Ensemble Methods

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Introduction to Machine Learning (CS771A)

November 8, 2018

Some Simple Ensembles

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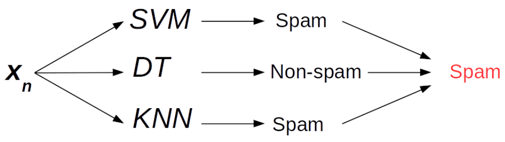
- Voting or Averaging of predictions of multiple pre-trained models



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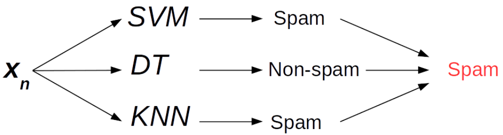
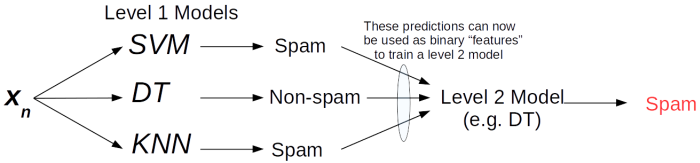


- "Stacking": Use predictions of multiple models as "features" to train a new model and use the new model to make predictions on test data



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- Bayesian Learning: Posterior weighted averaging of predictions by all possible parameter values

$$p(y_*|\boldsymbol{x}_*, \mathbf{X}, \boldsymbol{y}) = \int p(y_*|\boldsymbol{w}, \boldsymbol{x}_*)p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X})d\boldsymbol{w}$$

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- Train same model multiple times on different data sets, and "combine" these "different" models

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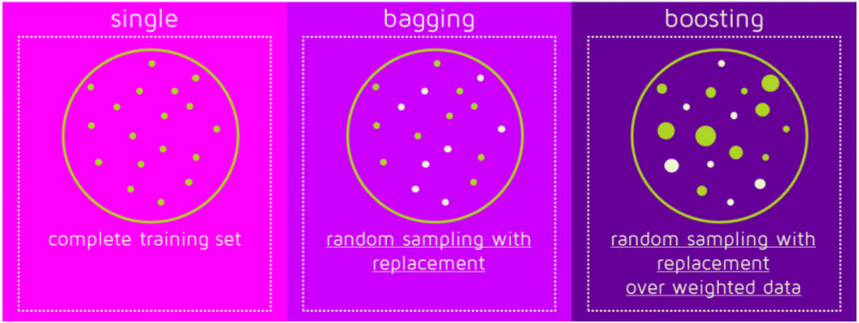

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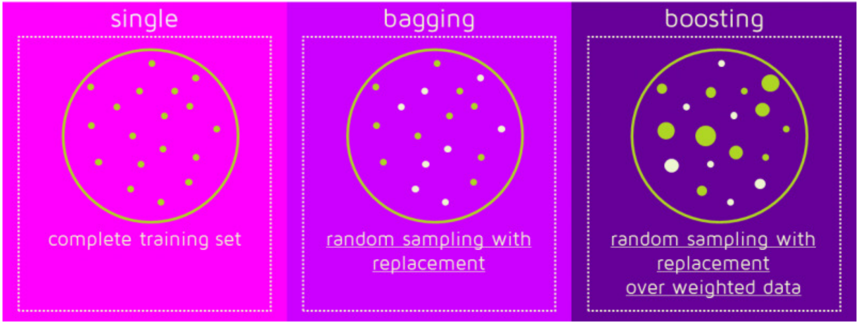

- Note: Bagging trains independent models; boosting trains them sequentially (we'll see soon)

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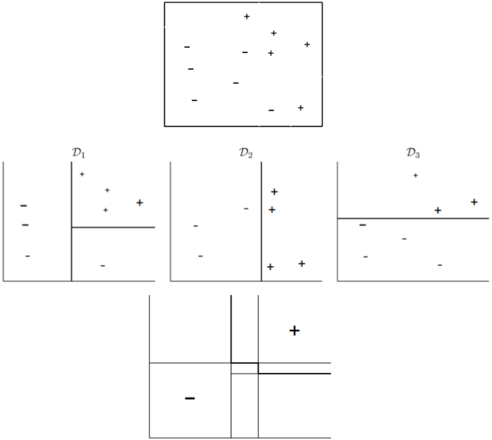
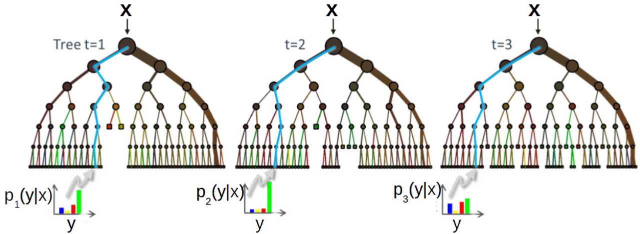
- High variance models = models whose prediction accuracies varies a lot across different data sets

