Machine Learning

Ensembles

Dan Goldwasser

dgoldwas@purdue.edu

Shattering

We say that a set S of examples is **shattered** by a set of functions H if for every partition of the examples in S into positive and negative examples there is a function in H that gives exactly these labels to the examples

Intuition: *A richer set of functions can shatter larger sets of points*

Determining the complexity of H:

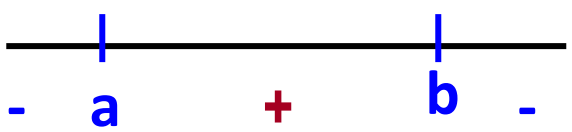
Show that there exists a set of points S of size K that functions in H are able to shatter

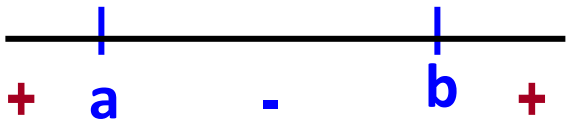
OR

Show that NO such set of points exists – all set of points of size K cannot be shattered by functions in H

Shattering

Intervals on the real axis: [a,b], for some real numbers b>a



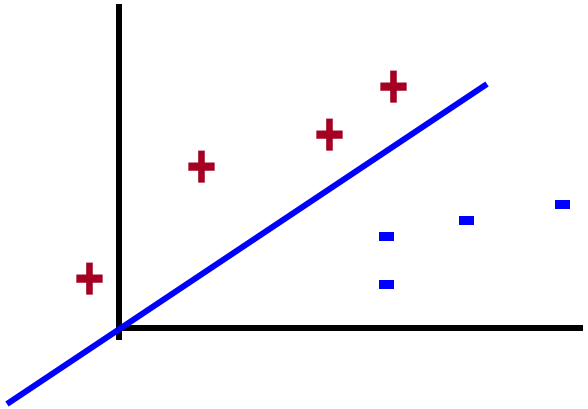


All sets of one or two points can be shattered
but sets of **three** points cannot be shattered

Shattering

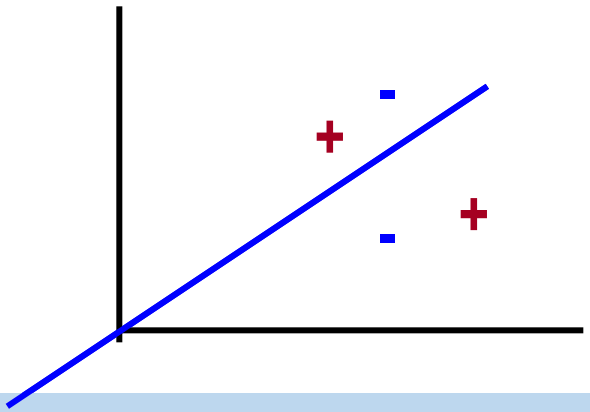
We say that a set S of examples is **shattered** by a set of functions H if for every partition of the examples in S into positive and negative examples there is a function in H that gives exactly these labels to the examples

Half-spaces in the plane:



Shattering

Half-spaces in the plane:



Can a set of one point be shattered?

Can a set of two points be shattered?

Can a set of three points be shattered?

Can a set of four points be shattered?

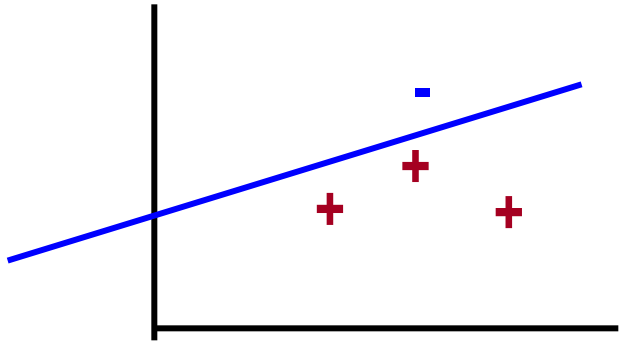
How can you show that a set of 4 points cannot be shattered?

1. If the 4 points form a convex polygon

2. If one point is in the convex hull defined by the other three

Shattering

Half-spaces in the plane:



Can a set of one point be shattered?

Can a set of two points be shattered?

Can a set of three points be shattered?

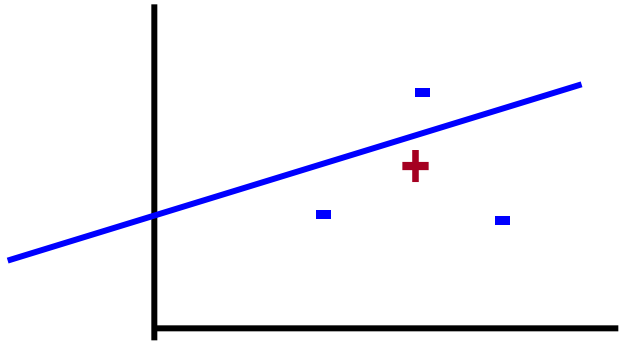
Can a set of four points be shattered?

How can you show that a set of 4 points cannot be shattered?

2. If one point is in the convex hull defined by the other three

Shattering

Half-spaces in the plane:



Can a set of one point be shattered?

Can a set of two points be shattered?

Can a set of three points be shattered?

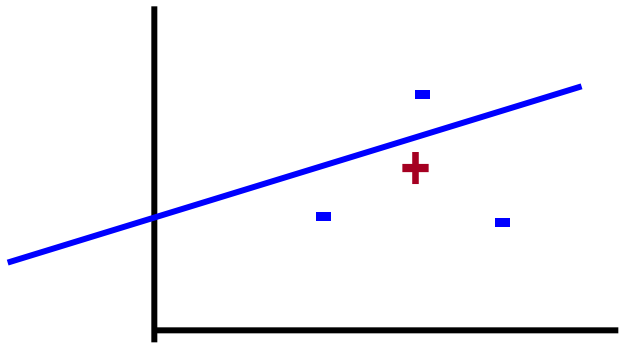
Can a set of four points be shattered?

How can you show that a set of 4 points cannot be shattered?

2. If one point is in the convex hull defined by the other three

Shattering

Half-spaces in the plane:



Conclusion for Half-spaces:

sets of one, two or three points can be shattered **but** there is no set of *four* points that can be shattered

VC Dimension

- A set S of examples is shattered by a set of functions H if for every partition of the examples in S into positive and negative examples there is a function in H that assigns similar labels.

