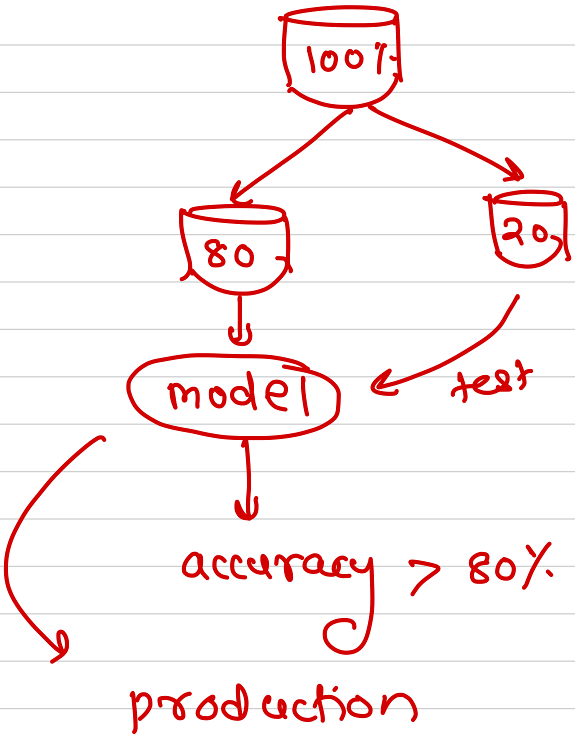
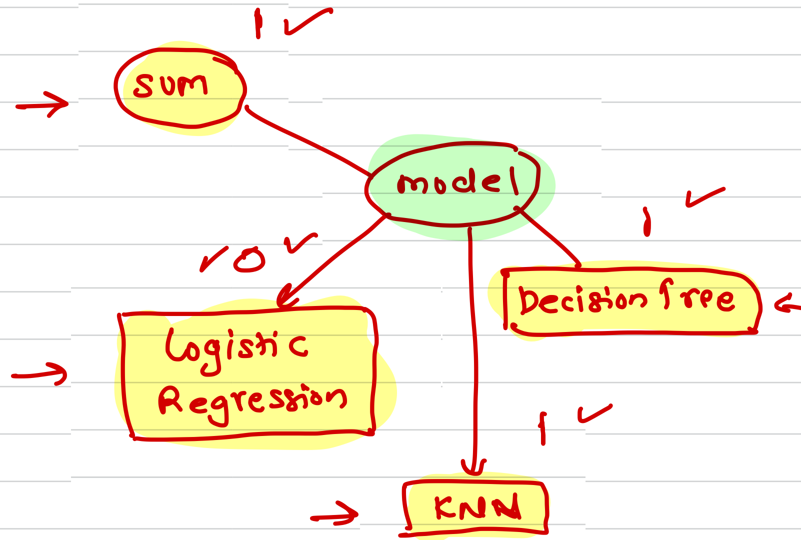
Machine Learning

Ensemble Learning

1


100%
80
20
model
test
accuracy > 80%
production


svm
model
Logistic Regression
Decision tree
KNN

Overview

models

- Ensemble is the art of combining diverse set of learners (individual models) together to improvise on the stability and predictive power of the model
- Primarily used to improve the (classification, prediction, function approximation, etc.) performance of a model, or reduce the likelihood of an unfortunate selection of a poor one
- Other applications of ensemble learning include assigning a confidence to the decision made by the model, selecting optimal (or near optimal) features, data fusion, incremental learning, nonstationary learning and error-correcting

