Boosting and Ensembles

Lecture 9

Machine Learning
Fall 2015

THE UNIVERSITY OF UTAH

Some slides based on materials by Yoav Freund, Rob Schapire, Dan Roth, Tommi Jakkola and others

Boosting and Ensembles

- What is boosting?
- AdaBoost
- Ensemble methods

Boosting and Ensembles

- What is boosting?
- AdaBoost
- Ensemble methods

Boosting

- A general learning approach for constructing a *strong learner*, given a collection of (possibly infinite) weak learners

- Historically: An answer to a theoretical question in PAC learning

The Strength of Weak Learnability

ROBERT E. SCHAPIRE 1989-90

Practically useful

- Boosting is a way to create a strong learner using only weak learners (also known as "rules of thumb")

- An *Ensemble method*
  - A class of learning algorithms that composes classifiers using other classifiers as building blocks
  - Boosting has stronger theoretical guarantees than other ensemble methods

Example: How may I help you?

Goal: Automatically categorize type of phone call requested by a phone customer

- "yes I'd like to place a collect call please" $\rightarrow$ `Collect`
- "Operator I need to make a call but need to bill it to my office" $\rightarrow$ `ThirdNumber`
- "I'd like to place my call on my master card please" $\rightarrow$ `CallingCard`

Important observation

"Rules of thumb" are *often* correct

Eg: If *card* occurs in the utterance, then predit `CallingCard`

But hard to find a single prediction rule

One boosting approach

- Select a small subset of examples
- Derive a rough rule of thumb
- Example a second set of examples
- Derive a second rule of thumb
- Repeat T times…
- Combine rules of thumb into a single prediction rule

Need to specify:
How to select these subsets?

Need to specify:
How to combine these rules of thumb?

Boosting: A general method for converting rough rules of thumb into accurate prediction classifiers

Boosting: The formal problem setup

- Strong PAC algorithm
  - For any distribution over examples,
  - For every $\epsilon > 0$, $\delta > 0$,
  - Given a polynomially many random examples
  - Finds a hypothesis with error $\leq \epsilon$ with probability $\geq 1 - \delta$
- Weak PAC algorithm
  - Same, but only for $\epsilon \geq ½ - \gamma$
- Question [Kearns and Valiant '88]:
  - Does weak learnability imply strong learnability?

History: Early boosting algorithms

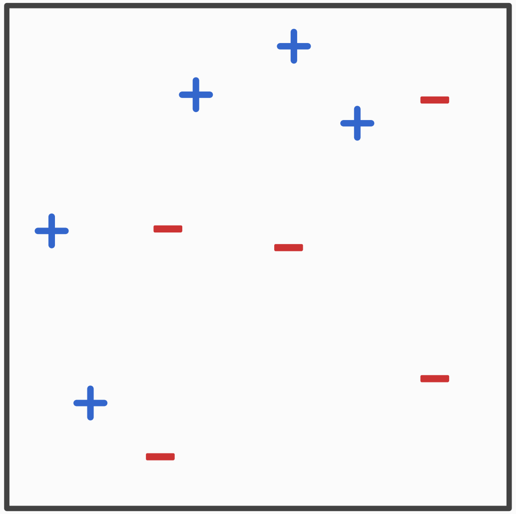
- [Schapire ’89]
  - First provable boosting algorithm
  - Call weak learner three times on three modified distributions
  - Get slight boost in accuracy
  - Apply recursively
- [Freund ’90]
  - “Optimal” algorithm that “boosts by majority”
- [Drucker, Schapire & Simard ’92]
  - First experiments using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

- AdaBoost was followed by a huge number of papers and practical applications
  - And a Gödel prize for Freund and Schapire

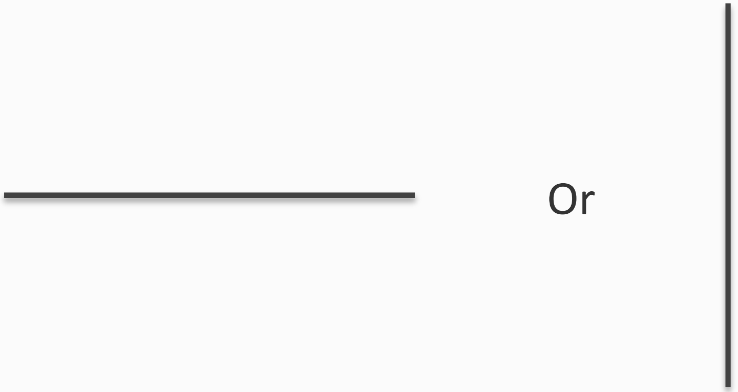
Boosting and Ensembles

- What is boosting?
- AdaBoost
  - Intuition
  - The algorithm
  - Why does it work
- Ensemble methods

