#### **Ensemble Methods**

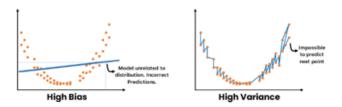
A. Sanchez, F. Reverter and E. Vegas

#### Outline

- Introduction to Ensembles
- Bagging and the Bootstrap
- Random Forests
- Boosting and its variants

#### Weak learners

- Models that perform only slightly better than random guessing are called *weak learners* (Bishop 2007).
- Weak learners low predictive accuracy may be due, to the predictor having high bias or high variance.



### Trees may be weak learners

- Trees use to be sensitive to small changes in training data which lead to very different tree structure.
- This implies predictions are highly variable
- This may be explained because they are greedy algorithms making locally optimal decisions at each node without considering the global optimal solution.
  - This can lead to suboptimal splits and ultimately a weaker predictive performance.

### There's room for improvement

- In many situations trees may be a good option (e.g. for simplicity and interpretability)
- But there are issues that, if solved, may improve performance.
- It is to be noted, too, that these problems are not unique to trees.
  - Other simple models such as linear regression may be considered as weakl learners in may situations.

#### The bias-variance trade-off

 When we try to improve weak learners we need to deal with the bias-variance trade-off.

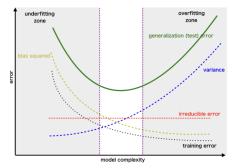


Figure 1: The bias-variance trade-off

#### How to deal with such trade-off

- How can a model be made less variable or less biased without this increasing its bias or variance?
- There are distinct appraches to deal with this problem
  - Regularization,
  - Feature engineering,
  - Model selection
  - Ensemble learning

#### Ensemble learners

- Ensemble learning takes a distinct based on "the wisdom of crowds".
- Predictors, also called, ensembles are built by fitting repeated (weak learners) models on the same data and combining them to form a single result.
- As a general rule, ensemble learners tend to improve the results obtained with the weak learners they are made of.

#### Ensemble methods

- If we rely on how they deal with the bias-variance trade-off we can consider distinct groups of ensemble methods:
  - Bagging
  - Boosting
  - Hybrid learners

Emnsemble methods cheatsheet

## Aggregating Trees

Bagging, Random Forests, and Random Patches reduce variance compared to individual decision trees by constructing multiple trees using different types of subsets:

- Subsets of observations (Bagging)
- Subsets of features (Random Forests)
- Subsets of both observations and features (Random Patches)

## Boosting & Stacking

- Boosting or Stacking combine distinct predictors to yield a model with an increasingly smaller error, and so reduce the bias.
- They differ on if do the combination
  - sequentially (1) or
  - using a meta-model (2) .

# Hybrid Techniques

- **Hybrid techniques** combine approaches in order to deal with both variance and bias.
- The approach should be clear from their name:
  - Gradient Boosted Trees with Bagging
  - Stacked bagging

### Bagging: bootstrap aggregation

- Decision trees suffer from high variance when compared with other methods such as linear regression, especially when n/p is moderately large.
- Given that this is intrinsic to trees, Breiman (1996) sugested to build multiple trees derived from the same dataset and, somehow, average them.

### Averaging decreases variance

- Bagging relies, informally, on the idea that:
  - $\bullet \ \ {\rm given} \ X \sim F() \text{, s.t. } Var_F(X) = \sigma^2 \text{,}$
  - given a s.r.s.  $X_1, ..., X_n$  from F then
  - if  $\overline{X} = \frac{1}{N} \sum_{i=1}^{n} X_i$  then  $var_F(\overline{X}) = \sigma^2/n$ .
- That is, relying on the sample mean instead of on simple observations, decreases variance by a factor of n.
- BTW this idea is still (approximately) valid for more general statistics where the CLT applies.

# What means averaging trees?

#### Two questions arise here:

- How to go from X to  $X_1,...,X_n$ ?
  - This will be done using bootstrap resampling.
- What means "averaging" in this context.
  - Depending on the type of tree:
    - Average predictions for regression trees.
    - Majority voting for classification trees.

