Ensemble Learning

Ensemble Learning

Consider a set of classifiers h_1, ..., h_L

Idea: construct a classifier $H(\mathbf{x})$ that combines the individual decisions of h_1, ..., h_L

- e.g., could have the member classifiers vote, or
- 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

[Based on slide by Léon Bottou]

Practical Application: Netflix Prize

Goal: predict how a user will rate a movie

- Based on the user's ratings for other movies
- and other peoples' ratings
- with no other information about the movies

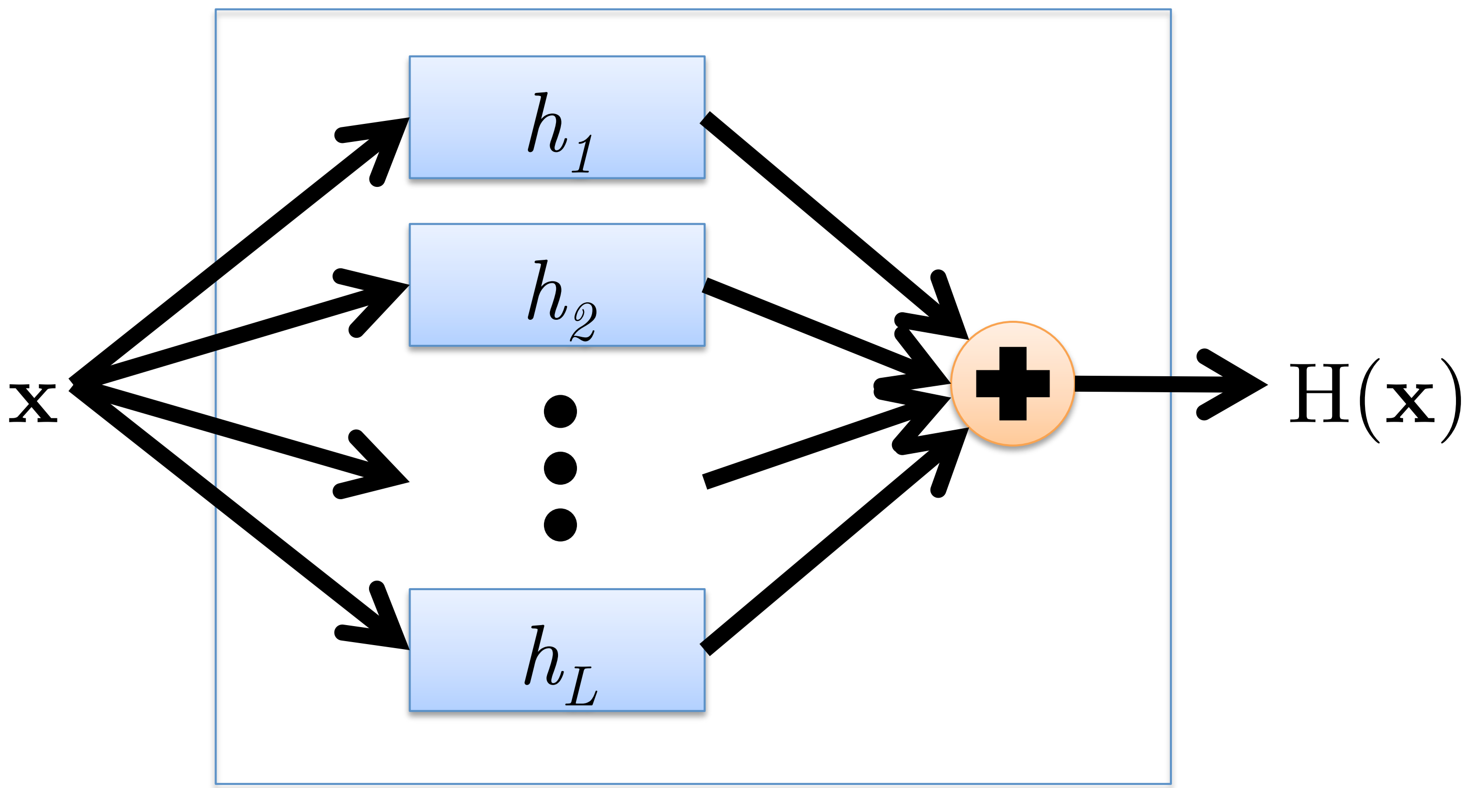
This application is called "collaborative filtering"

Netflix Prize: $1M to the first team to do 10% better then Netflix' system (2007-2009)

Winner: BellKor's Pragmatic Chaos – an ensemble of more than 800 rating systems

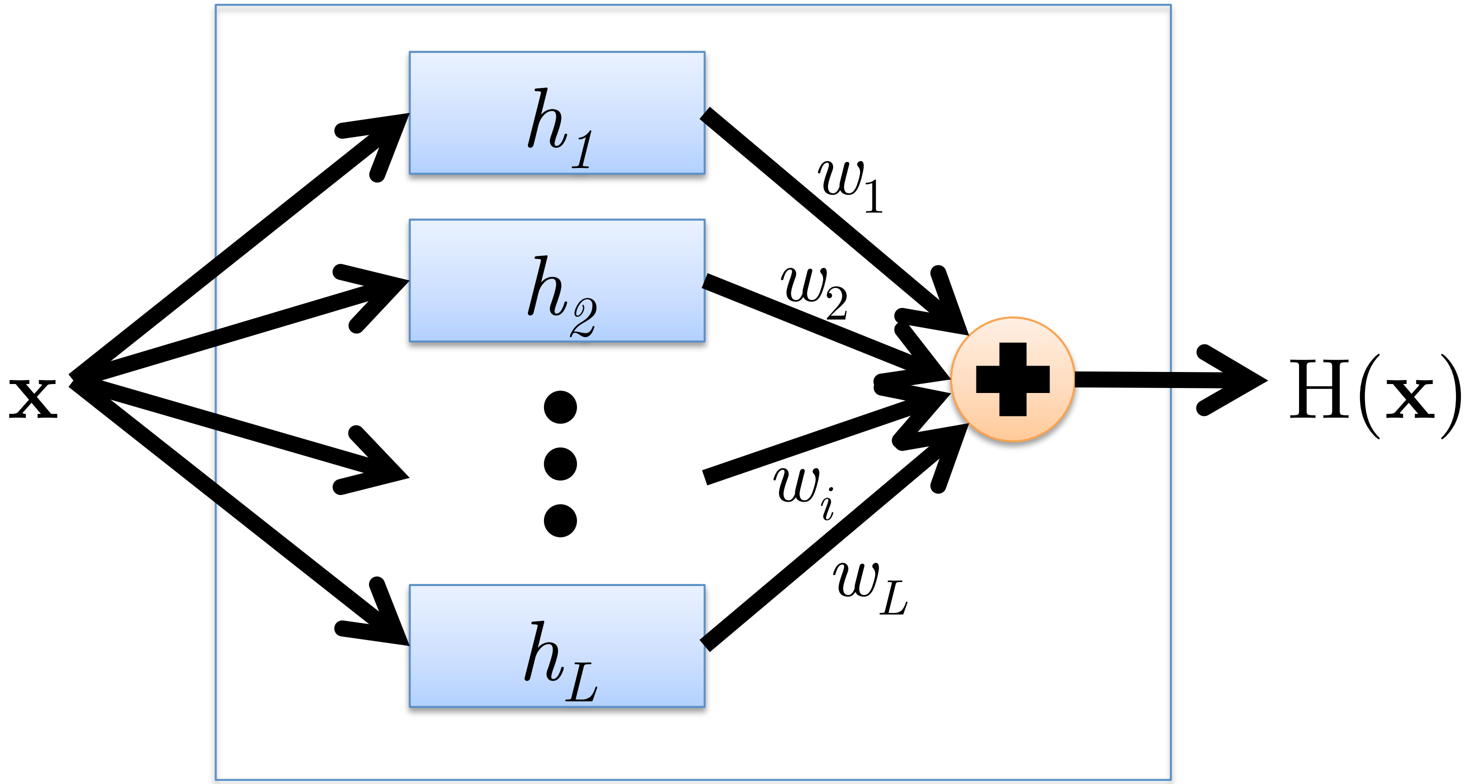
[Based on slide by Léon Bottou]

Combining Classifiers: Averaging



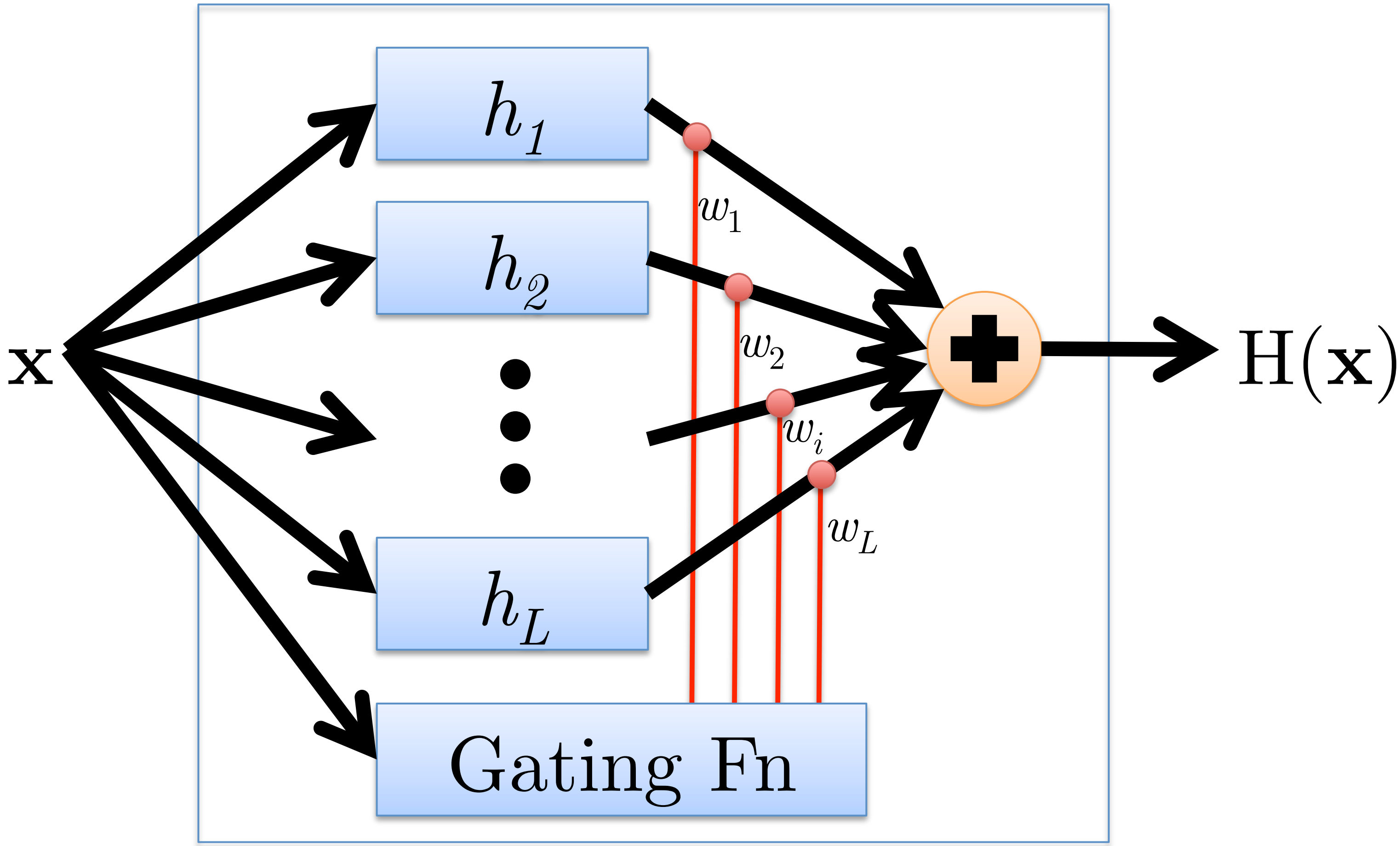
- Final hypothesis is a simple vote of the members

