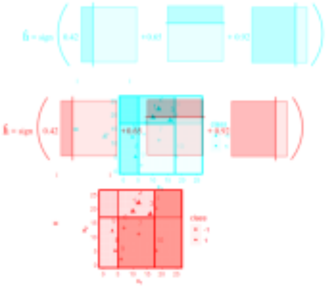
Introduction to Machine Learning

Gradient Boosting: Introduction and AdaBoost



Learning goals

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

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, 1988

- **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

Any weak (base) learner can be iteratively boosted to become a strong learner. The proof of this ground-breaking idea generated the first boosting algorithm.

- 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):
"Boosting is the best off-the-shelf classifier in the world."

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

Algorithm AdaBoost

Initialize observation weights: $w^{[1](i)} = \frac{1}{n} \quad \forall i \in \{1, \dots, n\}$

for $m = 1 \to M$ **do**

Fit classifier to training data with weights $w^{[m]}$ and get hard label classifier $\hat{b}^{[m]}$

Calculate weighted in-sample misclassification rate

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

Compute: $\hat{\beta}^{[m]} = \frac{1}{2} \log\left(\frac{1-\text{err}^{[m]}}{\text{err}^{[m]}}\right)$

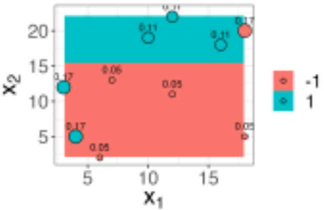
Set: $w^{[m+1](i)} = w^{[m](i)} \cdot \exp\left(-\hat{\beta}^{[m]} \cdot y^{(i)} \cdot \hat{b}^{[m]}(\mathbf{x}^{(i)})\right)$

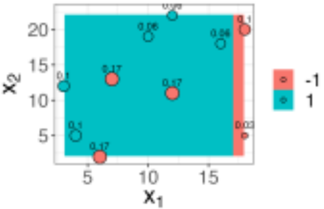
Normalize $w^{[m+1](i)}$ such that $\sum_{i=1}^{n} w^{[m+1](i)} = 1$

end for

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

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: $w^{[3](i)} = w^{[2](i)} \cdot \exp\left(-\hat{\beta}^{[2]} \cdot (-1)\right) \approx w^{[2](i)} \cdot 1.92$
- For correctly classified observations: $w^{[3](i)} = w^{[2](i)} \cdot \exp\left(-\hat{\beta}^{[2]} \cdot 1\right) \approx w^{[2](i)} \cdot 0.52$

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

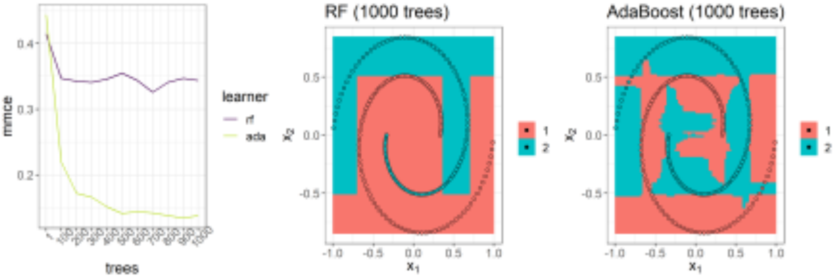
ADABOOST ILLUSTRATION / 3

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:

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

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.