Bagging: illustration

Top: Original data, Middle: 3 models (from some model class) learned using three data sets chosen via bootstrapping, Bottom: averaged model



A Decision Tree Ensemble: Random Forests



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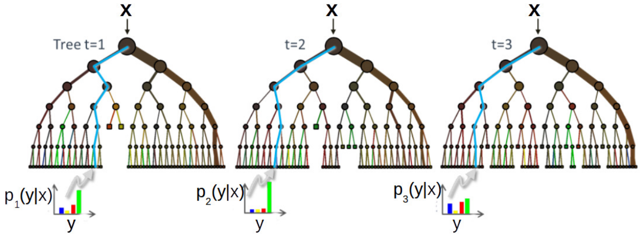

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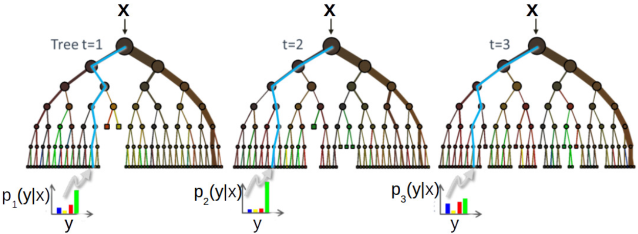

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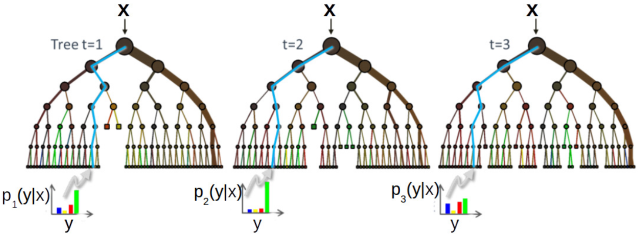

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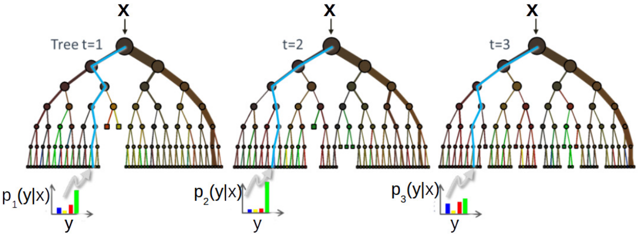

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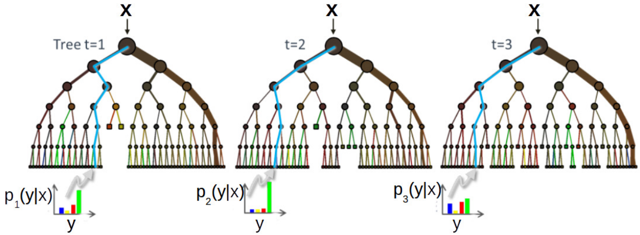

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- Prediction for a test example votes on/averages predictions from all the DTs

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- Note: Unlike bagging, boosting is a sequential algorithm (models learned in a sequence)

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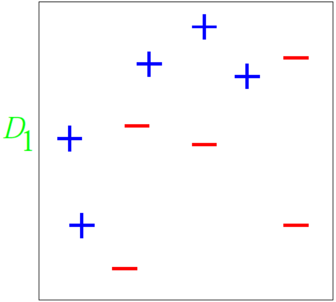
- Output the "boosted" final hypothesis $H(\boldsymbol{x}) = \text{sign}(\sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x}))$