## BAGGING: Bootstrap Aggregation

- Breiman (1996) combined the ideas of:
  - Averaging provides decreased variance estimates,
  - Bootstrap provides multiple (re)samples.
- He suggested: **b**ootstrap **agg**regat**ing**:
  - Take resamples from the original training dataset
  - Learn the model on each bootstrapped training set to get a prediction  $\hat{f}^{*b}(x).$
  - Average  $\hat{f}^{*b}(x)$  to obtain improved prediction/classification.

# Bagging prediction/classifier

• For regression (trees) the **bagged estimate** is the average prediction at x from these B trees.

$$\hat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}(x)$$

 For classification (trees) the bagged classifier selects the class with the most "votes" from the B trees:

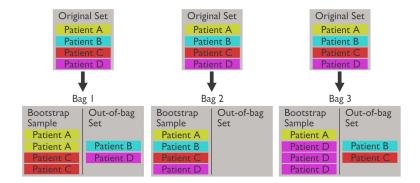
$$\hat{G}_{bag}(x) = \arg\max_{k} \hat{f}_{bag}(x).$$

### Resampling based estimators

- The bootstrap was introduced as a way to provide standard error estimators.
- When used to compute  $\hat{f}_{bag}(x)$  or  $\hat{G}_{bag}(x)$ , as described above, it provides direct estimators of a characteristic, not of their standard errors.
- However, the bagging process can also provide resampling based estimates of the precision of these estimators.

### Out-Of-Bag observations

 Every time a resample is taken with replacement, some observations are omitted, due to the multiple occurring of others.



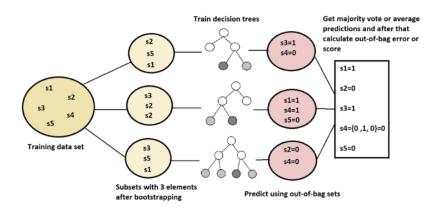
• These *out-of-bag* (OOB) observations can be used to build an estimate of prediction error.

### Out-Of-Bag error estimates

Since each out-of-bag set is not used to train the model, it can be used to evaluate performance.

- Find all trees that are not trained by the OOB instance.
- ② Take the majority vote of these trees for the OOB instance, compared to the true value of the OOB instance.
- 3 Compile OOB error for all instances in the OOB dataset.

#### Illustration of OOB EE



Source:

https://www.baeldung.com/cs/random-forests-out-of-bag-error



# Bagging in R

- We use the AmesHousing dataset on house prices in Ames, IA, to predict the "Sales price" of houses.
- Start by splitting the dataset in test/train subsets
- Build a bagged tree on the train subset and evaluate it on the test subset.
- Interpret the results using "Variable importance"
- Bagging is equivalent to RandomForest if each tree in a Random Forest considers all features at every split.
- So we use randomForest package setting mtry to total number of features.

### Bagging - Prepare data

```
# Prepare "clean" dataset from raw data
ames <- AmesHousing::make ames()</pre>
# Scale response variable to improve readability
ames$Sale Price <- ames$Sale Price/1000
# Split in test/training
set.seed(123)
train <- sample(1:nrow(ames), nrow(ames)/2)
# split <- rsample::initial_split(ames, prop = 0.7,
                          strata = "Sale_Price")
#
ames_train <- ames[train,]
ames_test <- ames[-train,]</pre>
```

### Bagging - Build bag of trees

### Bagging - Results

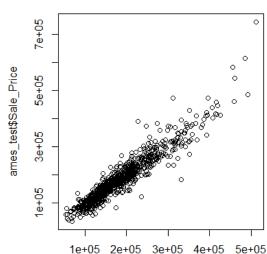
```
show(bag.Ames )
Call:
randomForest(formula = Sale_Price ~ ., data = ames_train,
               Type of random forest: regression
                     Number of trees: 100
No. of variables tried at each split: 80
          Mean of squared residuals: 771498315
                    % Var explained: 87.89
```

