Introduction to Machine Learning

Ensemble Learning

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Ensemble Learning

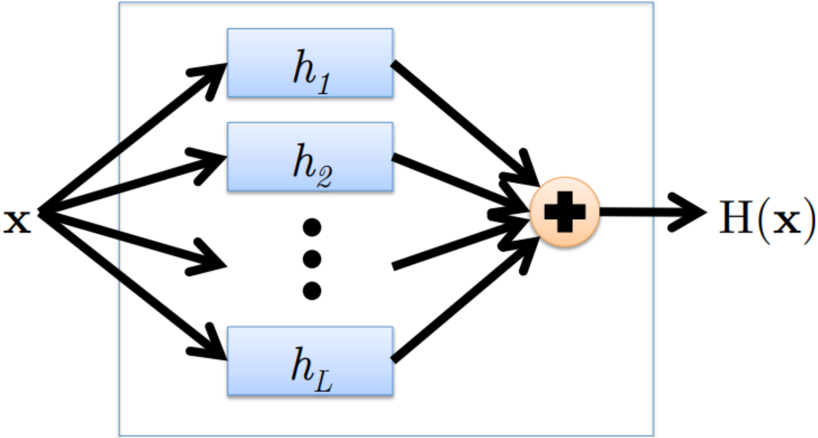
- Consider a set of classifiers $h_1, ..., h_L$
- Idea: construct a classifier $H(\boldsymbol{x})$ that combines the individual decisions of $h_1, ..., h_L$
  - e.g. could have the member classifiers vote
  - e.g. could use different members for different regions of the instance space
  - works well 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

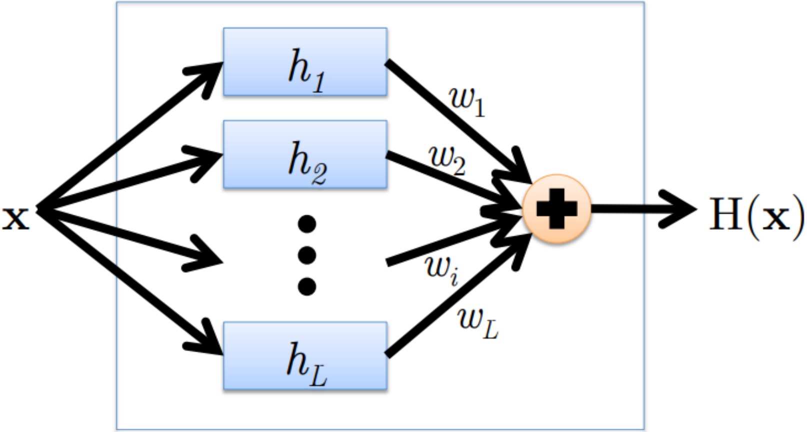
Combining Classifiers: Averaging

- Final hypothesis is a simple vote of the members



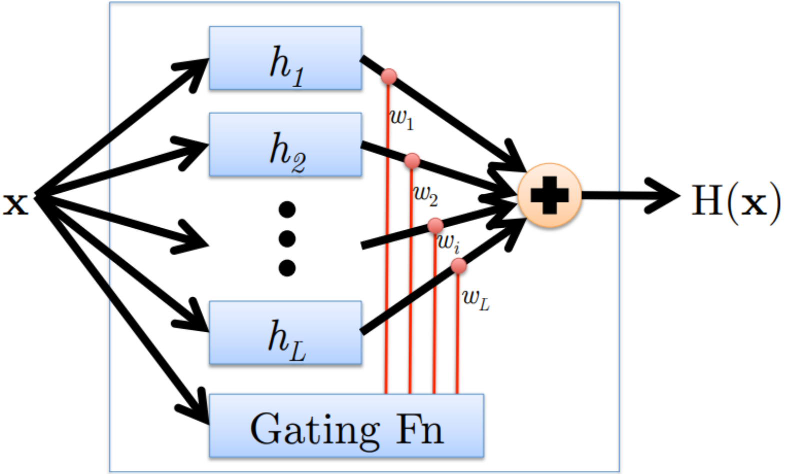
Combining Classifiers: Weighted Averaging

