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Random Forests

September 2024

Data Science Session Housekeeping

- The use of disrespectful language is prohibited in the questions, this is a supportive, learning environment for all - please engage accordingly.
- No question is daft or silly - **ask them!**
- There are **Q&A sessions** midway and at the end of the session, should you wish to ask any follow-up questions. Moderators are going to be answering questions as the session progresses as well.
- If you have any questions outside of this lecture, or that are not answered during this lecture, please do submit these for upcoming Academic Sessions. You can submit these questions here: **Questions**

Data Science Session Housekeeping cont.

- For all **non-academic questions**, please submit a query: www.hyperiondev.com/support

- Report a **safeguarding** incident: www.hyperiondev.com/safeguardreporting

- We would love your **feedback** on lectures: **Feedback on Lectures**

Learning Objectives

By the end of this lesson, learners should be able to:

- ❖ Understand fundamental concepts and advantages of **ensemble methods** to improve predictive performance and robustness of decision trees.
- ❖ Describe **bootstrapping** and its role in creating diverse subsets of training data for ensemble methods.
- ❖ Explain **bagging** (bootstrap aggregation) technique, highlighting how it reduces variance and improves the stability of predictions.

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Learning Objectives

❖ Identify the key difference between **random forests** and other **ensemble** methods, emphasizing **feature randomness**

❖ Interpret **feature importance** in random forests and determine the **most influential variables** for prediction.

Learning Objectives

- ❖ Apply **random forests** using Python libraries like *scikit-learn*, training models on **real-world datasets,** and comparing performances with individual decision trees and other ensemble methods.

- ❖ Experiment with **hyperparameter tuning** for random forests (n_estimators, max_depth), to **optimise model performance** and understand the impact of these parameters on the **bias-variance trade-off**.

Ensemble Methods

Introduction

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Ensemble Methods

- **Decision Trees** are easy to understand, apply, interpret and visualise. However, they are **not very robust**, **small perturbations in the training data** could give rise to **substantially different predictions** at test time.

- Predictions of decision trees have very **high variance.** Ideally, we'd like our models to capture general patterns, not to be **so dependent on the data** they have trained on that a bit of noise or a different sample changes predictions entirely.

Ensemble Methods

- **Ensemble techniques** work like a group of diverse experts teaming up to make decisions, and create a more robust solution than any individual could achieve alone.

- Ensemble methods **aggregate the predictions of multiple classifiers/regressors** into a single, improved prediction.

- Aside from **Random Forests**, **ensemble methods** can and do get applied to methods **other than decision trees,** but trees can benefit in particular due to how flexible they are.

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Ensemble Methods

Bagging: Bootstrap aggregation	Boosting
Trains multiple weak models in **parallel** on different subsets of the training data.	Trains multiple based models **sequentially**.
Each model is built independently.	New models are influenced by the performance of previously built models.
Training data subsets are selected using row sampling prediction is made by **averaging predictions** (regression) and **majority vote** (classification).	Each model tries to **correct the errors** made by the previous models and is **trained on a modified version of the dataset.**
Aim to **decrease variance**, solve the over-fitting problem, use for unstable models.	Aim to **decrease bias**, use for stable but simple models.
Each model receives **equal weight.**	Models **weighted** as per **performance**.

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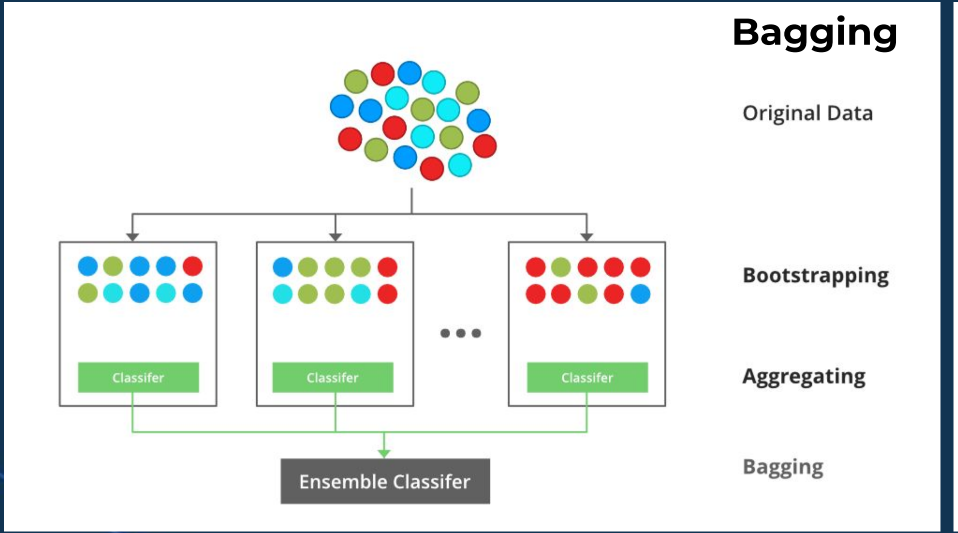
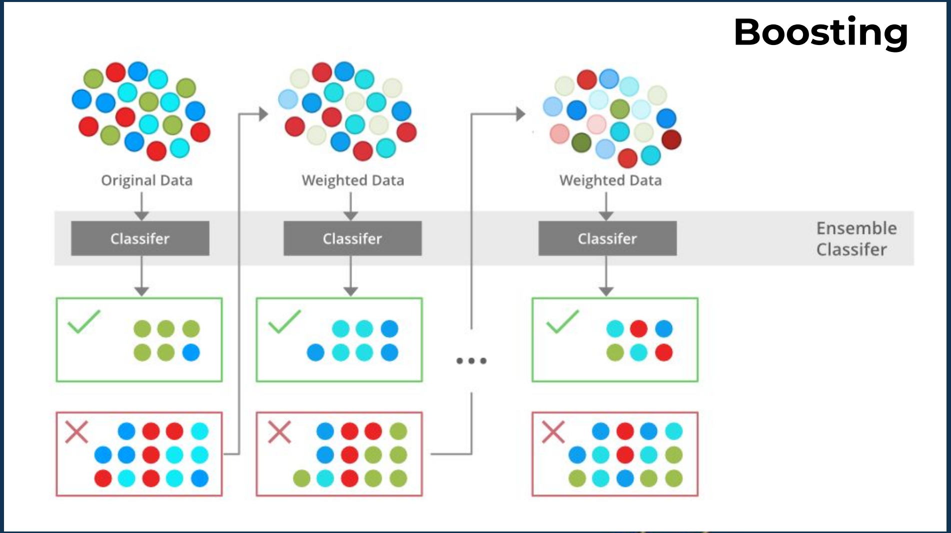
Ensemble Methods





