

# Statistical Machine Learning

**Pier Francesco Palamara**

Department of Statistics

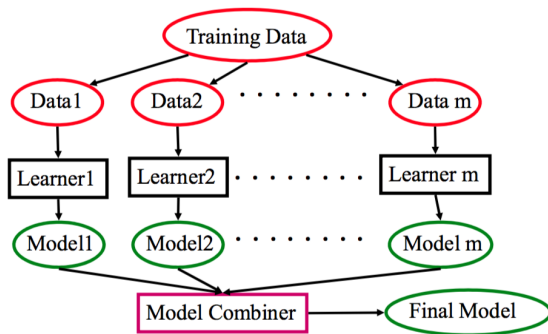
University of Oxford

Slide credits and other course material can be found at:

[http://www.stats.ox.ac.uk/~palamara/SML19\\_BDI.html](http://www.stats.ox.ac.uk/~palamara/SML19_BDI.html)

# Learning Ensembles

- Learn multiple alternative definitions of a concept using different training data or different learning algorithms.
- Combine decisions of multiple definitions, (e.g. using weighted voting).

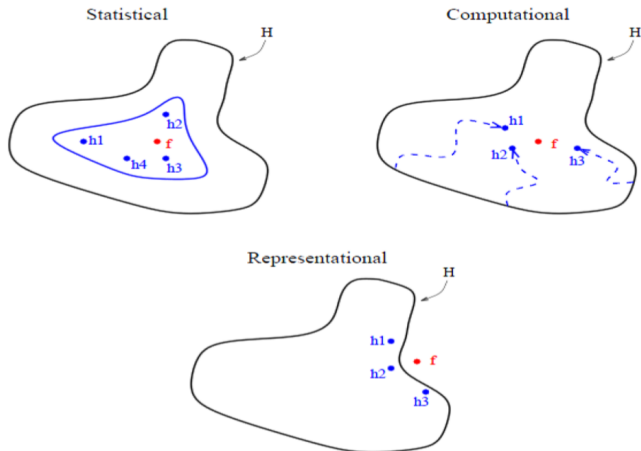


# Three fundamental reasons for good ensembles

- It is desirable to build good ensembles for three fundamental reasons. (Dietterich, 2000):
  - Statistical: if little data
  - Computational: enough data, but local optima produced by local search
  - Representational: when the true function  $f$  cannot be represented by any of the hypothesis in  $\mathcal{H}$  (weighted sums of hypotheses drawn from  $\mathcal{H}$  might expand the space)

# Three fundamental reasons for good ensembles

- It is desirable to build good ensembles for three fundamental reasons. (Dietterich, 2000):



# Value of Ensembles

- “No Free Lunch” Theorem
  - No single algorithm wins all the time
- When combining multiple independent and diverse decisions each of which is at least more accurate than random guessing, random errors cancel each other out, correct decisions are reinforced.
- Examples: Human ensembles are demonstrably better
  - How many jelly beans in the jar?: Individual estimates vs. group average.
  - Who want to be a millionaire: Audience vote.

# Homogeneous Ensembles

- Use a single arbitrary learning algorithm, but manipulate training data to make it learn multiple models.
  - Data 1  $\neq$  Data 2  $\neq \dots \neq$  Data  $m$
  - Lerner 1 = Lerner 2 =  $\dots$  = Lerner  $m$
- In this course, we consider two methods of this kind:
  - Bagging: Resample training data (last time)
  - Boosting: Reweight training data (today)

# Approach: Bagging (Bootstrap + Aggregating)

- Create ensembles by “bootstrap aggregation”, (i.e., repeatedly randomly resampling the training data) to generate training sets (Breiman, 1996).
- Bootstrap: draw  $N$  data points with replacement from original data set of size  $N$ .
- For each resampled data set, train base learners using an unstable<sup>1</sup> learning procedure (like decision trees).
- During test, combine learners by e.g. taking the average.
- This decreases error by decreasing the **variance** in the results due to unstable learners.