- Coefficients of individual members are tuned using a validation set



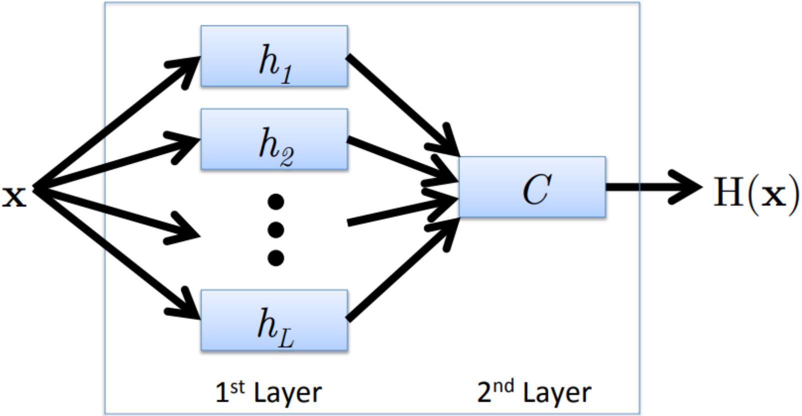
Combining Classifiers: Gating

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

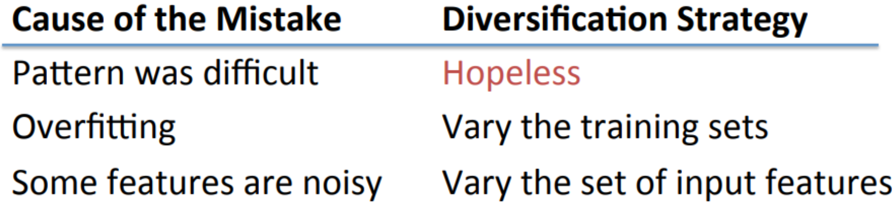


Combining Classifiers: Stacking

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



How to Achieve Diversity



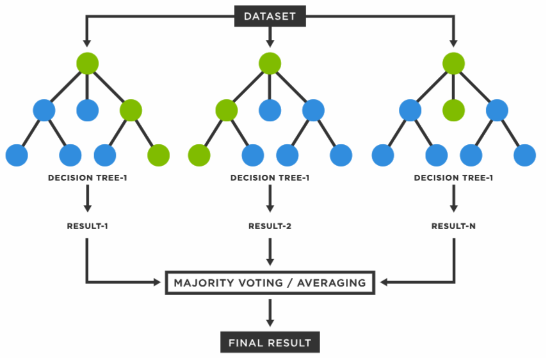
Cause of the Mistake	**Diversification Strategy**
Pattern was difficult	Hopeless
Overfitting	Vary the training sets
Some features are noisy	Vary the set of input features

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

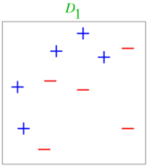
- Developed by Freund & Schapire in 1997
- A meta-learning algorithm with great theoretical and empirical performance
- Turns a base learner (e.g. “weak hypothesis”) into a high performance classifier
- Create an ensemble of weak hypotheses by repeatedly emphasizing mispredicted instances

Weak Learners and Classifiers

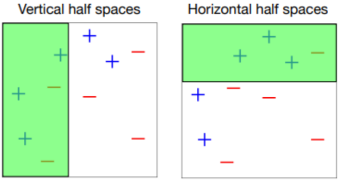
- (Informal) A weak learner is a learning algorithm that outputs a hypothesis (e.g. a classifier) that performs slightly better than chance.
  - e.g. it predicts the correct label with probability 0.51 in binary label case
- We are interested in weak learners that are computationally efficient
  - Decision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

Weak Classifiers

- Suppose these are the data

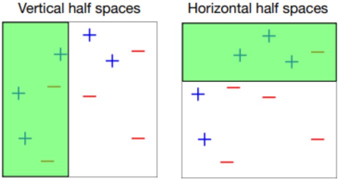


- These weak classifiers, which are decision stumps, consist of the set of horizontal and vertical half-spaces.