Random Forests

Gradient Boosting, XGBoost, AdaBoost

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https://www.geeksforgeeks.org/bagging-vs-boosting-in-machine-learning/

Random Forests

Bootstrapping and Bagging

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Random Forests

- **Random Forests:** created from **many decision trees** during training phase using **random subset of the dataset** to measure a **random subset of features** in each partition.

- Randomness introduces **variability** among individual trees, **reducing** the risk of **overfitting** and **improving** overall **prediction performance**.

- Aggregates predictions of all trees, either by **voting** (**classification problems**) or by **averaging** (**regression problems**).

- **Collaborative decision-making process**, supported by **multiple trees** with their insights, gives **stable** and **precise results.**

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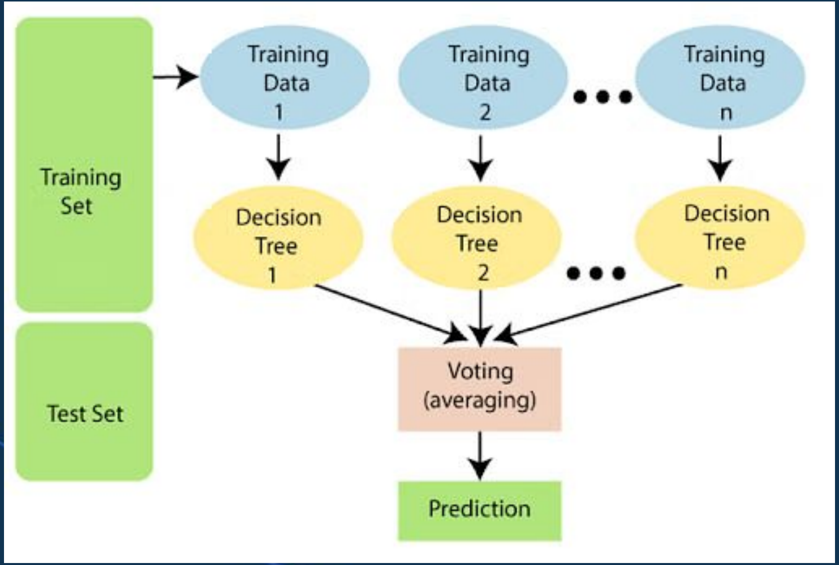
Random Forests



- ❖ **Ensemble of Decision Trees,** each operates independently, minimizing the risk of the model being overly influenced by a single tree.
- ❖ **Random Feature Selection** during each tree's training, randomness ensures focus on different aspects.
- ❖ **Bootstrap Aggregating or Bagging**
- ❖ **Decision Making and Voting:** Final prediction is the **majority voting** across all trees (classification) and **average** of individual predictions (regression).

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Bagging (Bootstrap Aggregation)

Ensemble technique in the **Random Forest** algorithm.

- **Selection of Subset:** Choose a random sample (size n), or subset, from entire dataset (size N, n < N).
- **Bootstrapping (Bootstrap row Sampling) with replacement:** Each model is then created from these samples (Bootstrap), which are taken from the original data with replacement (instance can occur in more than one sample).
- **Independent Model Training:** Each model is trained independently on its corresponding Bootstrap Sample, generating results for each model.
- **Aggregation:** Combine all the results and generate final output based on majority voting/averaging.

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Key features of Random Forests

Differences with other models

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Key Features of Random Forests

- **Diversity:** Not all attributes/variables/features are considered while making an individual tree; each tree is different.
- **Dimensionality reduction:** Feature space is reduced.
- **Parallelization:** Each tree is created independently out of different data and attributes, fully use the CPU to build random forests.
- **Train-Test split:** No train and test data splitting required as there is always 30% of data which is not seen by the decision tree.
- **Stability:** Stable as final results are based on majority voting/ averaging.

Differences with Decision Trees

Decision Trees	Random Forests
Can suffer from **overfitting** if allowed to grow without any control.	Created from subsets of data, and final output is based on average or majority ranking; **overfitting is mitigated.** Better **bias-variance trade-off.**
When a data set with features is taken as input by a decision tree, some **rules formulated to make predictions.**	**Randomly** selects observations, builds a decision tree, and takes the average result. Does not use any set of rules.
A single decision tree is **faster** in computation.	Comparatively **slower**.

