#### Chapter 9: Ensemble Learning

#### Reza Rezazadegan

Sharif University of Technology

Fall 2022

Reza Rezazadegan (Sharif University)

Introduction to Machine Learning

December 18, 2022

In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x).

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.
- Such an ensemble often outperforms the individual predictors in it.

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.
- Such an ensemble often outperforms the individual predictors in it.
- In hard voting we use the unweighted count or mean.

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.
- Such an ensemble often outperforms the individual predictors in it.
- In hard voting we use the unweighted count or mean.
- In **soft voting** we have an ensemble of probabilistic predictors and for a new instance **x** take the average of probabilities for each class for classification. Or the probability-weighted average of values for regression.

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.
- Such an ensemble often outperforms the individual predictors in it.
- In hard voting we use the unweighted count or mean.
- In **soft voting** we have an ensemble of probabilistic predictors and for a new instance **x** take the average of probabilities for each class for classification. Or the probability-weighted average of values for regression.
- For Ensemble Learning to work, the classifiers have to be independent of each other.

Reza Rezazadegan (Sharif University)

- In Ensemble Learning we train a set (ensemble) of different predictors (classifiers or regressors) {P<sub>1</sub>, P<sub>2</sub>, P<sub>3</sub>, ..., P<sub>N</sub>} and for a new instance x, ensemble's prediction is the aggregation of P<sub>i</sub>(x).
- For classification, aggregation is given by majority vote (or *mode*) of the P<sub>i</sub>(x). This means the class which gets most of the "votes" by these predictors is assigned to x.
- For regression, the mean of the predictions  $P_i(\mathbf{x})$  is used.
- Such an ensemble often outperforms the individual predictors in it.
- In hard voting we use the unweighted count or mean.
- In **soft voting** we have an ensemble of probabilistic predictors and for a new instance **x** take the average of probabilities for each class for classification. Or the probability-weighted average of values for regression.
- For Ensemble Learning to work, the classifiers have to be independent of each other. Otherwise they will repeat the same mistakes.

Reza Rezazadegan (Sharif University)

Introduction to Machine Learning

- In **Bagging**, we train the same classifier on different random samples of the training set.
- In **Boosting** we have a sequence  $\{P_i\}$  of predictors and in each step the instances misclassified by  $P_i$  are given a higher sampling weight, for  $C_{i+1}$ .

- In **Bagging**, we train the same classifier on different random samples of the training set.
- In **Boosting** we have a sequence  $\{P_i\}$  of predictors and in each step the instances misclassified by  $P_i$  are given a higher sampling weight, for  $C_{i+1}$ .
- In **Stacking**, instead of simple aggregation, a model is trained to give us the ensemble's prediction from those of individual *P<sub>i</sub>*'s.

• Bagging is the abbreviation of Bootstrap Aggregation.

æ

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.
- In these classes we can set:
  - estimator: the estimator used (default: Decision Tree)

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.
- In these classes we can set:
  - estimator: the estimator used (default: Decision Tree)
  - n\_estimators: the number of estimators in the ensemble, which is the same as the number of samples drawn from data.

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.
- In these classes we can set:
  - estimator: the estimator used (default: Decision Tree)
  - n\_estimators: the number of estimators in the ensemble, which is the same as the number of samples drawn from data.
  - max\_samples: the number of elements in each sample drawn from training data, and given to each estimator. Can be a float value as well.

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.
- In these classes we can set:
  - estimator: the estimator used (default: Decision Tree)
  - n\_estimators: the number of estimators in the ensemble, which is the same as the number of samples drawn from data.
  - max\_samples: the number of elements in each sample drawn from training data, and given to each estimator. Can be a float value as well.
  - max\_features: the number of features to randomly choose for each estimator. (Specially useful for high-dimensional data.)

- Bagging is the abbreviation of Bootstrap Aggregation.
- As mentioned above, in Bagging all the predictors *P<sub>i</sub>* are the same but they are trained on different random samples from the training data and/or different samples of features.
- In Bagging, *replacement* is allowed i.e. an instance can be sampled several times for the same classifier.
- sklearn.ensemble has two classes for bagging: BaggingClassifier and BaggingRegressor.
- In these classes we can set:
  - estimator: the estimator used (default: Decision Tree)
  - n\_estimators: the number of estimators in the ensemble, which is the same as the number of samples drawn from data.
  - max\_samples: the number of elements in each sample drawn from training data, and given to each estimator. Can be a float value as well.
  - max\_features: the number of features to randomly choose for each estimator. (Specially useful for high-dimensional data.)
  - Bootstrap: whether replacement (repetition) is allowed in sampling or not.