- The VC dimension of hypothesis space H over instance space X is the size of the largest finite subset of X that is shattered by H.
  - ***Even if only one subset of this size does it***

VC Dimension

Direct Implication:

If there exists a subset of size d that can be shattered, then VC(H) >=d, If **no** subset of size d can be shattered, then VC(H) < d

- VC(Half intervals) = 1 (*no subset of size 2 can be shattered*)
- VC(Intervals) = 2 (*no subset of size 3 can be shattered*)
- VC(Half-spaces in the plane) = 3 (*no subset of size 4 can be shattered*)

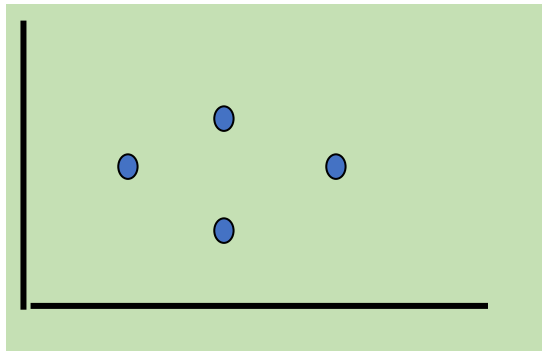
Sample Complexity & VC Dimension

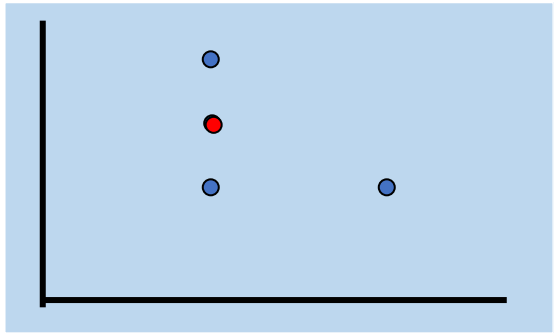
- Using VC(H) as a measure of expressiveness we have an Occam algorithm for infinite hypothesis spaces.
- Given a sample D of m examples, find some $h \in H$ that is consistent with all m examples

$$m > \frac{1}{\varepsilon}\{8VC(H)\log\frac{13}{\varepsilon} + 4\log(\frac{2}{\delta})\}$$

Learning Axis Parallel Rectangles

- Consider axis parallel rectangles
- Can we PAC learn it ?
  1. **What is the VC dimension ?**





Can a set of ***one*** point be shattered?

Can a set of ***two*** points be shattered?

Can a set of ***three*** points be shattered?

Can a set of ***four*** points be shattered?

We found one set of points that can be shattered! VC(H) >= 4

Learning Axis Parallel Rectangles

- Consider axis parallel rectangles
- Can we PAC learn it ?
  1. **What is the VC dimension ?**

Can a set of ***one*** point be shattered?

Can a set of ***two*** points be shattered?

Can a set of ***three*** points be shattered?

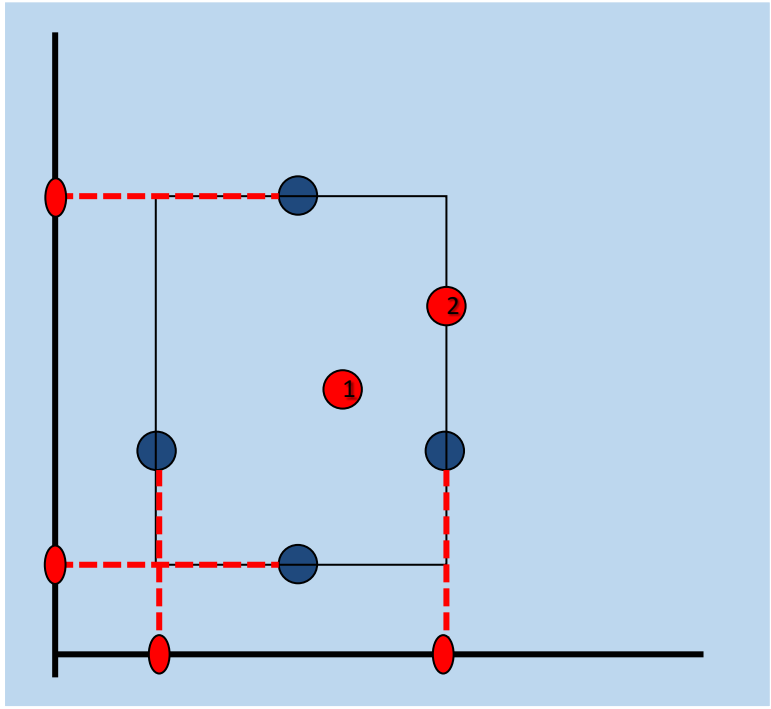
Can a set of ***four*** points be shattered?

Can a set of ***five*** points be shattered?

Learning Axis Parallel Rectangles

- Consider axis parallel rectangles
- Can we PAC learn it ?
  1. **What is the VC dimension ?**

Can a set of ***five*** points be shattered?

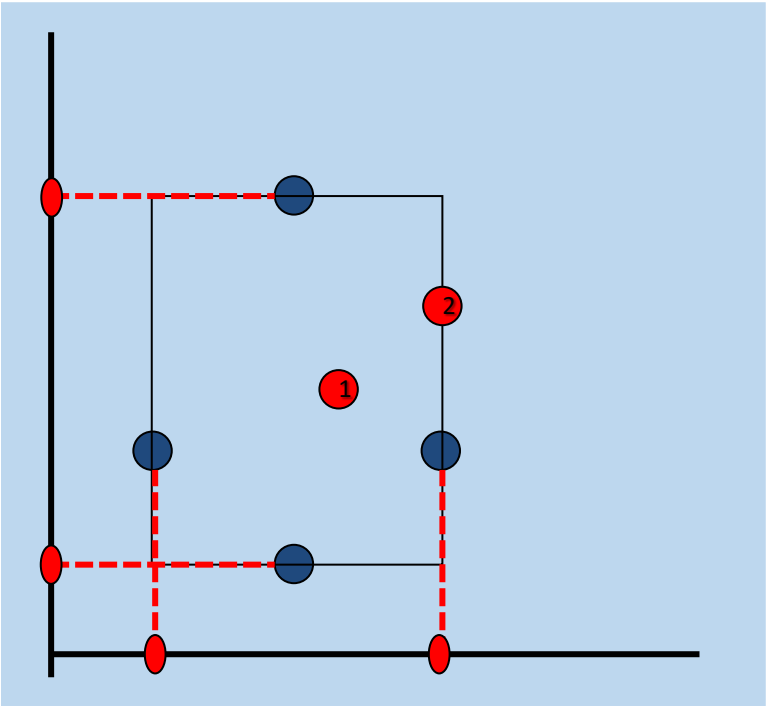


Consider the rectangle defined by *the min-x,max-x, min-y, max-y* values of the four extreme points. The fifth point must lie either inside the rectangle or on the edges

