Bagging

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

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Ensemble Methods

Voting Classifier

- same training set,
- $\neq$ algorithms.

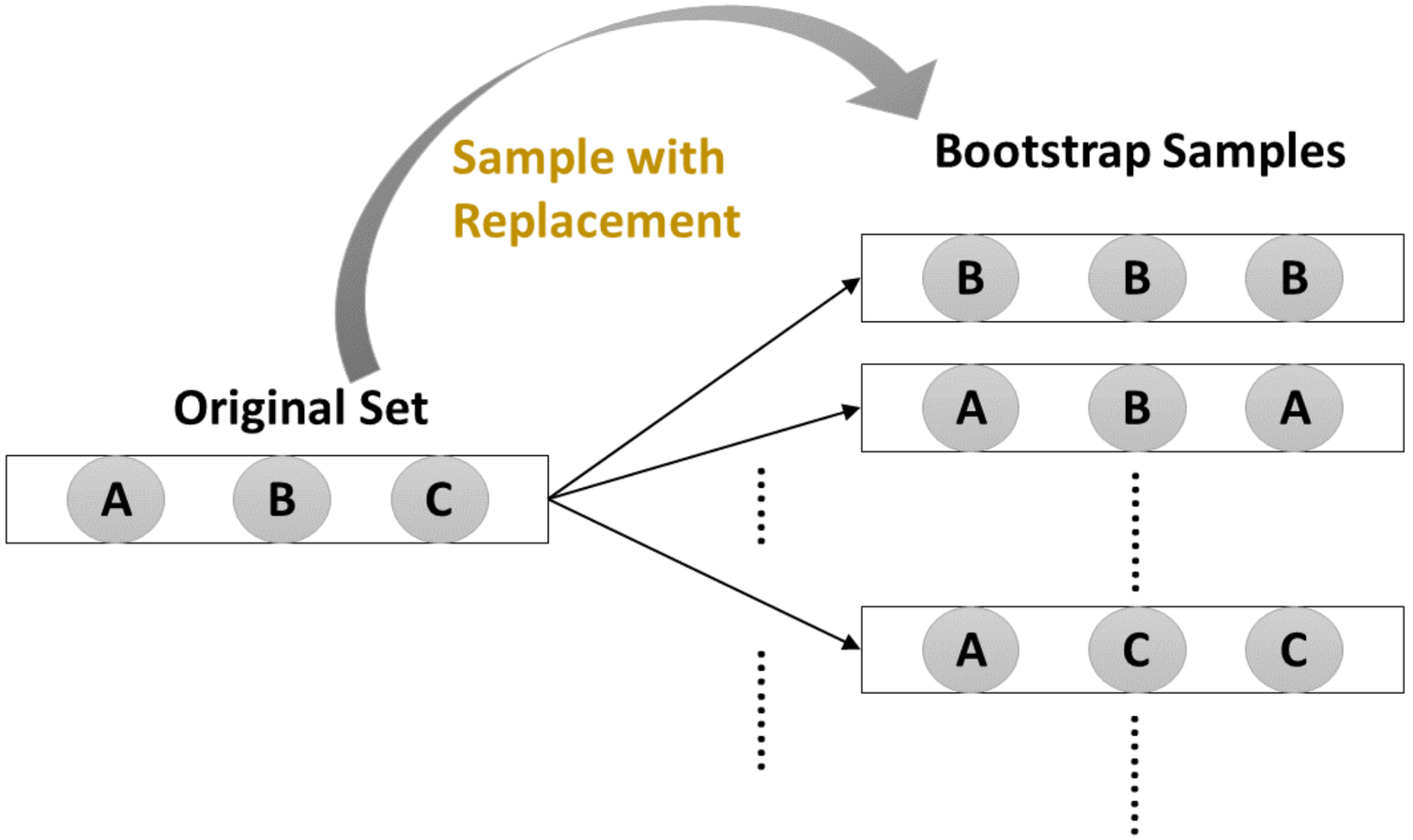
Bagging

- one algorithm,
- $\neq$ subsets of the training set.