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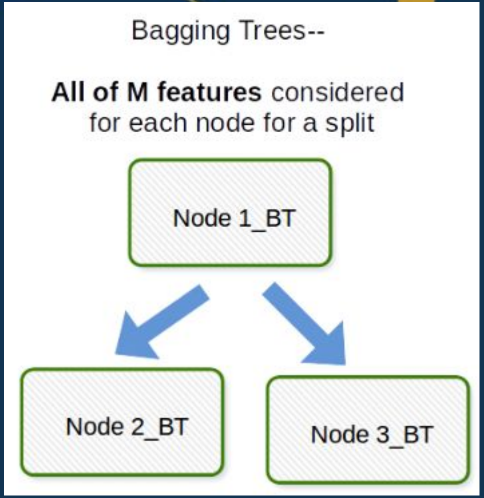
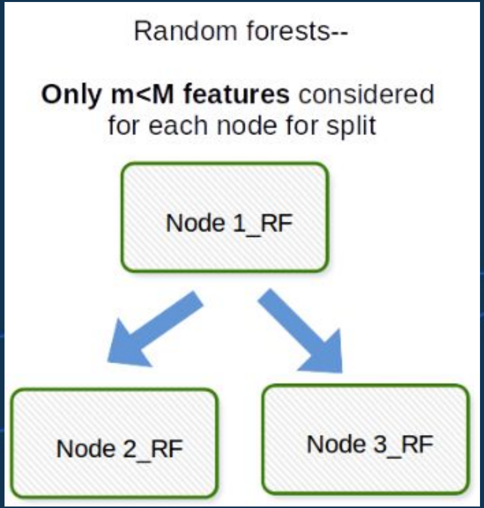
Differences with Bagged Trees

Bagged Trees	Random Forests
All features are selected.	**Randomly selected features.**
Highly correlated trees, can **reduce diversity** of model. More prone to **overfitting**.	**Randomness lowers correlation** between trees, results in **diverse set** of trees, **improving** model **accuracy** by **reducing overfitting** and increasing the **diversity** of the model.
Less computationally expensive.	More computationally expensive.





$m = \sqrt{M}$ is a good place to start

Feature Selection

Feature importance

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Feature importance

- **Feature importance** calculates a **score** for all the input features for a given model to establish the "**importance**" of each feature in the decision-making process. The **higher the score for a feature**, the **larger effect** it has on the model to predict a certain variable.

- Note: However, **bias** is a common problem in RF models, incorrect conclusions about the importance of features.
  - Algorithm uses gain in impurity reduction as proxy for feature importance.
  - A feature with more unique values, gain in impurity reduction is artificially inflated as the model is able to split on the feature more often.
  - Model tends to *overestimate importance of features with a high number of unique values*. So check if **feature** with many unique values is **relevant** to the model or not.

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Feature importance

Understanding feature importance offers several advantages

- ❖ **Enhanced Model Performance:** By identifying the most influential features, you can **prioritize** them during model training, leading to more **accurate predictions**.
- ❖ **Faster Training Times:** Focusing on the most relevant features streamlines the training process, saving valuable time and computational resources.
- ❖ **Reduced Overfitting:** Overfitting occurs when a model memorizes the training data instead of learning general patterns. By focusing on important features, you can prevent the model from becoming overly reliant on specific data points.

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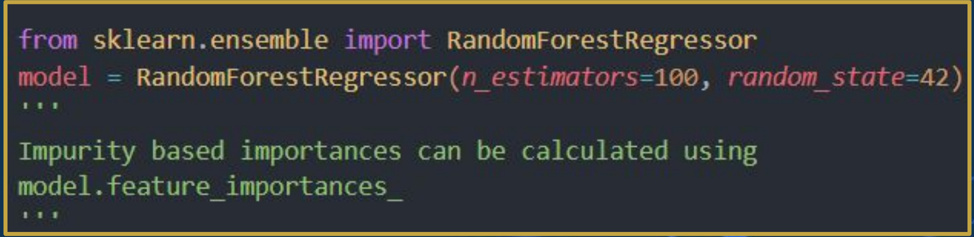
Feature Importance Methods

Random Forest Built-in Gini Importance: node impurity reduction, weighted by the number of samples that are reaching that node from the total number of samples.

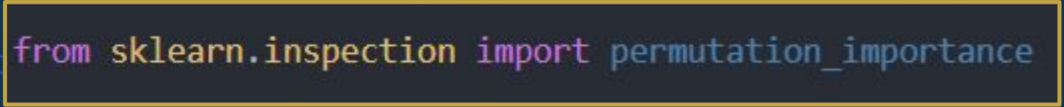
- ❖ More prone to **bias**, can inflate importance of numerical features
- ❖ Computed on statistics derived from the **training dataset,** the importances can be high even for features that are not predictive of the target variable.

Permutation Based: Calculated based on change in mean squared error (MSE) while permuting values of a feature. If permuting the values causes a huge change in the error, it means the feature is important for our model.

- ➢ Model agnostic, simple maths.



```
from sklearn.ensemble import RandomForestRegressor
model = RandomForestRegressor(n_estimators=100, random_state=42)
'''
Impurity based importances can be calculated using
model.feature_importances_
'''
```



```
from sklearn.inspection import permutation_importance
```