Weak Classifiers

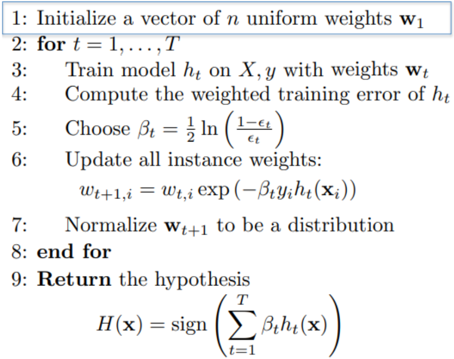
- A single weak classifier is not capable of making the training error small
- But if we can guarantee that it performs slightly better than chance
- Using it with AdaBoost gives us a universal function approximator



- 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



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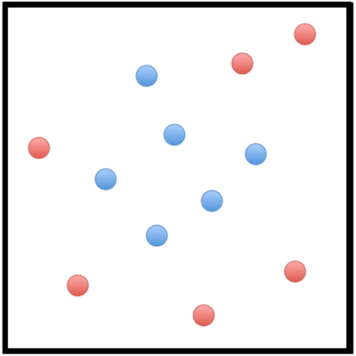
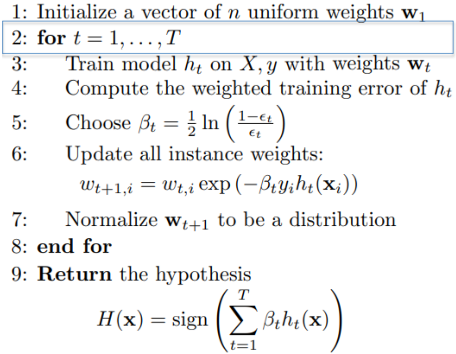


AdaBoost



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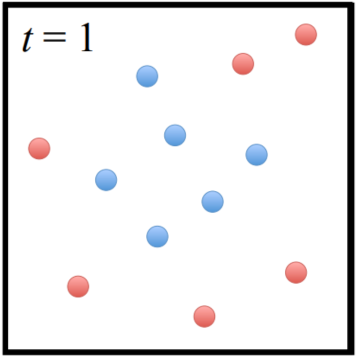

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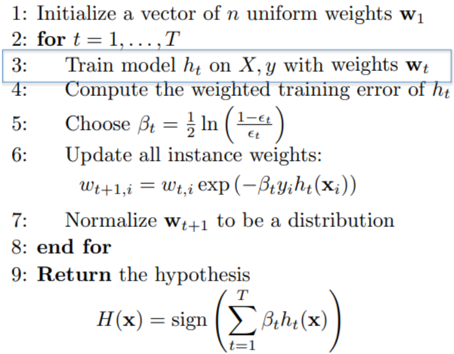

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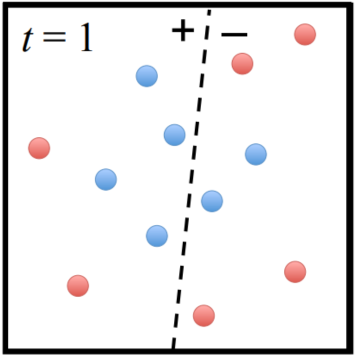

AdaBoost

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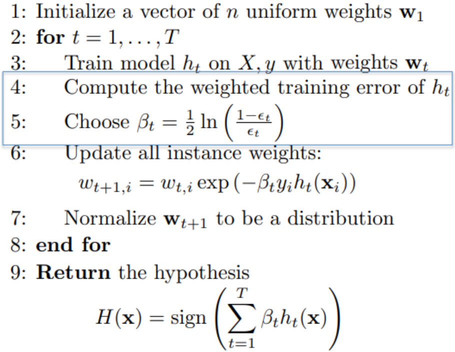
- if $\epsilon_t \leq 0.5$ then $\beta_t \geq 0$ (can trivially gurantee)