A toy example

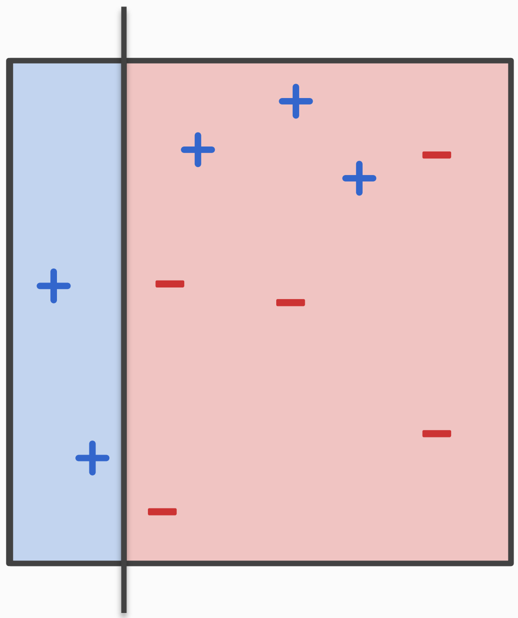


Our weak learner: An axis parallel line



Initially all examples are equally important

A toy example



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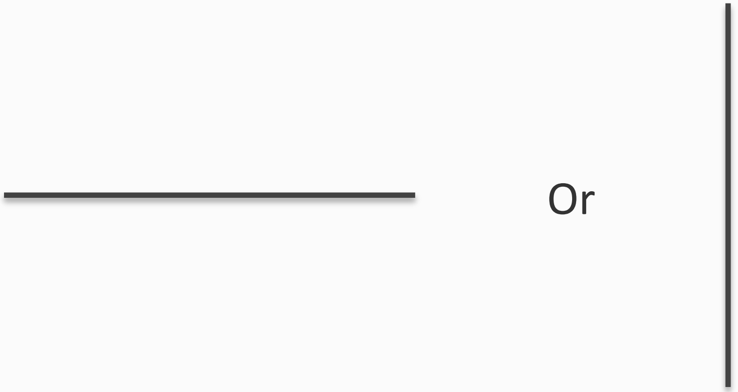
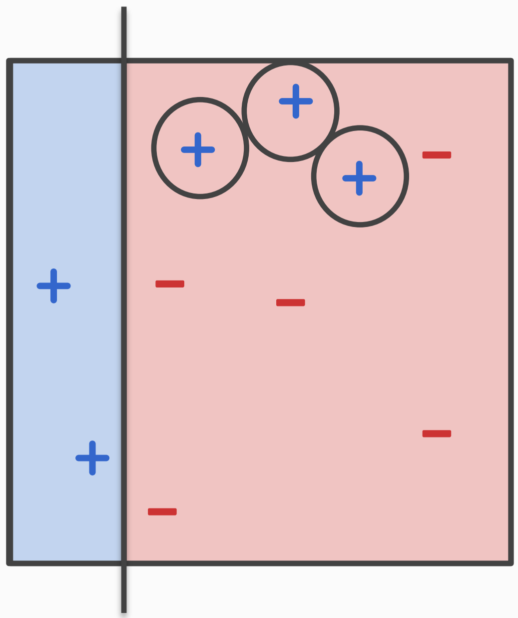


Initially all examples are equally important

h_1 = The best classifier on this data

A toy example



Our weak learner: An axis parallel line

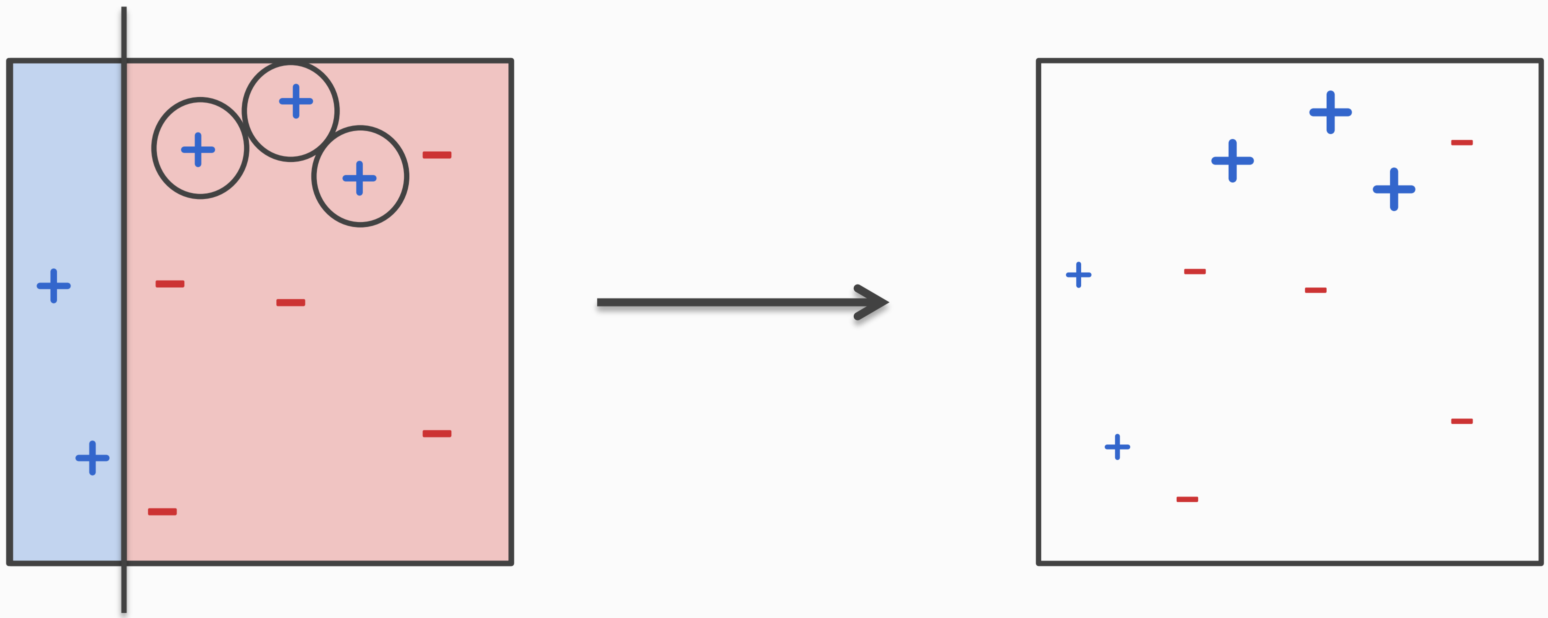
Or

Initially all examples are equally important

h_1 = The best classifier on this data

Clearly there are mistakes. Error ϵ_1 = 0.3

A toy example



Initially all examples are equally important

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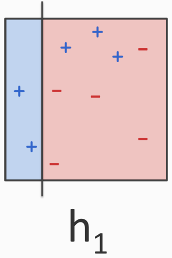
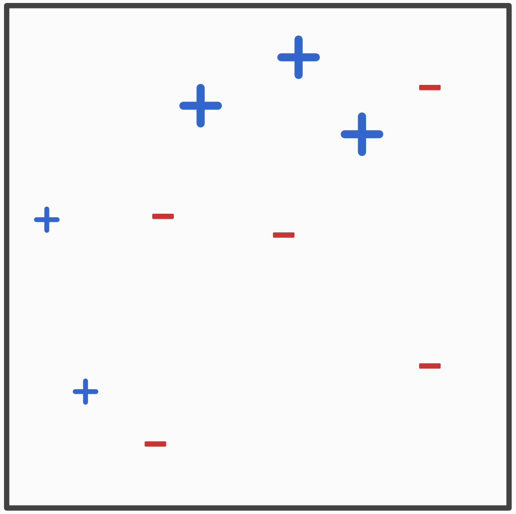
For the next round, increase the importance of the examples with mistakes and down-weight the examples that h_1 got correctly