ensemble

✓ Bagging

✓ Boosting

Stacking

Bagging

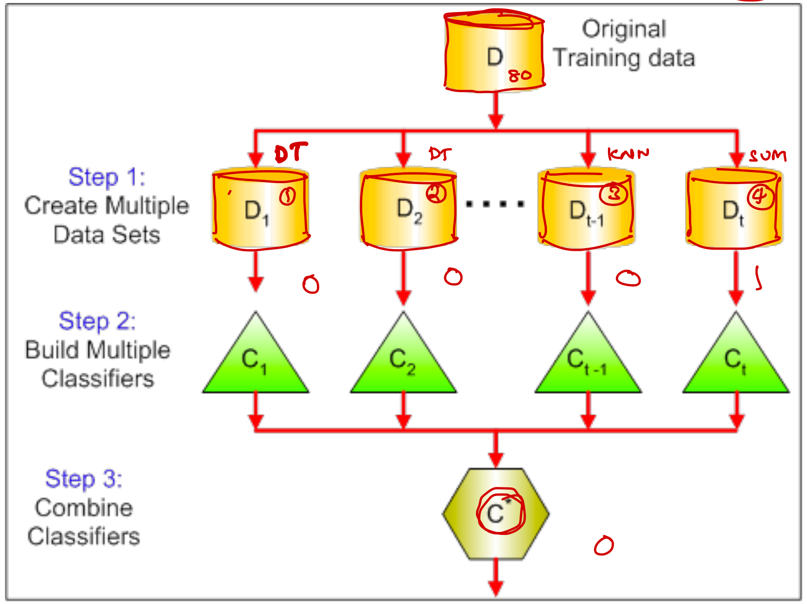
same models

- Bagging tries to implement similar learners on small sample populations and then takes a mean of all the predictions
- In generalized bagging, you can use different learners on different population
- This helps us to reduce the variance error
- Algorithm
  - Random Forest

100%

train-test-split()

20

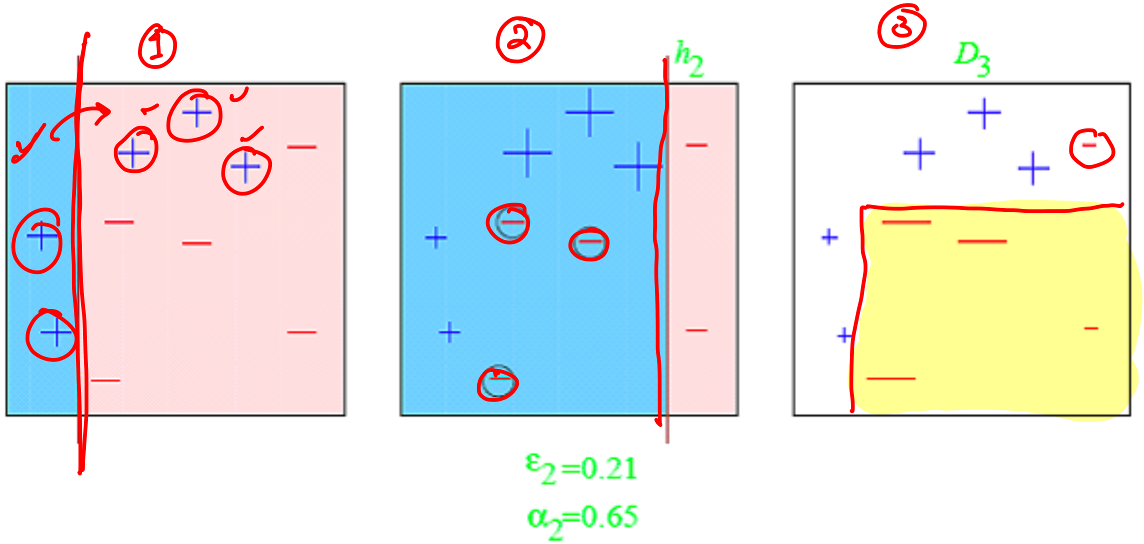


1. AdaBoost
2. CatBoost
3. Stockistic Gradient Boost
4. eXtreme Gradient Boost (XGBoost)

Boosting

Boosting

- Boosting refers to a family of algorithms that are able to convert weak learners to strong learners
  low accuracy — high accuracy
- Boosting is an iterative technique which adjust the weight of an observation based on the last classification
- If an observation was classified incorrectly, it tries to increase the weight of this observation and vice versa
- Boosting in general decreases the bias error and builds strong predictive models
- Algorithms
  - AdaBoost
  - Gradient Boosting
  - eXtreme Gradient Boosting (XGBoost)
  - * Stockistic Gradient Boosting
  - * Cat Boost