---

<sup>1</sup> Unstable algorithm: when small change in the training set causes a large difference in the base learners (high variance).

# Approach: Boosting

## Weak learners vs Strong learners

- In boosting, we actively try to generate complementary base-learners by training the next learner on the mistakes of the previous learners. We build a **strong learner** using **weak learners**.
- Example: in a binary classification problem, a weak learner does at least a bit better than random guessing, but not much better. A strong learner has arbitrarily small error probability.

In boosting, focus is on reducing **bias**, rather than variance.



# Approach: Boosting

## History

- In 1988 Kearns and Valiant posed the question of whether one can “boost” a weak learner to a strong learner.
- Two years later Rob Schapire published his landmark paper “The Strength of Weak Learnability” closing the theoretical question by providing the first “boosting” algorithm.
- Schapire and Yoav Freund worked together for the next few years to produce a simpler and more versatile algorithm called Adaboost.
- They received the 2003 Gödel Prize. “Best off-the-shelf classifier in the world” (Breiman 1998).

# AdaBoost: Overview

- Adaptive Boosting (AdaBoost)
- As in bagging, we will use the same training set over and over.
- Classifiers must be “simple” (i.e. **weak**) so they do not overfit.
- Can combine an arbitrary number of base learners. (parameters)
- When testing, given an instance, all the classifiers make predictions and a weighted vote is taken.
- The weights are proportional to the base learners' accuracies on the training set.

# Probably Approximately Correct (PAC)

- Definition: PAC (not examinable)

An algorithm  $A(\epsilon, \delta)$  is said to PAC-learn the concept class  $\mathcal{H}$  over the set  $\mathcal{X}$  if, for any distribution  $\mathcal{D}$  over  $\mathcal{X}$  and for any  $0 < \epsilon, \delta < 1/2$  and for any target concept  $c \in \mathcal{H}$ , the probability that  $A$  produces a hypothesis  $h$  of error at most  $\epsilon$  is at least  $1 - \delta$ . In symbols,  $P_{\mathcal{D}}(err_{c, \mathcal{D}}(h) \leq \epsilon) > 1 - \delta$ . Moreover,  $A$  must run in time polynomial in  $1/\epsilon, 1/\delta$  and  $n$ , where  $n$  is the size of an element  $x \in \mathcal{X}$ .

- Weak PAC-learning model requires the algorithm to have accuracy that is slightly better than random guessing. That is the algorithm will output a classification function which will correctly classify a random label with probability at least  $\frac{1}{2} + \eta$  for some small, but fixed,  $\eta > 0$ .

We call an algorithm that produces PAC guarantees a **strong learner**, while an algorithm with the latter guarantees is called a **weak learner**.

# Strong and Weak PAC-learning

- It turns out that strong learning and weak learning are equivalents! We can obtain a strong learner by combining weak learners. How?
- We can maintain a large number of separate instances of the weak learner, run them on our dataset, and then combine their hypotheses with a majority vote.

# Strong learners from weak learners

- This is a bit too simplistic: what if the majority of the weak learners are wrong?
- We can do better:  
Instead of taking a majority vote, we can take a weighted majority vote.
- That is, give the weak learner a random subset of your data, and then test its hypothesis on the data to get a good estimate of its error.
- Then you can use this error to say whether the hypothesis is any good, and give good hypotheses high weight and bad hypotheses low weight (proportionally to the error).
- Then the “boosted” hypothesis would take a weighted majority vote of all hypotheses on an example.

# Strong learners from weak learners

- Rather than use the estimated error just to say something about the hypothesis, we can identify the mislabeled examples in a round and somehow encourage  $A$  to do better at classifying those examples in later rounds.
- This turns out to be the key insight, and it's why the algorithm is called AdaBoost. (Ada stands for “adaptive”).
- We are adaptively modifying the distribution over the training data we feed to  $A$  based on which data  $A$  learns “easily” and which it does not.
- So as the boosting algorithm runs, the distribution given to  $A$  has more and more probability weight on the examples that  $A$  misclassified.