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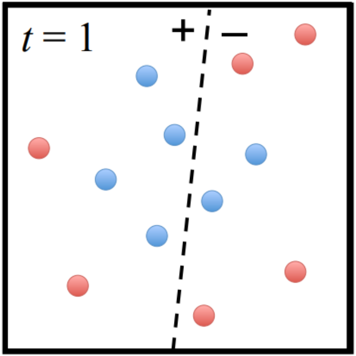

AdaBoost

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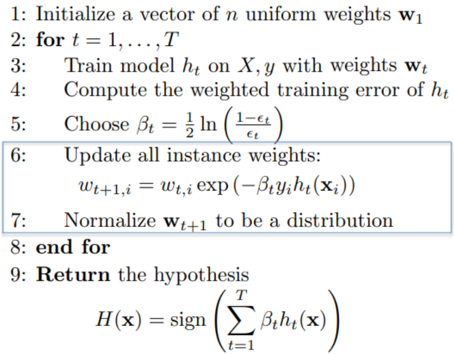

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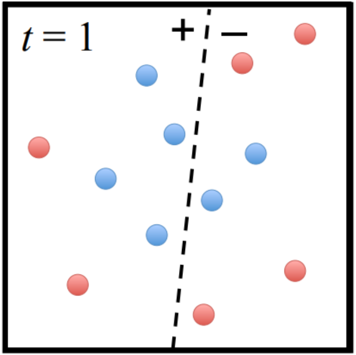
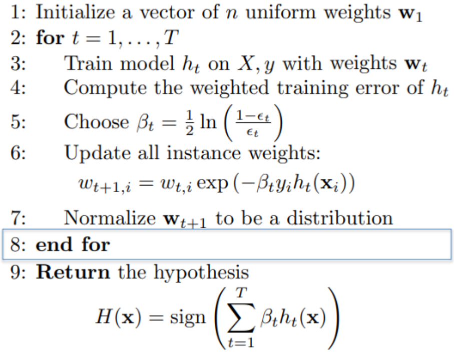


AdaBoost

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



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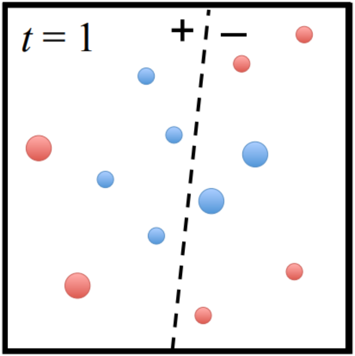

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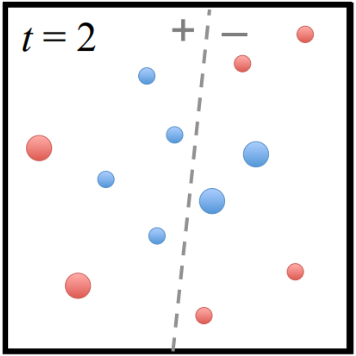

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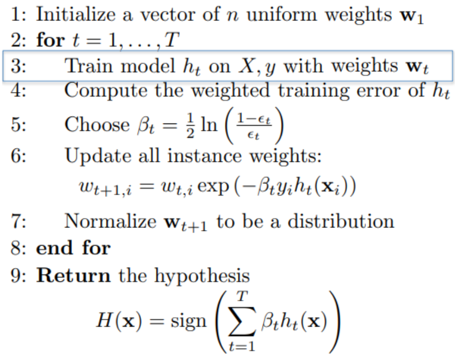

