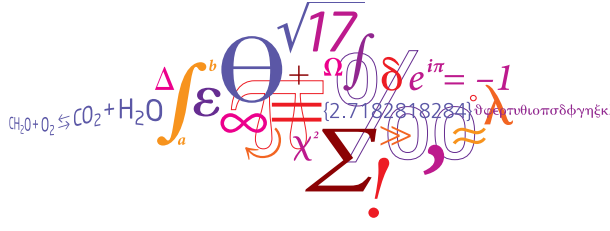
Nakul R Padalkar
GEORGETOWN UNIVERSITY

Tree Ensemble Methods

Bagging and Random Forests



Overview

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Classification Problem

In general, we want our classifier to have lowest generalized error.

- **Data** $(X, Y) \in \mathbb{R}^p \times \{0, 1\}$**.**
- ***X* is predictor, feature; *Y* is class label, response.**
- (X, Y) **have joint probability distribution** $\mathcal{D}$**.**
- **Goal: Based on *N* training pairs** (X_i, Y_i) **drawn.**
- **from** $\mathcal{D}$ **produce a classifier** $\hat{C}(X) \in \{0, 1\}$**.**
- **Goal: choose** $\hat{C}$ **to have low generalization error.**

Generative Methods

$$\underbrace{\mathbb{E}_D[(h(x|D) - y)^2]}_{ExpectedError} = \underbrace{\mathbb{E}_D[(\theta - \hat{\theta})^2]}_{Variance} + \underbrace{\hat{\theta}^2}_{Bias}$$

- Boosting - converts weak learners to strong learners. Intuitively, a weak learner is just slightly better than a random guess, while a strong learner is very close to perfect performance.
- **Goal:** Reduce Bias.
- Bagging or bootstrap aggregation averages a given procedure over many samples to reduce its variance — a poor man's Bayes.
- **Goal:** Reduce Variance.

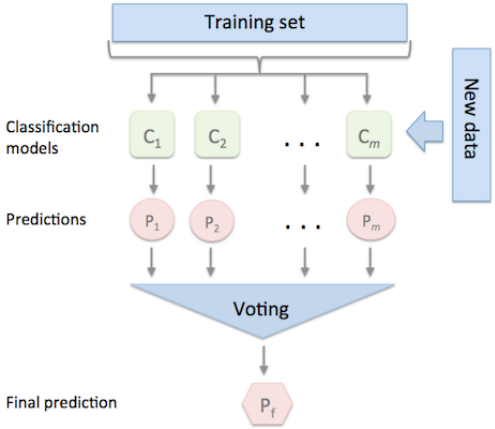
Weak and Strong Learners

Learners

- A weak learner produces a classifier that is only slightly more accurate than random classification.
- A class of concepts is learnable (or strongly learnable) if a polynomial-time algorithm achieves low error with high confidence for all concepts in the class.

Principle of Averaging

Voting Classifier: Average the predictions of a collection of classifiers.



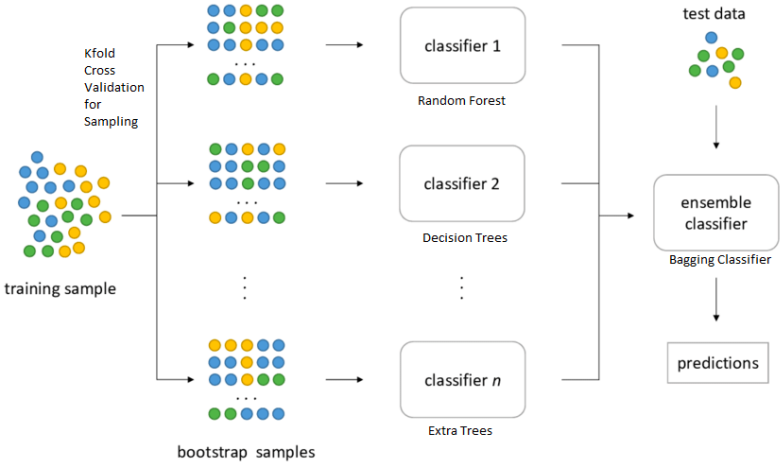
Principle of Averaging

- Instead of training different models on the same data, train the same model multiple times on different data sets and “combine” these “different” models
- We can use some simple/weak models as the base model
- **How do we get multiple training data sets?** (in practice, we only have one data set at training time)

Bootstrap Aggregating

- Bagging or bootstrap aggregation averages a given procedure over many samples, to reduce its variance — a poor man's Bayes.
- Bagging classifier helps in reducing the variance of individual estimators by introducing randomization into the training stage of each of the estimators and making an ensemble out of all the estimators. Note that the high variance means that changing the training data set results in the constructed or trained estimator by a great deal.