# Adaboost Algorithm

- Given:  $N$  samples  $\{\mathbf{x}_n, y_n\}$ , where  $y_n \in \{+1, -1\}$ , and some way of constructing weak (or base) classifiers.
- Notation: we indicate the weak learner using  $h(\cdot)$ .
- Initialize weights  $w_1(n) = \frac{1}{N}$  for every training sample
- For  $t = 1$  to  $T$ 
  - Train a weak classifier  $h_t(\mathbf{x})$  using current weights  $w_t(n)$ , by minimizing the weighted classification error

$$\epsilon_t = \sum_n w_t(n) \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)]$$

- Compute contribution for this classifier:  $\beta_t = \frac{1}{2} \ln \frac{1-\epsilon_t}{\epsilon_t}$
- Update weights on training points

$$w_{t+1}(n) \propto w_t(n) e^{-\beta_t y_n h_t(\mathbf{x}_n)}$$

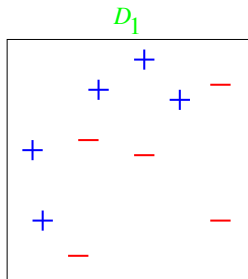
and normalize them such that  $\sum_n w_{t+1}(n) = 1$

- Output the final classifier

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

# Example

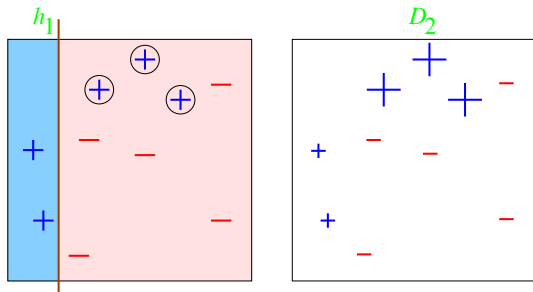
## 10 data points and 2 features



- The data points are clearly not linear separable
- In the beginning, all data points have equal weights (the size of the data markers “+” or “-”)
- Base classifier  $h(\cdot)$ : either horizontal or vertical lines
  - These ‘decision stumps’ are just trees with a single internal node, i.e., they classifying data based on a single attribute

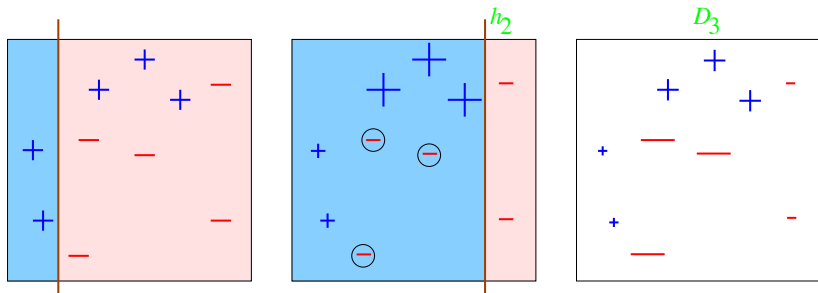


# Round 1: $t = 1$



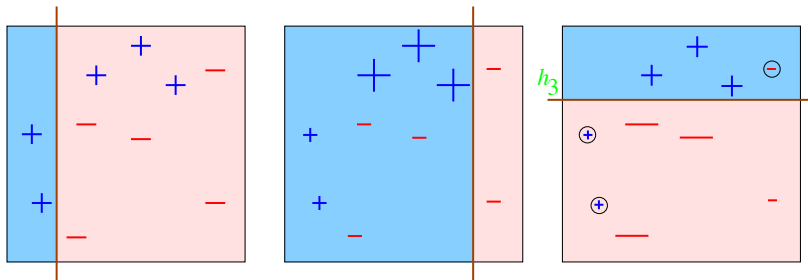
- 3 misclassified (with circles):  $\epsilon_1 = 0.3 \rightarrow \beta_1 = 0.42$ .
- Weights recomputed; the 3 misclassified data points receive larger weights