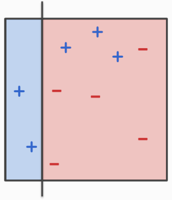
A toy example



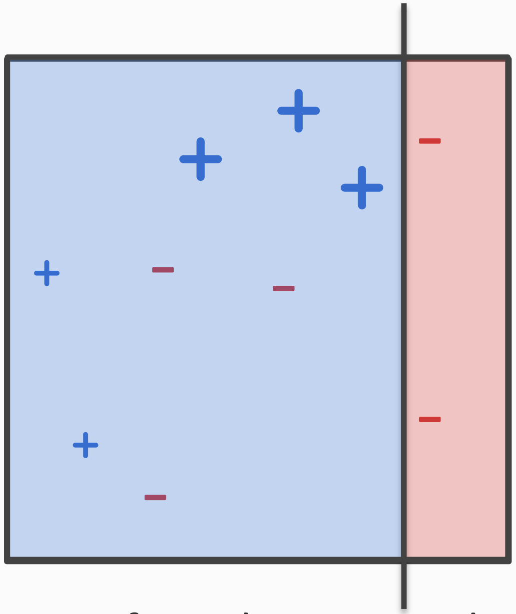


D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

A toy example



h_1



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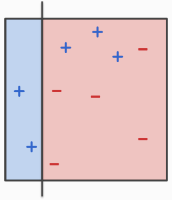
A toy example



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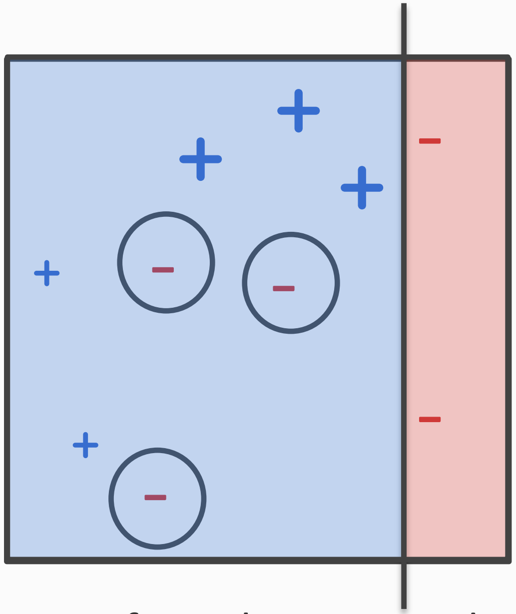


$$\epsilon_t = \frac{1}{2} - \frac{1}{2}\left(\sum_{i=1}^{m} D_t(i)\; y_i h(x_i)\right)$$

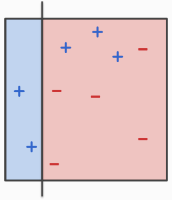
Why is this a reasonable definition?

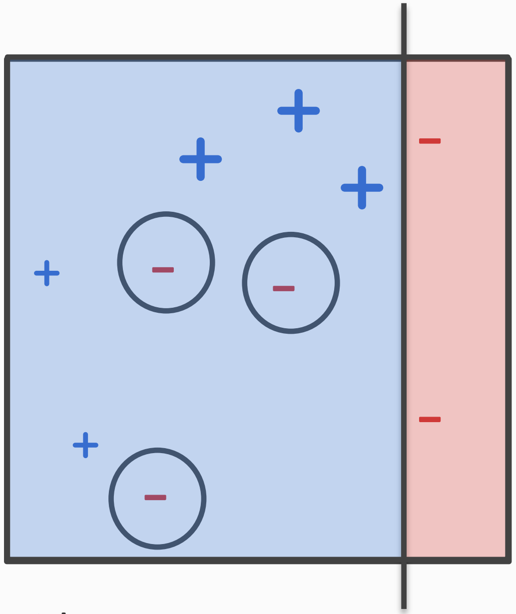
D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

h_2 = A classifier learned on this data. *Has an error ϵ_2 = 0.21*

Why not 0.3? Because while computing error, we will weight each example x_i by its $D_t(i)$

A toy example





$$\epsilon_t = \frac{1}{2} - \frac{1}{2}\left(\sum_{i=1}^{m} D_t(i)\ y_i h(x_i)\right)$$

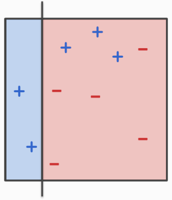
Why is this a reasonable definition?

Consider two cases

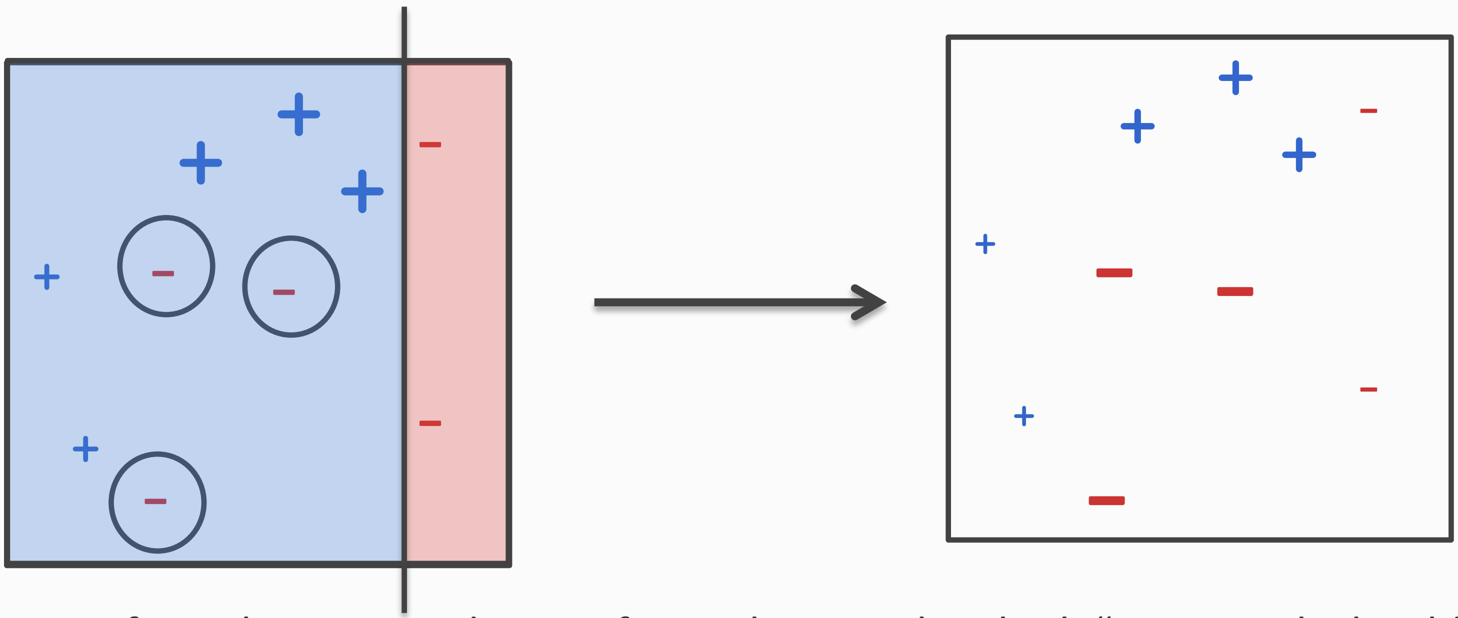
Case 1: When y = +1, $h(x)$ = –1 OR y = –1, $h(x)$ = +1