➔ For either case it is possible to come up with a label assignment that cannot be represented using an axis parallel rectangle

Learning Axis Parallel Rectangles

- Consider axis parallel rectangles
- Can we PAC learn it ?
  1. **What is the VC dimension ?**



Can a set of ***five*** points be shattered?

No set of five points can be shattered!

➔ VC(H) = 4

As far as sample complexity, *PAC learnability* is guaranteed.

And now to something completely different

…. Ensemble methods

Ensemble Learning Algorithms

- **Simple idea**: *combine the predictions of multiple classifiers*
- *Don't repeat the same classification multiple times*
  - *combine different classifiers, train over different datasets, use different feature representation.*
- **Intuition**: *"wisdom of the crowds" principle*
  - *Many non-experts can perform better*

Ensemble Learning Algorithms

- **Simple idea**: *combine the predictions of multiple classifiers*
- *Many ways to combine the classifiers:*
  - *Majority vote, weighted vote, confidence-based,..*
- *For example:*

$$y_1 = f_1(x, w)$$
$$y_2 = f_1(x, w) \quad \Rightarrow \quad y_{final} = Sign\left(\sum_i \alpha_i y_i\right)$$
$$y_3 = f_1(x, w)$$
$$\ldots$$

Where have we seen it before?

Ensemble Learning Algorithms

- In this lecture we will talk about two ensembles
  - Boosting
  - Bagging

- Both combine classifiers of the **same type**, multiple times by modifying the training set

- **Big idea**: *The methods will be used to help control the **bias** and **variance** in a different way*

http://cseweb.ucsd.edu/~yfreund/adaboost/

Boosting

- Boosting is a general learning paradigm for putting together a **Strong Learner**, given a collection of Weak Learners.
- The original Boosting Algorithm was proposed as an answer to a theoretical question in PAC learning.
  - [The Strength of Weak Learnability; Schapire, 89]
- Importance: Theoretical and Practical
  - Strong and weak learners in the **PAC framework**
- **Intuition:** reducing bias by increasing the complexity of simple classifiers

Boosting Motivation

Example: "How May I Help You?"

[Gorin et al.]

- goal: automatically categorize type of call requested by phone customer (Collect, CallingCard, PersonToPerson, etc.)
  - `yes I'd like to place a collect call long distance please` (Collect)
  - `operator I need to make a call but I need to bill it to my office` (ThirdNumber)
  - `yes I'd like to place a call on my master card please` (CallingCard)
  - `I just called a number in sioux city and I musta rang the wrong number because I got the wrong party and I would like to have that taken off of my bill` (BillingCredit)
- observation:
  - easy to find "rules of thumb" that are "often" correct
    - e.g.: "IF '`card`' occurs in utterance THEN predict 'CallingCard' "
  - hard to find single highly accurate prediction rule

Rules-of-thumb are accurate but have a **low** recall

The Boosting Approach

- **Algorithm**
  - Select a small subset of examples
  - Derive a rough rule of thumb
  - Examine 2nd set of examples
  - Derive 2nd rule of thumb
  - Repeat T times
  - Combine the learned rules into a single hypothesis
- **Questions**:
  - *How to choose subsets of examples to examine on each round?*
    - ***Emphasize*** *subsets instead of selecting subsets*
  - How to combine all the rules into single prediction rule?
- **Boosting**
  - General method of converting rough rules of thumb into highly accurate prediction rule

Note the design decisions made:
- Rules-of-thumb
- Small sub-set of examples

Theoretical Motivation

- **"Strong" PAC algorithm *(for class H):***
  - for *any distribution*
  - $\forall\ \varepsilon, \delta > 0$
  - Given polynomially many random examples
  - Finds hypothesis with error $\leq \varepsilon$ with probability $\geq (1-\delta)$

- **"Weak" PAC algorithm**
  - Same, but only for $\varepsilon \geq \frac{1}{2} - \gamma$

Not trivial: for any distribution you can find a hypothesis that performs better than chance (for any training set)

- [Kearns & Valiant '88]:
  - *Does weak learnability imply strong learnability?*
    - *I.e., "can we boost a better-than-chance learner to be as good as we want it to be?"*

History

- [Schapire ’89]:
  - **First provable boosting algorithm**
    - Call weak learner three times on three modified distributions
    - Get slight boost in accuracy
    - apply recursively
- [Freund ’90]:
  - “Optimal” algorithm that “**boosts by majority**”
- [Drucker, Schapire & Simard ’92]:
  - **First practical experiments** using boosting
  - Limited by *practical drawbacks*
- [Freund & Schapire ’95]:
  - Introduced “AdaBoost” algorithm
  - Strong practical advantages over previous algorithms
  - AdaBoost was followed by a huge number of papers and practical applications

A Formal View of Boosting

- Given training set $(x_1, x_1), \ldots, (x_m, y_m)$
- $y_i \in \{-1, +1\}$ is the correct label of instance $x_i \in X$
- For t = 1, …, T
  - Construct a distribution D_t on {1,…m}
  - Find weak hypothesis ("*rule of thumb*") $h_t : X \to \{-1, +1\}$

with small error ϵ_t on D_t: $\epsilon_t = P_{D_t}[h_t(x_i) \neq y_i]$

Error is measured according to the distribution at step t!

- **Output**: final hypothesis H_{final}

Source: A Tutorial on Boosting Yoav Freund, Rob Schapire

How can we construct the distribution?

Constructing D_t on {1,..,m}:

$$D_1(i) = \frac{1}{m}$$

Initialization : Construct the **uniform distribution**

Given D_t and h_t :

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if} \quad y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if} \quad y_i \neq h_t(x_i) \end{cases}$$

$$= \frac{D_t(i)}{Z_t} \cdot e^{(-\alpha_t y_i h_t(x_i))}$$

Next : Given the old distribution (D_t), construct the new distribution (D_{t+1}), by **assigning weight to each example**

How can we construct the distribution?

