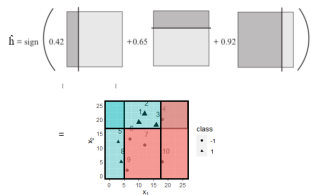


Introduction to Machine Learning

Boosting

Gradient Boosting: Introduction and AdaBoost



Learning goals

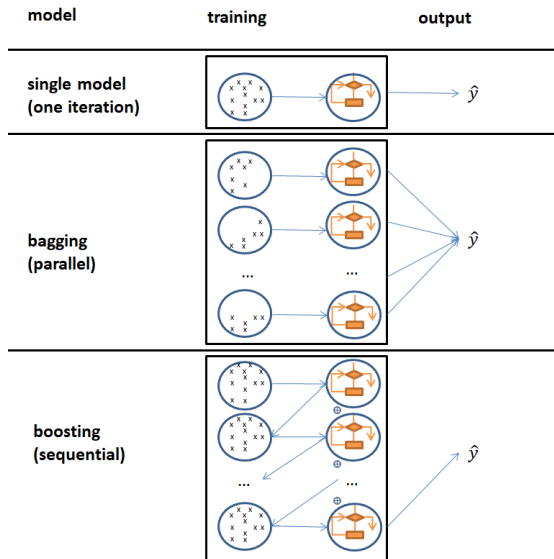
- Understand general idea of boosting
- Learn AdaBoost algorithm
- Understand difference between bagging and boosting

INTRODUCTION TO BOOSTING

- Boosting is considered to be one of the most powerful learning ideas within the last twenty years.
- Originally designed for classification, (especially gradient) boosting handles regression (and many other supervised tasks) naturally nowadays.
- Homogeneous ensemble method (like bagging), but fundamentally different approach.
- **Idea:** Take a weak classifier and sequentially apply it to modified versions of the training data.
- We will begin by describing an older, simpler boosting algorithm designed for binary classification, the popular “AdaBoost”.



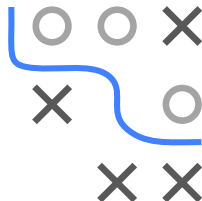
BOOSTING VS. BAGGING



THE BOOSTING QUESTION

The first boosting algorithm ever was in fact no algorithm for practical purposes, but the solution for a theoretical problem:

“Does the existence of a weak learner for a certain problem imply the existence of a strong learner?” ▶ Kearns n.d.



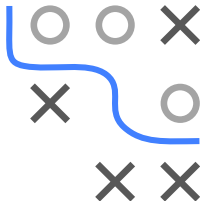
- **Weak learners** are defined as a prediction rule with a correct classification rate that is at least slightly better than random guessing ($> 50\%$ accuracy on a balanced binary problem).
- We call a learner a **strong learner** “if there exists a polynomial-time algorithm that achieves low error with high confidence for all concepts in the class” ▶ Schapire 1990 .

In practice it is typically easy to construct weak learners, but difficult to build a strong one.

THE BOOSTING ANSWER - ADABOOST

- The **AdaBoost** (Adaptive Boosting) algorithm is a **boosting** method for binary classification by ▶ Freund, Schapire, et al. 1996 .
- The base learner is sequentially applied to weighted training observations.
- After each base learner fit, currently misclassified observations receive a higher weight for the next iteration, so we focus more on instances that are harder to classify.

