

Boosting

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Introduction

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 - ▶ Many trees trained on slightly different data contribute to the model's predictions
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Introduction

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 - ▶ Many trees trained on slightly different data contribute to the model's predictions
 - ▶ This is an *aggregation* approach, as each base model is *trained separately* and the predictions are aggregated
- ▶ Today we will discuss *boosting* approaches, where the base models in the ensemble are *trained sequentially*
 - ▶ Boosting was originally developed as a classifier aimed at combining many “weak” classifiers into a more powerful “committee” by Freund and Schapire (1997) as “Adaptive Boosting” or “AdaBoost.M1”

Bagging vs. Boosting

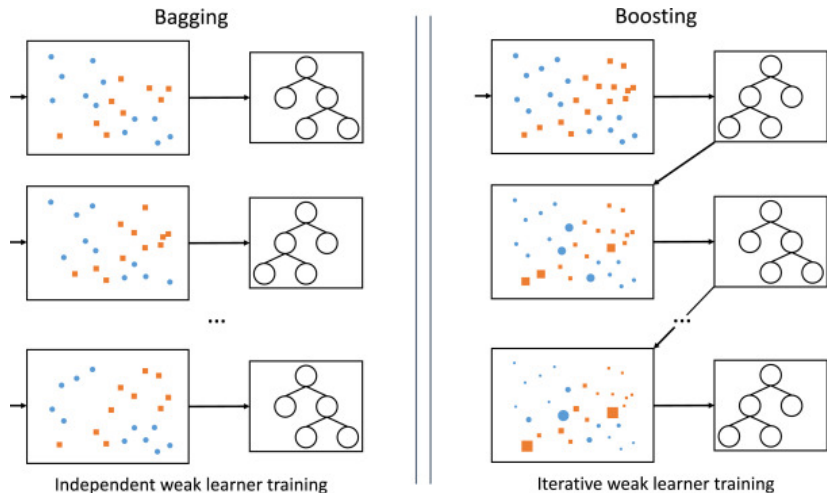


Image Credit: <https://www.sciencedirect.com/science/article/pii/S1566253520303195>

To begin, suppose Y is a binary variable encoded by $\{-1, 1\}$, and define the error rate as:

$$\text{error} = \frac{1}{n} \sum_{i=1}^n I(y_i \neq G(\mathbf{x}_i))$$

- ▶ Here, $G(\mathbf{x}_i)$ represents the predicted class for an observation with predictors \mathbf{x}_i
 - ▶ Notice that if y_i does not match the predicted class the summation increases by 1
 - ▶ Thus, we see that error = 1 – classification accuracy

AdaBoost

In AdaBoost, $G()$ is a sum of M sequentially built classifiers trained on differently weighted versions of the data:

$$G(x) = \text{Sign}\left(\sum_{m=1}^M \alpha_m G_m(x)\right)$$

- ▶ $\alpha_1, \dots, \alpha_M$ allow each classifier to contribute differently to the final prediction (thereby allowing some models to contribute more)
- ▶ Each training data-point, (\mathbf{x}_i, y_i) is also given a different weight, w_{im} , at each iteration
 - ▶ At the first step of the algorithm, these weights are set to $\frac{1}{n}$, so that all observations contribute equally
 - ▶ At step m , the weights of observations misclassified by $G_{m-1}(x)$ are increased by a factor of $\exp(\alpha_m)$

AdaBoost (algorithm)

Pseudocode for the original AdaBoost algorithm:

```
w = 1/n # initialize weights
for i in 1:M:
    G_m = model.fit(X, w, y) # fit using weighted data
    err_m = error(G_m) # calculate error
    alpha_m = log((1-err_m)/err_m)
    w_i = w_i*exp(alpha_m*(y_i != G_m(x_i))) # reweight
```

- ▶ Each model's contribution in the ensemble is based upon its accuracy (notice $\log((1-0.5)/0.5) = 0$)
- ▶ If an observation was misclassified, its weight in the next model is increased by a factor of $\exp(\alpha_m)$

AdaBoost (diagram)