Constructing D_t on {1,..,m}:

$$D_1(i) = \frac{1}{m}$$

The **old distribution** divided by a **normalization factor** (constant)

Given D_t and h_t:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if} \quad y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if} \quad y_i \neq h_t(x_i) \end{cases}$$

$$= \frac{D_t(i)}{Z_t} \cdot e^{(-\alpha_t y_i h_t(x_i))}$$

Multiplied by **penalty** term for **correct** classification, and a **promotion** term for **mistakes**

Where:

Z_t = Normalization constant

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right) > 0$$

Positive due to the weak learning assumption

Examples that we predicted correctly are demoted, others promoted

How can we construct the distribution?

Constructing D_t on {1,..,m}:

$$D_1(i) = \frac{1}{m}$$

Given D_t and h_t:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if} \quad y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if} \quad y_i \neq h_t(x_i) \end{cases}$$

$$= \frac{D_t(i)}{Z_t} \cdot e^{(-\alpha_t y_i h_t(x_i))}$$

Where:

Z_t = Normalization constant

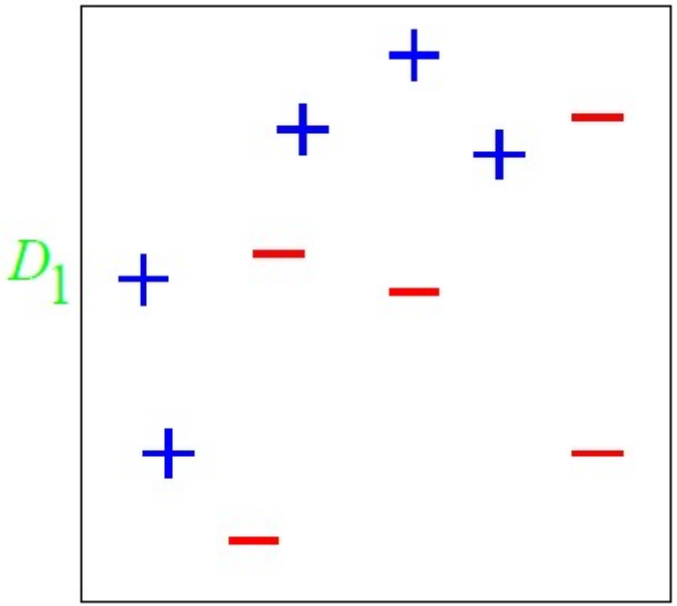
$$\alpha_t = \frac{1}{2} \ln \left(\frac{1-\epsilon_t}{\epsilon_t}\right) > 0$$

Note that the weight of each hypothesis correlates with its error

Final Hypothesis:

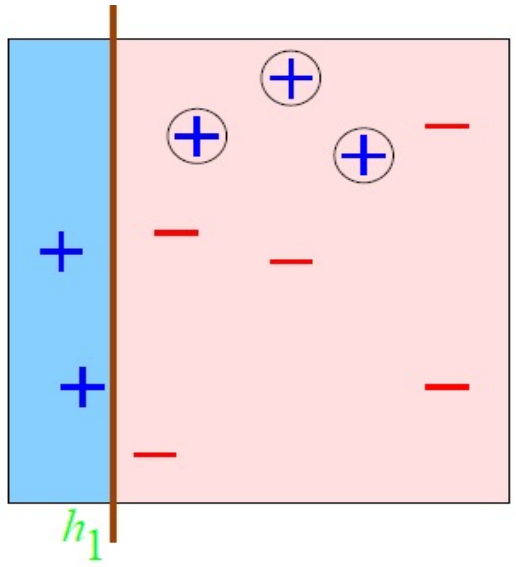
$$H_{\text{final}}(x) = \text{sign}\left(\sum_t \alpha_t h_t(x)\right)$$

A Toy Example



Weak learner: axis parallel lines

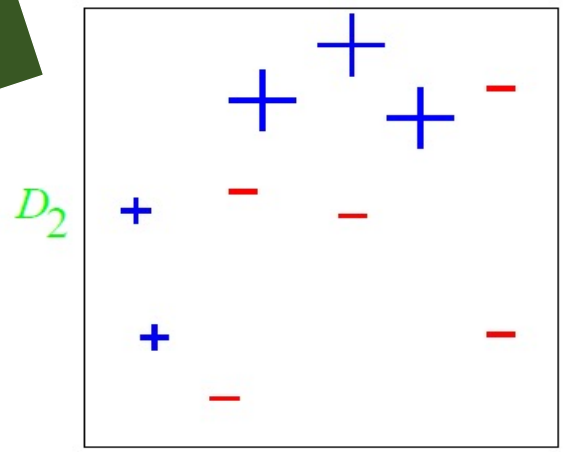
A Toy Example: **Round 1**



Weak learner h_1
Three mistakes under the **uniform** distribution

$$\epsilon_1 = 0.3$$
$$\alpha_1 = 0.42$$

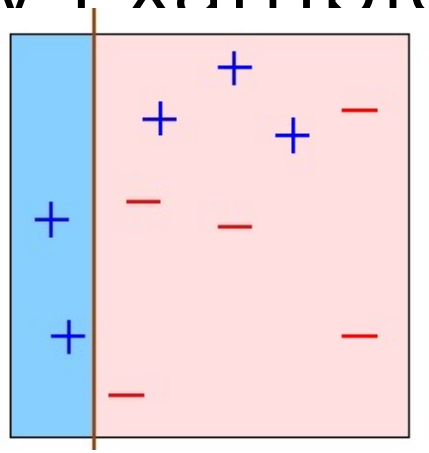
Generate a **new probability distribution** over the data



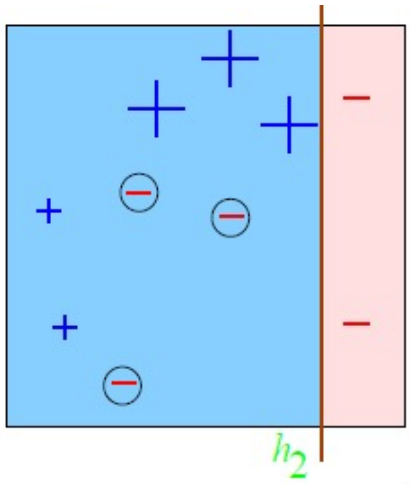
What is the effect of increasing the probability of examples with wrong classification?