Bagging Sequence



Bagging Algorithm

Algorithm 1: Bagged Averaging

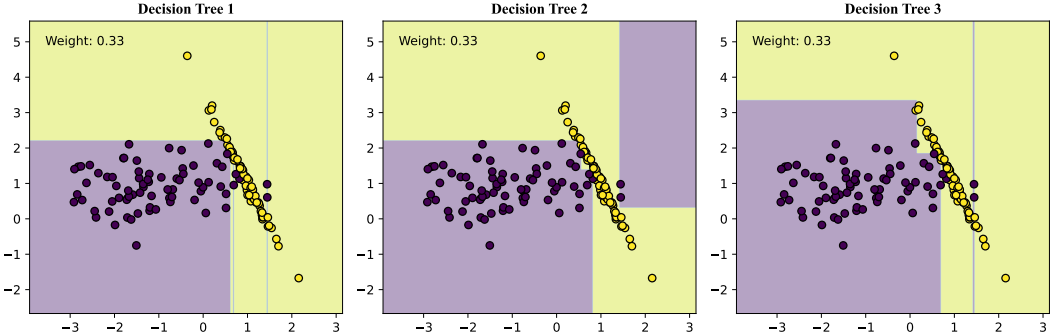
Input : Original dataset $\mathcal{D}$, Number of classifiers T
Output: Aggregated prediction

Initialize empty set of classifiers $\mathcal{C}$;
Initialize empty set of predictions $\mathcal{P}$;

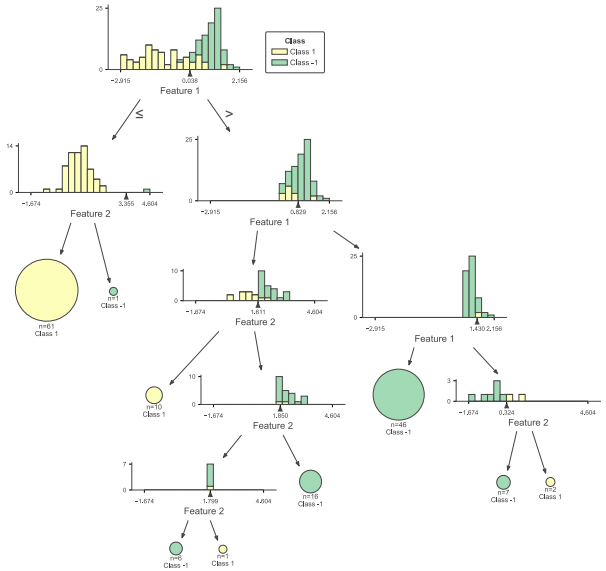
for $t = 1$ **to** T **do**
    Sample a bootstrap dataset $\mathcal{D}_t$ from the original dataset $\mathcal{D}$;
    Train a classifier C_t using $\mathcal{D}_t$;
    Make predictions $\mathcal{P}_t$ using classifier C_t;
    $\mathcal{C} \leftarrow \mathcal{C} \cup C_t$;
    $\mathcal{P} \leftarrow \mathcal{P} \cup \mathcal{P}_t$;
end

Aggregate predictions in $\mathcal{P}$ using averaging or voting;
return *Aggregated prediction*;

