotheses
  - Can be susceptible to noise
  - When there are a large number of outliers

Boosted Decision Tree

- Boosted decision trees are one of the best "off-the-shelf" classifiers
  - i.e. no parameter tunning
- Limit member hypothesis complexity by limiting tree depth

Quote

"AdaBoost with trees is the best off-the-shelf classifier in the world"
- Breiman

- Also, see results by Caruana & Niculescu-Mizil, ICML 2006