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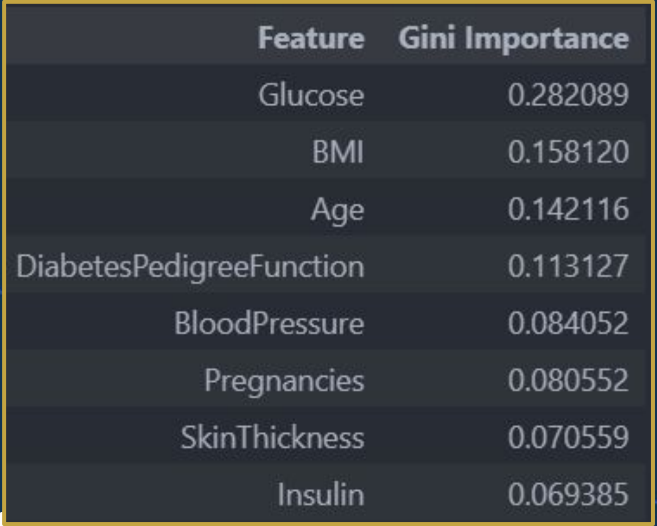
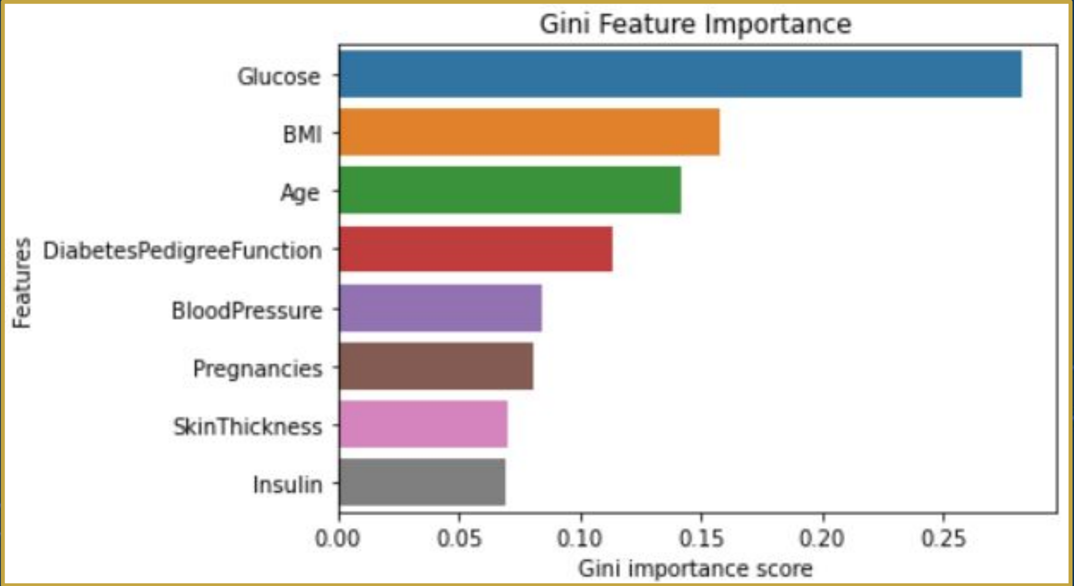
Feature importance

Built-in Gini importance

```python
#Finding the important features using the built-in Gini importance
importances = rf.feature_importances_
feature_imp_df = pd.DataFrame({'Feature': feature_names, 'Gini Importance': importances}).sort_values('Gini Importance', ascending=False)
feature_imp_df
```



Feature	Gini Importance
Glucose	0.282089
BMI	0.158120
Age	0.142116
DiabetesPedigreeFunction	0.113127
BloodPressure	0.084052
Pregnancies	0.080552
SkinThickness	0.070559
Insulin	0.069385



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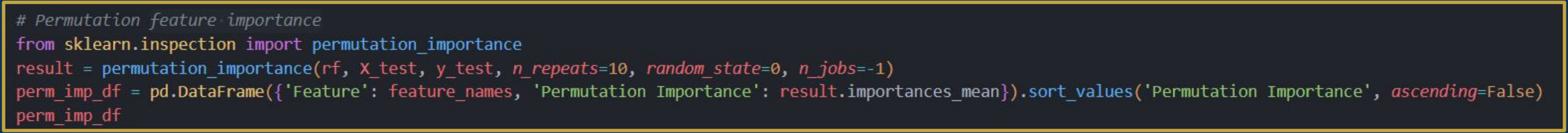
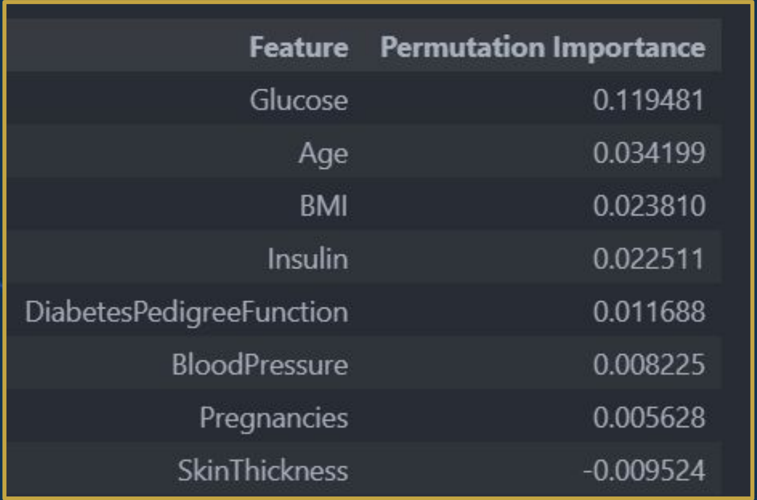
Feature importance