AdaBoost: A Toy Example

Consider binary classification with 10 training examples

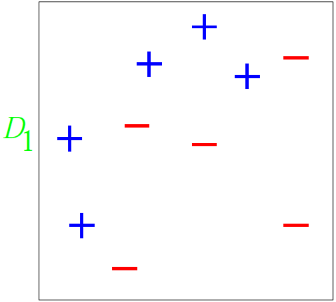
Initial weight distribution D_1 is uniform (each point has equal weight $= 1/10$)



AdaBoost: A Toy Example

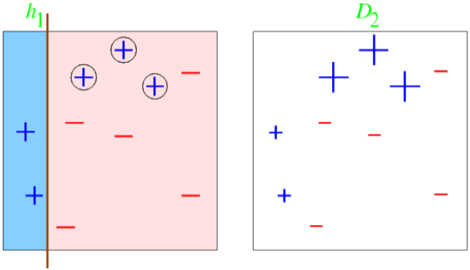
Consider binary classification with 10 training examples

Initial weight distribution D_1 is uniform (each point has equal weight $= 1/10$)



Let's assume each of our weak classifers is a very simple **axis-parallel linear classifier**

After Round 1



- Error rate of h_1: $\epsilon_1 = 0.3$

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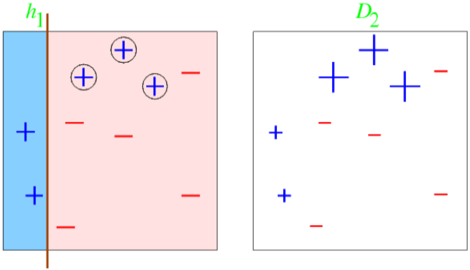

- Error rate of h_1: $\epsilon_1 = 0.3$; weight of h_1: $\alpha_1 = \frac{1}{2}\ln((1-\epsilon_1)/\epsilon_1) = 0.42$

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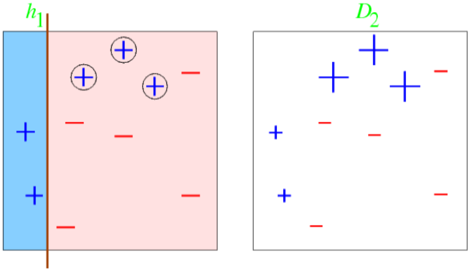

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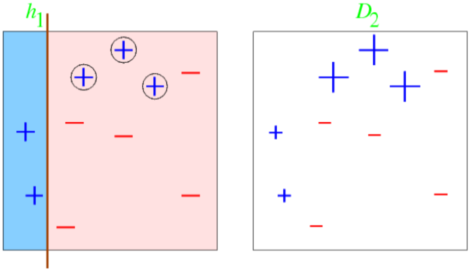

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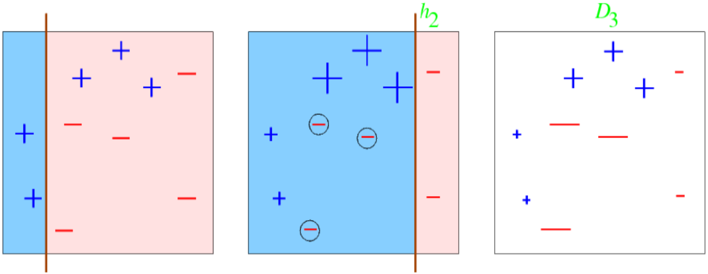

- Error rate of h_2: $\epsilon_2 = 0.21$

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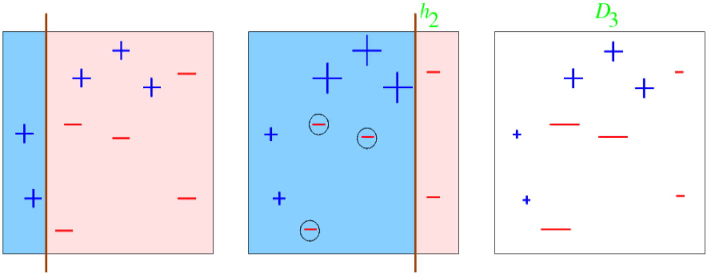