Combining Classifiers: Weighted Average



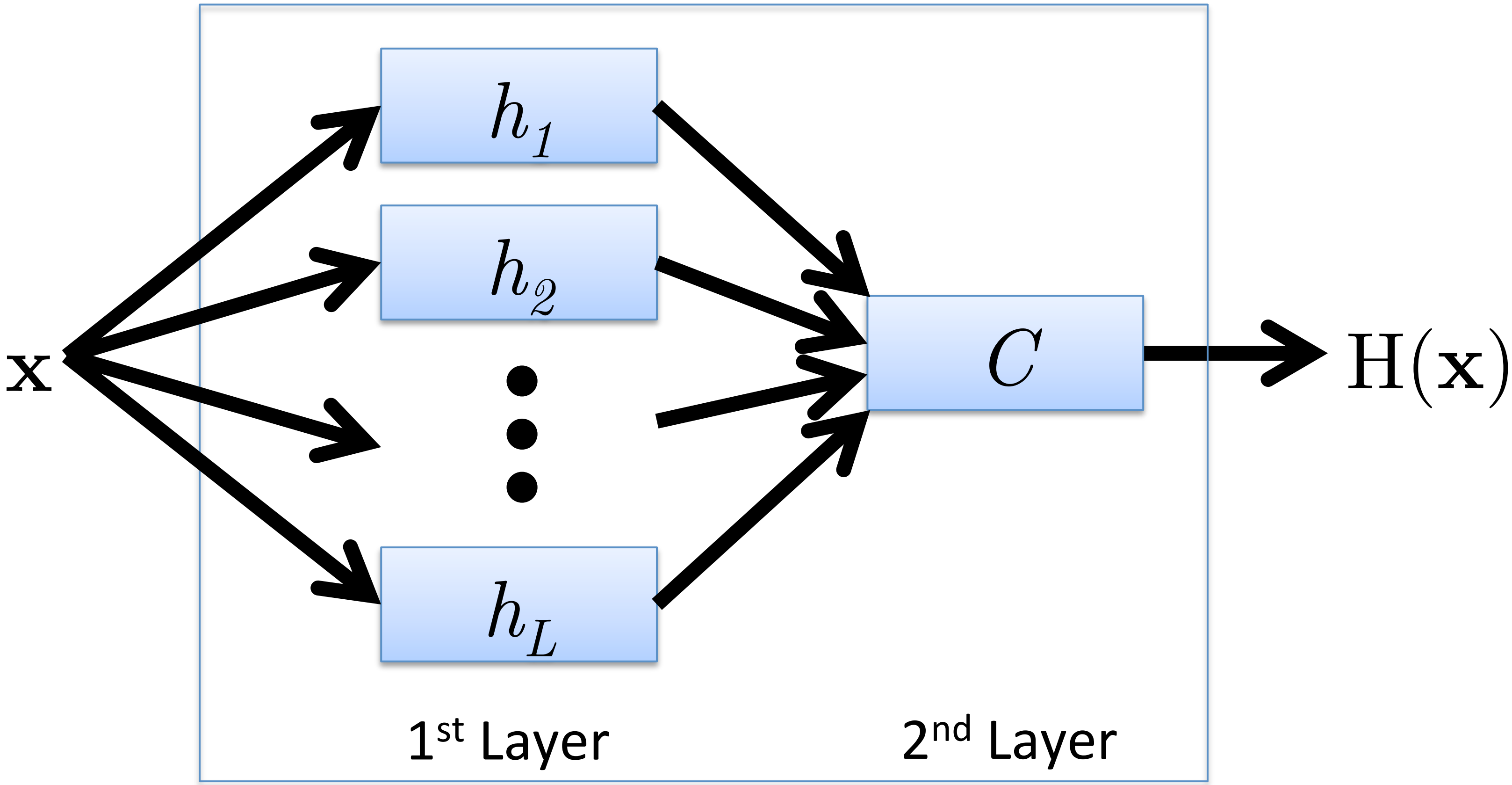
- Coefficients of individual members are trained using a validation set

Combining Classifiers: Gating



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

Combining Classifiers: Stacking



- Predictions of 1st layer used as input to 2nd layer
- Train 2nd layer on 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

[Based on slide by Léon Bottou]

Manipulating the Training Data

Bootstrap replication:

- Given n training examples, construct a new training set by sampling n instances with replacement
- Excludes ~30% of the training instances

Bagging:

- Create bootstrap replicates of 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

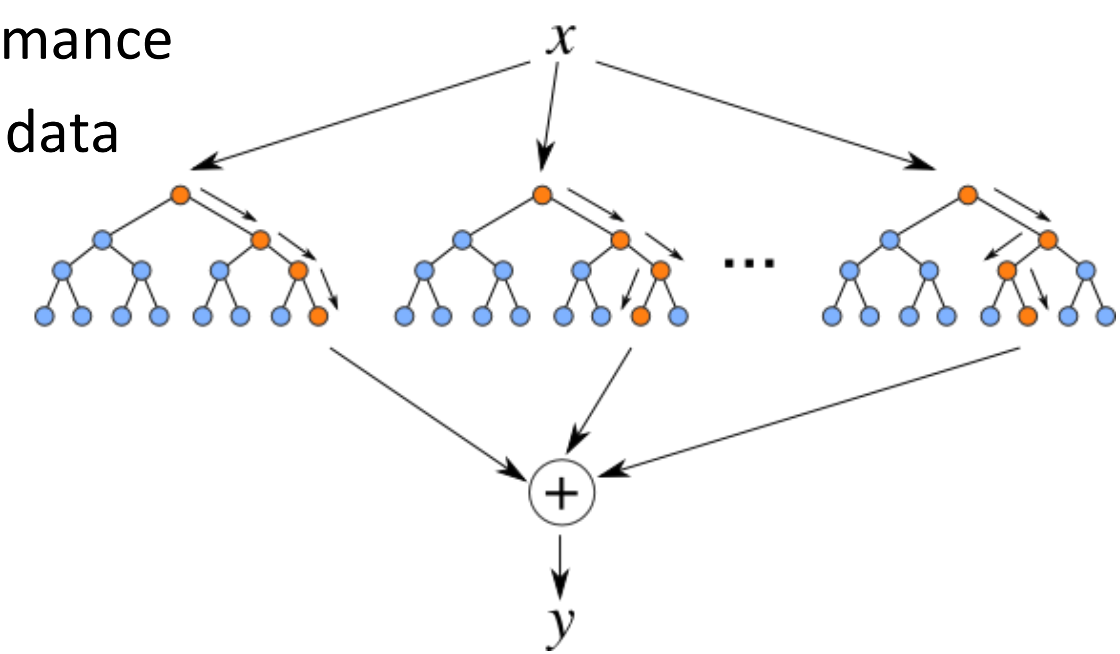
Boosting: (in just a minute...)

[Based on slide by Léon Bottou]

Manipulating the Features

Random Forests

- 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 trees
  - Estimate tree performance on out-of-bootstrap data
- Average the output of all trees



[Based on slide by Léon Bottou]

Boosting

AdaBoost

[Freund & Schapire, 1997]

- A meta-learning algorithm with great theoretical and empirical performance
- Turns a base learner (i.e., a “weak hypothesis”) into a high performance classifier
- Creates an ensemble of weak hypotheses by repeatedly emphasizing mispredicted instances

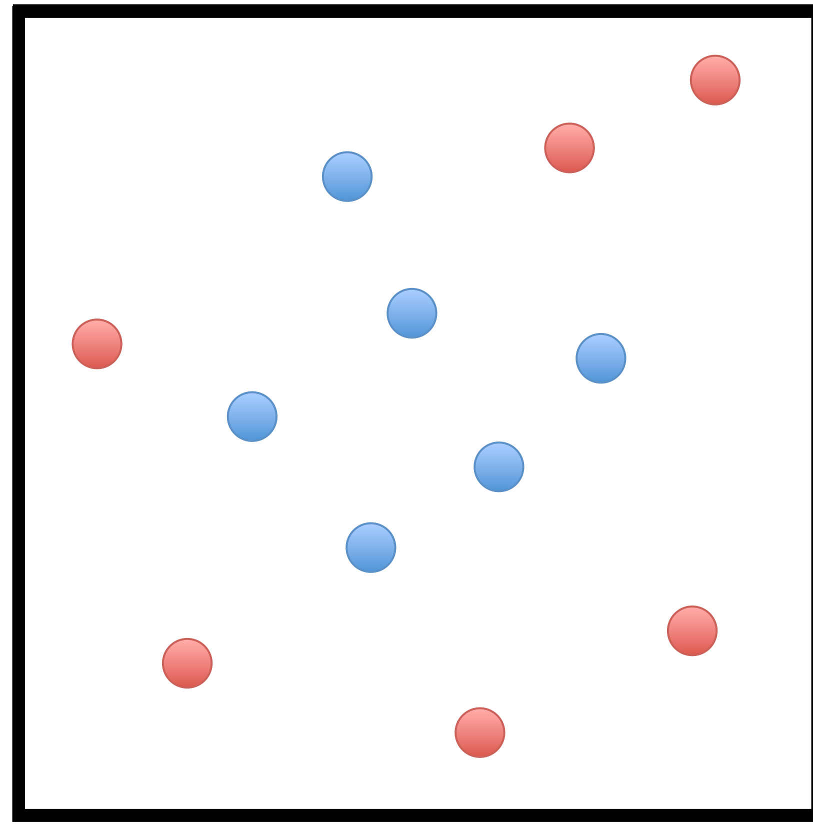
AdaBoost

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

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

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

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



- Size of point represents the instance's weight

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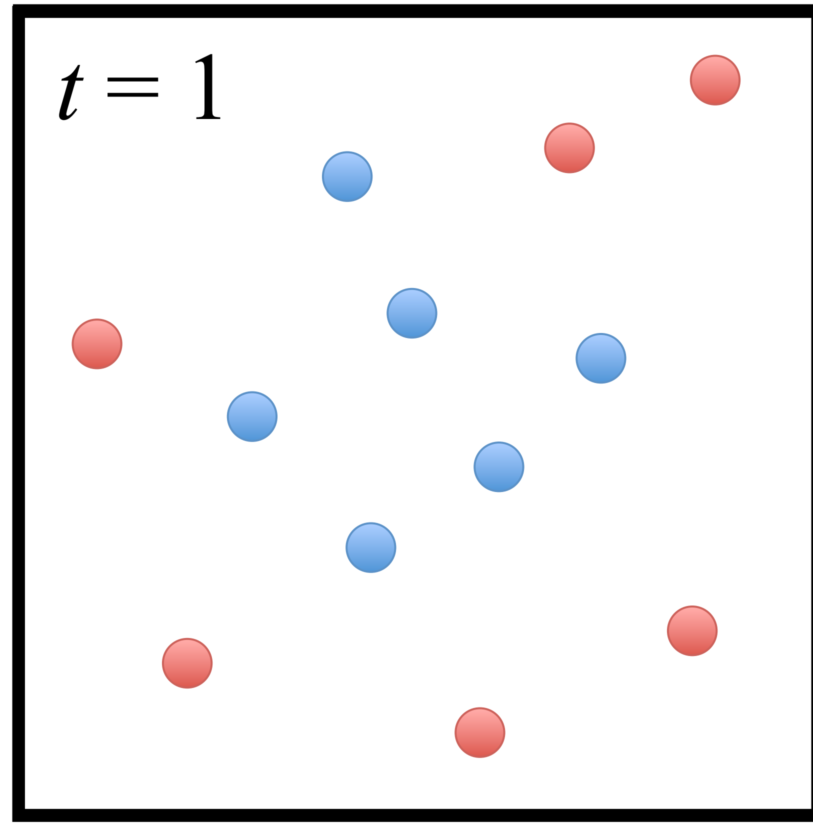