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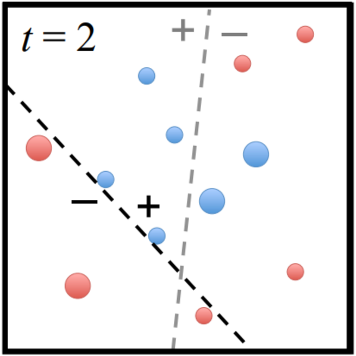

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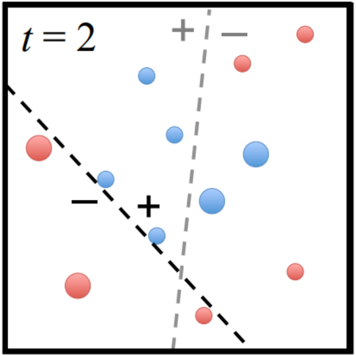

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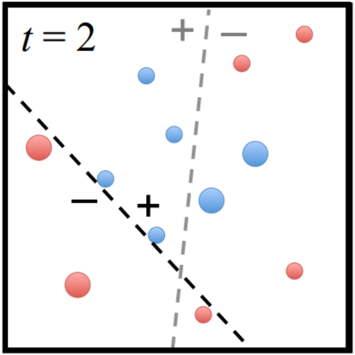

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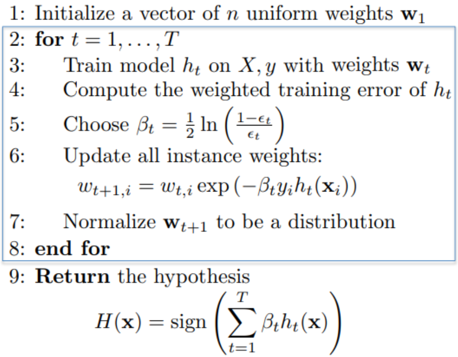

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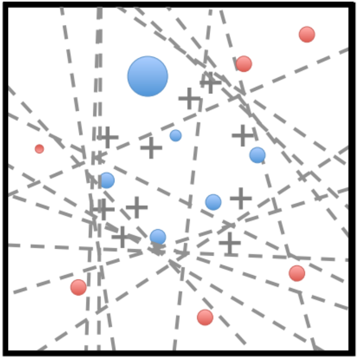

AdaBoost

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

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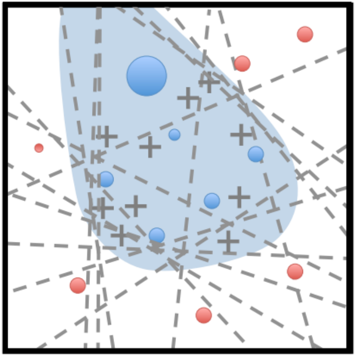

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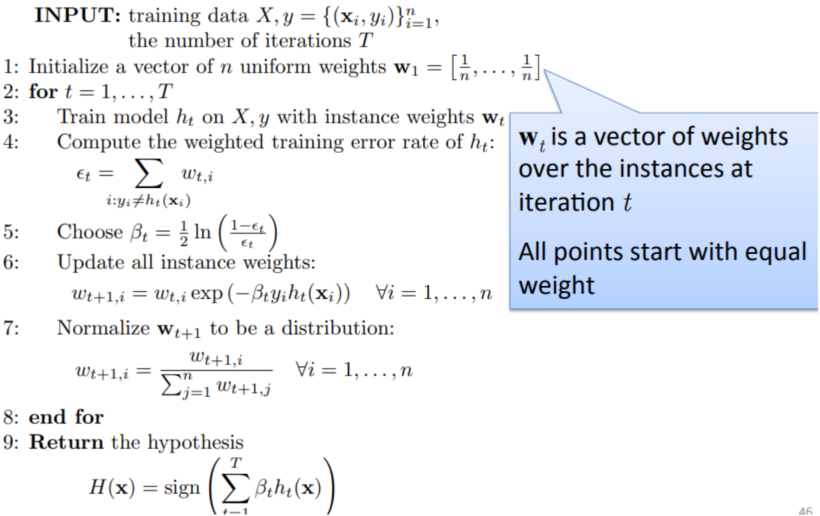