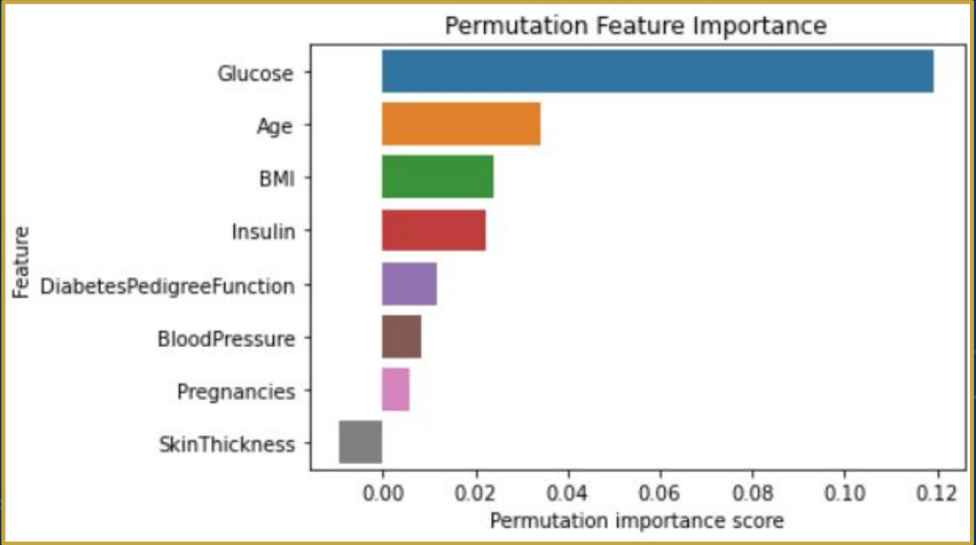
Permutation feature importance



```
# Permutation feature importance
from sklearn.inspection import permutation_importance
result = permutation_importance(rf, X_test, y_test, n_repeats=10, random_state=0, n_jobs=-1)
perm_imp_df = pd.DataFrame({'Feature': feature_names, 'Permutation Importance': result.importances_mean}).sort_values('Permutation Importance', ascending=False)
perm_imp_df
```



Feature	Permutation Importance
Glucose	0.119481
Age	0.034199
BMI	0.023810
Insulin	0.022511
DiabetesPedigreeFunction	0.011688
BloodPressure	0.008225
Pregnancies	0.005628
SkinThickness	-0.009524



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Implementing Random Forests

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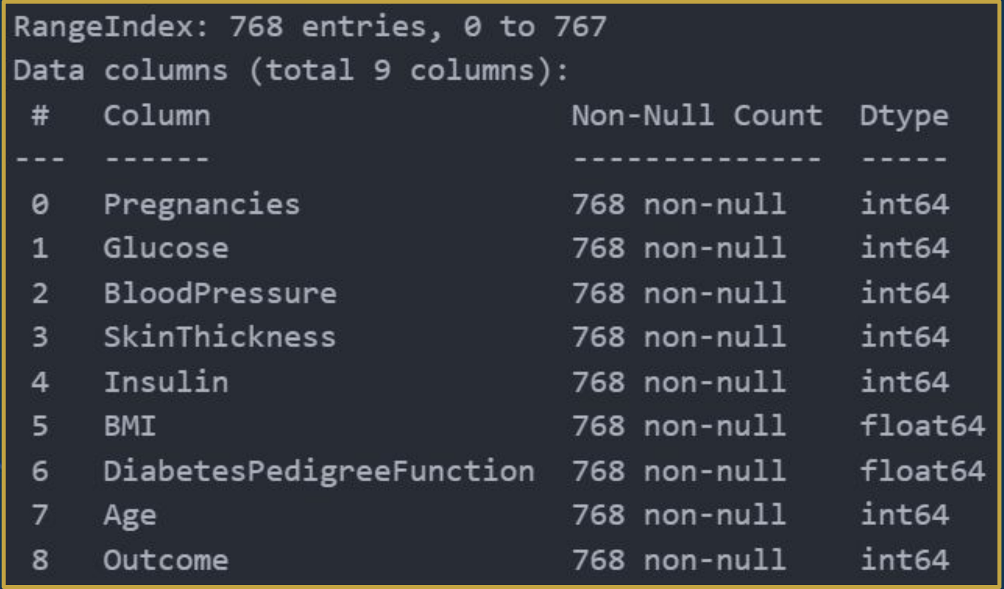
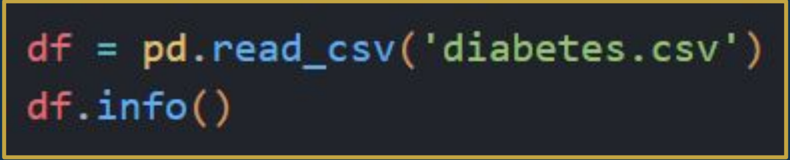
Random Forests with Diabetes dataset

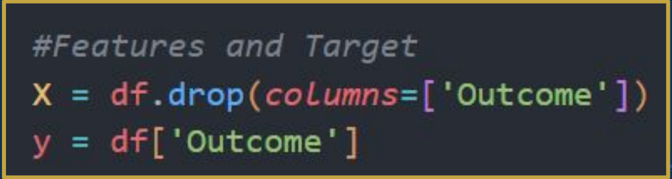


```
RangeIndex: 768 entries, 0 to 767
Data columns (total 9 columns):
 #   Column                    Non-Null Count  Dtype
---  ------                    --------------  -----
 0   Pregnancies               768 non-null    int64
 1   Glucose                   768 non-null    int64
 2   BloodPressure             768 non-null    int64
 3   SkinThickness             768 non-null    int64
 4   Insulin                   768 non-null    int64
 5   BMI                       768 non-null    float64
 6   DiabetesPedigreeFunction  768 non-null    float64
 7   Age                       768 non-null    int64
 8   Outcome                   768 non-null    int64
```