## Bagging - Prediction and accuracy

```
yhat.bag <- predict(bag.Ames, newdata = ames_test)
MSE= mean((yhat.bag -ames_test$Sale_Price)^2)
plot(yhat.bag, ames_test$Sale_Price, main=c("MSE= ", MSE))
abline(0, 1)</pre>
```

### Bagging - Prediction and accuracy

MSE= 658769103.178802





### Interpetability: The "achiles heel"

- Trees may have a straightforward interpretation,
  - Plotting the tree provides information about
    - which variables are important
    - how they act on the prediction
- Ensembles are less intuitive because
  - there is no consensus tree.
  - not clear which variables are most important.

### Feature importance from Trees

- To measure feature importance, the reduction in the loss function (e.g., SSE) attributed to each variable at each split is tabulated.
- The total reduction in the loss function across all splits by a variable are summed up and used as the total feature importance.

### Feature importance for Ensembles

 Variable importance measures can be extended to an ensemble simply by adding up variable importance over all trees built.

```
%IncMSE IncNodePurity
Gr_Liv_Area
               28.539804
                           1.104450e+12
Overall_Qual
               28.512566
                           6.776106e+12
Neighborhood
               16.369936
                           1.526868e+12
Total Bsmt SF
               11.254286
                           6.535928e+11
First Flr SF
               11.077080
                           4.336448e+11
MS_SubClass
                9.303874
                           8.894513e+10
                 8.390321
                           1.105019e+11
Garage_Area
Overall Cond
                 6.517383
                           4.146669e+10
Year_Remod_Add
                6.440552
                           5.582591e+10
Kitchen_Oual
                6.340537
                           4.133352e+10
```

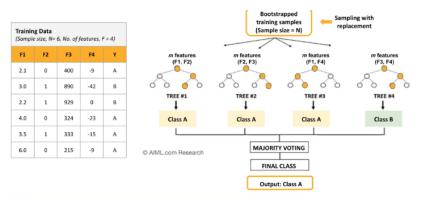
### Random forests: decorrelating predictors

- Bagged trees, based on re-samples (of the same sample) tend to be highly correlated.
- Leo Breimann, again, introduced a modification to bagging, he called Random forests, that aims at decorrelating trees as follows:
  - When growing a tree from one bootstrap sample,
  - At each split use only a randomly selected subset of predictors.

### Split variable randomization

- While growing a decision tree, during the bagging process,
- Random forests perform split-variable randomization:
  - each time a split is to be performed,
  - the search for the split variable is limited to a random subset of  $m_{try}$  of the original p features.

#### Random forests



Key parameters of Random Forest Model are: (a) Number of trees, (b) Maximum depth of the trees (c) Size of the random subset of features In this example, No. of trees = 4, Depth = 2, and Feature subset size, m = 2 (no. of features/2)

Source: AIML.com research



### How many variables per split?

- ullet m can be chosen using cross-validation, but
- The usual recommendation for random selection of variables at each split has been studied by simulation:
  - For regression default value is m=p/3
  - For classification default value is  $m = \sqrt{p}$ .
- If m=p, we have bagging instead of RF.

# Random forest algorithm (1)

```
1. Given a training data set
Select number of trees to build (n trees)
for i = 1 to n trees do
      Generate a bootstrap sample of the original data
      Grow a regression/classification tree to the bootstrapped data
     for each split do
      | Select m_try variables at random from all p variables
8. | Pick the best variable/split-point among the m try
      | Split the node into two child nodes
10. | end
11. | Use typical tree model stopping criteria to determine when a
    | tree is complete (but do not prune)
12. end
13. Output ensemble of trees
```

Figure 2: RF Algorithm, from ch. 11 in (Boehmke and Greenwell 2020)