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    Train model $h_t$ on $X, y$ with instance weights $\mathbf{w}_t$
    Compute the weighted training error rate of $h_t$:
        $\epsilon_t = \sum_{i : y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$
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Return the hypothesis
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$\mathbf{w}_t$ is a vector of weights over the instances at iteration t

All points start with equal weight

AdaBoost

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```

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

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

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

- 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

AdaBoost

```
INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$,
       the number of iterations $T$
Initialize a vector of $n$ uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \dots, \frac{1}{n}\right]$
for $t = 1, \dots, T$
    Train model $h_t$ on $X, y$ with instance weights $\mathbf{w}_t$
    Compute the weighted training error rate of $h_t$:
        $\epsilon_t = \sum_{i: y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$
    Choose $\beta_t = \frac{1}{2} \ln \left( \frac{1-\epsilon_t}{\epsilon_t} \right)$
    Update all instance weights:
        $w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right) \quad \forall i = 1, \dots, n$
    Normalize $\mathbf{w}_{t+1}$ to be a distribution:
        $w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^{n} w_{t+1,j}} \quad \forall i = 1, \dots, n$
end for
Return the hypothesis
    $H(\mathbf{x}) = \text{sign}\left( \sum_{t=1}^{T} \beta_t h_t(\mathbf{x}) \right)$
```

Error is the sum the weights of all misclassified instances

AdaBoost

```
INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$,
       the number of iterations $T$
Initialize a vector of n uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$
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    Train model $h_t$ on $X, y$ with instance weights $\mathbf{w}_t$
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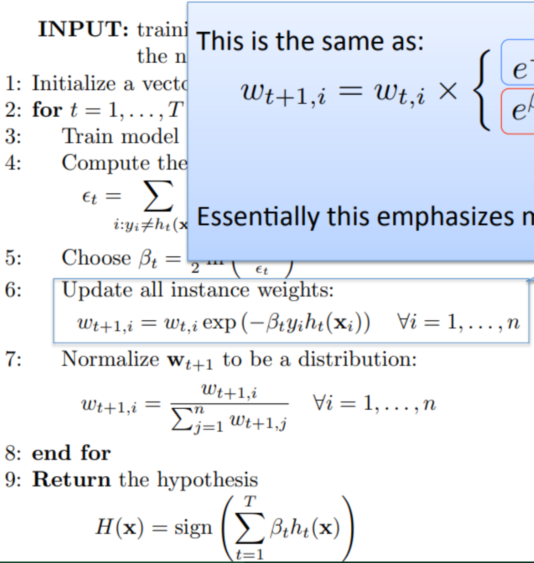
        $\epsilon_t = \sum_{i: y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$
    Choose $\beta_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
    Update all instance weights
        $w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t($
    Normalize $\mathbf{w}_{t+1}$ to be a dis
        $w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^{n} w_{t+1,j}}$    ∀
end for
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
Initialize a vect
for $t = 1, \dots, T$
    Train model
    Compute the
    $\epsilon_t = \sum_{i: y_i \neq h_t(\mathbf{x}}$
    Choose $\beta_t = \frac{}{2} \ln \left( \frac{}{\epsilon_t} \right)$
    Update all instance weights:
        $w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right) \quad \forall i = 1, \dots, n$
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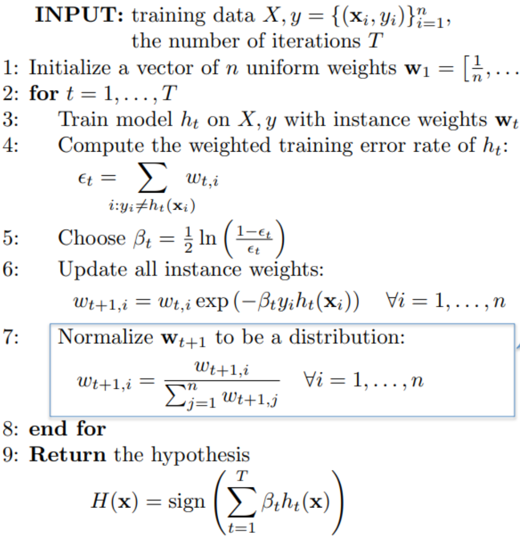
end for
Return the hypothesis
    $H(\mathbf{x}) = \text{sign}\left( \sum_{t=1}^{T} \beta_t h_t(\mathbf{x}) \right)$
```