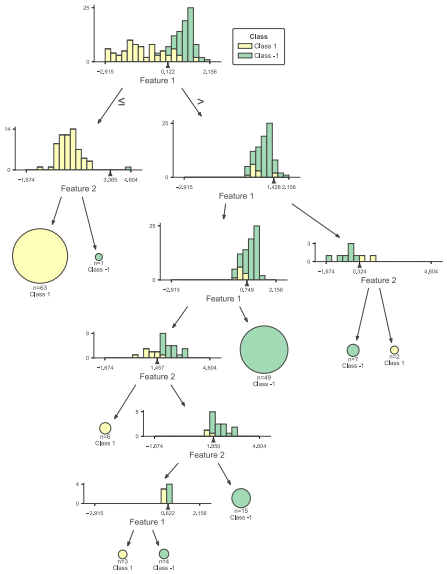
Average Bagged Classifier



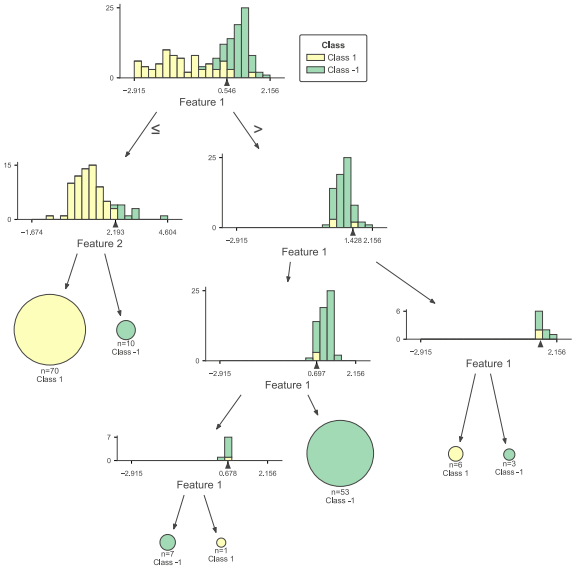
Bagged Classifier Trees



Bagged Classifier Trees



Bagged Classifier Trees



Classifier Aggregation I

- The bagged classifier is an ensemble learning method that combines multiple individual classifiers, known as decision trees, to make predictions.
- Each decision tree in the ensemble is trained on a different subset of the original training dataset, created through bootstrap sampling (sampling with replacement).
- During the training process, the bagged classifier fits each decision tree to a random subset of the training data, allowing each tree to learn different patterns and reduce overfitting.
- When making predictions, the bagged classifier combines the predictions from all decision trees by averaging the predicted probabilities (for classification problems) or taking the majority vote (for binary classification).

Classifier Aggregation II

- The weights of the individual decision trees in the bagged classifier are calculated as $1/N$, where N is the ensemble's total number of decision trees. This ensures that each decision tree contributes equally to the final prediction.
- By aggregating the predictions of multiple decision trees, the bagged classifier aims to improve the overall accuracy, robustness, and generalization ability compared to using a single decision tree.
- The bagged classifier can be used for both classification and regression tasks, depending on the type of base classifier (e.g., decision trees, random forests) used in the ensemble.

Building Random Forests

- Randomly select k features from the total m features.
- Among the k features, calculate the node d using the best split point.
- Split the node into daughter nodes using the best split.
- Repeat steps 1 to 3 until the number of nodes n in the tree exceeds a specified minimum.
- Build forest by repeating steps 1 to 4 for N times to create N number of trees.
- For a new data point, make each tree in the forest predict the class to which the data points belong. The forest chooses the class that gets the most votes.

Random Forest Algorithm

Algorithm 2: Random Forest Algorithm

Input : X: Input features (training data)
Input : y: Output labels (training data)
Input : $n\_estimators$: Number of decision trees to include in the forest
Input : $max\_features$: Maximum number of features to consider for each split
Output: $RandomForest$: Trained random forest model

$RandomForest \leftarrow \emptyset$;
for $i \leftarrow 1$ **to** $n\_estimators$ **do**
    # Bootstrap the training data:;
    $X\_bootstrap, y\_bootstrap \leftarrow$ `RandomlySelectSamplesWithReplacement`(X, y);
    # Construct a decision tree:;
    $tree \leftarrow$ `DecisionTreeAlgorithm`$(X\_bootstrap, y\_bootstrap, max\_features)$;
    # Append the tree to the RandomForest:;
    $RandomForest \leftarrow RandomForest \cup \{tree\}$;
end
return $RandomForest$;