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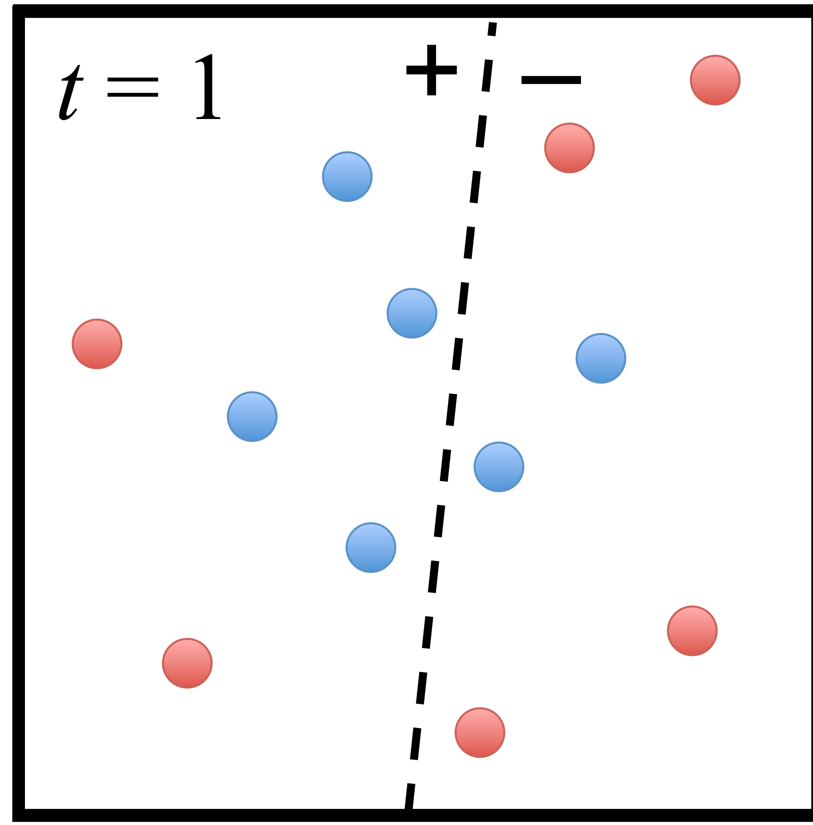

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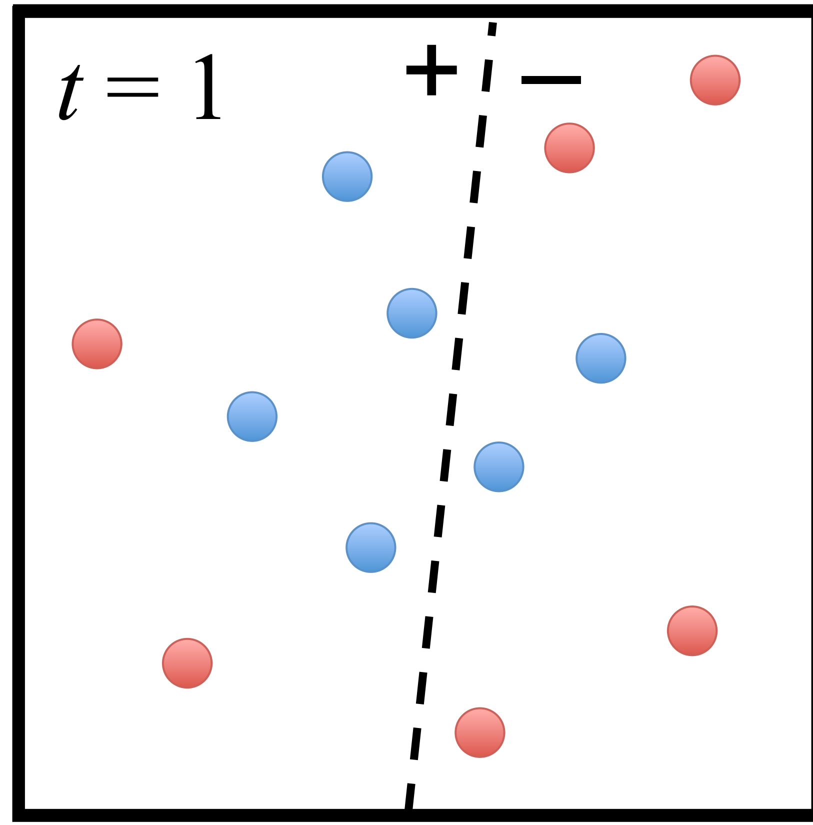

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- If $\epsilon_t \leq 0.5$, then $\beta_t \geq 0$ (can trivially guarantee)

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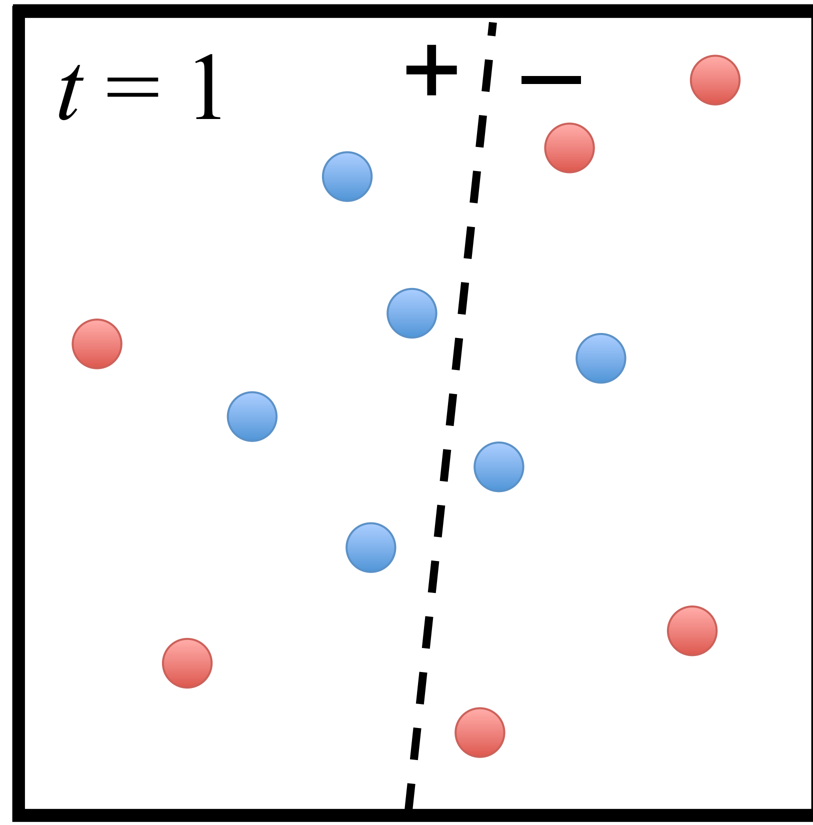

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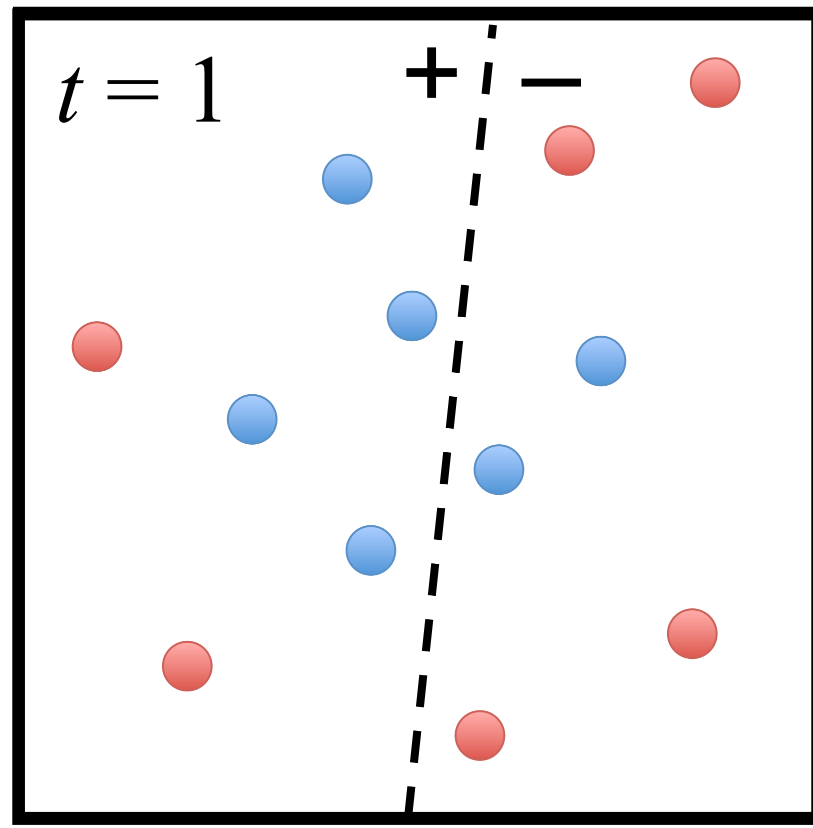

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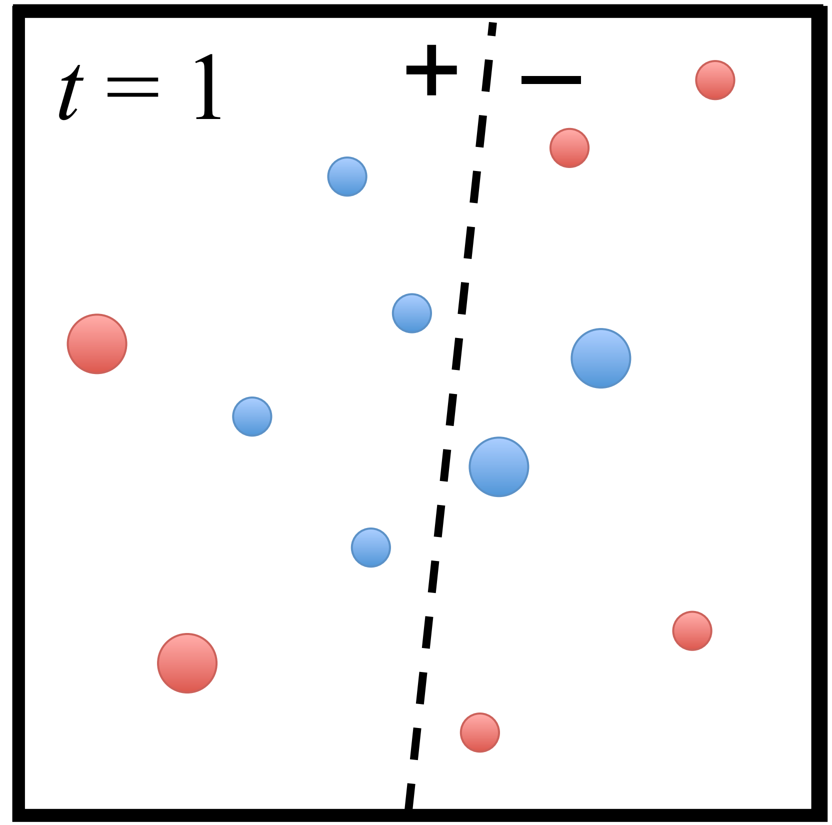