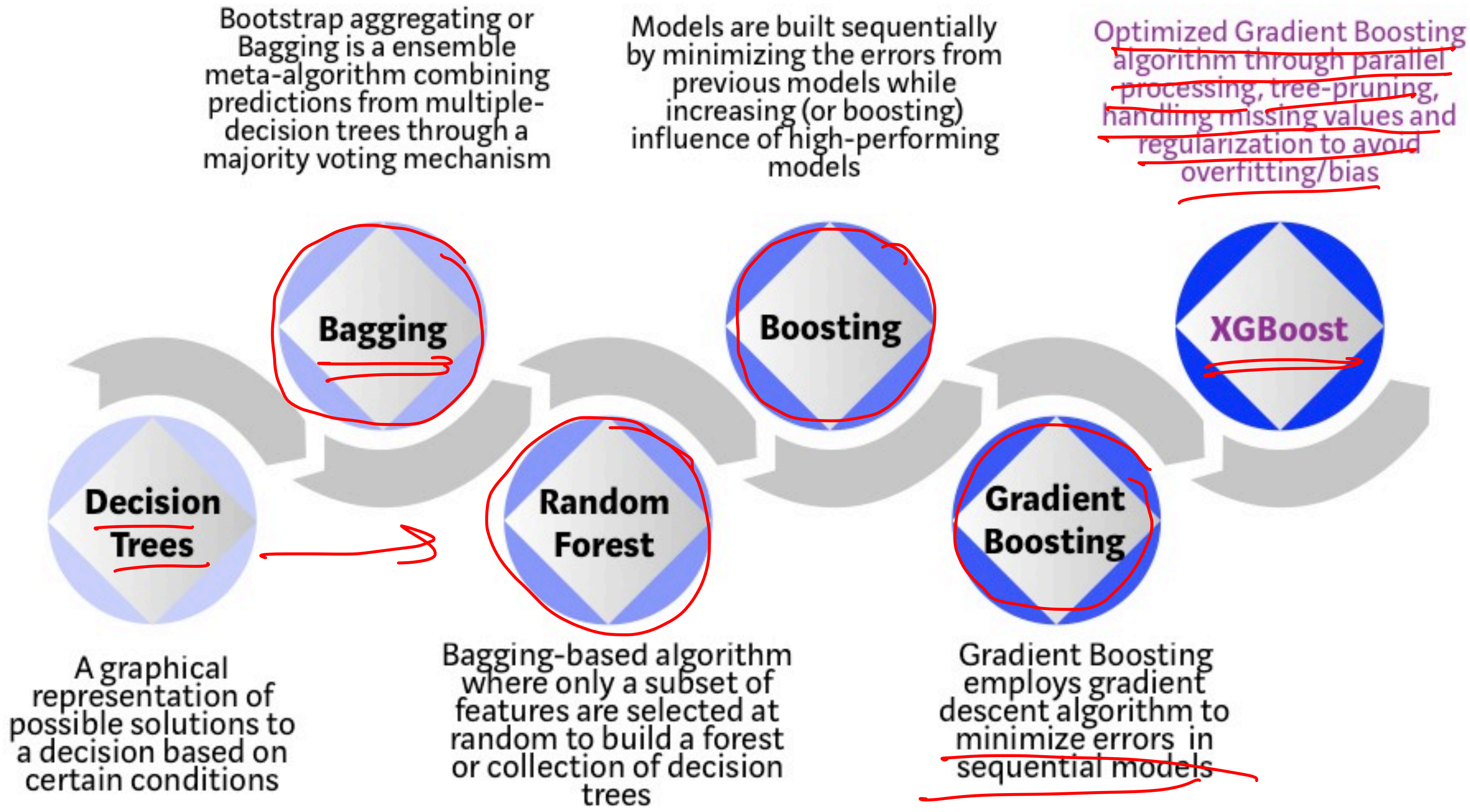


XGBoost

Overview

- XGBoost is a decision-tree-based ensemble Machine Learning algorithm that uses a gradient boosting framework
- XGBoost algorithm was developed as a research project at the University of Washington
- Since its introduction, this algorithm has not only been credited with winning numerous Kaggle competitions but also for being the driving force under the hood for several cutting-edge industry applications
- As a result, there is a strong community of data scientists contributing to the XGBoost open source projects with ~350 contributors and ~3,600 commits on GitHub