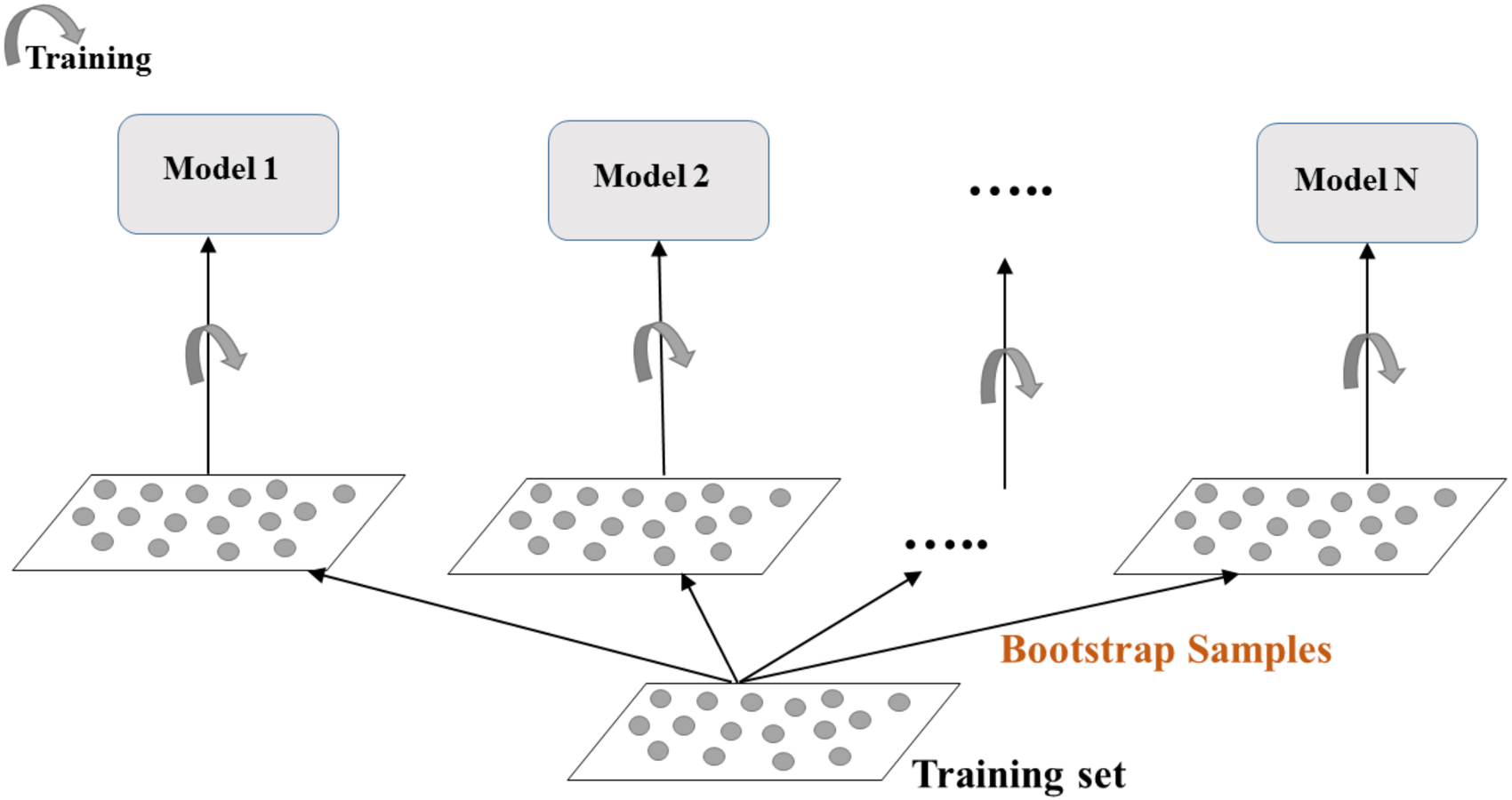
Bagging

- Bagging: Bootstrap Aggregation.
- Uses a technique known as the bootstrap.
- Reduces variance of individual models in the ensemble.