Leo Breiman (referring to the success of AdaBoost):

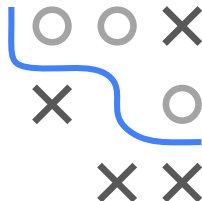


THE BOOSTING ANSWER - ADABOOST / 2

- Assume a target variable y encoded as $\{-1, +1\}$, and weak base learners (e.g., tree stumps) from a hypothesis space \mathcal{B} .
- Base learner models $b^{[m]}$ are binary classifiers that map to $\mathcal{Y} = \{-1, +1\}$. We might sometimes write $b(\mathbf{x}, \theta^{[m]})$ instead.
- Predictions from all base models $b^{[m]}$ over M iterations are combined in an additive manner by the formula:

$$f(\mathbf{x}) = \sum_{m=1}^M \beta^{[m]} b^{[m]}(\mathbf{x}).$$

- Weights $\beta^{[m]}$ are computed by the boosting algorithm. Their purpose is to give higher weights to base learners with higher predictive accuracy.
- The number of iterations M is the main tuning parameter.
- The discrete prediction function is $h(\mathbf{x}) = \text{sign}(f(\mathbf{x})) \in \{-1, +1\}$.



THE BOOSTING ANSWER - ADABOOST / 3

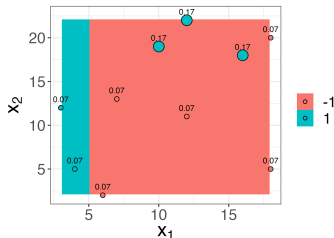
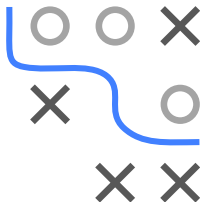
- 1: Initialize observation weights: $w^{[1](i)} = \frac{1}{n} \quad \forall i \in \{1, \dots, n\}$
- 2: **for** $m = 1 \rightarrow M$ **do**
- 3: Fit classifier to training data with weights $w^{[m]}$ and get hard label classifier $\hat{b}^{[m]}$
- 4: Calculate weighted in-sample misclassification rate

$$\text{err}^{[m]} = \sum_{i=1}^n w^{[m](i)} \cdot \mathbb{1}_{\{y^{(i)} \neq \hat{b}^{[m]}(\mathbf{x}^{(i)})\}}$$

ADABOOST ILLUSTRATION

Example description

- $n = 10$ observations and two features x_1 and x_2
- Tree stumps as base learners $b^{[m]}(\mathbf{x})$
- Balanced classification task with y encoded as $\{-1, +1\}$
- $M = 3$ iterations \Rightarrow initial weights $w^{[1](i)} = \frac{1}{10} \quad \forall i \in 1, \dots, 10$.



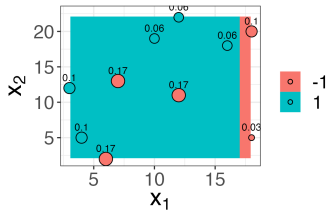
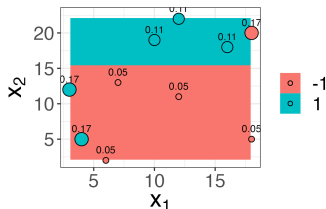
New observation weights:

- Prediction correct:
 $w^{[2](i)} = w^{[1](i)} \cdot \exp(-\hat{\beta}^{[1]} \cdot 1)$
 ≈ 0.065 .
- For 3 misclassified observations:
 $w^{[2](i)} = w^{[1](i)} \cdot \exp(-\hat{\beta}^{[1]} \cdot (-1))$
 ≈ 0.15 .
- After normalization:
 - correctly classified: $w^{[2](i)} \approx 0.07$
 - misclassified: $w^{[2](i)} \approx 0.17$

Iteration $m = 1$:

- $\text{err}^{[1]} = 0.3$
- $\hat{\beta}^{[1]} = \frac{1}{2} \log\left(\frac{1-0.3}{0.3}\right) \approx 0.42$

ADABOOST ILLUSTRATION / 2



Iteration $m = 2$:

- $\text{err}^{[2]} \approx 3 \cdot 0.07 = 0.21$

- $\hat{\beta}^{[2]} \approx 0.65$

New observation weights (before normalization):