Evolution

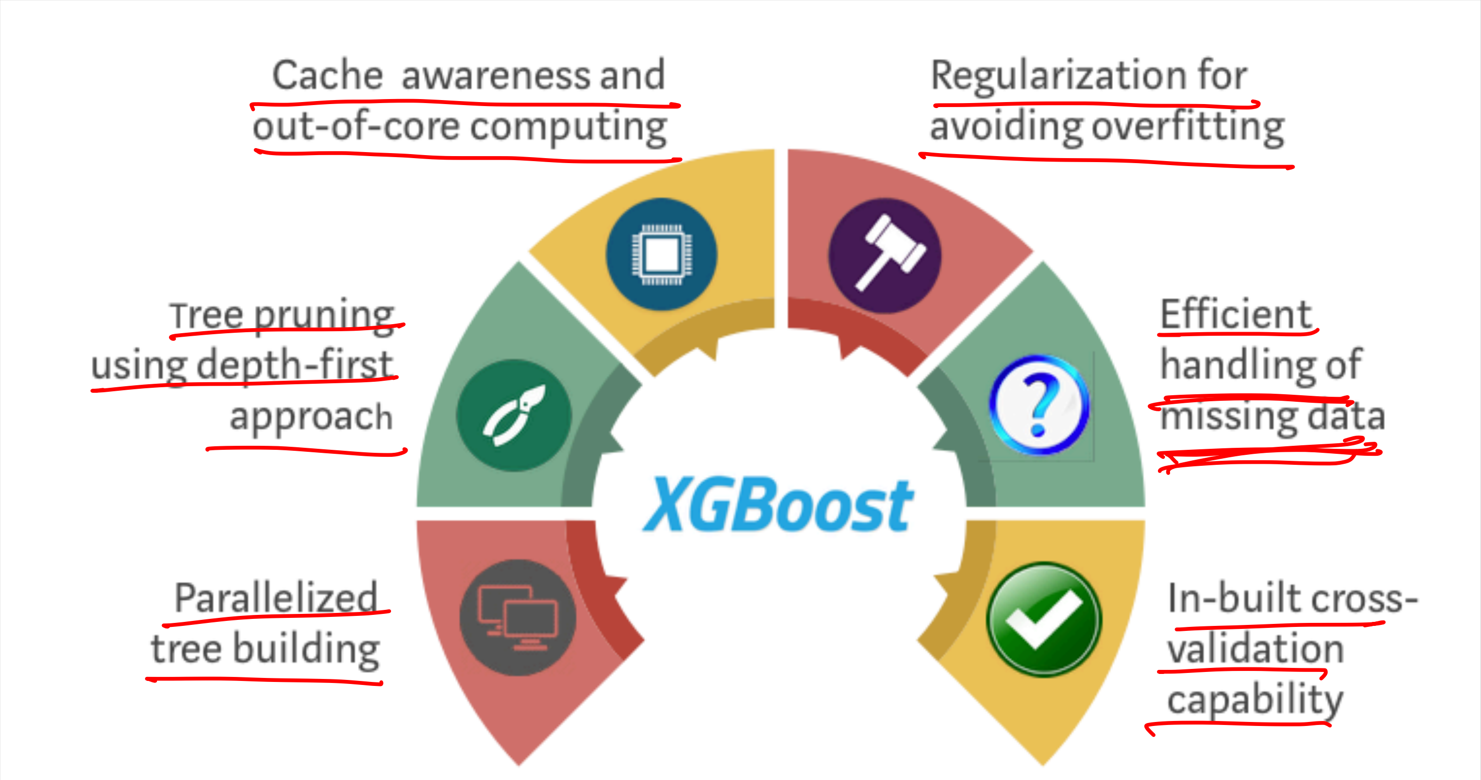

Bootstrap aggregating or Bagging is a ensemble meta-algorithm combining predictions from multiple-decision trees through a majority voting mechanism
Models are built sequentially by minimizing the errors from previous models while increasing (or boosting) influence of high-performing models
Optimized Gradient Boosting algorithm through parallel processing, tree-pruning, handling missing values and regularization to avoid overfitting/bias
Bagging
Boosting
XGBoost
Decision Trees
Random Forest
Gradient Boosting
A graphical representation of possible solutions to a decision based on certain conditions
Bagging-based algorithm where only a subset of features are selected at random to build a forest or collection of decision trees
Gradient Boosting employs gradient descent algorithm to minimize errors in sequential models

How does it work?

- XGBoost belongs to a family of boosting algorithms that convert weak learners into strong learners
- A weak learner is one which is slightly better than random guessing

Why does it perform so well?

- XGBoost and Gradient Boosting Machines (GBMs) are both ensemble tree methods that apply the principle of boosting weak learners using the gradient descent architecture
- However, XGBoost improves upon the base GBM framework through systems optimization and algorithmic enhancements.



System Optimization

- **Parallelization**
  - XGBoost approaches the process of sequential tree building using parallelized implementation
  - This is possible due to the interchangeable nature of loops used for building base learners; the outer loop that enumerates the leaf nodes of a tree, and the second inner loop that calculates the features
  - This nesting of loops limits parallelization because without completing the inner loop (more computationally demanding of the two), the outer loop cannot be started
  - Therefore, to improve run time, the order of loops is interchanged using initialization through a global scan of all instances and sorting using parallel threads