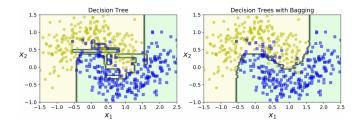


Figure: A single decision tree (left) vs a bagging ensemble of 500 decision trees (right). Credit: Aurelien Geron

• The estimators in a bagging ensemble can be trained in parallel.

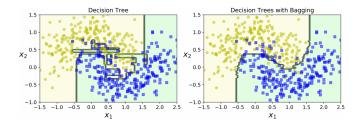


Figure: A single decision tree (left) vs a bagging ensemble of 500 decision trees (right). Credit: Aurelien Geron

- The estimators in a bagging ensemble can be trained in parallel.
- Aggregation reduces both bias and variance.

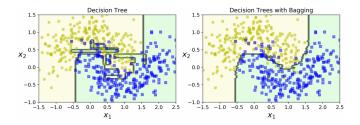


Figure: A single decision tree (left) vs a bagging ensemble of 500 decision trees (right). Credit: Aurelien Geron

- The estimators in a bagging ensemble can be trained in parallel.
- Aggregation reduces both bias and variance.
- Consequently, the ensemble's bias is similar to the base predictor but it has a lower variance.

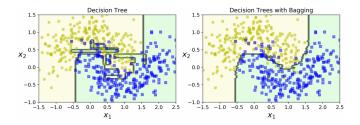


Figure: A single decision tree (left) vs a bagging ensemble of 500 decision trees (right). Credit: Aurelien Geron

- The estimators in a bagging ensemble can be trained in parallel.
- Aggregation reduces both bias and variance.
- Consequently, the ensemble's bias is similar to the base predictor but it has a lower variance.
- Thus, Bagging works better with model with low bias and high variance such as Decision Trees.

Reza Rezazadegan (Sharif University)

Introduction to Machine Learning

• A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.
- Random Forests can be used to measure the importance of features.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.
- Random Forests can be used to measure the importance of features.
- The importance of a feature is given by the weighted sum of the information gain, over all the nodes in the forest that use that feature.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.
- Random Forests can be used to measure the importance of features.
- The importance of a feature is given by the weighted sum of the information gain, over all the nodes in the forest that use that feature. The weights are given by the number of samples in the node.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.
- Random Forests can be used to measure the importance of features.
- The importance of a feature is given by the weighted sum of the information gain, over all the nodes in the forest that use that feature. The weights are given by the number of samples in the node. The results are normalized so that the sum of the feature importances is 1.

- A **Random Forest** is a bagging ensemble of decision trees. It is provided by classes RandomForestClassifier and RandomForestRegressor.
- The Random Forest algorithm searches among a random subset of features at each node of each tree.
- In *Extremely Randomized Trees* (or *Extra-Trees*), instead of finding the best threshold at each node, a random threshold is used.
- This makes Extra-Trees much faster, and with lower variance.
- Random Forests can be used to measure the importance of features.
- The importance of a feature is given by the weighted sum of the information gain, over all the nodes in the forest that use that feature. The weights are given by the number of samples in the node. The results are normalized so that the sum of the feature importances is 1.
- Feature importances can be accessed using member variable feature\_importances\_.

### Boosting

 Boosting is similar to Bagging, but instead of using independently sampled subsets of training data for each estimator, sampling is modified, at each step, to emphasize the mistakes of the previous estimator.

### Boosting

- Boosting is similar to Bagging, but instead of using independently sampled subsets of training data for each estimator, sampling is modified, at each step, to emphasize the mistakes of the previous estimator.
- At the first step (i.e. for  $P_1$ ) all instances have weight (probability) 1/n to be sampled, where n is the size of the dataset.

# Boosting

- Boosting is similar to Bagging, but instead of using independently sampled subsets of training data for each estimator, sampling is modified, at each step, to emphasize the mistakes of the previous estimator.
- At the first step (i.e. for  $P_1$ ) all instances have weight (probability) 1/n to be sampled, where n is the size of the dataset.
- At the 2nd step, the items misclassified by P<sub>1</sub> are given a higher sampling weight and so on.