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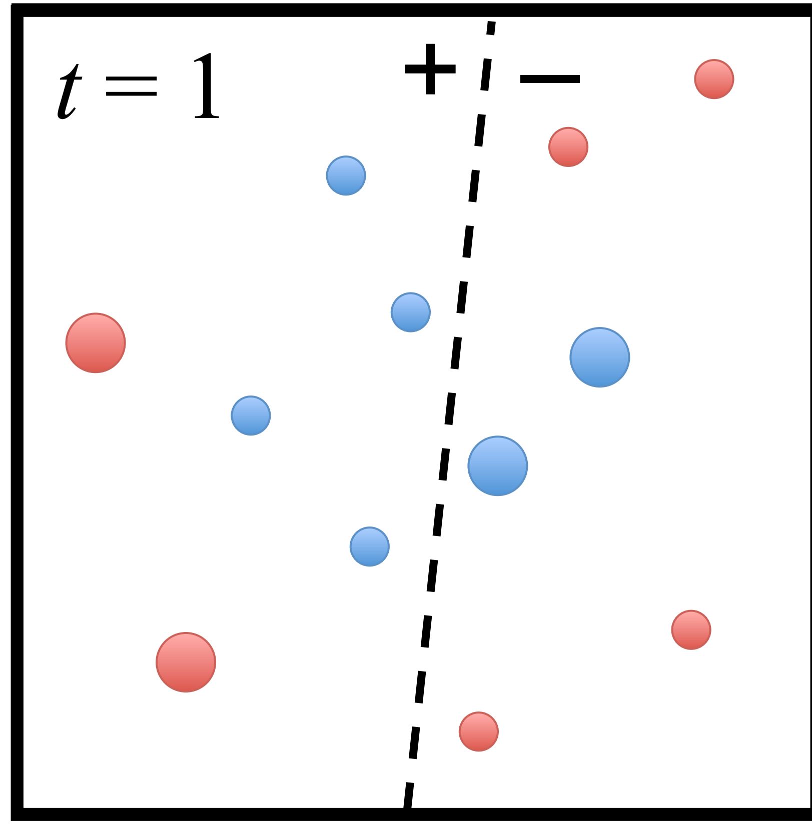

Disclaimer: Note that resized points in the illustration above are not necessarily to scale with β_t

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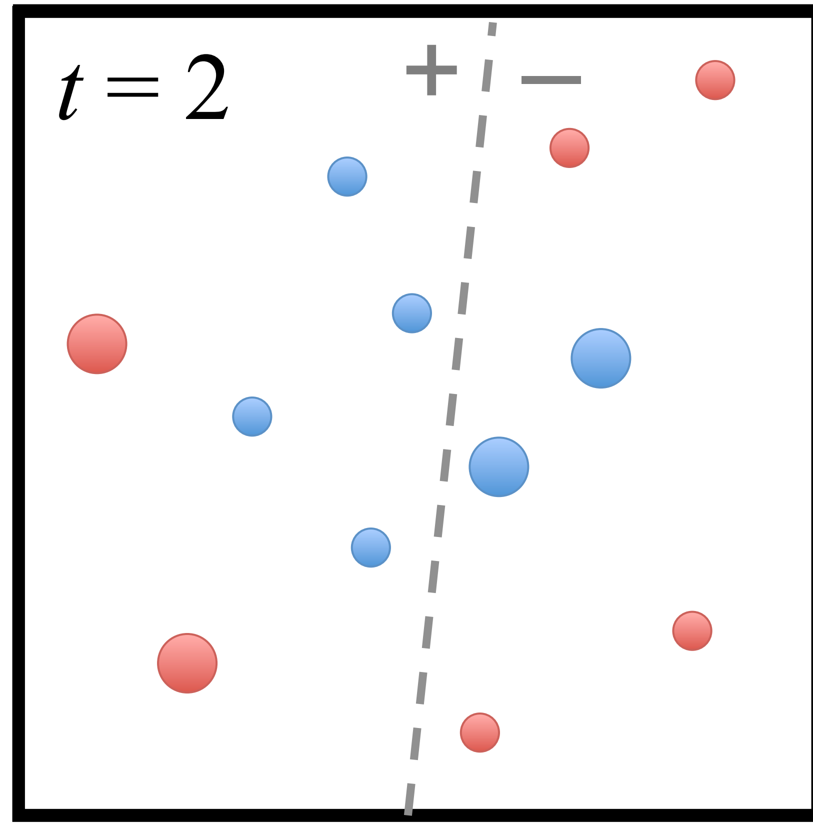

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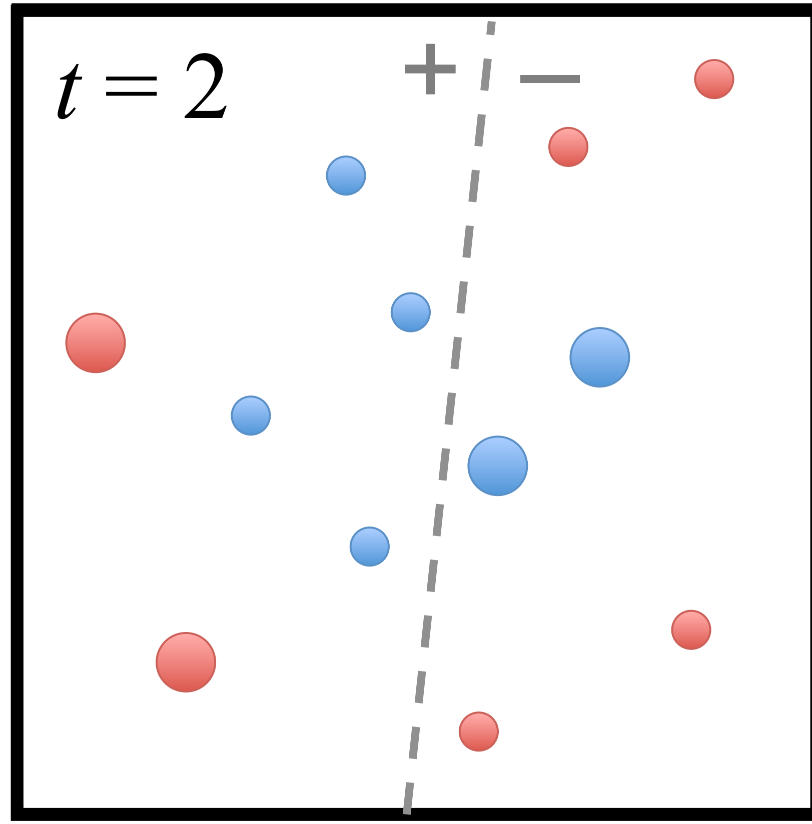

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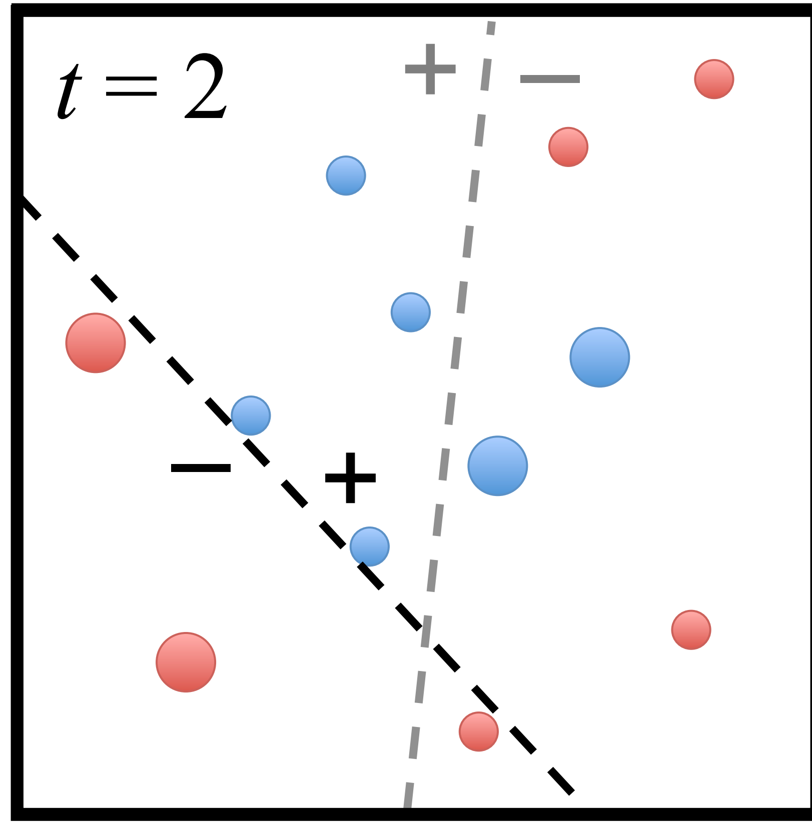

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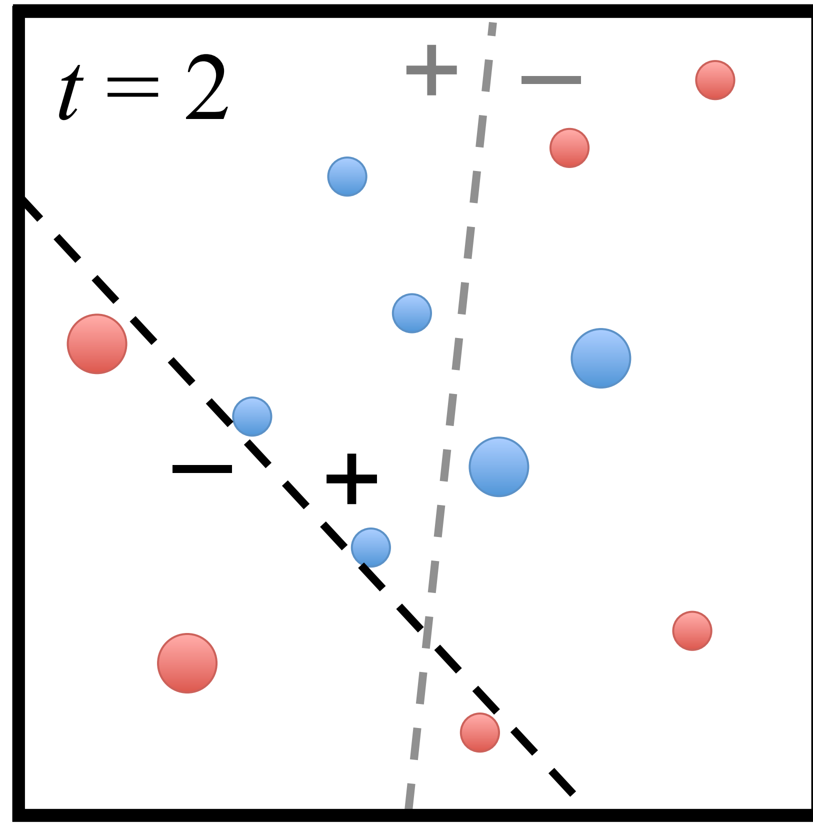