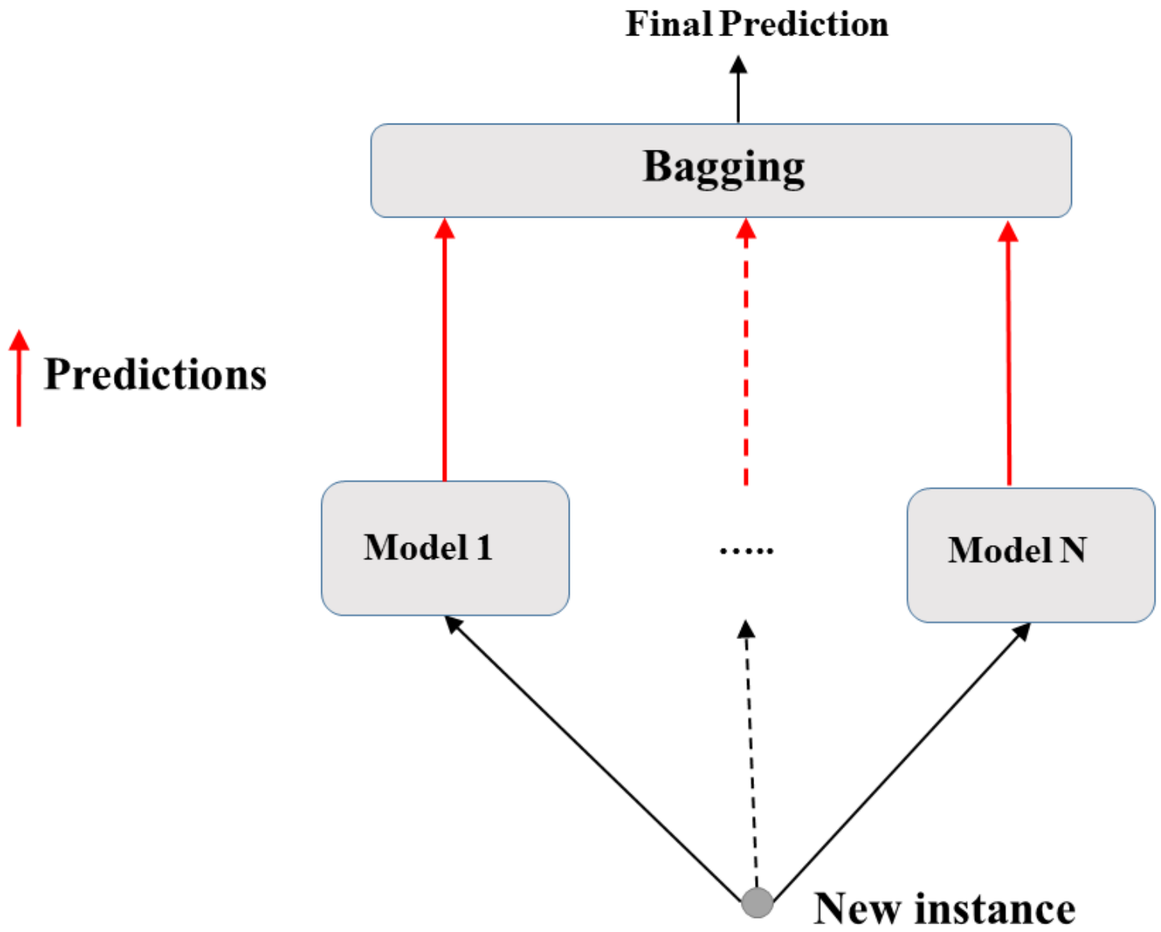
Bootstrap


Sample with
Replacement
Bootstrap Samples
Original Set
A
B
C
B
B
B
A
B
A
A
C
C

Bagging: Training



Bagging: Prediction



Bagging: Classification & Regression

Classification:

- Aggregates predictions by majority voting.
- `BaggingClassifier` in scikit-learn.

Regression:

- Aggregates predictions through averaging.
- `BaggingRegressor` in scikit-learn.

Bagging Classifier in sklearn (Breast-Cancer dataset)

```
# Import models and utility functions
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split

# Set seed for reproducibility
SEED = 1

# Split data into 70% train and 30% test
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3,
                                                    stratify=y,
                                                    random_state=SEED)
```

```
# Instantiate a classification-tree 'dt'
dt = DecisionTreeClassifier(max_depth=4, min_samples_leaf=0.16, random_state=SEED)
# Instantiate a BaggingClassifier 'bc'
bc = BaggingClassifier(base_estimator=dt, n_estimators=300, n_jobs=-1)
# Fit 'bc' to the training set
bc.fit(X_train, y_train)
# Predict test set labels
y_pred = bc.predict(X_test)

# Evaluate and print test-set accuracy
accuracy = accuracy_score(y_test, y_pred)
print('Accuracy of Bagging Classifier: {:.3f}'.format(accuracy))
```

```
Accuracy of Bagging Classifier: 0.936
```

Let's practice!