# Boosting

- Boosting is similar to Bagging, but instead of using independently sampled subsets of training data for each estimator, sampling is modified, at each step, to emphasize the mistakes of the previous estimator.
- At the first step (i.e. for  $P_1$ ) all instances have weight (probability) 1/n to be sampled, where n is the size of the dataset.
- At the 2nd step, the items misclassified by P<sub>1</sub> are given a higher sampling weight and so on.
- This way, correctly classified items are less likely to be sampled again and thus, their predictions are likely to stay correct.

- **Boosting** is similar to Bagging, but instead of using independently sampled subsets of training data for each estimator, sampling is modified, at each step, to emphasize the mistakes of the previous estimator.
- At the first step (i.e. for  $P_1$ ) all instances have weight (probability) 1/n to be sampled, where n is the size of the dataset.
- At the 2nd step, the items misclassified by P<sub>1</sub> are given a higher sampling weight and so on.
- This way, correctly classified items are less likely to be sampled again and thus, their predictions are likely to stay correct.
- On the other hand, misclassified items (i.e. the ones that are difficult to classify) are more likely to be sampled until correct predictions for the is obtained.

< □ > < □ > < □ > < □ > < □ > < □ >

# Boosting

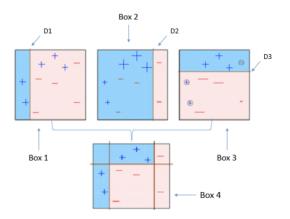


Figure: Schematic depiction of Boosting. In each box we train a classifier on a sample of data. The misclassified items get a higher sampling weight (probability) in the next box. Credit: Kaggle

• More precisely, in **AdaBoost (Adaptive Boost)**, the *error rate*  $r_k$  of  $P_k$  is the sum of the weights of the items it misclassified divided by the sum of the weights of all items in dataset.

- More precisely, in **AdaBoost (Adaptive Boost)**, the *error rate*  $r_k$  of  $P_k$  is the sum of the weights of the items it misclassified divided by the sum of the weights of all items in dataset.
- The predictor weight of  $P_k$  is defined as  $\alpha_k = \eta \log \frac{1-r_k}{r_k}$

- More precisely, in **AdaBoost (Adaptive Boost)**, the *error rate*  $r_k$  of  $P_k$  is the sum of the weights of the items it misclassified divided by the sum of the weights of all items in dataset.
- The predictor weight of  $P_k$  is defined as  $\alpha_k = \eta \log \frac{1-r_k}{r_k}$
- Then (for P<sub>k+1</sub>), the weights are updated, only for items misclassified by P<sub>k</sub>, by multiplying them with e<sup>α<sub>k</sub></sup>.

- More precisely, in **AdaBoost (Adaptive Boost)**, the *error rate*  $r_k$  of  $P_k$  is the sum of the weights of the items it misclassified divided by the sum of the weights of all items in dataset.
- The predictor weight of  $P_k$  is defined as  $\alpha_k = \eta \log \frac{1-r_k}{r_k}$
- Then (for  $P_{k+1}$ ), the weights are updated, only for items misclassified by  $P_k$ , by multiplying them with  $e^{\alpha_k}$ . They are then normalized to sum to 1.

- More precisely, in **AdaBoost (Adaptive Boost)**, the *error rate*  $r_k$  of  $P_k$  is the sum of the weights of the items it misclassified divided by the sum of the weights of all items in dataset.
- The predictor weight of  $P_k$  is defined as  $\alpha_k = \eta \log \frac{1-r_k}{r_k}$
- Then (for  $P_{k+1}$ ), the weights are updated, only for items misclassified by  $P_k$ , by multiplying them with  $e^{\alpha_k}$ . They are then normalized to sum to 1.
- $\eta$  is a constant called *learning rate* which defaults to 1.

## Ada Boost cont

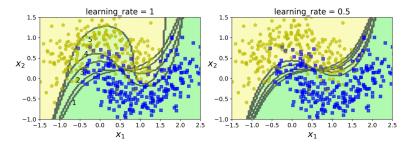


Figure: Five iterations of Ada Boost with an SVM classifier with RBF kernel. Credit: Aurelien Geron

 Unlike Bagging, in Boosting, different weights α<sub>i</sub> are associated to the predictors P<sub>i</sub>.