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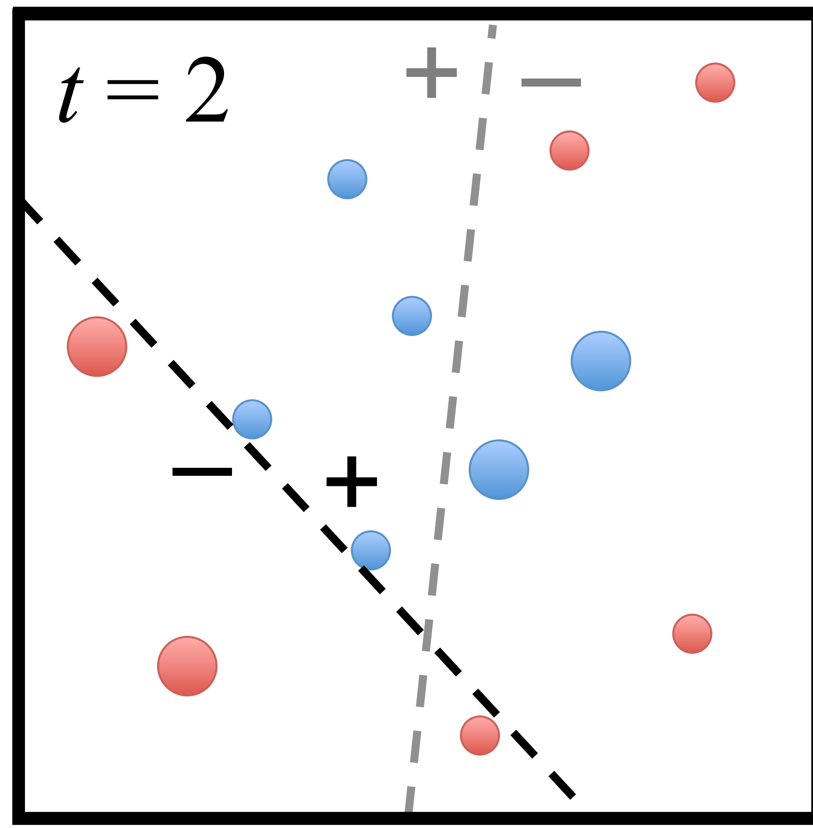

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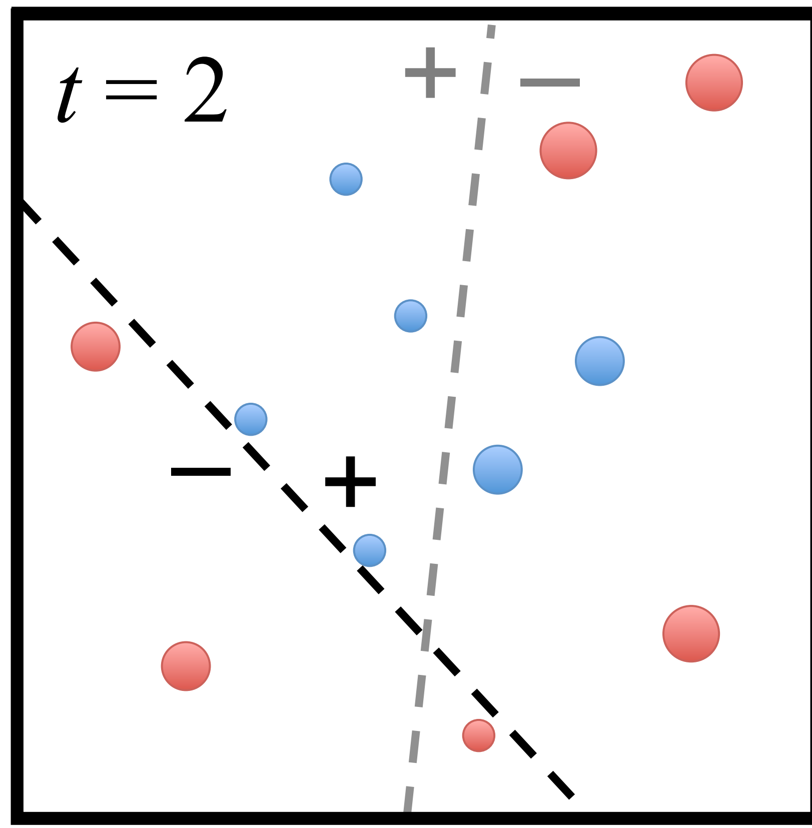

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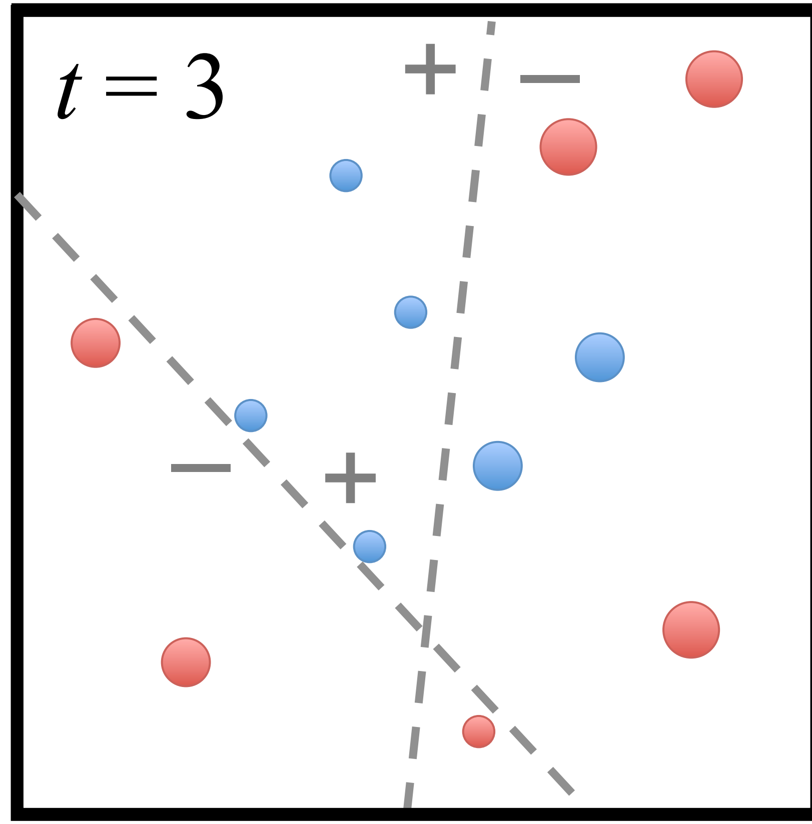