## Round 2: $t = 2$



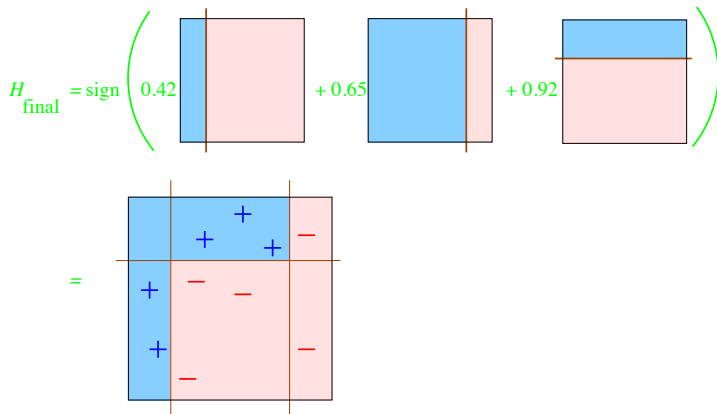
- 3 misclassified (with circles):  $\epsilon_2 = 0.21 \rightarrow \beta_2 = 0.65$ .  
Note that  $\epsilon_2 \neq 0.3$  as those 3 data points have weights less than  $1/10$
- 3 misclassified data points get larger weights
- Data points classified correctly in both rounds have small weights

## Round 3: $t = 3$



- 3 misclassified (with circles):  $\epsilon_3 = 0.14 \rightarrow \beta_3 = 0.92$ .
- Previously correctly classified data points are now misclassified, hence our error is low; what's the intuition?
  - Since they have been consistently classified correctly, this round's mistake will hopefully not have a huge impact on the overall prediction

# Final classifier: combining 3 classifiers



- All data points are now classified correctly!

# Why AdaBoost works?

It minimizes a loss function related to classification error.

## Classification loss

- Suppose we want to have a classifier

$$h(\mathbf{x}) = \text{sign}[f(\mathbf{x})] = \begin{cases} 1 & \text{if } f(\mathbf{x}) > 0 \\ -1 & \text{if } f(\mathbf{x}) < 0 \end{cases}$$

- Our loss function is thus

$$\ell(h(\mathbf{x}), y) = \begin{cases} 0 & \text{if } yf(\mathbf{x}) > 0 \\ 1 & \text{if } yf(\mathbf{x}) < 0 \end{cases}$$

Namely, the function  $f(\mathbf{x})$  and the target label  $y$  should have the same sign to avoid a loss of 1.

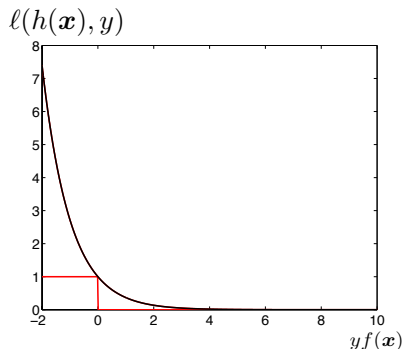
# Surrogate loss

As we discussed for logistic regression, the  $0 - 1$  loss function  $\ell(h(\mathbf{x}), y)$  is non-convex and difficult to optimize. But as we did with logistic regression, we can come up with a tractable approximation of the  $0 - 1$  loss:

## Exponential Loss

$$\ell^{\text{EXP}}(h(\mathbf{x}), y) = e^{-yf(\mathbf{x})}$$

$\ell^{\text{EXP}}(h(\mathbf{x}), y)$  is easier to handle numerically as it is differentiable



# Choosing the $t$ -th classifier

Suppose we have built a classifier  $f_{t-1}(\mathbf{x})$ , and we want to improve it by adding a weak learner  $h_t(\mathbf{x})$

$$f(\mathbf{x}) = f_{t-1}(\mathbf{x}) + \beta_t h_t(\mathbf{x})$$

How can we choose optimally the new classifier  $h_t(\mathbf{x})$  and the combination coefficient  $\beta_t$ ?