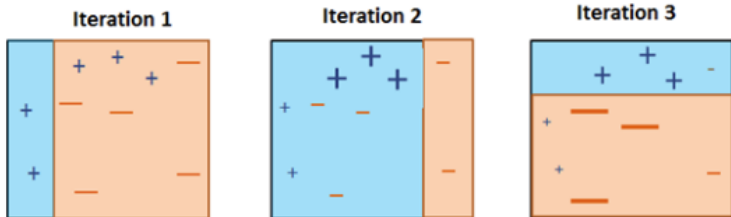


Image Credit: Packt Big data and Business Intelligence

Gradient Boosting

- ▶ AdaBoost re-weights observations that are misclassified before training the next model
 - ▶ Gradient boosting takes a more general approach - train subsequent models to the *residuals* (or loss contributions for cost functions other than squared error)
- ▶ At each iteration, t , of gradient boosting, the algorithm finds a base model (estimates \hat{f}_t):

$$\hat{f}_t(\mathbf{X}) = \arg \min_{f_t} (L(y, \hat{y}_{t-1} + \alpha f_t(\mathbf{X})))$$

- ▶ For the squared error cost function, this amounts to fitting the base model to the residuals

Gradient Boosting

Consider squared error as the objective function:

$$\frac{1}{n}(\mathbf{y} - (\hat{\mathbf{y}}_{t-1} + \alpha f_t(\mathbf{X})))^T (\mathbf{y} - (\hat{\mathbf{y}}_{t-1} + \alpha f_t(\mathbf{X})))$$

If we disregard terms without f_t , we have:

$$\frac{1}{n}(2\alpha \mathbf{y}^T f_t(\mathbf{X}) - 2\alpha \hat{\mathbf{y}}_{t-1}^T f_t(\mathbf{X}) + \alpha^2 f_t(\mathbf{X})^T f_t(\mathbf{X}))$$

After differentiating WRT $f_t(\mathbf{X})$:

$$\frac{2\alpha}{n}(\mathbf{y} - \hat{\mathbf{y}}_{t-1} + \alpha f_t(\mathbf{X}))$$

If $\alpha = 1$ and we substitute $\mathbf{r} = \mathbf{y} - \hat{\mathbf{y}}_{t-1}$, we have $\frac{1}{n}(\mathbf{r} - f_t(\mathbf{X}))$, which is minimized when f_t is fit to the residuals.

Gradient Boosting (pseudocode)

```
r = y ## Initialize residuals
f = 0 ## Initialize model to zero

for i in 1:M:
    f_m = model.fit(X, r) ## Fit model to residuals
    f = f + alpha*f_m ## Add new model to ensemble
    r = r - alpha*f_m ## Update residuals
```

- ▶ The output is f , the ensemble model consisting of M different base models.
- ▶ The learning rate, α , is a small positive number that controls how quickly boosting learns (by limiting how much a model can contribute to the ensemble)

Gradient Boosting vs AdaBoost (diagram)

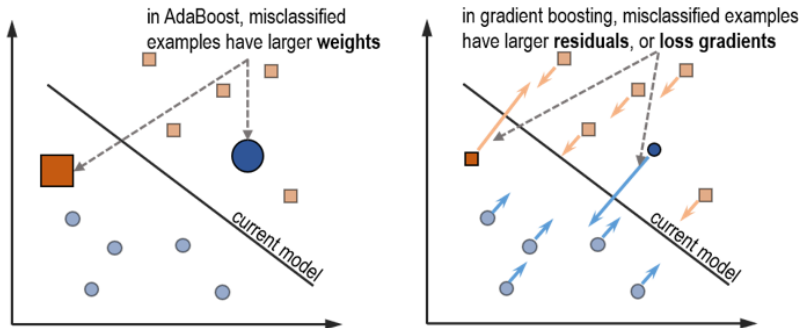


Image credit: Ensemble Methods for Machine Learning (textbook)

Gradient Boosting (comments)

- ▶ Unlike bagging (random forests), boosting can overfit if too many base models are used, so the number of boosting iterations should be carefully chosen.
 - ▶ The learning rates (value of α) and the number of boosting iterations work jointly to dictate whether a model ends up being overfit or underfit
- ▶ Like random forests, boosting tends to work best using shallow simple decision trees (max depths of either 1 or 2)