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    Train model h_t on X, y with weights w_t
    Compute the weighted training error of h_t
    Choose β_t = 1/2 ln((1 − ε_t) / ε_t)
    Update all instance weights:
        w_{t+1,i} = w_{t,i} exp(−β_t y_i h_t(x_i))
    Normalize w_{t+1} to be a distribution
end for
Return the hypothesis
    H(x) = sign( Σ_{t=1}^{T} β_t h_t(x) )
```

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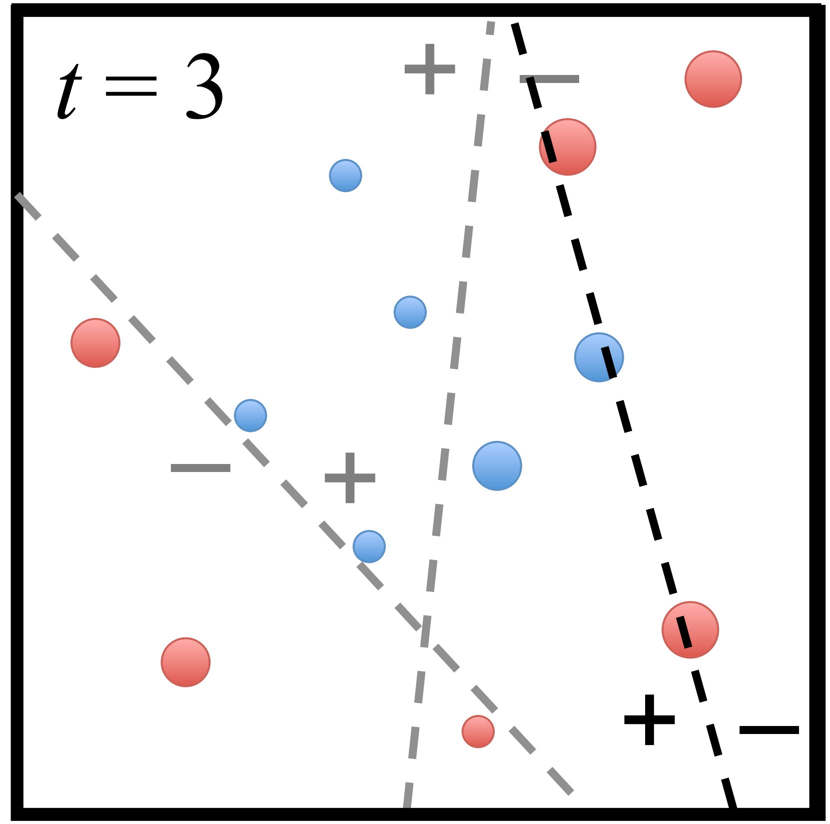

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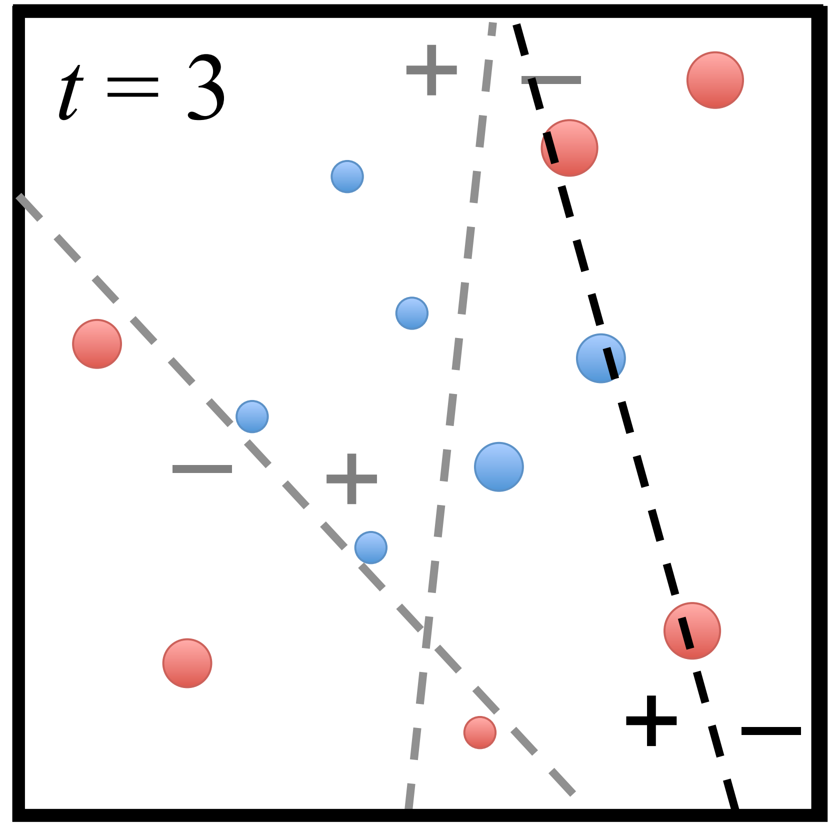

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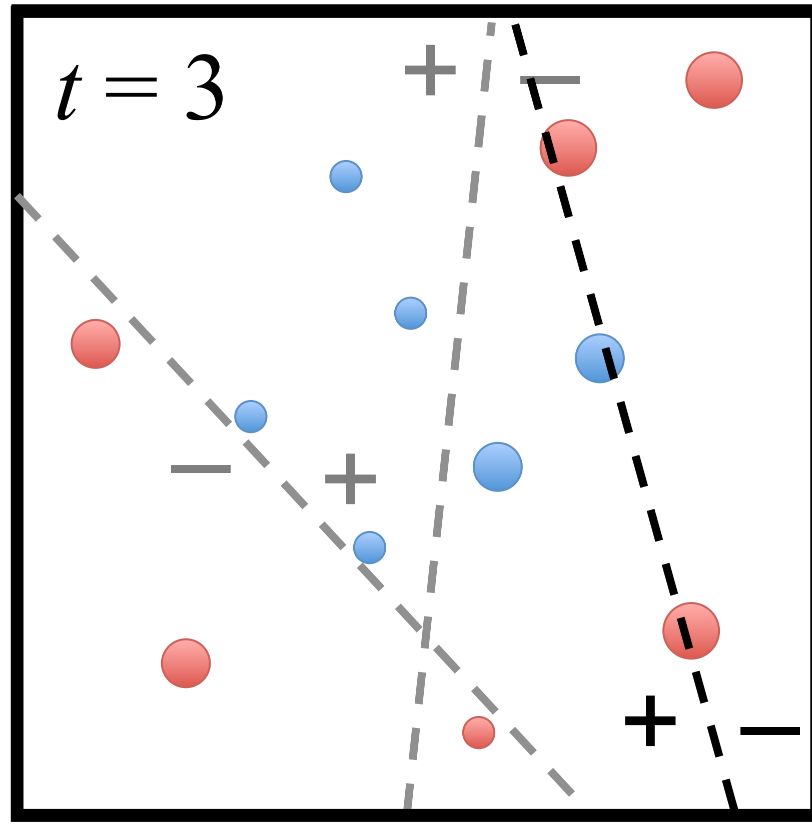

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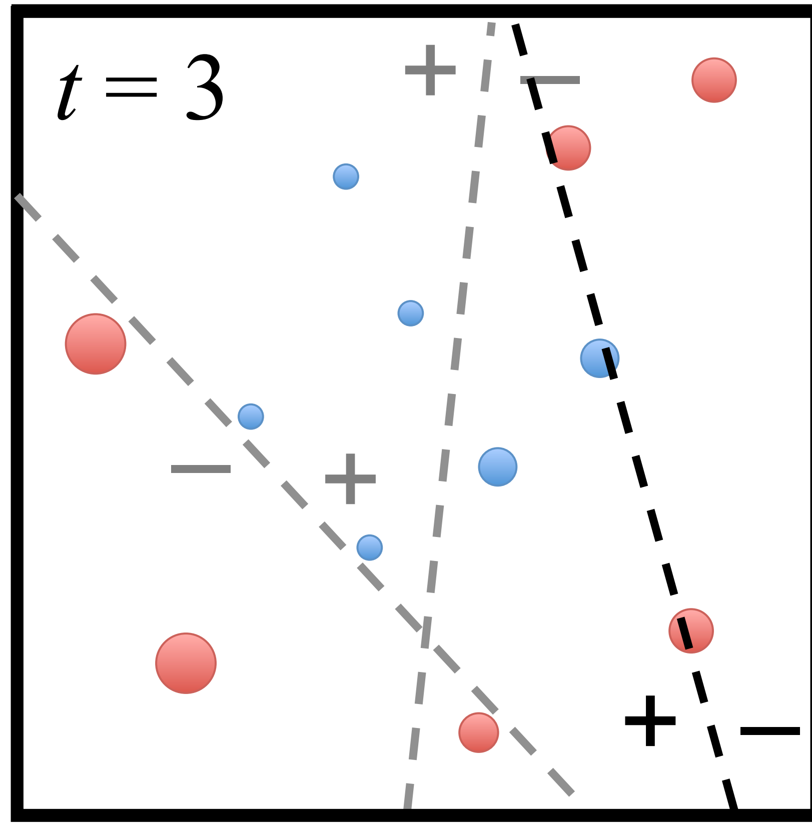

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AdaBoost

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:

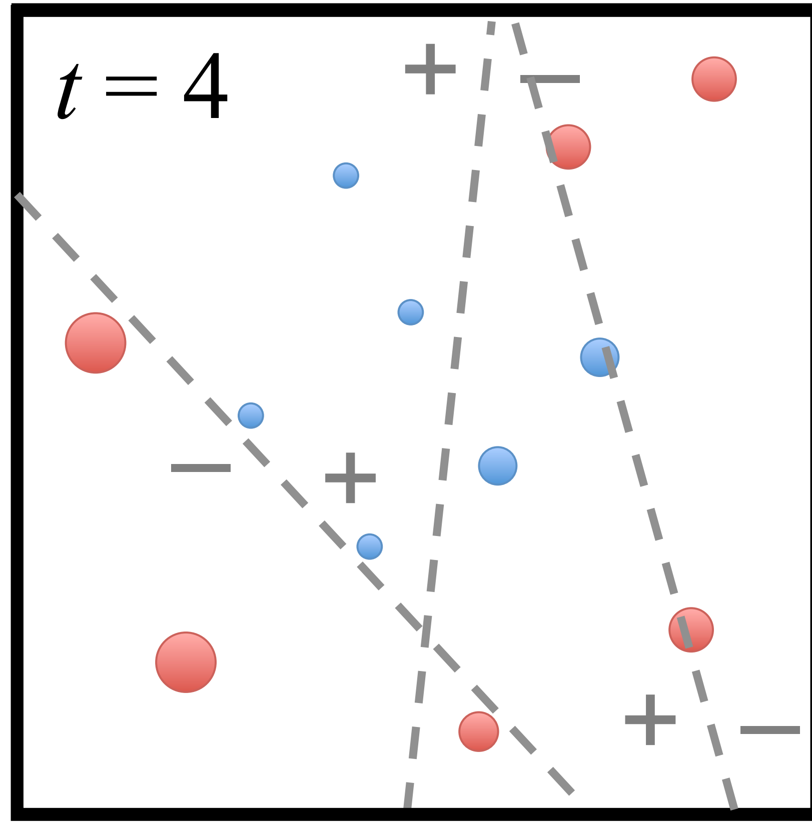
$$w_{t+1,i} = w_{t,i} \exp\left(-\beta_t y_i h_t(\mathbf{x}_i)\right)$$

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

8: **end for**

9: **Return** the hypothesis

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



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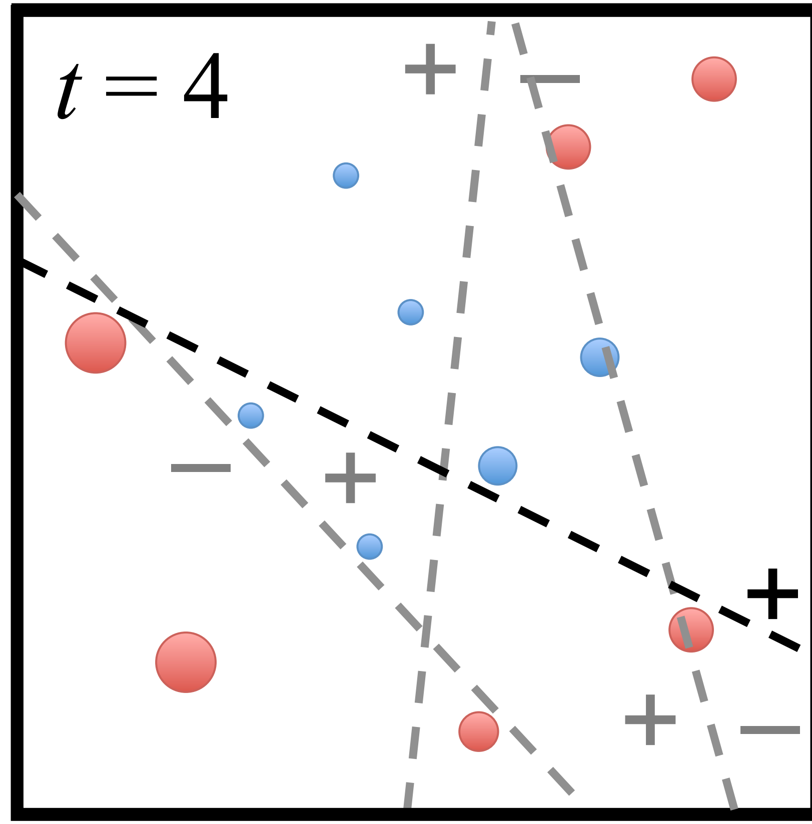

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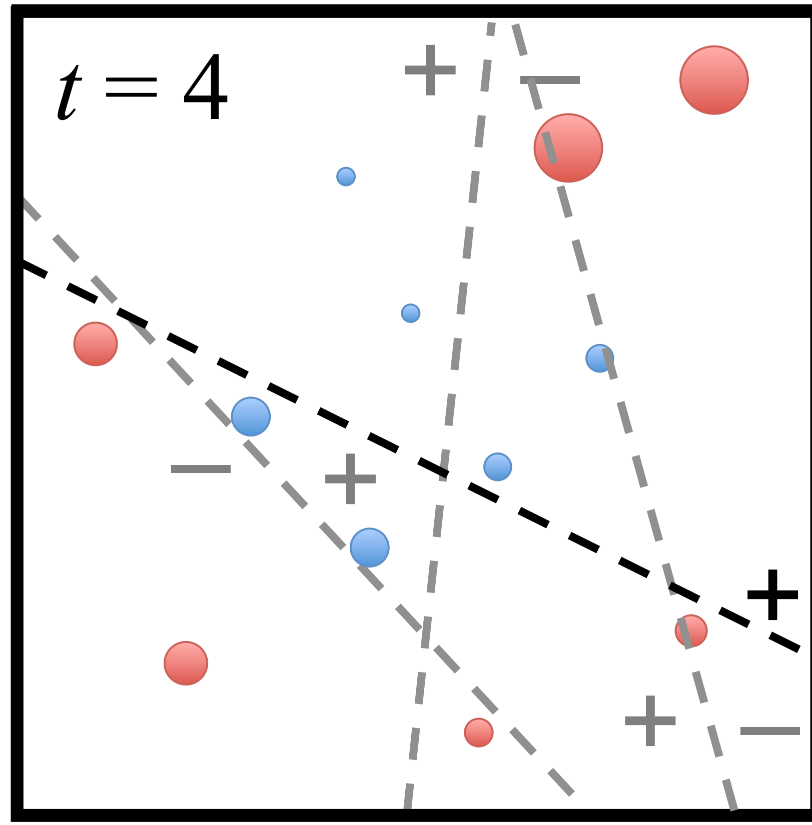

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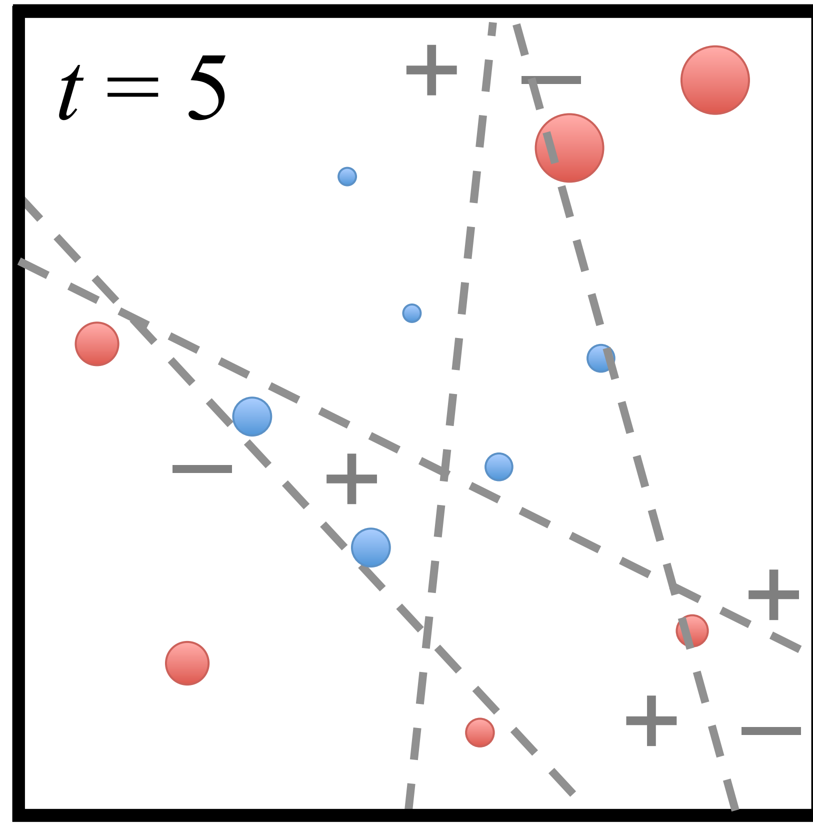

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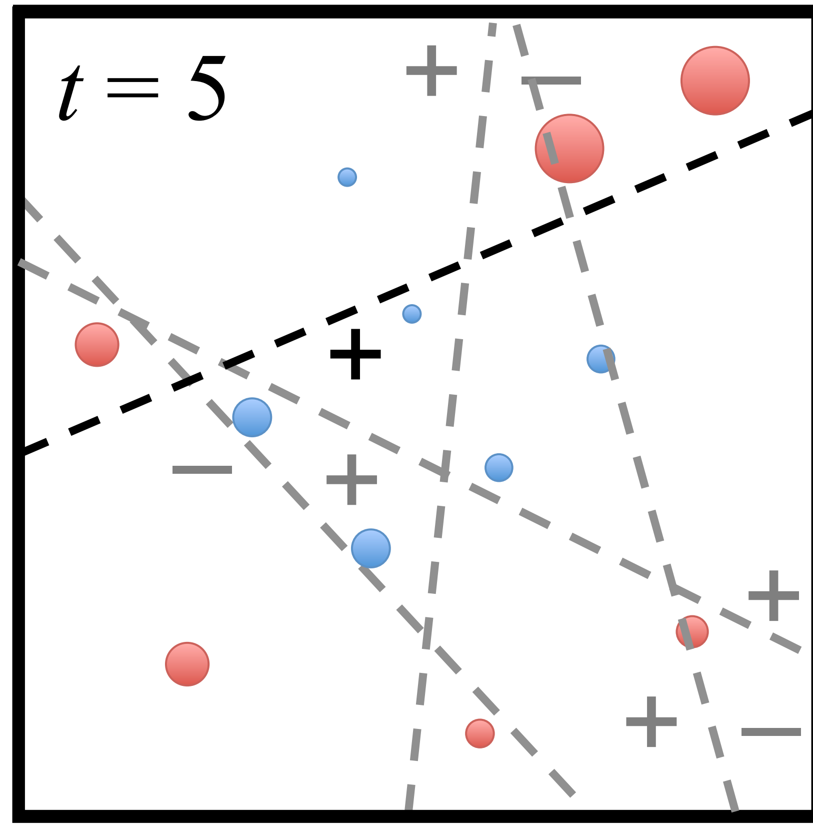

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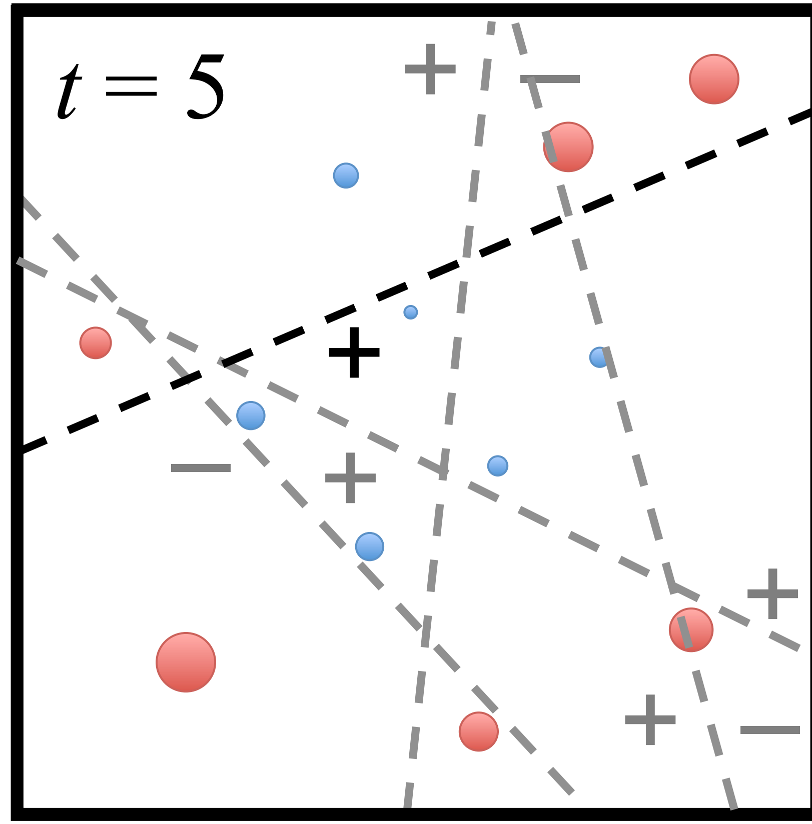

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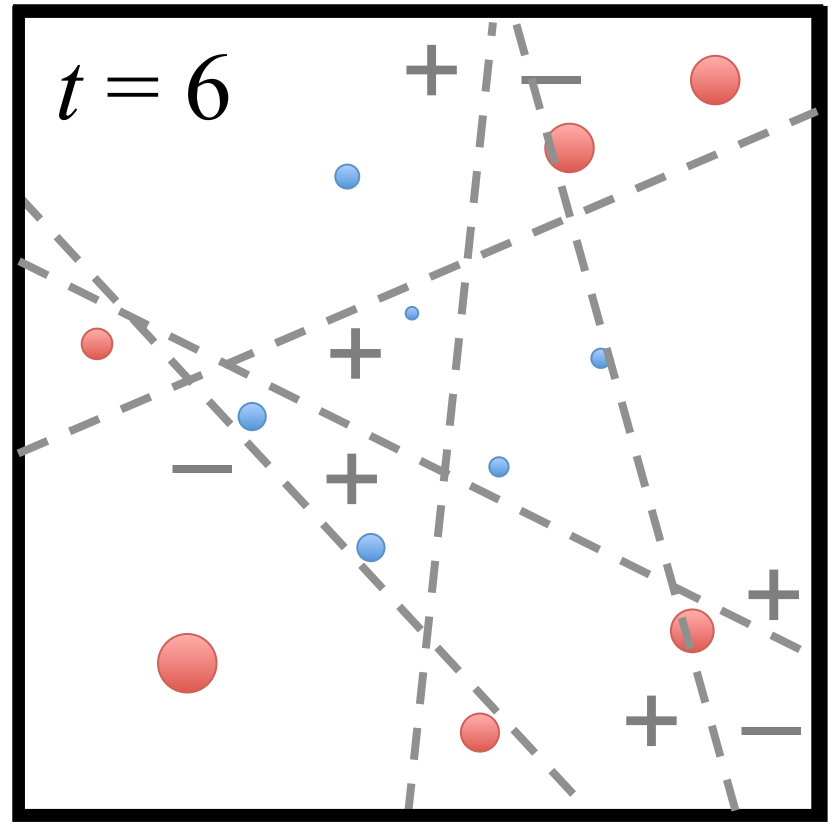

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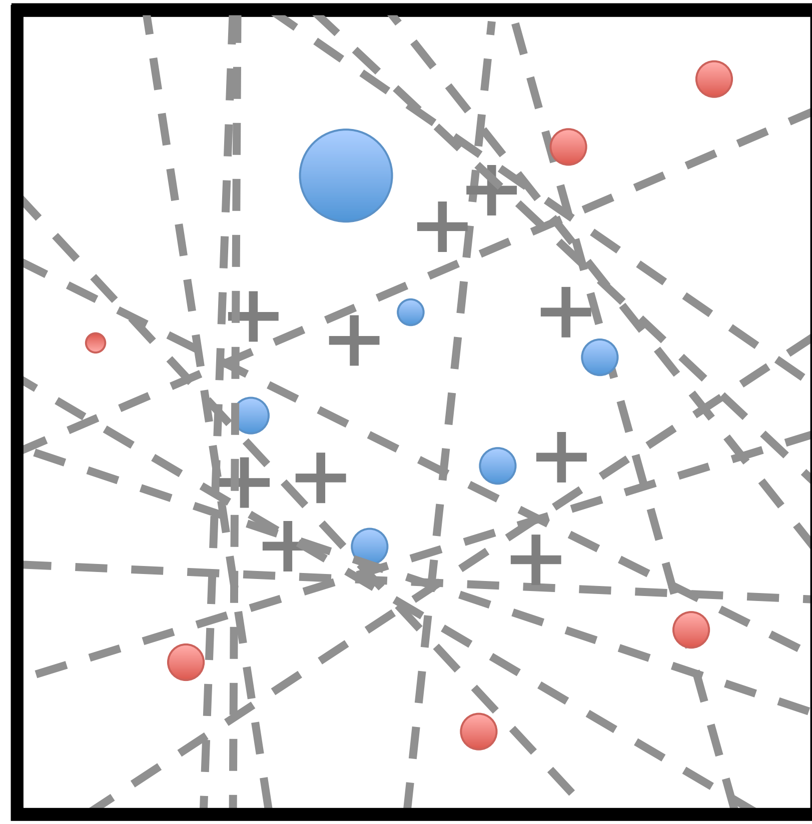

AdaBoost

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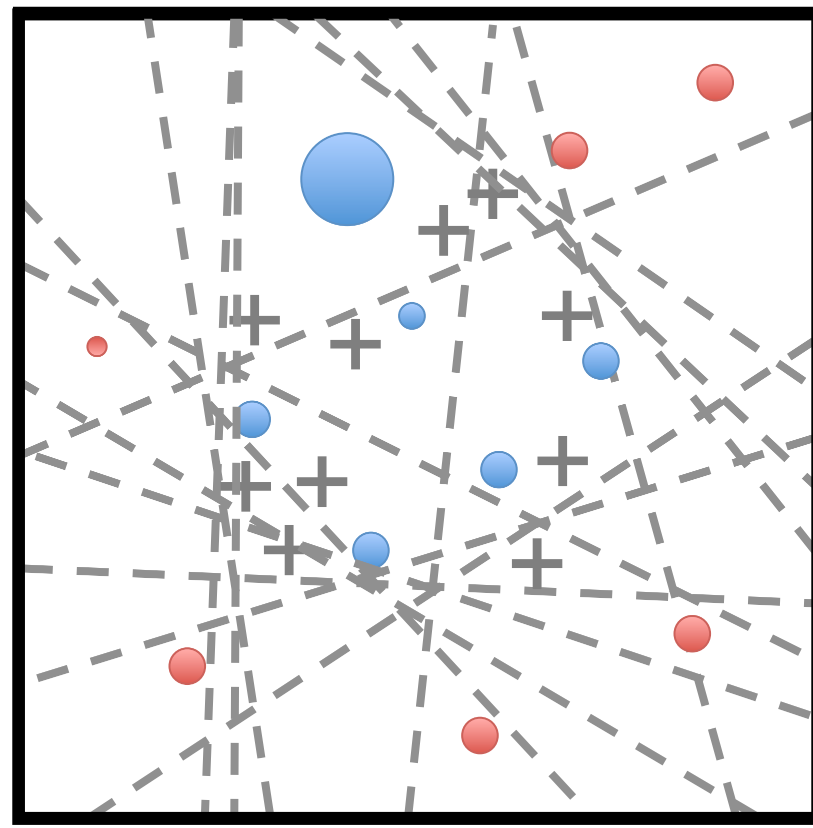

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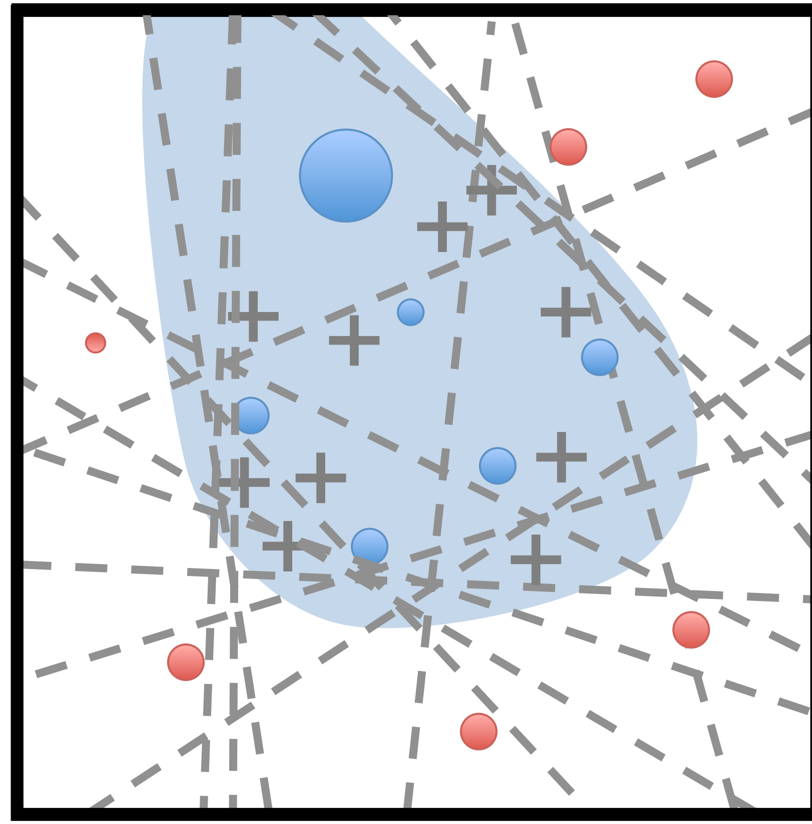

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    Normalize $\mathbf{w}_{t+1}$ to be a distribution
end for
Return the hypothesis

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

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

AdaBoost

[Freund & Schapire, 1997]