Case 2: When y = $h(x)$

A toy example



h_1



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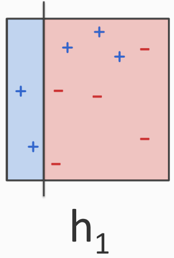
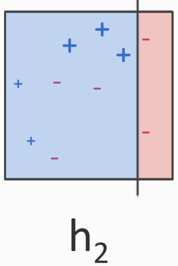
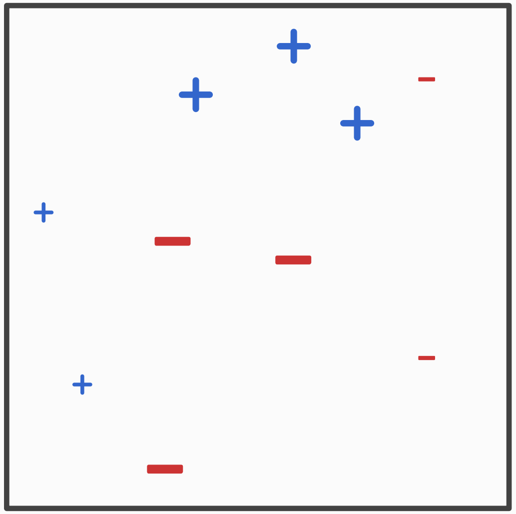
h_2 = A classifier learned on this data. *Has an error $\epsilon_2 = 0.21$*

For the next round, increase the importance of the mistakes and down-weight the examples that h_2 got correctly

A toy example







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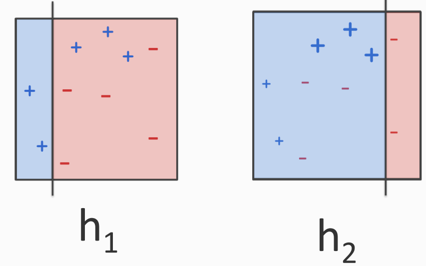
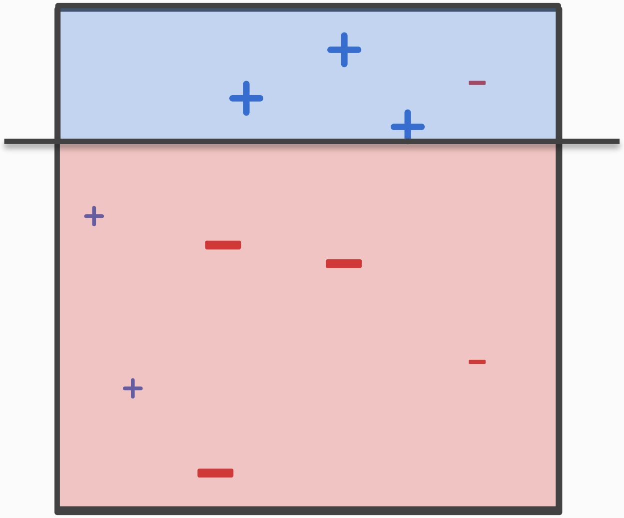




$$\epsilon_t = \frac{1}{2} - \frac{1}{2}\left(\sum_{i=1}^{m} D_t(i)\ y_i h(x_i)\right)$$

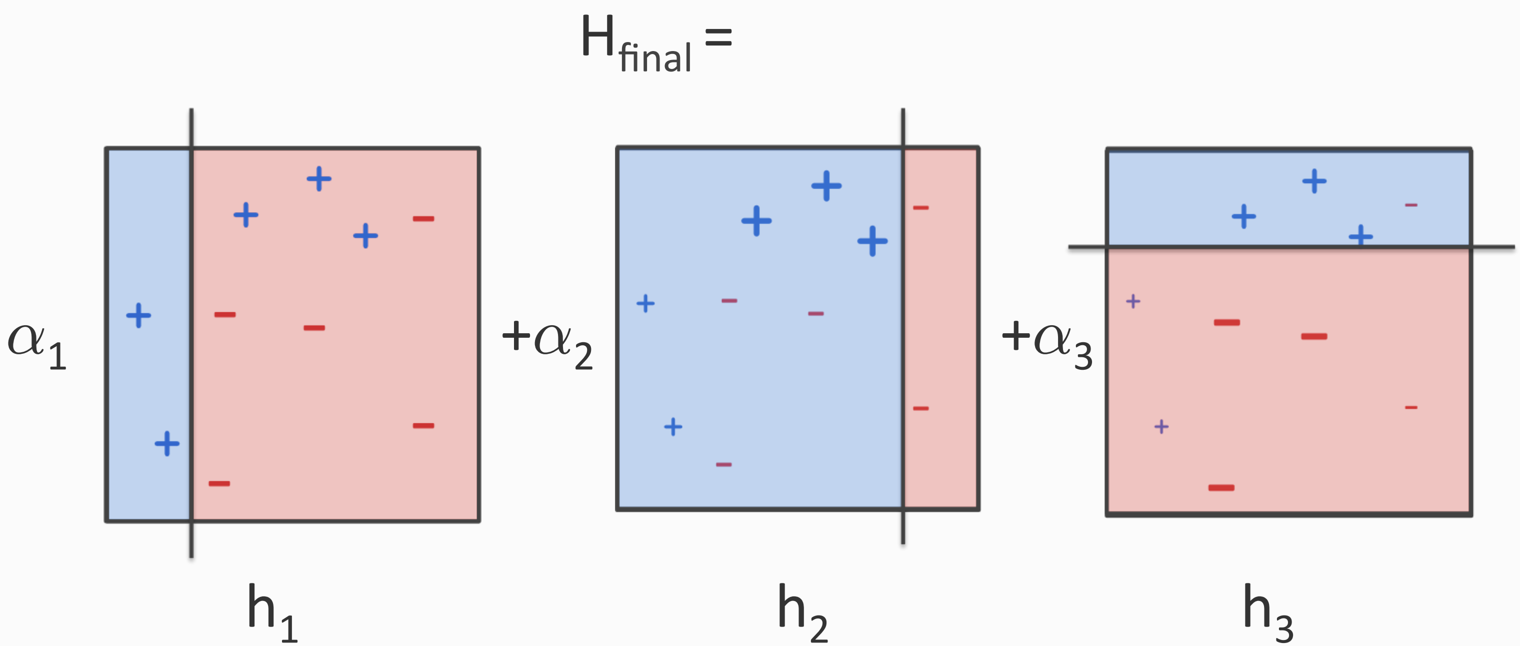
D_t = Set of weights at round t, one for each example. Think "How much should the weak learner care about this example in its choice of the classifier?"