The error of the current classifier will rise over the new distribution
(So what?)

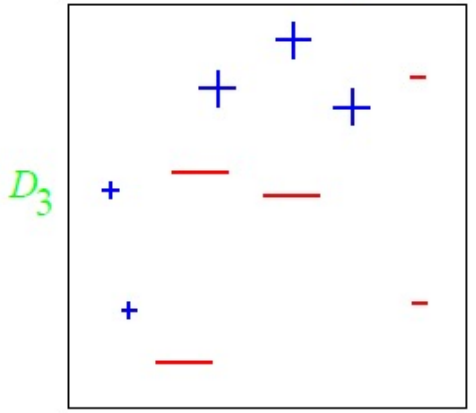
A Toy Example: Round 2



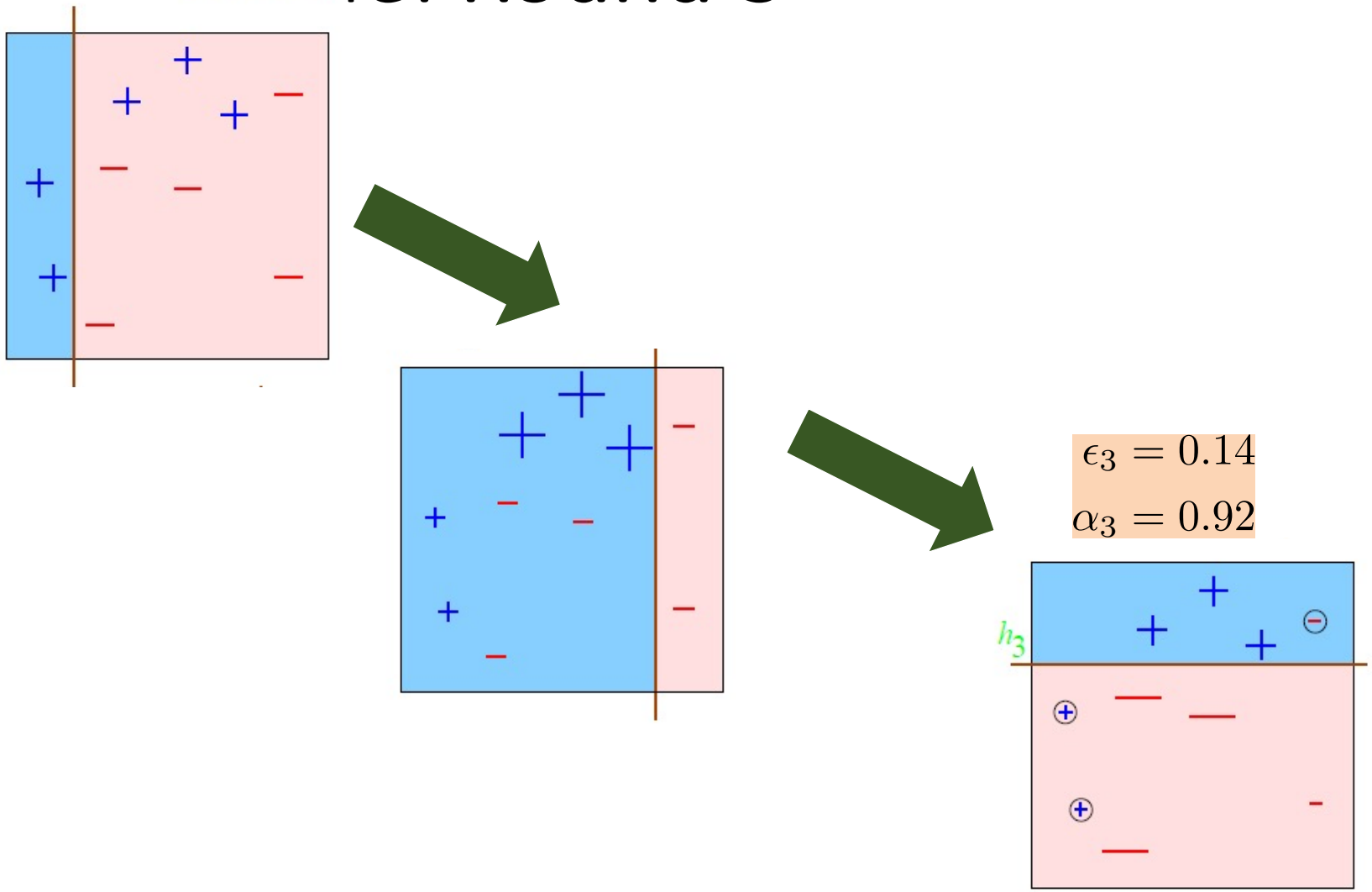
Weak learner h_1
Three mistakes under the **uniform** distribution