  - This switch improves algorithmic performance by offsetting any parallelization overheads in computation
- **Tree Pruning**
  - The stopping criterion for tree splitting within GBM framework is greedy in nature and depends on the negative loss criterion at the point of split
  - XGBoost uses 'max_depth' parameter as specified instead of criterion first, and starts pruning trees backward
  - This 'depth-first' approach improves computational performance significantly.

System Optimization

- **Hardware Optimization**
  - This algorithm has been designed to make efficient use of hardware resources
  - This is accomplished by cache awareness by allocating internal buffers in each thread to store gradient statistics
  - Further enhancements such as 'out-of-core' computing optimize available disk space while handling big data-frames that do not fit into memory.

Benefits

- **Parallel Computing:** It is enabled with parallel processing (using OpenMP); i.e., when you run xgboost, by default, it would use all the cores of your laptop/machine.
- **Regularization:** I believe this is the biggest advantage of xgboost. GBM has no provision for regularization. Regularization is a technique used to avoid overfitting in linear and tree-based models.
- **Enabled Cross Validation:** In R, we usually use external packages such as caret and mlr to obtain CV results. But, xgboost is enabled with internal CV function (we'll see below).
- **Missing Values:** XGBoost is designed to handle missing values internally. The missing values are treated in such a manner that if there exists any trend in missing values, it is captured by the model.
- **Flexibility:** In addition to regression, classification, and ranking problems, it supports user-defined objective functions also. An objective function is used to measure the performance of the model given a certain set of parameters. Furthermore, it supports user defined evaluation metrics as well.