# Random forest algorithm (2)

#### Algorithm 17.1 RANDOM FOREST.

- 1 Given training data set d = (X, y). Fix  $m \le p$  and the number of trees B.
- 2 For b = 1, 2, ..., B, do the following.
- (a) Create a bootstrap version of the training data  $d_b^*$ , by randomly sampling the n rows with replacement n times. The sample can be represented by the bootstrap frequency vector  $\boldsymbol{w}_{b}^{*}$ .
- (b) Grow a maximal-depth tree  $\hat{r}_b(x)$  using the data in  $d_b^*$ , sampling m of the p features at random prior to making each split.
- (c) Save the tree, as well as the bootstrap sampling frequencies for each of the training observations.
- 3 Compute the random-forest fit at any prediction point  $x_0$  as the average

$$\hat{r}_{rf}(x_0) = \frac{1}{B} \sum_{b=1}^{B} \hat{r}_b(x_0).$$

4 Compute the  $OOB_i$  error for each response observation  $y_i$  in the training data, by using the fit  $\hat{r}_{rf}^{(i)}$ , obtained by averaging only those  $\hat{r}_b(x_i)$  for which observation i was not in the bootstrap sample. The overall OOB error is the average of these  $OOB_i$ .

### Out-of-the box performance

- Random forests tend to provide very good out-of-the-box performance, that is:
  - Although several hyperparameters can be tuned,
  - Default values tend to produce good results.
- Moreover, among the more popular machine learning algorithms, RFs have the least variability in their prediction accuracy when tuning (Probst, Wright, and Boulesteix 2019).

### Out of the box performance

- A random forest trained with all hyperparameters set to their default values can yield an OOB RMSE that is better than many other classifiers, with or without tuning.
- This combined with good stability and ease-of-use has made it the option of choice for many problems.

# Out of the box performance example

```
# number of features
n_features <- length(setdiff(names(ames_train), "Sale Price
# train a default random forest model
ames rf1 <- ranger(
  Sale Price ~ .,
  data = ames_train,
  mtry = floor(n_features / 3),
  respect.unordered.factors = "order",
  seed = 123
# get OOB RMSE
(default_rmse <- sqrt(ames_rf1$prediction.error))</pre>
## [1] 24859.27
```

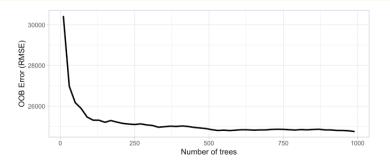
# Tuning hyperparameters

There are several parameters that, appropriately tuned, can improve RF performance.

- Number of trees in the forest.
- ② Number of features to consider at any given split  $(m_{try})$ .
- Omplexity of each tree.
- Sampling scheme.
- Splitting rule to use during tree construction.
- 1 & 2 usually have largest impact on predictive accuracy.

### 1. Number of trees





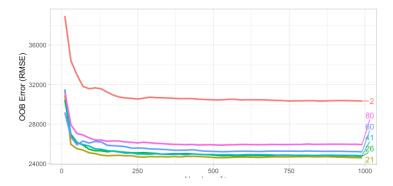
- The number of trees needs to be sufficiently large to stabilize the error rate.
- More trees provide more robust and stable error estimates
- ullet But impact on computation time increases linearly with  $n_{t}ree$



# 2. Number of features $(m_{trn})$ .



Start with five evenly spaced values of  $m_{try}$  across the range 2–p centered at the recommended default as illustrated in Figure 11.2.



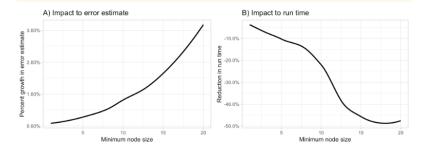
- $\bullet$   $m_{try}$  helps to balance low tree correlation with reasonable predictive strength.
- Sensitive to total number of variables. If high /low, better



### 3. Complexity of each tree.



When adjusting node size start with three values between 1–10 and adjust depending on impact to accuracy and run time.