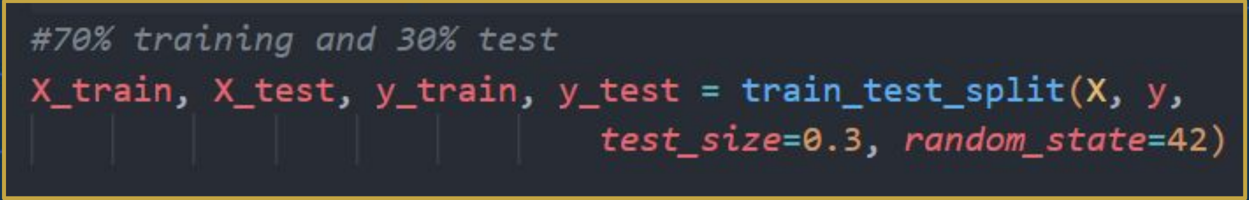
Classify and predict diabetes based on **features**.
Target is Outcome = 0 for not diabetic and 1 for diabetic.



```python
df = pd.read_csv('diabetes.csv')
df.info()
```



```python
#Features and Target
X = df.drop(columns=['Outcome'])
y = df['Outcome']
```



```python
#70% training and 30% test
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.3, random_state=42)
```

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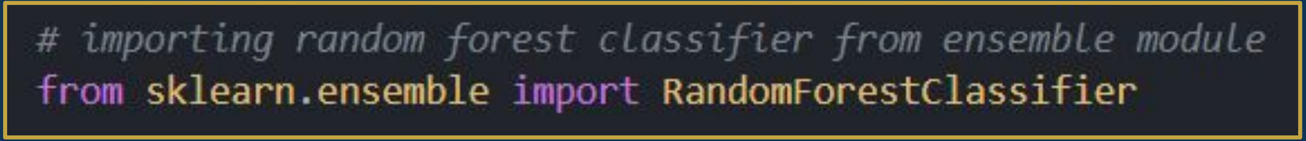
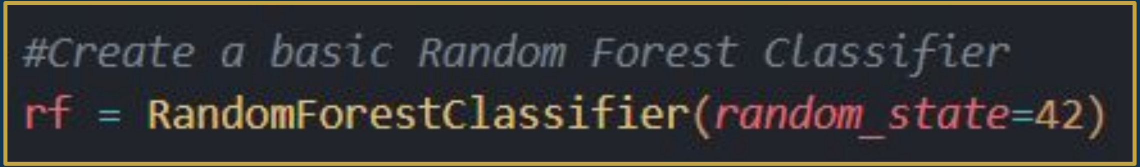
Implementing Random Forests

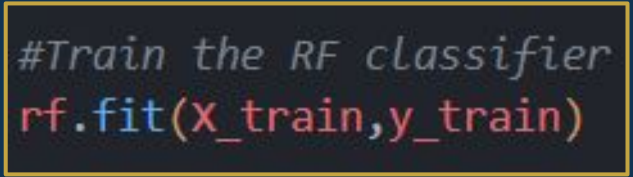


```python
# importing random forest classifier from ensemble module
from sklearn.ensemble import RandomForestClassifier
```

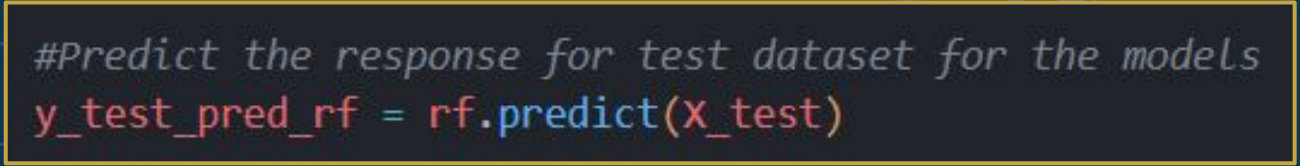
`RandomForestRegressor` for Regression models (will see an example in Tutorial)



```python
#Create a basic Random Forest Classifier
rf = RandomForestClassifier(random_state=42)
```



```python
#Train the RF classifier
rf.fit(X_train,y_train)
```



```python
#Predict the response for test dataset for the models
y_test_pred_rf = rf.predict(X_test)
```

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Hyperparameter Tuning

Optimisation and Bias-Variance Trade Off

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Hyperparameter Tuning

Hyperparameter to increase the Predictive Power

❖ **n_estimators:** number of trees the algorithm builds before taking the maximum voting or taking the averages of predictions. In general, a higher number of trees increases the performance and makes the predictions more stable, but it also slows down the computation.

❖ **max_features**: maximum number of features RF considers to split a node.

❖ **min_sample_leaf**: minimum number of leafs to split an internal node.

Hyperparameters to increase the RF model's speed
n_jobs, random_stat, oob_score (out-of-bag sampling).