$$\epsilon_2 = 0.21$$
$$\alpha_2 = 0.65$$

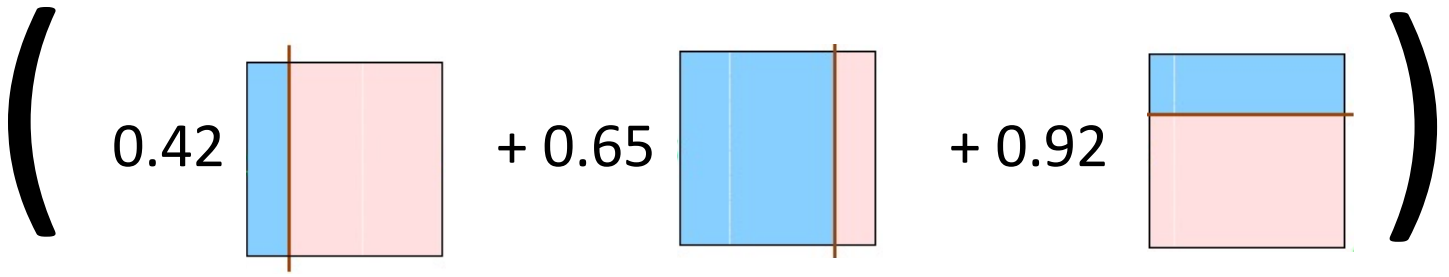


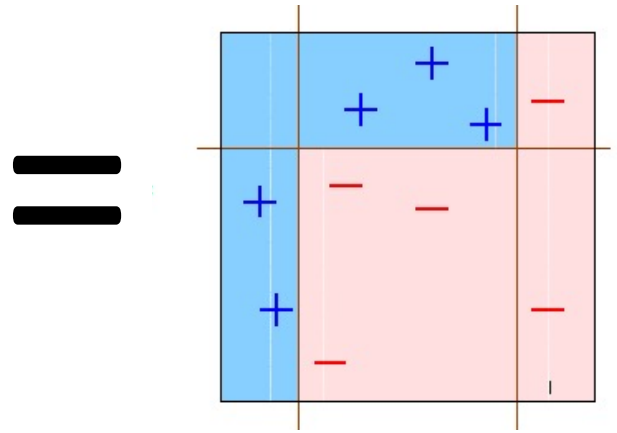
A Toy Example: Round 3



A Toy Example: Final Hypothesis

$$H_{Final} =$$





Note: It is possible that the combined hypothesis makes no mistakes on the training data, but boosting can still learn, by adding more weak hypotheses.

Analyzing Adaboost

Theorem:

- Run AdaBoost for T rounds
- Let $\epsilon_t = ½ - \gamma_t$
- Let $0 < \gamma \leq \gamma_t$ for all t
- Then: *Training error* (H_{final}) $\leq \prod_t \left[2\sqrt{\epsilon_t(1-\epsilon_t)}\right]$

$$= \prod_t \sqrt{1-4\gamma_t^2}$$

$$\leq e^{(-2\sum_t \gamma^2)}$$

Do we care about the training error?

As T (number of iterations) increases, the training error drop exponentially!

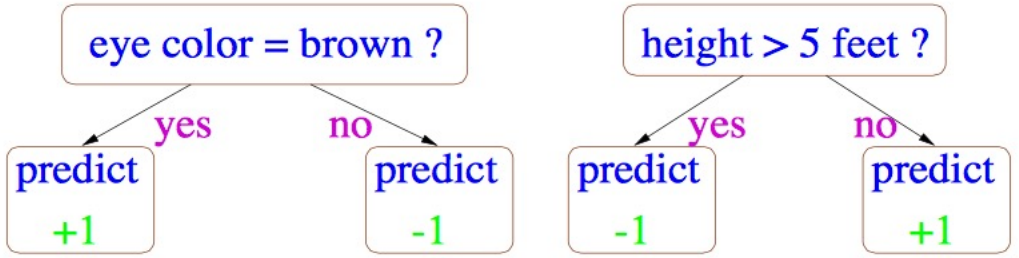
AdaBoost in practice

- **Initialization**:
  - *Weigh all training samples equally*
- **Iteration Step:**
  - Train model on (weighted) train set
  - Compute error of model on train set
  - Increase weights on training cases model gets wrong
    - Focus the next classifier on “difficult” examples
- *Slow convergence*
  - *Typically requires 100’s to 1000’s of iterations*
- **Return final model:**
  - Carefully weighted prediction of each model

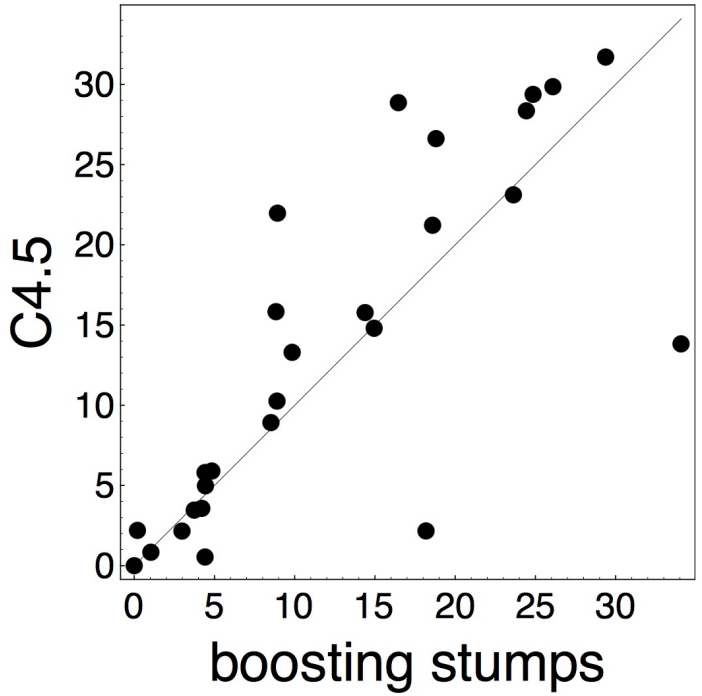
Key idea: change the distribution during training

36

AdaBoost in practice: Boosting Decision Stumps



Decision Stumps:
decision rule splitting on one attribute

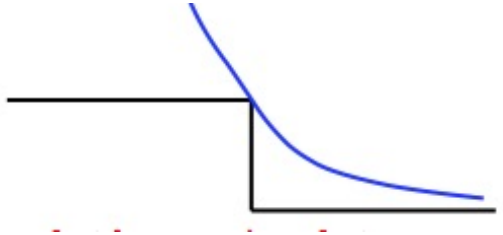


AdaBoost in practice: Loss minimization

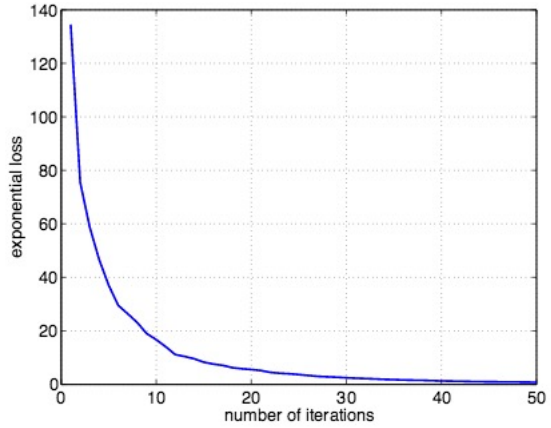
- *AdaBoost corresponds to minimizing the Exponential loss function*