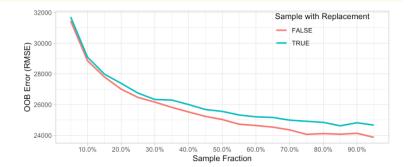


- The complexity of underlying trees influences RF performance.
- Node size has strong influence on error and time.

### 4. Sampling scheme.



Assess 3–4 values of sample sizes ranging from 25%–100% and if you have unbalanced categorical features try sampling without replacement.



- Default: Bootstrap sampling with replacement on 100% observations. - Sampling size and replacement or not can affect diversity and reduce bias.
- Node size has strong influence on error and time.

### 5. Splitting rule

- *Default splitting rules* favor features with many splits, potentially biasing towards certain variable types.
- Conditional inference trees offer an alternative to reduce bias, but may not always improve predictive accuracy and have longer training times.
- Randomized splitting rules, like extremely randomized trees (which draw split points completely randomly), improve computational efficiency but may not enhance predictive accuracy and can even reduce it.

### Tuning hyperparameters

- RF are a good example of a common situachion in ML:
  - As the number of parameter increases,
  - finding their optimal values requires more effort
  - and can even become computationally unfeasible.
- As more complex algorithms with greater number of hyperparameters are introduced tuning strategies should also be considered.

### Tuning strategies

- **Grid Search**: Systematically searches through (*all possible combinations*) a predefined grid of hyperparameter values to find the combination that maximizes performance.
- Random Search: Randomly samples hyperparameter values from predefined distributions. Faster than Grid Search, but less prone to find optimum.
- Model-Based Optimization leverages probabilistic models, often Gaussian processes, to model the objective function and iteratively guide the search for optimal hyperparameters.

### Random forests in bioinformatics

- Random forests have been thoroughly used in Bioinformatics (Boulesteix et al. 2012).
- Bioinformatics data are often high dimensional with
  - dozens or (less often) hundreds of samples/individuals
  - thousands (or hundreds of thousands) of variables.

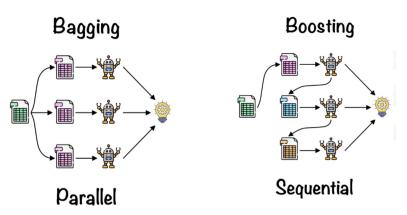
### Application of Random forests

- Random forests provide robust classifiers for:
  - Distinguishing cancer from non cancer,
  - Predicting tumor type in cancer of unknown origin,
  - Selecting variables (SNPs) in Genome Wide Association Studies...
- Some variation of Random forests are used only for variable selection

### Improving predictors iteratively

- The idea of *improving weak learners by aggregation* has moved historically along two distinct lines:
  - Build similar learners on resamples from the original sample and average the predictions.
  - This entails Bagging and Random Forests
  - ② Build a learner progressively, improving it at every step using weak learners, until the desired possible quality is obtained.
    - This is what Boosting is about.

### Bagging vs Boosting



Source: Ensemble Learning: Bagging & Boosting

### So what is Boosting

- Idea: create a model that is better than any of its individual components by combining their strengths and compensating for their weaknesses.
  - Multiple weak models are trained sequentially.
  - Each new model is trained to improve the errors made by the previous model.
- The final model is a weighted combination of all the models where the weights are determined by the accuracy of each model.

# Historical background

- The *boosting technique* was proposed by Robert Schapire (Schapire 1989) and Yoav Freund in the 1990s.
- They introduced AdaBoost, the first widely-used Boosting algorithm.
  - It achieved significant success in various applications, including face detection and handwriting recognition.
- Other Boosting algorithms have become popular: Gradient Boosting, XGBoost, and LightGBM.