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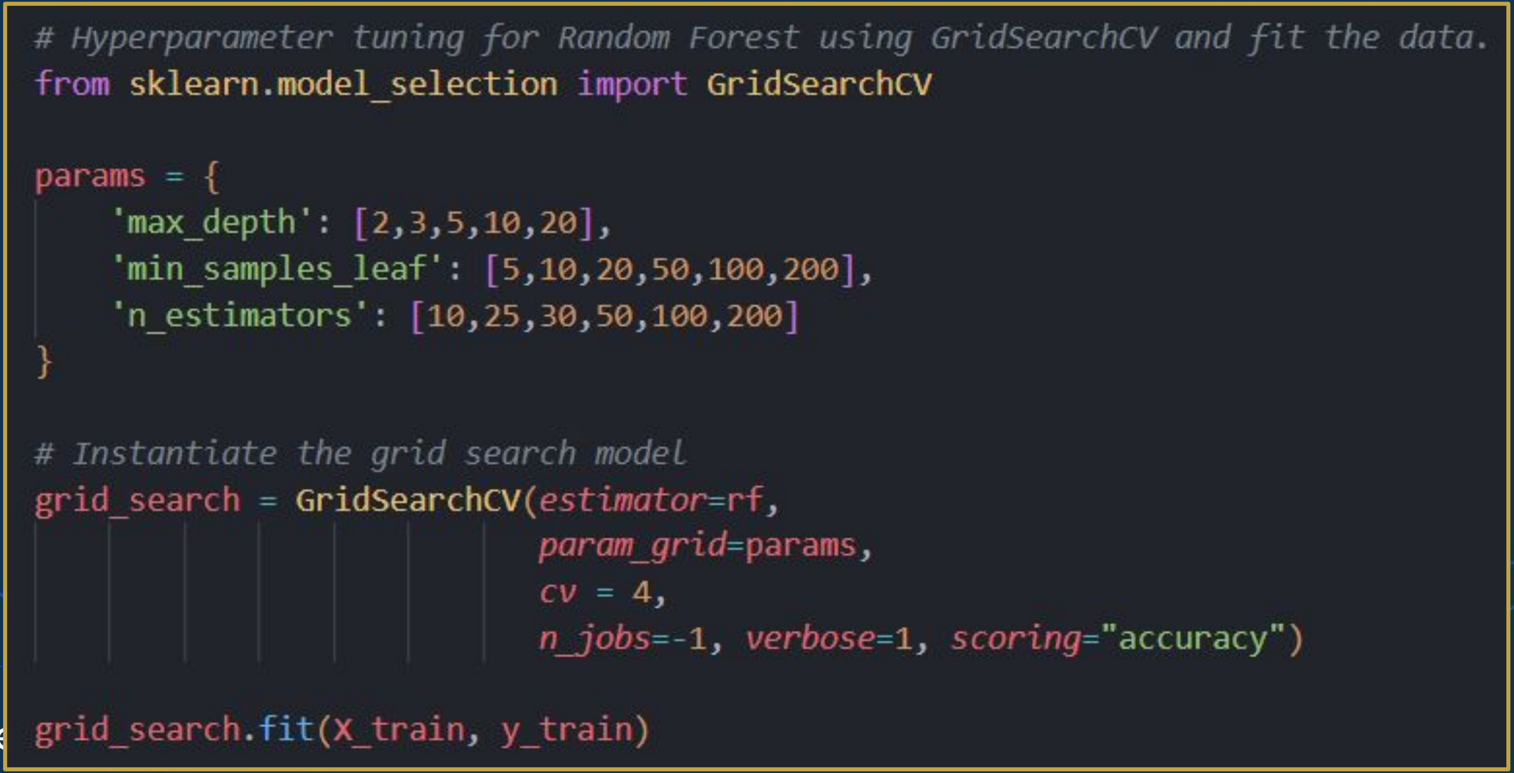
https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html

Hyperparameter Tuning

Exhaustive search over specified parameter values for an estimator



```
# Hyperparameter tuning for Random Forest using GridSearchCV and fit the data.
from sklearn.model_selection import GridSearchCV

params = {
    'max_depth': [2,3,5,10,20],
    'min_samples_leaf': [5,10,20,50,100,200],
    'n_estimators': [10,25,30,50,100,200]
}

# Instantiate the grid search model
grid_search = GridSearchCV(estimator=rf,
                           param_grid=params,
                           cv = 4,
                           n_jobs=-1, verbose=1, scoring="accuracy")

grid_search.fit(X_train, y_train)
```

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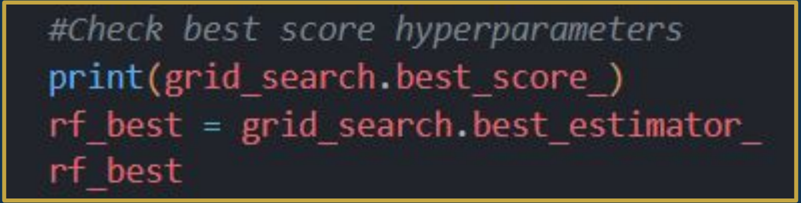
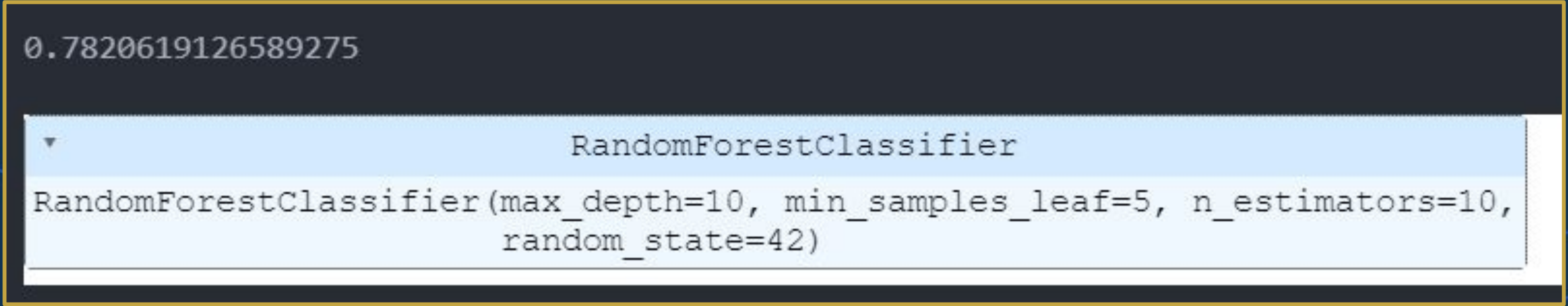
Hyperparameter Tuning