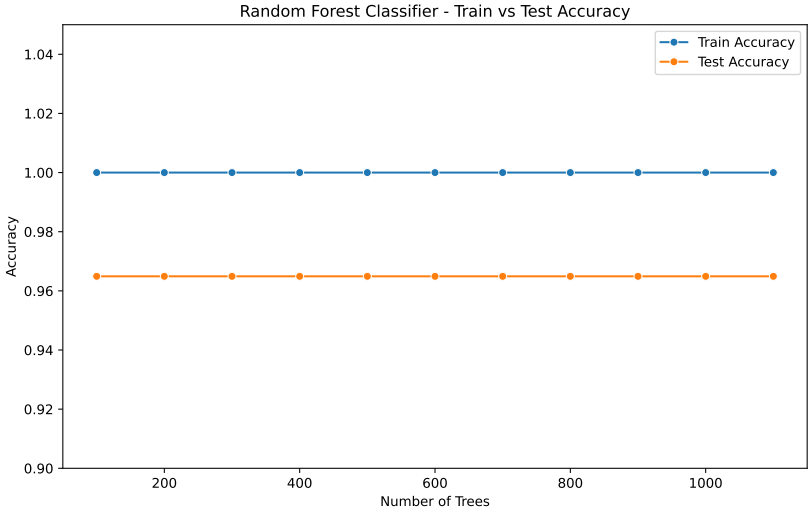
Scikit-Learn Python vs. R I

- `n_estimators`: The number of trees in the random forest.
- `max_depth`: The maximum depth of each decision tree in the ensemble.
- `min_samples_split`: The minimum number of samples required to split an internal node.
- `min_samples_leaf`: The minimum number of samples required to be at a leaf node.
- `max_features`: The number of features to consider when looking for the best split.
- `bootstrap`: Whether bootstrap samples should be used when building trees.
- `random_state`: The seed used by the random number generator.

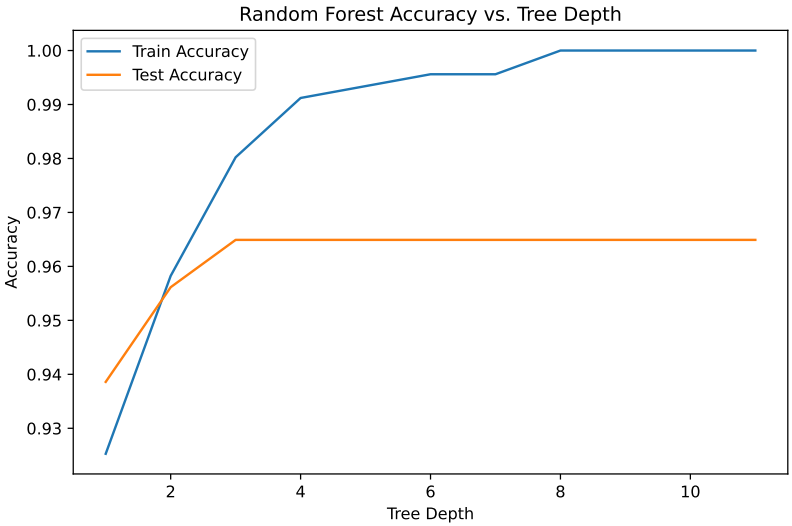
Scikit-Learn Python vs. R II

- `ntree`: The number of trees in the random forest.
- `mtry`: The number of variables randomly sampled as candidates at each split.
- `maxdepth`: The maximum depth of each tree in the ensemble.
- `nodesize`: The minimum number of samples required for a node to be split further.
- `sampsize`: The number of samples randomly drawn for each tree.
- `importance`: Whether to compute variable importance measures.

Effect of Number of Trees



Effect of Tree Depth



Advanced Uses of Random Forests

- **Feature Importance**: Random Forests can be used to compute feature importance scores that indicate the relative importance of each feature in the dataset.
- **Outlier Detection**: Random Forests can be used to identify outliers in a dataset.
- **Missing Value Imputation**: Random Forests can be used to impute missing values in a dataset.
- **Anomaly Detection**: Random Forests can be used to identify anomalies in a dataset.
- **Semi-Supervised Learning**: Random Forests can be used for semi-supervised learning, where only a subset of the training data has labels.
- **Unsupervised Learning**: Random Forests can be used for unsupervised learning, where the goal is to discover patterns and structures in a dataset.

Benefits I

- **Reduced Overfitting**: Random Forest reduces the risk of overfitting by diversifying the trees in the ensemble.
- **Highly Accurate**: Random Forest provides high predictive accuracy by averaging the predictions of multiple trees.
- **Handles High-Dimensional Data**: Random Forest performs well with high-dimensional data, handling large feature spaces effectively.
- **Implicit Feature Selection**: Random Forest performs feature selection by evaluating feature importance during training.
- **Resistant to Overfitting**: Random Forest resists overfitting due to random subsampling and the ensemble averaging effect.
- **Efficient Parallelization**: Random Forest training can be parallelized for improved performance.
- **Outliers and Missing Data Handling**: Random Forest is relatively robust to outliers and can handle missing data.