#### Adaboost

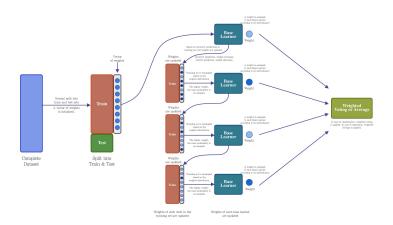
- AdaBoost (*Adaptive Boosting*) is a direct implementation of the "boosting" idea.
- It trains models sequentially, new models focusing on correcting the errors of the previous ones.
- Final Decision is made by combining models, giving more influence to the most reliable ones through
  - A weighted majority vote (classification) or
  - Weighted sum (regression).

# Running Adaboost

- Adaboost proceeds iteratively by, at each iteration:
  - Fit the weak learner using initial weights.
  - Predict and identify misclassified observations.
  - Update observation weights:
    - decrease for correctly classified
    - increase for misclassified.
  - Assign a learner weight to the weak learner based on its accuracy.
- The final prediction is a weighted combination of all weak learners.



### Adaboost Architecture



Source: Ensemble Learning: Bagging & Boosting



### Adaboost pseudo-code

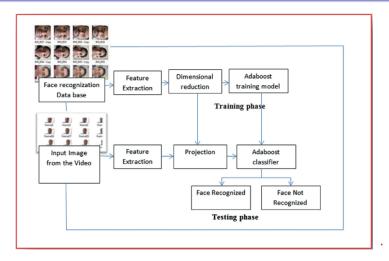
- Initialize sample weights:  $w_i = 1/N$ , where N = # of training samples.
- 2 For each iteration t = 1, 2, ..., T do:
  - Train weak classifier  $h_t(x)$  on training set weighted by  $w_i$ .
  - Compute the weighted error rate:

$$\epsilon_t = \sum_{i=1}^N w_i I(y_i \neq h_t(x_i)) \Bigg/ \sum_{i=1}^N w_i$$

- Compute the classifier weight:  $\alpha_t = \frac{1}{2} \log \frac{1 \epsilon_t}{\epsilon_t}$ .
- Update the sample weights:  $w_i \leftarrow w_i^{-\alpha_t I(y_i \neq h_t(x_i))}$ .
- Normalize the sample weights:  $w_i \leftarrow \frac{w_i}{\sum_{i=1}^{N} w_i}$ .
- Output the final classifier:  $H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$ .



### Adaboost applications



source: Evaluating the AdaBoost Algorithm for Biometric-Based Face Recognition



#### Adaboost has limitations

- Adaboost was a breakthrough algorithm that significantly improved the accuracy of ML models.
- However, Adaboost has its limitations.
  - It does not handle continuous variables very well.
  - Can be sensitive to noisy data and outliers,
  - May not perform well with complex datasets.
  - Its performance can reach a "plateau": it will no longer improve after a certain number of iterations.
- In order to deal with some of these drawbacks different variants of boosting have been proposed.



# **Gradient Boosting**

- Developed to overcome the limitations of Adaboost.
- Takes a different approach that can be linked with Optimization by Gradient Descent.
- Several advantages over Adaboost
  - Can handle continuous variables much better,
  - It is more robust to noisy data and outliers.
  - Can handle complex datasets and
  - Can continue to improve its accuracy even after Adaboost's performance has "plateaued".

# **Gradient Boosting Algorithm**

- Train a first weak learner  $f_1$ , which predicts the response variable y, and calculate the residuals  $y-f_1(x)$ .
- Next, train a new model  $f_2$ , to predict the residuals of the previous model, that is, to correct the errors made by model  $f_1$ .
  - $f_1(x) \approx y$
  - $\bullet \ f_2(x) \approx y f_1(x)$
- Iterate calculating residuals of the two models together  $y-f_1(x)-f_2(x)$  and train a third model  $f_3$  to correct them.
  - $\bullet \ f_3(x) \approx y f_1(x) f_2(x)$
- ullet Repeat the process M times, so that each new model minimizes the residuals (errors) of the previous one.