Exhaustive search over specified parameter values for an estimator



```
#Check best score hyperparameters
print(grid_search.best_score_)
rf_best = grid_search.best_estimator_
rf_best
```



```
0.7820619126589275

▾ RandomForestClassifier
RandomForestClassifier(max_depth=10, min_samples_leaf=5, n_estimators=10,
                       random_state=42)
```

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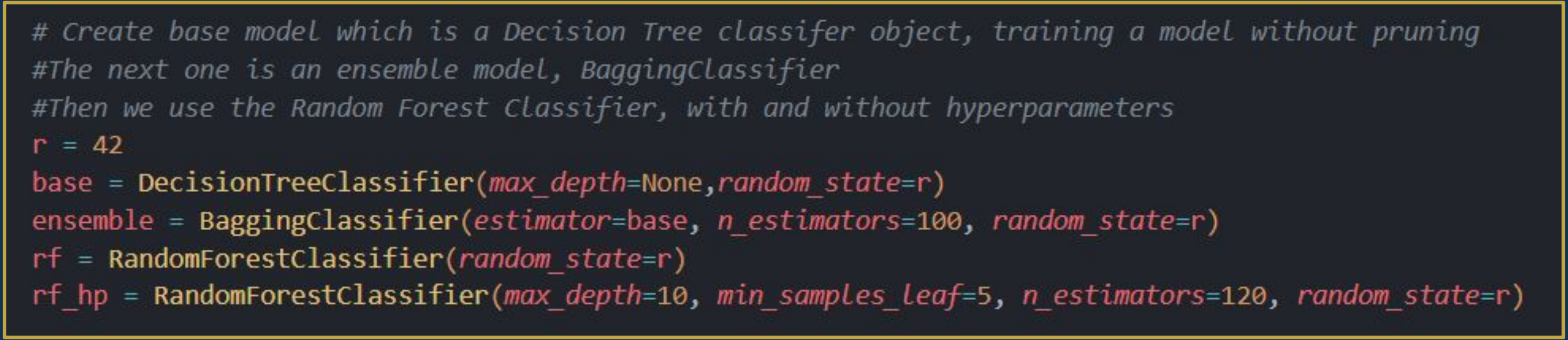
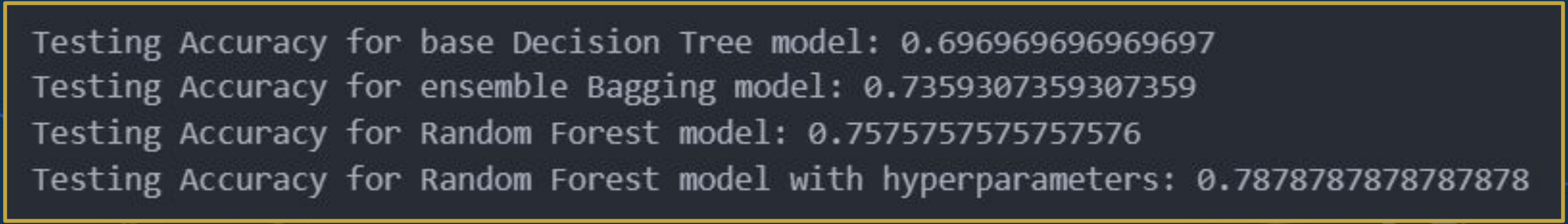
Hyperparameter Tuning



```python
# Create base model which is a Decision Tree classifer object, training a model without pruning
#The next one is an ensemble model, BaggingClassifier
#Then we use the Random Forest Classifier, with and without hyperparameters
r = 42
base = DecisionTreeClassifier(max_depth=None,random_state=r)
ensemble = BaggingClassifier(estimator=base, n_estimators=100, random_state=r)
rf = RandomForestClassifier(random_state=r)
rf_hp = RandomForestClassifier(max_depth=10, min_samples_leaf=5, n_estimators=120, random_state=r)
```



```
Testing Accuracy for base Decision Tree model: 0.696969696969697
Testing Accuracy for ensemble Bagging model: 0.7359307359307359
Testing Accuracy for Random Forest model: 0.7575757575757576
Testing Accuracy for Random Forest model with hyperparameters: 0.7878787878787878
```

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Bias Variance Trade-Off

- **Balance between underfitting and overfitting.** Random Forest is better at managing bias-variance trade-off than Decision Tree.

- Decision Tree tends to have high variance, which can lead to overfitting, while Random Forest has a lower variance, which results in better generalisation.

- **max_features** and **min_samples_leaf** reduce correlation between trees, but might increase bias, since each tree now has less data to work with.

- Choose set of hyperparameters that nagivates this tradeoff between bias and variance to minimize error.

Summary

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Key Takeaways

1. Decision tree is more simple and interpretable but prone to overfitting, but a random forest is **complex** and **prevents** the risk of **overfitting**, better at **managing bias-variance trade-off**.
2. Random forest: more **robust** and **generalised** performance on new data, widely used in various domains, finance, healthcare, and deep learning.
3. **Features** that are ranked highly have a significant influence on the model's decision-making, improving its performance.
4. Random Forests are fast to train, but quite **slow** to create **predictions** once they are trained. In some real-world cases where **run-time performance** is important, other approaches would be preferred.
5. It is a **predictive** modeling tool, **not a descriptive tool.** For a description of the relationships in the data, other approaches would be better.

Further Resources

- https://www.geeksforgeeks.org/bagging-vs-boosting-in-machine-learning/
- https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html
- Understanding Random Forests: From Theory to Practice https://arxiv.org/abs/1407.7502
- https://www.geeksforgeeks.org/random-forest-algorithm-in-machine-learning/

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Questions and Answers

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Thank you for attending

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