h_3 = A classifier learned on this data. *Has an error $\epsilon_3 = 0.14$*

Why not 0.3? Because while computing error, we will weight each example x_i by its $D_t(i)$

A toy example

The final hypothesis is a combination of all the h_i's we have seen so far



A toy example

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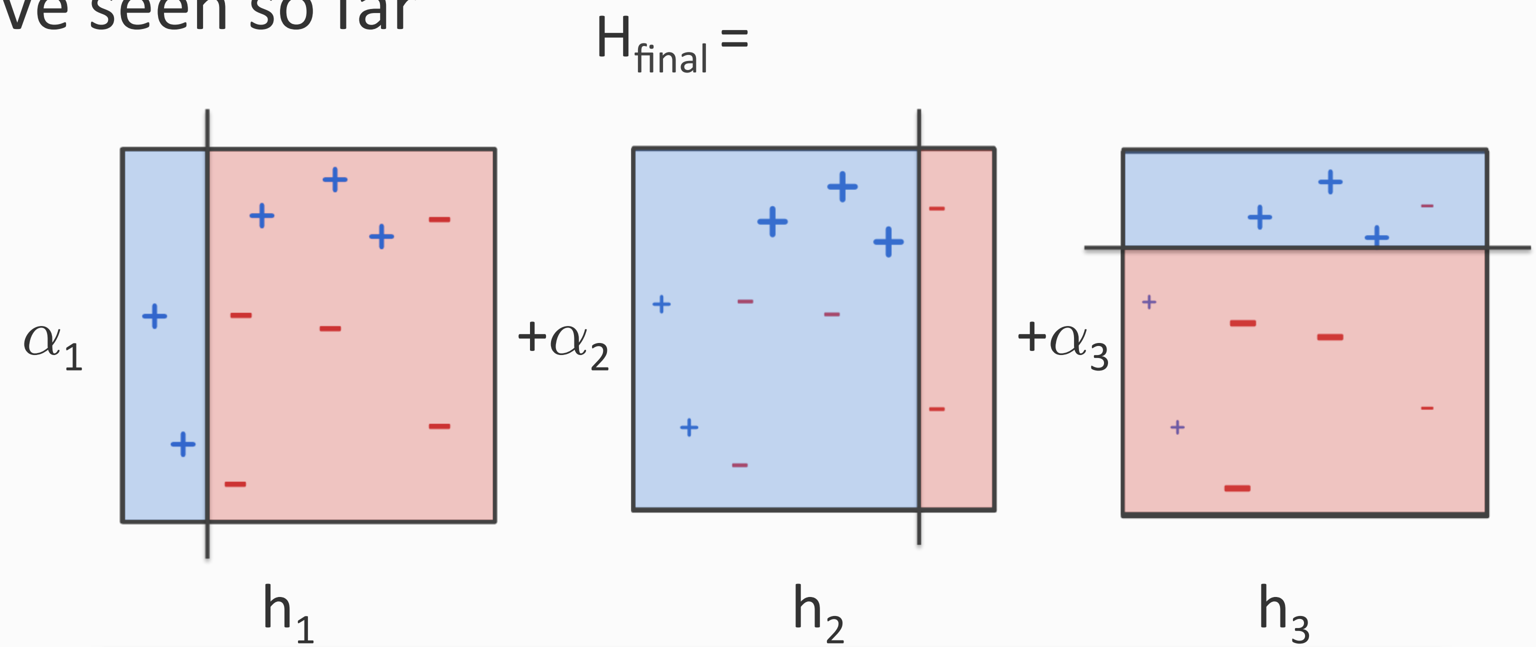

Think of the α values as the vote for each weak classifier and the boosting algorithm has to somehow specify them

An outline of Boosting

Given a training set $(x_1, y_1), \cdots, (x_m, y_m)$

– Instances $x_i \in X$ labeled with $y_i \in \{-1, +1\}$

- For $t = 1, 2, \cdots, T$:
  – Construct a distribution D_t on $\{1, 2, \cdots, m\}$
  – Find a weak hypothesis (rule of thumb) h_t such that it has a small *weighted* error ϵ_t
- Construct a final output H_{final}

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Need to specify these two to get a complete algorithm

AdaBoost: Constructing D_t

We have m examples

D_t is a set of weights over the examples

$$D_t(1), D_t(2), \cdots D_t(m)$$

At every round, the weak learner looks for hypotheses h_t that emphasizes examples that have a higher D_t

AdaBoost: Constructing D_t

Initially ($t = 1$), use the uniform distribution over all examples

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

AdaBoost: Constructing D_t

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

After t rounds

- What we have
  - D_t and the hypothesis h_t that was learned
  - The error ϵ_t of that hypothesis on the training data

- What we want from the $(t+1)^{th}$ round
  - Find a hypothesis so that examples that were incorrect in the previous round are correctly predicted by the new one
  - That is, increase the importance of misclassified examples and decrease the importance of correctly predicted ones

AdaBoost: Constructing D_t

Initially (t = 1), use the uniform distribution over all examples

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

After t rounds, we have some D_t and a hypothesis h_t that the weak learner produced

Create D_{t+1} as follows:

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

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Demote correctly predicted examples

Promote incorrectly predicted examples

AdaBoost: Constructing D_t

After t rounds, we have some D_t and a hypothesis h_t that the weak learner produced

Create D_{t+1} as follows:

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

$$= \frac{D_t(i)}{Z_t} \cdot \exp\left(-\alpha_t \cdot y_i h_t(x_i)\right)$$

Z_t: A normalization constant. Ensures that the weights D_{t+1} add up to 1

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

The classifier h_t gets a vote of α_t in the final classifier

An outline of Boosting

Given a training set $(x_1, y_1), \cdots, (x_m, y_m)$

– Instances $x_i \in X$ labeled with $y_i \in \{-1, +1\}$

- For $t = 1, 2, \cdots, T$:
  – Construct a distribution D_t on $\{1, 2, \cdots, m\}$
  – Find a weak hypothesis (rule of thumb) h_t such that it has a small weighted error ϵ_t
- Construct a final output H_{final}

Need to specify these two to get a complete algorithm

The final hypothesis

- After T rounds, we have
  - T weak classifiers h_1, h_2, $\cdots$ h_T
  - T values of α_t

- Recall that each weak classifier is takes an example x and produces a -1 or a +1