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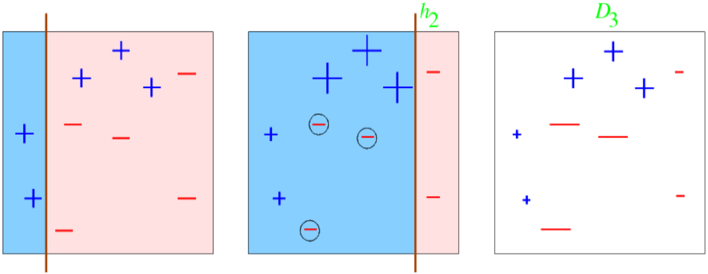

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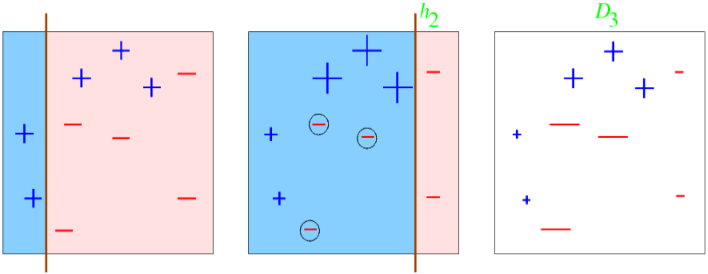

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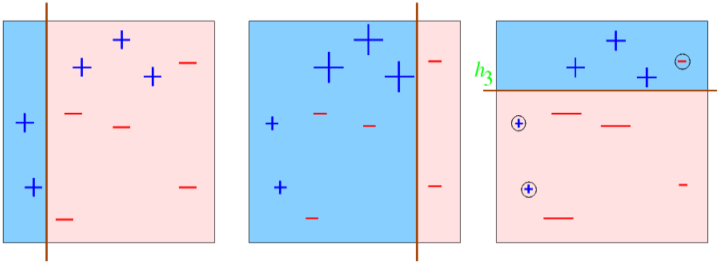
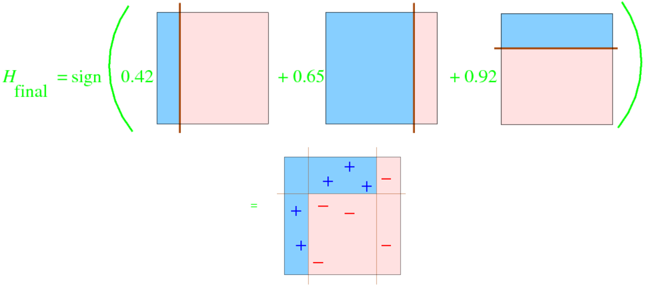
After Round 3



- Error rate of h_3: $\epsilon_3 = 0.14$; weight of h_3: $\alpha_3 = \frac{1}{2}\ln((1-\epsilon_3)/\epsilon_3) = 0.92$
- Suppose we decide to stop after round 3
- Our ensemble now consists of 3 classifiers: h_1, h_2, h_3

The Final Classifier

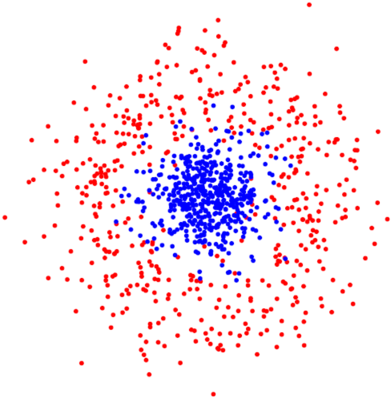
- Final classifier is a weighted linear combination of all the classifiers
- Classifier h_i gets a weight α_i



- Multiple weak, linear classifiers **combined** to give a strong, nonlinear classifier

Another Example

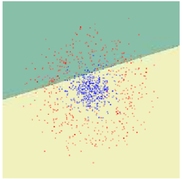
- Given: A nonlinearly separable dataset
- We want to use Perceptron (linear classifier) on this data

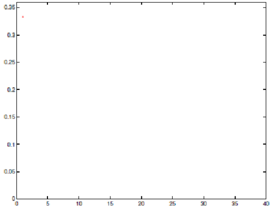


AdaBoost: Round 1

- After round 1, our ensemble has 1 linear classifier (Perceptron)
- Bottom figure: X axis is number of rounds, Y axis is training error

$t = 1$

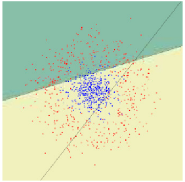


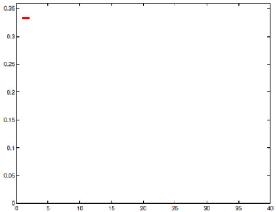


AdaBoost: Round 2

- After round 2, our ensemble has 2 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