Benefits

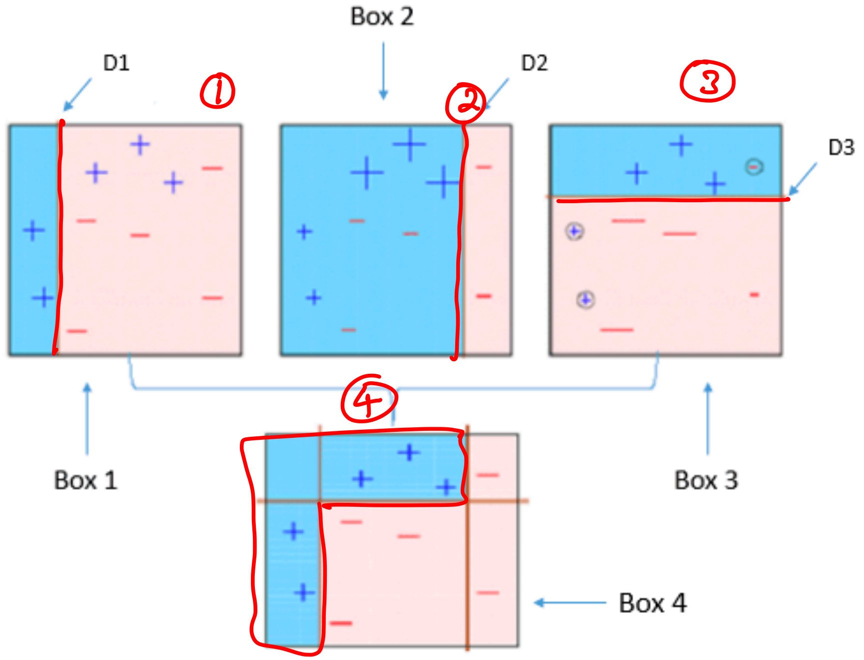
- **Availability:** Currently, it is available for programming languages such as R, Python, Java, Julia, and Scala.
- **Save and Reload:** XGBoost gives us a feature to save our data matrix and model and reload it later. Suppose, we have a large data set, we can simply save the model and use it in future instead of wasting time redoing the computation.
- **Tree Pruning:** Unlike GBM, where tree pruning stops once a negative loss is encountered, XGBoost grows the tree upto max_depth and then prune backward until the improvement in loss function is below a threshold.

How does it work?

- It combines a set of weak learners and delivers improved prediction accuracy
- At any instant t, the model outcomes are weighed based on the outcomes of previous instant t-1
- The outcomes predicted correctly are given a lower weight and the ones miss-classified are weighted higher
- Note that a weak learner is one which is slightly better than random guessing

How does it work?

- **1. Box 1**: The first classifier (usually a decision stump) creates a vertical line (split) at D1. It says anything to the left of D1 is **+** and anything to the right of D1 is **-**. However, this classifier misclassifies three **+** points.
- **Note** a Decision Stump is a Decision Tree model that only splits off at one level, therefore the final prediction is based on only one feature.
- **2. Box 2**: The second classifier gives more weight to the three **+** misclassified points (see the bigger size of **+**) and creates a vertical line at D2. Again it says, anything to the right of D2 is **-** and left is **+**. Still, it makes mistakes by incorrectly classifying three **-** points.
- **3. Box 3**: Again, the third classifier gives more weight to the three **-** misclassified points and creates a horizontal line at D3. Still, this classifier fails to classify the points (in the circles) correctly.
- **4. Box 4**: This is a weighted combination of the weak classifiers (Box 1,2 and 3). As you can see, it does a good job at classifying all the points correctly.



Stacking

Stacking

- Stacking is an ensemble learning technique that combines multiple classification or regression models via a meta-classifier or a meta-regressor
- The base level models are trained based on a complete training set, then the meta-model is trained on the outputs of the base level model as features
- The base level often consists of different learning algorithms and therefore stacking ensembles are often heterogeneous