- Define the final hypothesis H_{final} as

$$H_{final}(x) = \operatorname{sgn}\left(\sum_t \alpha_t h_t(x)\right)$$

AdaBoost: The full algorithm

Given a training set $(x_1, y_1), \cdots, (x_m, y_m)$

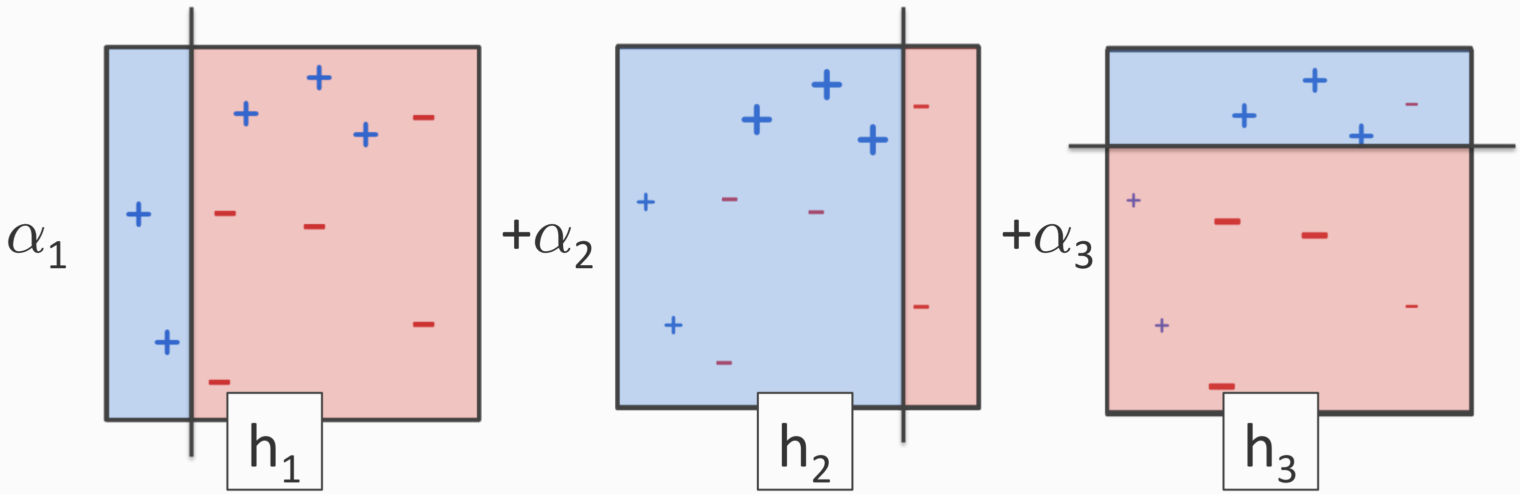
Instances $x_i \in X$ labeled with $y_i \in \{-1, +1\}$

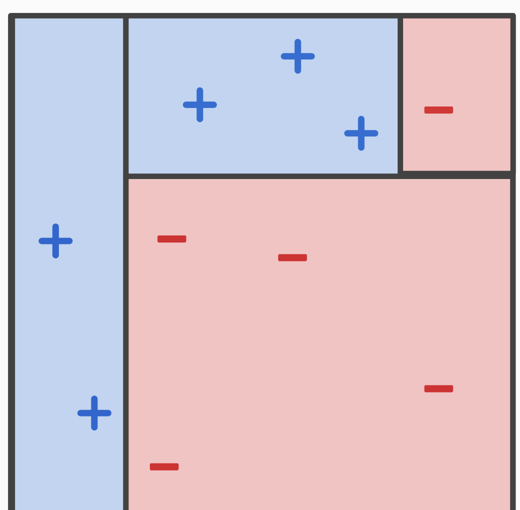
T: a parameter to the learner

1. Initialize $D_1(i) = 1/m$ for all $i = 1, 2, \cdots, m$
2. For $t = 1, 2, \cdots T$:
   1. Find a classifier h_t whose *weighted classification error* is better than chance
   2. Compute its vote
   $$\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$$
   3. Update the values of the weights for the training examples
   $$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \exp\left(-\alpha_t \cdot y_i h_t(x_i)\right)$$
3. Return the final hypothesis $H_{final}(x) = \mathrm{sgn}\left(\sum_t \alpha_t h_t(x) \right)$

Back to the toy example

$H_{final} =$





Analyzing the training error

Theorem:

- Run AdaBoost for T rounds
- Let ϵ_t = ½ - γ_t
- Let 0 < $\gamma \leq \gamma_t$ for all t
- Then,

$$\text{Training error}(H_{final}) \leq e^{-2\gamma^2 T}$$

We have a weak learner

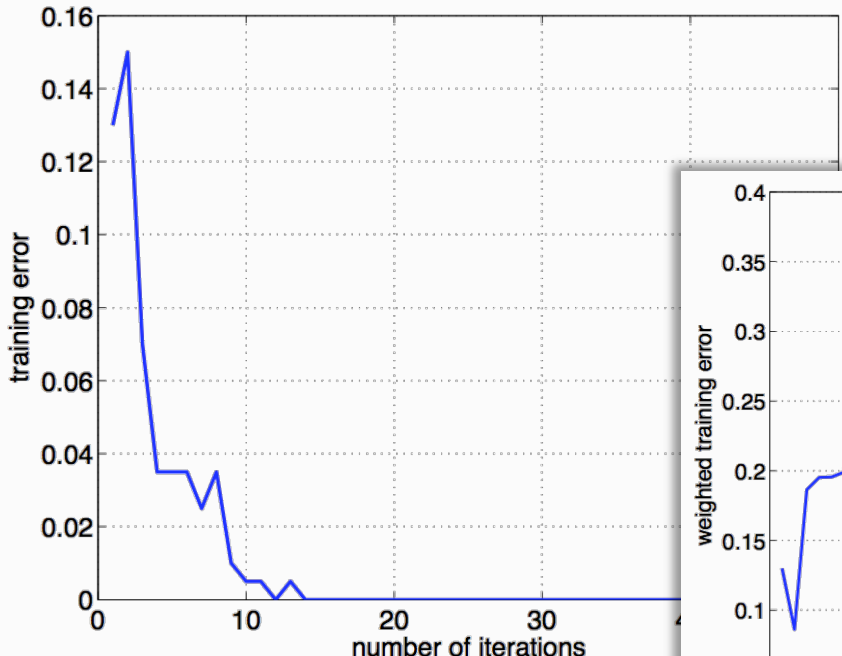
As T increases, the training error drops exponentially

Is it sufficient to upper bound the training error?