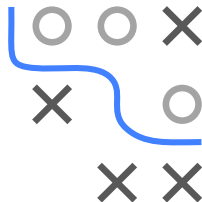
- For misclassified observations: $w^{[3](i)} = w^{[2](i)} \cdot \exp(-\hat{\beta}^{[2]} \cdot (-1)) \approx w^{[2](i)} \cdot 1.92$

- For correctly classified observations: $w^{[3](i)} = w^{[2](i)} \cdot \exp(-\hat{\beta}^{[2]} \cdot 1) \approx w^{[2](i)} \cdot 0.52$

Iteration $m = 3$:

- $\text{err}^{[3]} \approx 3 \cdot 0.05 = 0.15$

- $\hat{\beta}^{[3]} \approx 0.92$



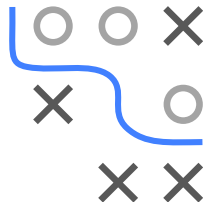
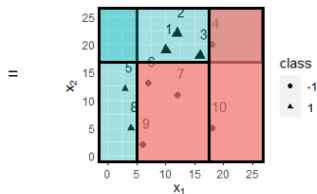
Note: the smaller the error rate of a base learner, the larger the weight, e.g.,

$$\text{err}^{[3]} \approx 0.15 < \text{err}^{[1]} \approx 0.3 \text{ and } \hat{\beta}^{[3]} \approx 0.92 > \hat{\beta}^{[1]} \approx 0.42.$$

ADABOOST ILLUSTRATION / 3

With $\hat{f}(\mathbf{x}) = \sum_{m=1}^M \hat{\beta}^{[m]} \hat{b}^{[m]}(\mathbf{x})$ and $h(\mathbf{x}) = \text{sign}(f(\mathbf{x})) \in \{-1, +1\}$, we get:

$$\hat{h} = \text{sign} \left(\begin{array}{c} \text{[Diagram 1]} \\ 0.42 \end{array} + \begin{array}{c} \text{[Diagram 2]} \\ +0.65 \end{array} + \begin{array}{c} \text{[Diagram 3]} \\ +0.92 \end{array} \right)$$



Hence, when all three base classifiers are combined, all samples are classified correctly.

BAGGING VS BOOSTING

Random forest

- Base learners are typically deeper decision trees (not only stumps!)
- Equal weights for base learners
- Base learners independent of each other
- Aim: variance reduction
- Tends **not** to overfit

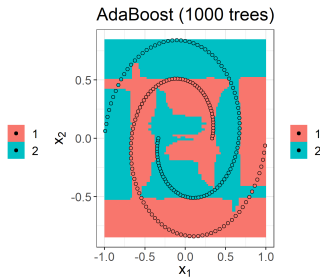
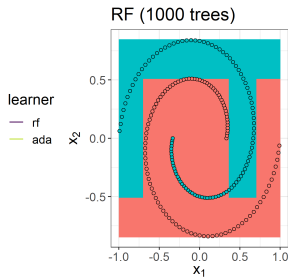
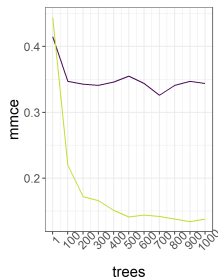
AdaBoost

- Base learners are weak learners, e.g., only stumps
- Base learners have different weights depending on their predictive accuracy
- Sequential algorithm, hence order matters
- Aim: bias and variance reduction
- Tends to overfit



BAGGING VS BOOSTING STUMPS

Random forest versus AdaBoost (both with stumps) on Spirals data from `mlbench` ($n = 200$, $sd = 0$), with 5×5 repeated CV.



Weak learners do not work well with bagging as only variance, but no bias reduction happens.

OVERFITTING BEHAVIOR

Historically, the overfitting behavior of AdaBoost was often discussed. Increasing standard deviation to $sd = 0.3$ and allowing for more flexibility in the base learners, AdaBoost overfits with increasing number of trees while the RF only saturates. The overfitting of AdaBoost here is quite typical as data is very noisy.