$t = 2$

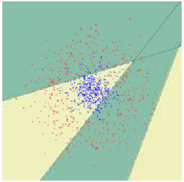


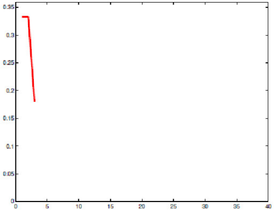


AdaBoost: Round 3

- After round 3, our ensemble has 3 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

$t = 3$

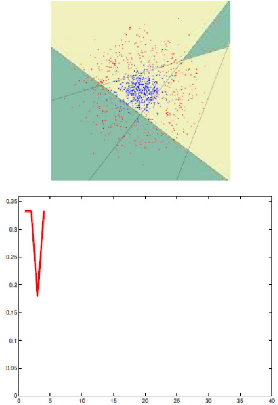




AdaBoost: Round 4

- After round 4, our ensemble has 4 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

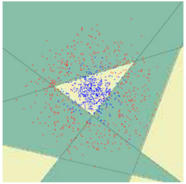
$t = 4$

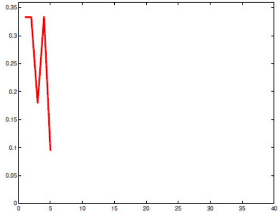


AdaBoost: Round 5

- After round 5, our ensemble has 5 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

$t = 5$

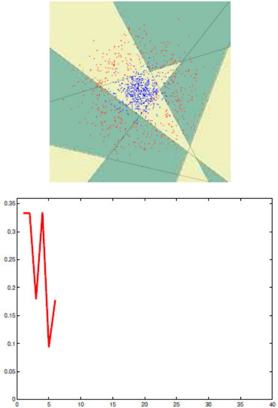




AdaBoost: Round 6

- After round 6, our ensemble has 6 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

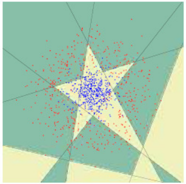
$t = 6$

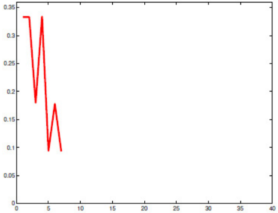


AdaBoost: Round 7

- After round 7, our ensemble has 7 linear classifiers (Perceptrons)
- Bottom figure: X axis is number of rounds, Y axis is training error

$t = 7$





AdaBoost: Round 40

- After round 40, our ensemble has 40 linear classifiers (Perceptrons)
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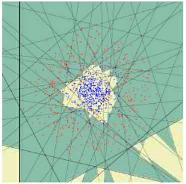
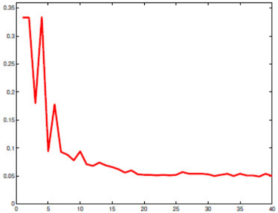
$t = 40$





AdaBoost: The Loss Function

- AdaBoost can be shown to be optimizing the following loss function

$$\mathcal{L} = \sum_{n=1}^{N} \exp\{-y_n H(\boldsymbol{x}_n)\}$$

where $H(\boldsymbol{x}) = \text{sign}(\sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x}))$, given weak base classifiers $h_1, \ldots, h_T$

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- Extensions for classification and ranking problems as well
- A very fast, parallel implementation of GBM is XGBoost (eXtreme Gradient Boosing)

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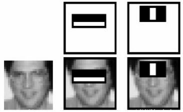

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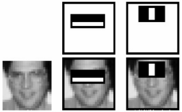

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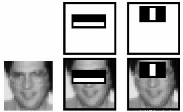

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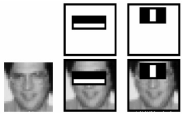

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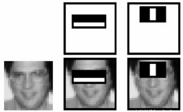

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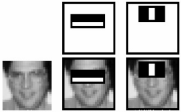

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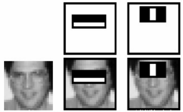

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- Help reduces bias or/and variance of machine learning models
  - High bias: very simple models have high bias. Boosting can reduce it
  - High variance: very complex models have high variance. Bagging can reduce it