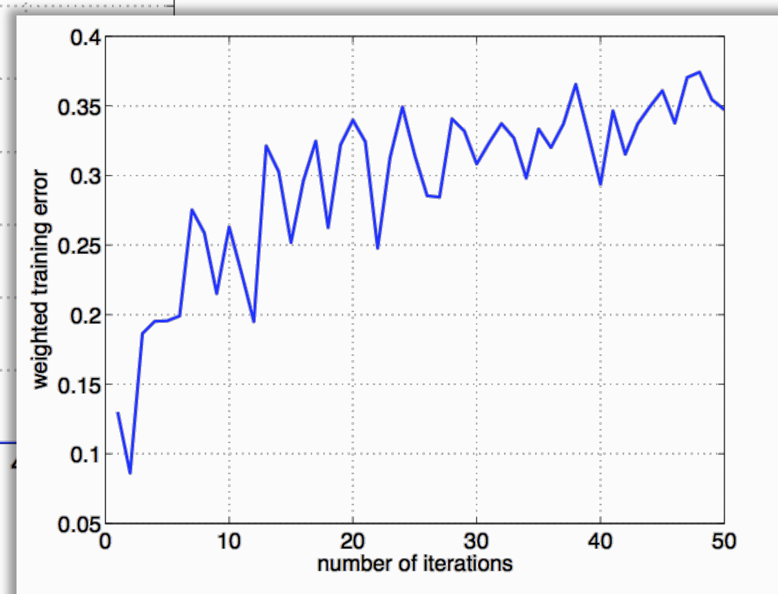
Proof is simple, see pointer on website

Adaboost: Training error

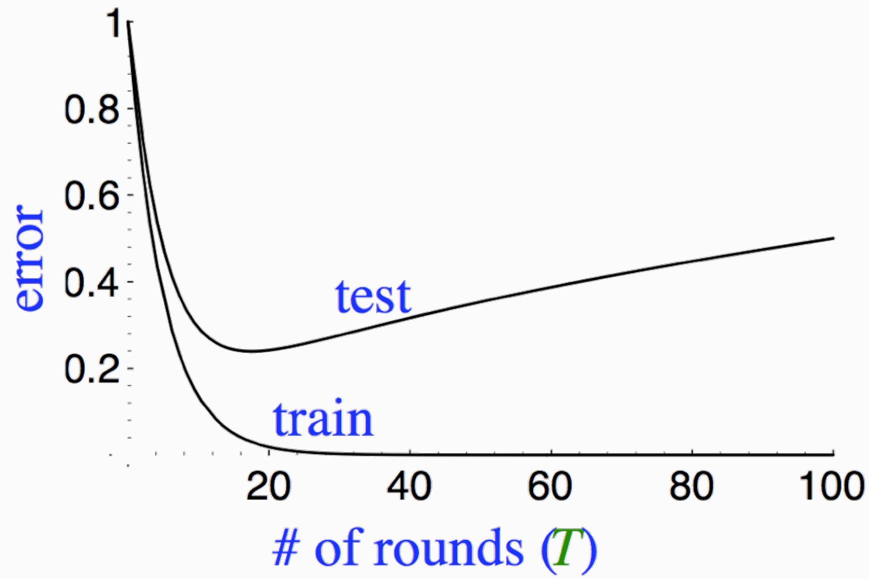
The training error of the combined classifier decreases exponentially fast if the errors of the weak classifiers (the ϵ_t) are strictly better than chance



The individual classifier errors (ϵ_t) tend to increase



What about the test error?



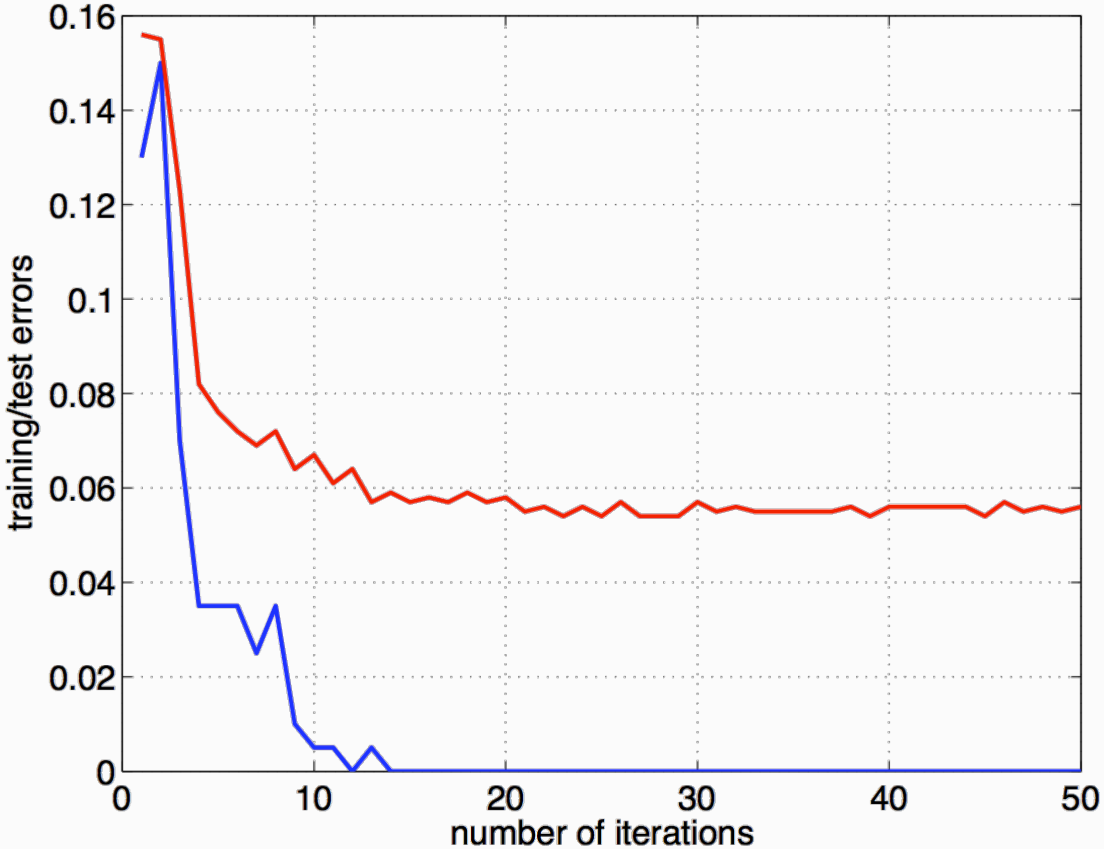
What the theory tells us:

Training error will keep decreasing or reach zero (the AdaBoost theorem)

Test error will increase after the H_{final} becomes too "complex"

- Think about Occam's razor and overfitting

In practice



Strange observation: Test error may decrease even after training error has hit zero!
Why? (One possible explanation in [Schapire, Freund, Bartlett, Lee, 1997])