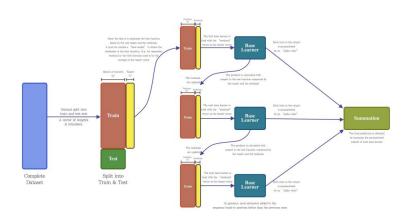


# Gradient Boosting may overfit

- Since the goal of Gradient Boosting is to minimize the residuals iteration by iteration, it is susceptible to overfitting.
- One way to avoid this problem is by using a regularization value, also known as the learning rate  $(\lambda)$ , which limits the influence of each model on the ensemble.
- As a result of this regularization, more models are needed to form the ensemble, but better results are achieved.
  - $f_1(x) \approx y$
  - $\bullet \ f_2(x) \approx y \lambda f_1(x)$
  - $f_3(x) \approx y \lambda f_1(x) \lambda f_2(x)$
  - $y \approx \lambda f_1(x) + \lambda f_2(x) + \lambda f_3(x) + ... + \lambda f_m(x)$



### Gradient boosting architechture



Source: Ensemble Learning: Bagging & Boosting



# Gradient Boosting pseudo-code

- Initialize the model with a constant value:  $f_0(x) = \frac{1}{n} \sum_{i=1}^n y_i$
- ② For t = 1 to T:
  - **Our condition of the loss function at the current fit:**  $r_{ti} = -\frac{\partial L(y_i, f_{t-1}(x_i))}{\partial f_{t-1}(x_i)}$
  - $\bullet$  Train a new model to predict the negative gradient values:

$$h(x; \theta_t) = \arg\min_{h} \sum_{i=1}^{n} (r_{ti} - h(x_i; \theta))^2$$

Compute the optimal step size:

$$\gamma_t = \arg\min_{\gamma} \sum_{i=1}^n L(y_i, f_{t-1}(x_i) + \gamma h(x_i; \theta_t))$$

- $\textbf{ 0} \quad \text{Update the model: } f_t(x) = f_{t-1}(x) + \gamma_t h(x;\theta_t)$
- **3** Output the final model:  $F(x) = f_T(x)$

### Relation with Gradient Descent

- Gradient Boosting can be seen as an extension of Gradient Descent, a popular optimization algorithm used to find the minimum of a function.
  - In Gradient Descent, the weights of the model are updated in the opposite direction of the gradient of the cost function.
  - In Gradient Boosting, the new model is trained on the negative gradient of the loss function, which is equivalent to minimizing the loss function in the direction of steepest descent.

### **Gradient Boosting Variations**

• Multiple extensions from Gradient Boosting.

#### XGBoost

- Optimized implementation that uses regularization to control overfitting and provide better accuracy.
- Won many competitions.

#### LightGBM

- Relies on a technique to reduce the number of samples used in each iteration
- Faster training, good for large datasets.

### Boosting applications

- Fraud Detection
- Image and Speech Recognition
- Anomaly Detection
- Medical Diagnosis
- Amazon's recommendation engine
- Models that predict protein structures from amino acid sequences
- Pattern identification in fMRI brain scans.

### Advantages of Boosting

- Boosting, like other Ensemble methods, improves the accuracy of weak learners and achieve better predictive performance than individual models.
- Boosting also reduces overfitting by improving the generalization ability of models.
- Available in many flavors,
- Can be parallelized
- Strong experience in Real world applications and industry.

### Limitations of Boosting

- Can be computationally expensive, especially when dealing with large datasets and complex models.
- Can be sensitive to noisy data and outliers,
- May not work well with certain types of data distributions.
- Not so good as "out-of-the-box": Requires careful tuning of hyperparameters to achieve optimal performance, which can be time-consuming and challenging.

### Boosting application with R and Python

- Many R packages implement the many variations of boosting:
  - ada,
  - adabag,
  - mboost,
  - gbm,
  - xgboost
  - An interesting option is to rely on the caret package which allows to run the distinct methods with a common interface.
- Inpython we usually rely on scikit-learn libraries although there are many alternative implementations
  - Scikit-learn ensemble
  - https://python-course.eu/machine-learning/boostingalgorithm-in-python.php



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