$$C_{ada} = \sum_i \exp[-y^{(i)} f(x^i)]$$

- *Convex and smooth surrogate loss function*

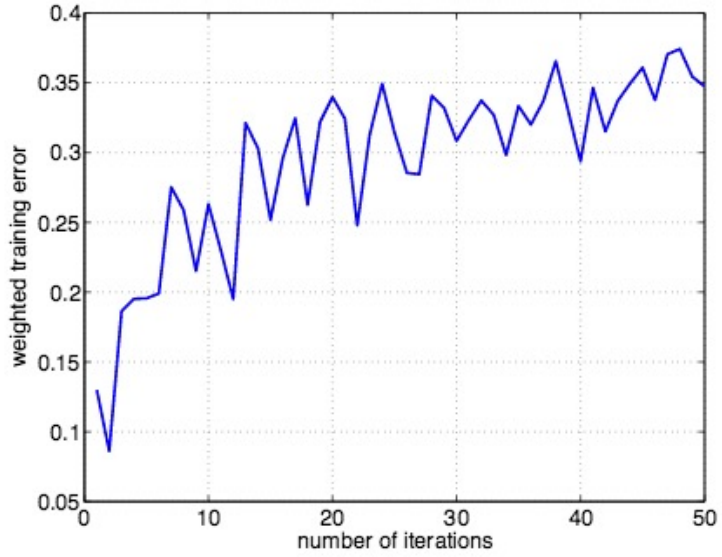


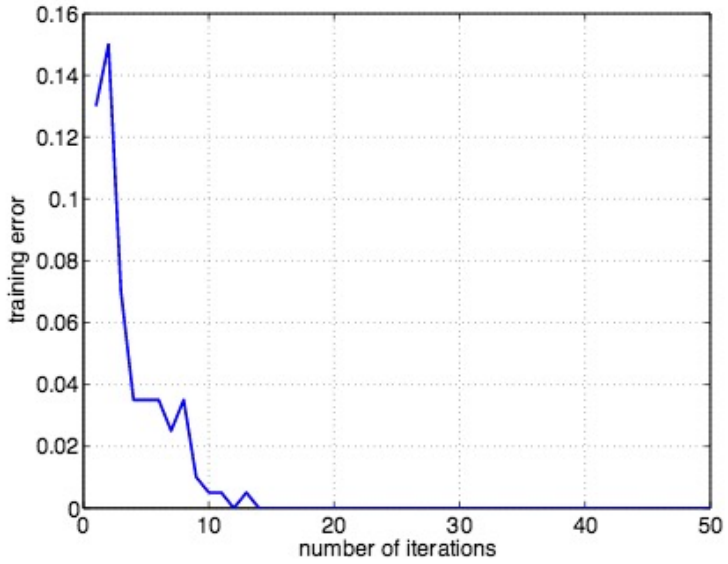
- At each iteration, it will have a lower exponential loss



AdaBoost in practice

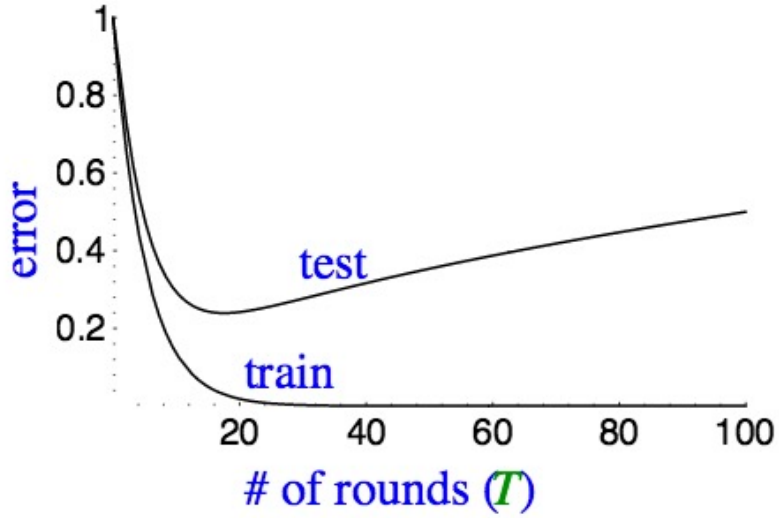
- *Note the difference between the **individual classifiers** (that tend to get worse over time), and the **combined hypothesis** (that improves over time)*