AdaBoost: Summary

- What is good about it
  - Simple, fast and only one additional parameter to tune (T)
  - Use it with any weak learning algorithm
    - Which means that we only need to look for classifiers that are slightly better than chance
- Caveats
  - Performance often depends on dataset and the weak learners
  - Can fail if the weak learners are too complex (overfitting)
  - Can fail if the weak learners are too weak (underfitting)

- Empirical evidence [Caruana and Niculescu-Mizil, 2006] that boosted decision stumps are the best approach to try if you have a small number of features (no more than hundreds)

Boosting and Ensembles

- What is boosting?
- AdaBoost
- Ensemble methods
  - Boosting, Bagging and Random Forests

Ensemble methods

- In general, meta algorithms that combine the output of multiple classifiers
- Often tend to be empirically robust
- Eg: The winner of the Netflix challenge was a giant ensemble

Boosting

- 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!!!
- Typically requires 100’s to 1000’s of iterations
- Return final model:
  - Carefully weighted prediction of each model

Boosting: Different Perspectives

- Boosting is a maximum-margin method (Schapire et al. 1998, Rosset et al. 2004)
  - Trades lower margin on easy cases for higher margin on harder cases

- Boosting is an additive logistic regression model (Friedman, Hastie and Tibshirani 2000)
  - Tries to fit the logit of the true conditional probabilities

- Boosting is an *equalizer* (Breiman 1998) (Friedman, Hastie, Tibshirani 2000)
  - Weighted proportion of the number of times an example is misclassified by base learners tends to be the same for all training cases

- Boosting is a linear classifier, but does not give well calibrated probability estimate.

Bagging

Also known as ***Boot**strap **agg**regat**ing*** [Breiman, 1994]

- Given a training set with m examples
- Repeat t = 1, 2, ⋯, m:
  - Draw m’ (< m) samples with replacement from the training set
  - Train a classifier (any classifier) C_i

- Construct final classifier by taking votes from each C_i

Bagging

Also known as ***B**ootstrap **agg**regat**ing***

- A method for generating multiple versions of a predictor and using these to get an aggregated predictor.
  - Averages over the versions when predicting a numerical outcome (regression)
  - Does a plurality vote when predicting a class (classification)

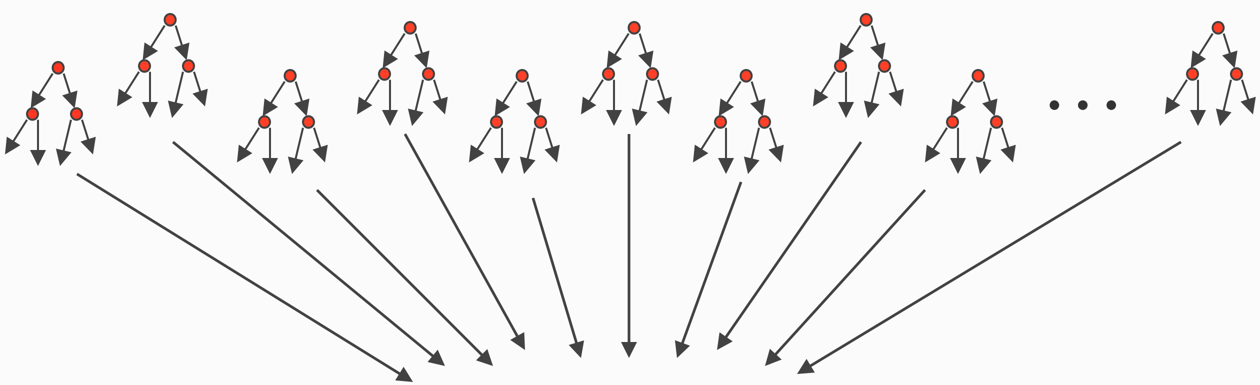
- The multiple versions are constructed by making bootstrap replicates of the learning set and using these as training sets
  - That is, use samples of the data, with repetition

- Tests on real and simulated data sets using classification and regression trees and subset selection in linear regression show that bagging can give substantial gains in accuracy

- Instability of the prediction method: If perturbing the training set can cause significant changes in the learned classifier *then* bagging can improve accuracy

Example: Bagged Decision Trees

- Draw T bootstrap samples of data
- Train trees on each sample $\rightarrow$ T trees
- Average prediction of trees on out-of-bag samples

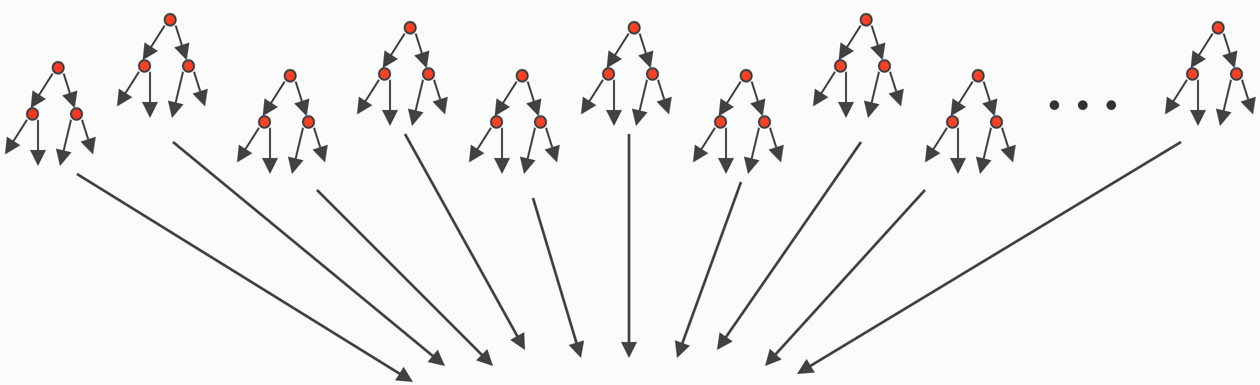


Average prediction

(0.23 + 0.19 + 0.34 + 0.22 + 0.26 + … + 0.31) / # Trees = 0.24

Random Forests (Bagged Trees++)

- Draw T (possibly ***1000s***) bootstrap samples of data
- ***Draw sample of available attributes at each split***
- Train trees on each sample/attribute set $\rightarrow$ T trees
- Average prediction of trees on out-of-bag samples



Average prediction

(0.23 + 0.19 + 0.34 + 0.22 + 0.26 + … + 0.31) / # Trees = 0.24

Boosting and Ensembles: What have we seen?

- What is boosting?
  - Does weak learnability imply strong learnability?
- AdaBoost
  - Intuition
  - The algorithm
  - Why does it work
- Ensemble methods
  - Boosting, Bagging and Random Forests