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:

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

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

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

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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  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

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

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

All points start with equal weight

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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end for
Return the hypothesis

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

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

Training a Model with Weighted Instances

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

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

- For algorithms that don't directly support instance weights (e.g., ID3 decision trees, etc.), use weighted bootstrap sampling
  - Form training set by resampling instances with replacement according to $\mathbf{w}$

Base Learner Requirements

- AdaBoost works best with "weak" learners
  - Should not be complex
  - Typically high bias classifiers
  - Works even when 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:

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

Error is the sum the weights of all misclassified instances

    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

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

AdaBoost

INPUT: training data $X, y = \{(\mathbf{x}_i, y_i)\}_{i=1}^{n}$,
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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 $\beta_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t} \right)$

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

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

end for

Return the hypothesis

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

- 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 vecto

for $t = 1, \ldots, T$

Train model

Compute the

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

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

Update all instance weights:

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

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

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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:

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

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:

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

end for

Return the hypothesis

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end for
Return the hypothesis

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

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 parts of the instance space
  - Instances with highest weight are often outliers

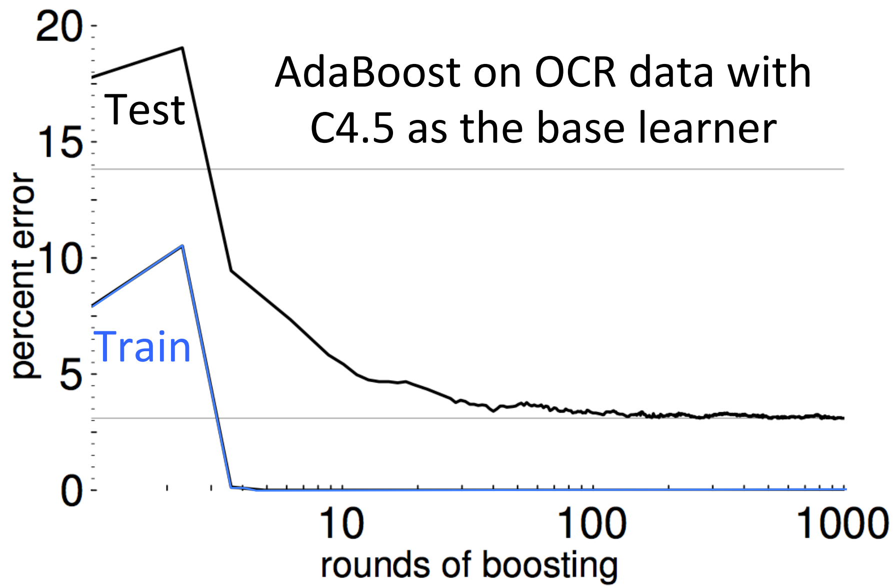
AdaBoost and Overfitting

- VC 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 VC theory

- Also, AdaBoost does not explicitly regularize the model

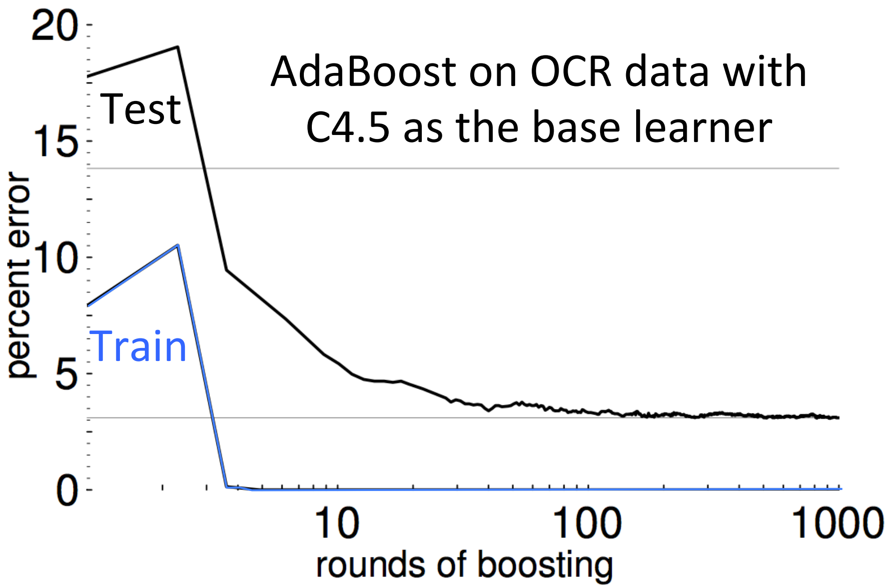
Explaining Why AdaBoost Works

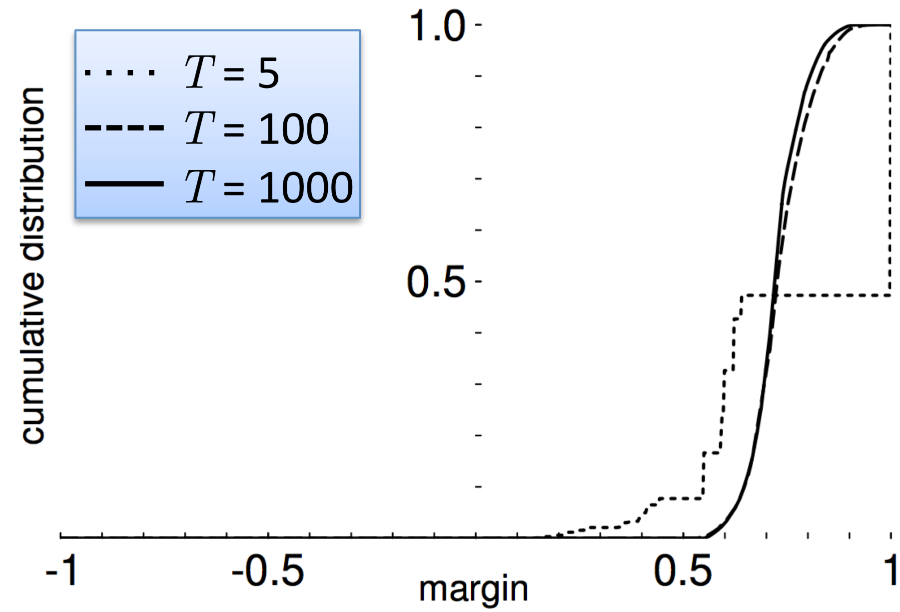


- Empirically, boosting resists overfitting
- Note that it continues to drive down the test error even AFTER the training error reaches zero

[Figure from Schapire: "Explaining AdaBoost"]

Explaining Why AdaBoost Works





- The "margins explanation" shows that boosting tries to increase the confidence in its predictions over time
  - Improves generalization performance
  - Effectively, boosting maximizes the margin!

[Figures from Schapire: "Explaining AdaBoost"]

AdaBoost in Practice

Strengths:

- Fast and simple to program
- No parameters to tune (besides T)
- No assumptions on weak learner

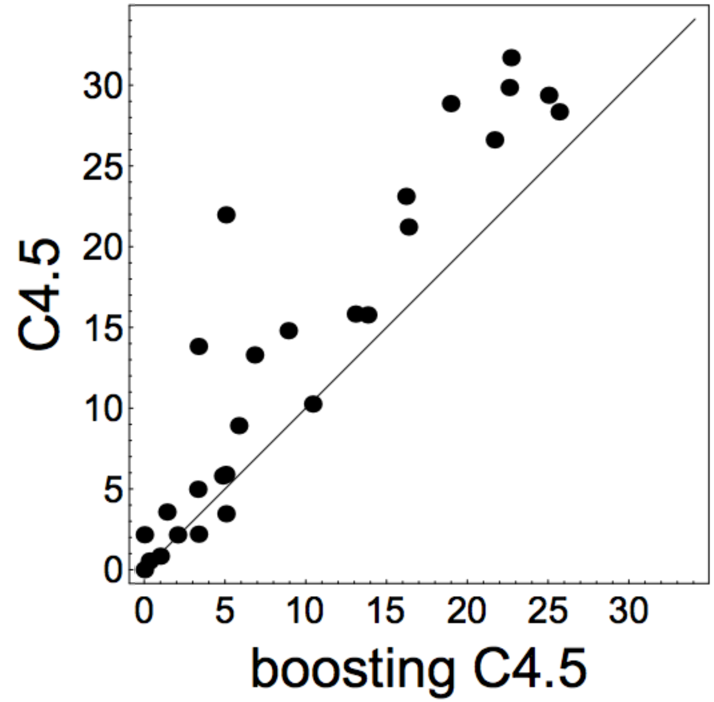
When boosting can fail:

- Given insufficient data
- Overly complex weak hypotheses
- Can be susceptible to noise
- When there are a large number of outliers

Boosted Decision Trees

- Boosted decision trees are one of the best "off-the-shelf" classifiers
  - i.e., no parameter tuning
- Limit member hypothesis complexity by limiting tree depth
- Gradient boosting methods are typically used with trees in practice

Error Rates on 27 Benchmark Data Sets



"AdaBoost with trees is the best off-the-shelf classifier in the world" -Breiman, 1996
(Also, see results by Caruana & Niculescu-Mizil, ICML 2006)

[Figure from Freud and Schapire: "A Short Introduction to Boosting"]