Adaboost greedily **minimizes the exponential loss function**.

$$\begin{aligned}(h_t^*(\mathbf{x}), \beta_t^*) &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} \sum_n e^{-y_n f(\mathbf{x}_n)} \\ &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} \sum_n e^{-y_n [f_{t-1}(\mathbf{x}_n) + \beta_t h_t(\mathbf{x}_n)]} \\ &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} \sum_n w_t(n) e^{-y_n \beta_t h_t(\mathbf{x}_n)}\end{aligned}$$

where we have used  $w_t(n)$  as a shorthand for  $e^{-y_n f_{t-1}(\mathbf{x}_n)}$

# The new classifier

We can decompose the **weighted** loss function into two parts

$$\begin{aligned} & \sum_n w_t(n) e^{-y_n \beta_t h_t(\mathbf{x}_n)} \\ &= \sum_n w_t(n) e^{\beta_t} \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)] + \sum_n w_t(n) e^{-\beta_t} \mathbb{I}[y_n = h_t(\mathbf{x}_n)] \\ &= \sum_n w_t(n) e^{\beta_t} \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)] + \sum_n w_t(n) e^{-\beta_t} (1 - \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)]) \\ &= (e^{\beta_t} - e^{-\beta_t}) \sum_n w_t(n) \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)] + e^{-\beta_t} \sum_n w_t(n) \end{aligned}$$

We have used the following properties to derive the above

- $y_n h_t(\mathbf{x}_n)$  is either 1 or -1 as  $h_t(\mathbf{x}_n)$  is the output of a binary classifier
- The indicator function  $\mathbb{I}[y_n = h_t(\mathbf{x}_n)]$  is either 0 or 1, so it equals  $1 - \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)]$



# Finding the optimal weak learner

## Summary

$$\begin{aligned}(h_t^*(\mathbf{x}), \beta_t^*) &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} \sum_n w_t(n) e^{-y_n \beta_t h_t(\mathbf{x}_n)} \\ &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} (e^{\beta_t} - e^{-\beta_t}) \sum_n w_t(n) \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)] \\ &\quad + e^{-\beta_t} \sum_n w_t(n)\end{aligned}$$

**What term(s) must we optimize to choose  $h_t(\mathbf{x}_n)$ ?**

$$h_t^*(\mathbf{x}) = \operatorname{argmin}_{h_t(\mathbf{x})} \epsilon_t = \sum_n w_t(n) \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)]$$

Minimize weighted classification error as noted in step 1 of Adaboost!

# How to choose $\beta_t$ ?

## Summary

$$\begin{aligned}
 (h_t^*(\mathbf{x}), \beta_t^*) &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} \sum_n w_t(n) e^{-y_n \beta_t h_t(\mathbf{x}_n)} \\
 &= \operatorname{argmin}_{(h_t(\mathbf{x}), \beta_t)} (e^{\beta_t} - e^{-\beta_t}) \sum_n w_t(n) \mathbb{I}[y_n \neq h_t(\mathbf{x}_n)] \\
 &\quad + e^{-\beta_t} \sum_n w_t(n)
 \end{aligned}$$

## What term(s) must we optimize?

We need to minimize the entire objective function with respect to  $\beta_t$ !

We can do this by taking derivative with respect to  $\beta_t$ , setting to zero, and solving for  $\beta_t$ . After some calculation and using  $\sum_n w_t(n) = 1$ , we find:

$$\beta_t^* = \frac{1}{2} \log \frac{1 - \epsilon_t}{\epsilon_t}$$

which is precisely step 2 of Adaboost! (**Exercise – verify the solution**)

# Updating the weights

Once we find the optimal weak learner we can update our classifier:

$$f(\mathbf{x}) = f_{t-1}(\mathbf{x}) + \beta_t^* h_t^*(\mathbf{x})$$

We then need to compute the weights for the above classifier as:

$$\begin{aligned} w_{t+1}(n) &= e^{-y_n f(\mathbf{x}_n)} = e^{-y_n [f_{t-1}(\mathbf{x}_n) + \beta_t^* h_t^*(\mathbf{x}_n)]} \\ &= w_t(n) e^{-y_n \beta_t^* h_t^*(\mathbf{x}_n)} = \begin{cases} w_t(n) e^{\beta_t^*} & \text{if } y_n \neq h_t^*(\mathbf{x}_n) \\ w_t(n) e^{-\beta_t^*} & \text{if } y_n = h_t^*(\mathbf{x}_n) \end{cases} \end{aligned}$$