## Ada Boost cont

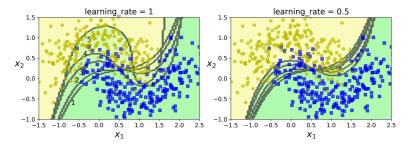


Figure: Five iterations of Ada Boost with an SVM classifier with RBF kernel. Credit: Aurelien Geron

- Unlike Bagging, in Boosting, different weights α<sub>i</sub> are associated to the predictors P<sub>i</sub>.
- For a new instance **x** and a class  $C_k$  we take the sum of the weights  $\alpha_i$  of the predictors  $P_i$  which predict  $C_k$  for **x**.

## Ada Boost cont

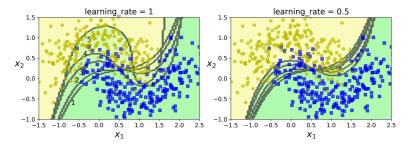


Figure: Five iterations of Ada Boost with an SVM classifier with RBF kernel. Credit: Aurelien Geron

- Unlike Bagging, in Boosting, different weights α<sub>i</sub> are associated to the predictors P<sub>i</sub>.
- For a new instance x and a class C<sub>k</sub> we take the sum of the weights α<sub>i</sub> of the predictors P<sub>i</sub> which predict C<sub>k</sub> for x. The class assigned to x by the ensemble is the one whose sum is highest.

Reza Rezazadegan (Sharif University)

Introduction to Machine Learning

 In Gradient Boosting we have a sequence of predictors h<sub>1</sub>, h<sub>2</sub>, h<sub>3</sub>,... and h<sub>i+1</sub> is trained on the residuals (errors) of h<sub>i</sub> i.e. {y<sub>i</sub> - h<sub>i</sub>(x<sub>j</sub>)}<sup>N</sup><sub>i=1</sub>.

- In Gradient Boosting we have a sequence of predictors h<sub>1</sub>, h<sub>2</sub>, h<sub>3</sub>,... and h<sub>i+1</sub> is trained on the residuals (errors) of h<sub>i</sub> i.e. {y<sub>i</sub> - h<sub>i</sub>(x<sub>j</sub>)}<sup>N</sup><sub>i=1</sub>.
- Ensemble prediction for **x** is given by  $\sum_i h_i(\mathbf{x})$ .

- In Gradient Boosting we have a sequence of predictors h<sub>1</sub>, h<sub>2</sub>, h<sub>3</sub>,... and h<sub>i+1</sub> is trained on the residuals (errors) of h<sub>i</sub> i.e. {y<sub>i</sub> - h<sub>i</sub>(x<sub>j</sub>)}<sup>N</sup><sub>i=1</sub>.
- Ensemble prediction for **x** is given by  $\sum_i h_i(\mathbf{x})$ .
- The Python library XGBoost is a fast and scalable implementation of Gradient Boosting.

## Gradient Boosting example

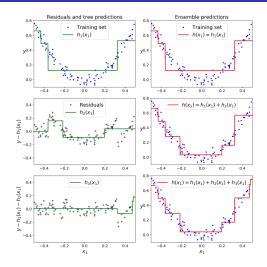


Figure: Example of Gradient Boosting for regression. The base estimator is a decision tree of depth 2. Credit: Aurelien Geron.

Reza Rezazadegan (Sharif University)

December 18, 2022

• Unlike bagging, in Boosting the goal is to decrease model bias.

3 N 3

• Unlike bagging, in Boosting the goal is to decrease model bias. Therefore it is used with models with less variance such as SVM or Decision Trees with shallow depth.

- Unlike bagging, in Boosting the goal is to decrease model bias. Therefore it is used with models with less variance such as SVM or Decision Trees with shallow depth.
- Unlike Bagging, Boosting cannot be parallelized.

- Unlike bagging, in Boosting the goal is to decrease model bias. Therefore it is used with models with less variance such as SVM or Decision Trees with shallow depth.
- Unlike Bagging, Boosting cannot be parallelized.
- Boosting has more parameters to tune (learning rate and tree depth).

- Unlike bagging, in Boosting the goal is to decrease model bias. Therefore it is used with models with less variance such as SVM or Decision Trees with shallow depth.
- Unlike Bagging, Boosting cannot be parallelized.
- Boosting has more parameters to tune (learning rate and tree depth).
- Boosting ensembles tend to overfit if too many iterations are used.
  Lower error with larger ensembles

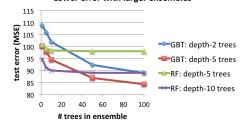


Figure: Comparison of the accuracy of Random Forest (RF) and Gradient Boosted Tree (GBT) estimators. Credit: DataBricks

Reza Rezazadegan (Sharif University)