This is the same as:

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

Essentially this emphasizes misclassified instances.

AdaBoost



```
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        $\epsilon_t = \sum_{i: y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$
    Choose $\beta_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
    Update all instance weights:
        $w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right) \quad \forall i = 1, \ldots, n$
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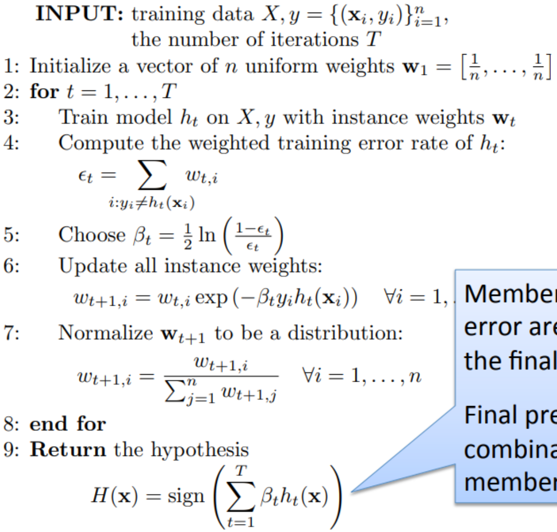
end for
Return the hypothesis
    $H(\mathbf{x}) = \text{sign}\left(\sum_{t=1}^{T} \beta_t h_t(\mathbf{x})\right)$
```

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 $T$
Initialize a vector of $n$ uniform weights $\mathbf{w}_1 = \left[\frac{1}{n}, \ldots, \frac{1}{n}\right]$
for $t = 1, \ldots, T$
    Train model $h_t$ on $X, y$ with instance weights $\mathbf{w}_t$
    Compute the weighted training error rate of $h_t$:
        $\epsilon_t = \sum_{i : y_i \neq h_t(\mathbf{x}_i)} w_{t,i}$
    Choose $\beta_t = \frac{1}{2} \ln \left( \frac{1-\epsilon_t}{\epsilon_t} \right)$
    Update all instance weights:
        $w_{t+1,i} = w_{t,i} \exp \left( -\beta_t y_i h_t(\mathbf{x}_i) \right) \quad \forall i = 1,$
    Normalize $\mathbf{w}_{t+1}$ to be a distribution:
        $w_{t+1,i} = \frac{w_{t+1,i}}{\sum_{j=1}^{n} w_{t+1,j}} \quad \forall i = 1, \ldots, n$
end for
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

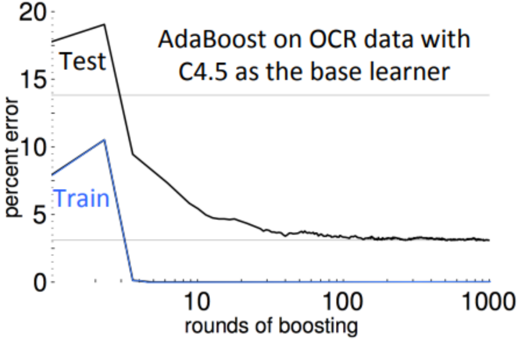
- If a point is repeatedly misclassified
    - Each time, its weight is increased
    - Eventually it will be emphasized enough to generate a hypothesis that correctly predicts it
- Successive member hypotheses focus on the hardest part of the instance space
    - Instances with the highest weight are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