**Intuition** Misclassified data points will get their weights increased, while correctly classified data points will get their weight decreased

# Meta-Algorithm

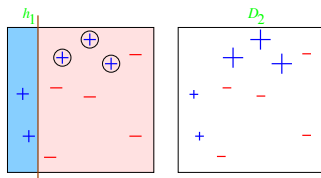
Note that the AdaBoost algorithm itself never specifies how we would get  $h_t^*(\mathbf{x})$  as long as it minimizes the weighted classification error

$$\epsilon_t = \sum_n w_t(n) \mathbb{I}[y_n \neq h_t^*(\mathbf{x}_n)]$$

In this aspect, the AdaBoost algorithm is a meta-algorithm and can be used with any type of classifier

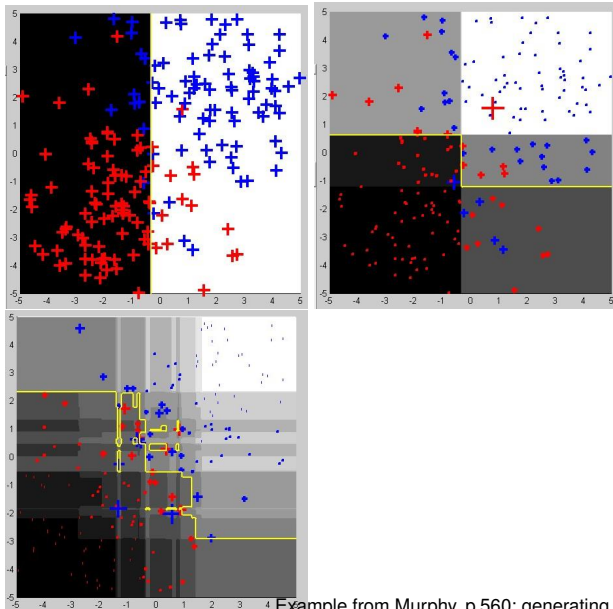
## E.g., Decision Stumps

How do we choose the decision stump classifier given the weights at the second round of the following distribution?



- Presort data by each feature in  $O(dN \log N)$  time
- Evaluate  $N + 1$  thresholds for each feature at each round in  $O(dN)$  time
- In total  $O(dN \log N + dNT)$  time – this efficiency is an attractive quality of boosting!

# Interpreting boosting as learning nonlinear basis



Example from Murphy, p.560; generating script written by R.Stapenhurst

# Example: Netflix



- The Netflix Prize: improve the accuracy of predictions about how much someone is going to love a movie based on their movie preferences.
- <http://www.netflixprize.com>
- Training data is a set of users and past ratings (1 to 5 stars).
- Construct a classifier that predicts user rating for unrated movies.
- Winning team (BellKor's Pragmatic Chaos) employed boosting. They received 1M\$.

FIN



# Syllabus I

## Part I: Introduction to unsupervised learning

- Dimensionality reduction
  - Principal component analysis, SVD, Biplots, Multidimensional scaling, Isomap
- Clustering
  - K-means
  - Hierarchical clustering

# Syllabus II

## Part II: Supervised learning

- Empirical risk minimization
- Regression
  - Linear
  - Non-linear basis functions
  - Gradient descent
- Overfitting, cross-validation
- Regularization
- Bias/variance tradeoff
- Classification
  - Discriminant analysis
  - Logistic regression
  - Naïve Bayes
  - K-nearest neighbors
- Generative vs discriminative methods
- Performance evaluation

# Syllabus III

## Part III: Useful algorithms for supervised learning

- Decision trees
- Bagging/Random forests
- Neural networks
- Deep learning
- Boosting