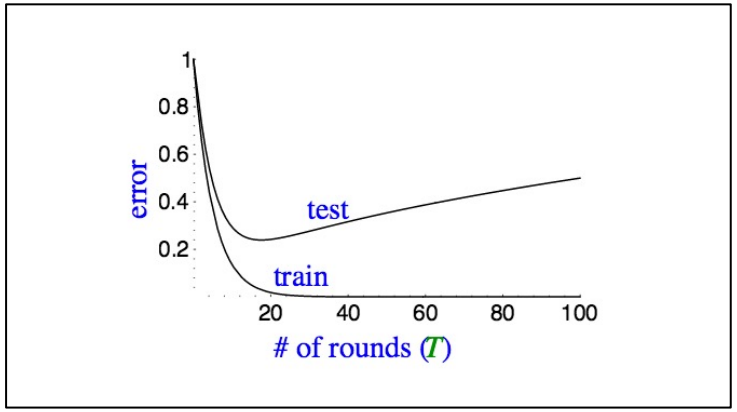
AdaBoost at Test time

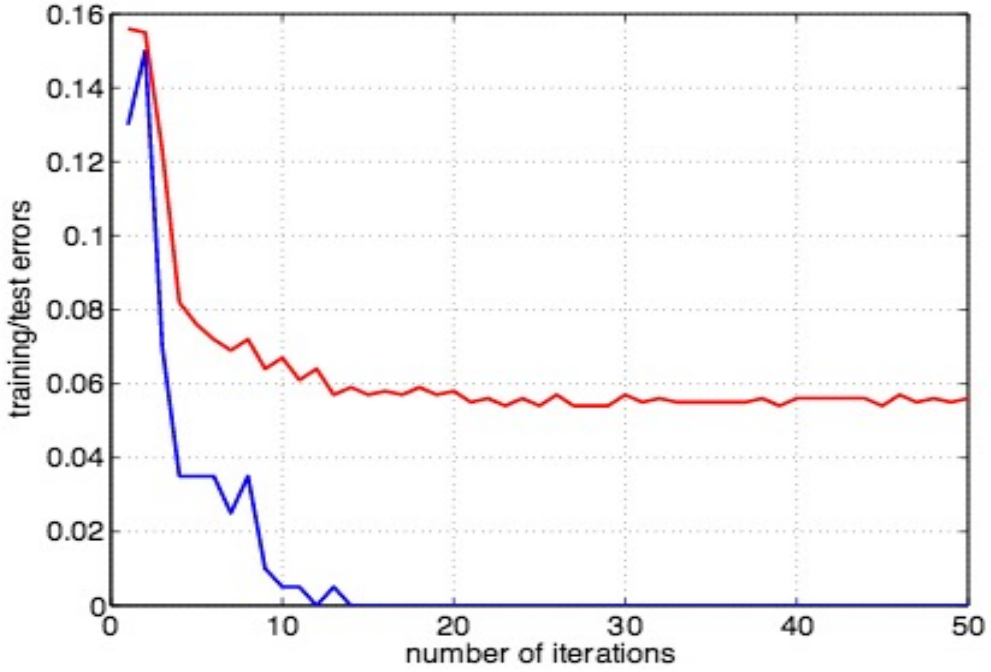
- The training error will reach zero (or keep decreasing) as we make the hypothesis more complex
- As a result, the test error will start increasing as the final hypothesis becomes overly complex



AdaBoost in practice

Interestingly, it does not happen!





Two observations:

(1) Adaboost does not over fit easily

(2)The *test error* can continue to decrease even when we already have *zero training error*

Boosting Summary

- Combine weak learners into a powerful learner
- Reduce bias without increasing variance!
- **Strong points**:
  - Effective and easy to implement
  - You can plug in your favorite learner
  - Only hyperparameter is T
- **Caveats**
  - Will overfit if the weak learners are too complex
  - Will underfit if the weak learners are too weak
    - $\gamma_t \rightarrow 0$ too quickly

Bagging

- **Bagging Intuition:**
  - Overfitting occurs when the model start memorizing the data (no generalization)
  - Variations in the data will results in different models
  - Bagging: **bootstrapped Aggregation**
    - Sample smaller sets of the data, each specific learner cannot memorize the entire dataset
  - Appropriate for: *Low bias-High Variance learners* (e.g., expressive learners)
    - Helps reduce variance!

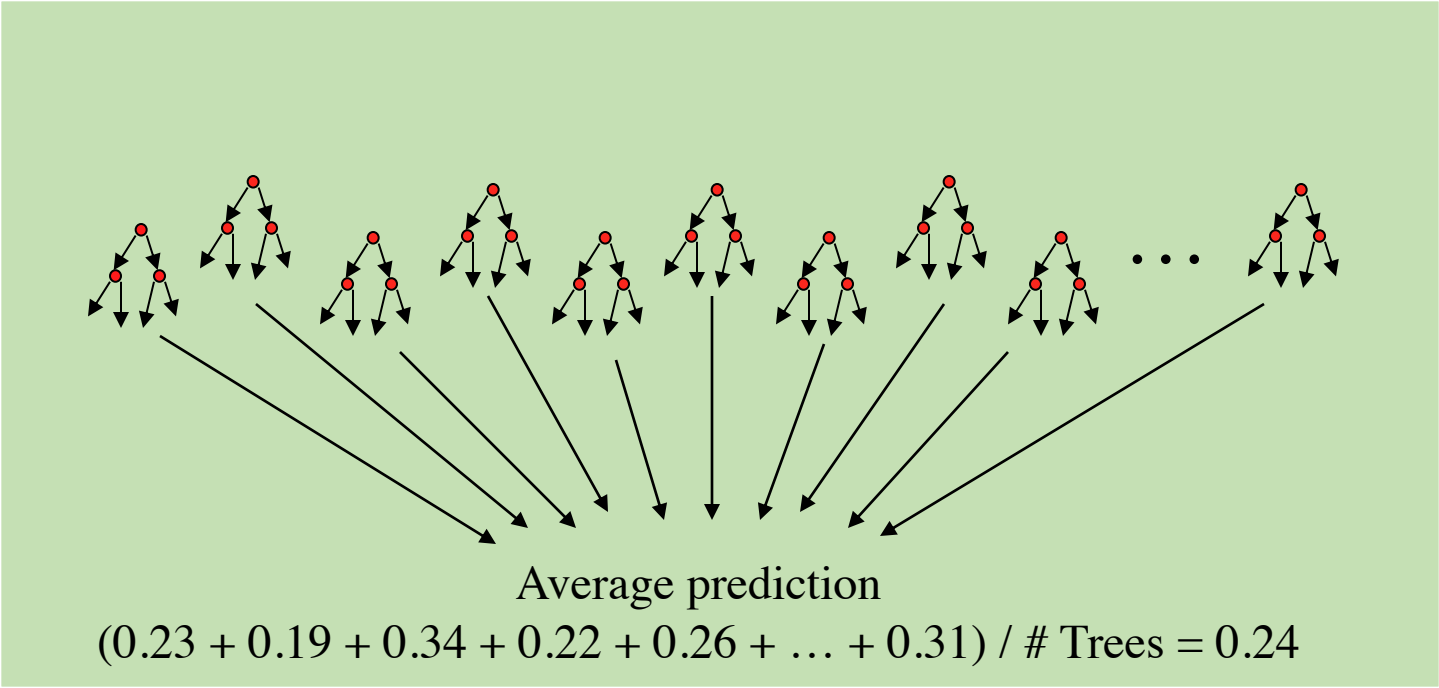
Bagging

- Bagging predictors generates multiple versions of a predictor and uses these to get an **aggregated predictor**
- The aggregation **averages over the versions** when predicting a numerical value and a **majority vote** when predicting a class.
- The multiple versions are formed by making bootstrap replicates of the learning set and using these as new learning sets.
  - *That is, use samples of the data, with repetition*

- The vital element is the **instability of the prediction** method. If perturbing the learning set can cause significant changes in the predictor constructed then bagging can improve accuracy.

Example: Bagged Decision Trees

- Draw 100 bootstrap samples of data
- Train trees on each sample → 100 trees
- Average prediction of trees on test examples (or majority vote)



Random Forests (*Bagged Trees*++)

Key idea: sample data (bagging) + sample features

- Draw ***1000+*** bootstrap samples of data
- ***Draw sample of available attributes at each split***
- Train trees on each sample/attribute set → ***1000+*** trees
- Average prediction of trees on out-of-bag samples