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Out Of Bag Evaluation

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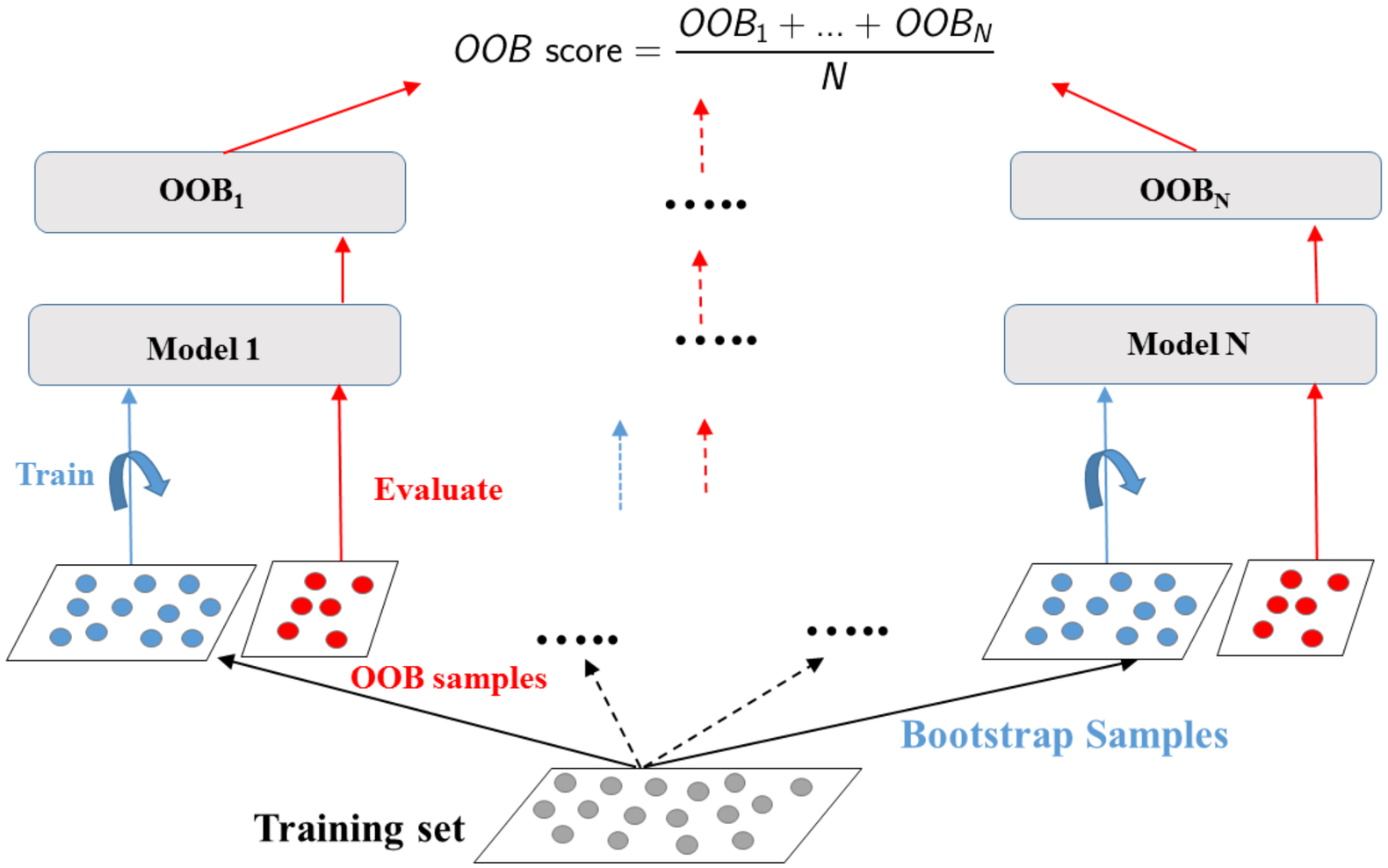
Bagging

- some instances may be sampled several times for one model,
- other instances may not be sampled at all.

Out Of Bag (OOB) instances

- On average, for each model, 63% of the training instances are sampled.
- The remaining 37% constitute the OOB instances.

OOB Evaluation



OOB Evaluation in sklearn (Breast Cancer Dataset)

```
# Import models and split utility function
from sklearn.ensemble import BaggingClassifier
from sklearn.tree import DecisionTreeClassifier
from sklearn.metrics import accuracy_score
from sklearn.model_selection import train_test_split

# Set seed for reproducibility
SEED = 1

# Split data into 70% train and 30% test
X_train, X_test, y_train, y_test =  train_test_split(X, y, test_size= 0.3,
                                                     stratify= y,
                                                     random_state=SEED)
```

```
# Instantiate a classification-tree 'dt'
dt = DecisionTreeClassifier(max_depth=4,
                            min_samples_leaf=0.16,
                            random_state=SEED)
# Instantiate a BaggingClassifier 'bc'; set oob_score = True
bc = BaggingClassifier(base_estimator=dt, n_estimators=300,
                       oob_score=True, n_jobs=-1)

# Fit 'bc' to the training set
bc.fit(X_train, y_train)

# Predict the test set labels
y_pred = bc.predict(X_test)
```

```
# Evaluate test set accuracy
test_accuracy = accuracy_score(y_test, y_pred)
# Extract the OOB accuracy from 'bc'
oob_accuracy = bc.oob_score_

# Print test set accuracy
print('Test set accuracy: {:.3f}'.format(test_accuracy))
```

```
Test set accuracy: 0.936
```

```
# Print OOB accuracy
print('OOB accuracy: {:.3f}'.format(oob_accuracy))
```

```
OOB accuracy: 0.925
```

Let's practice!

MACHINE LEARNING WITH TREE-BASED MODELS IN PYTHON

Random Forests

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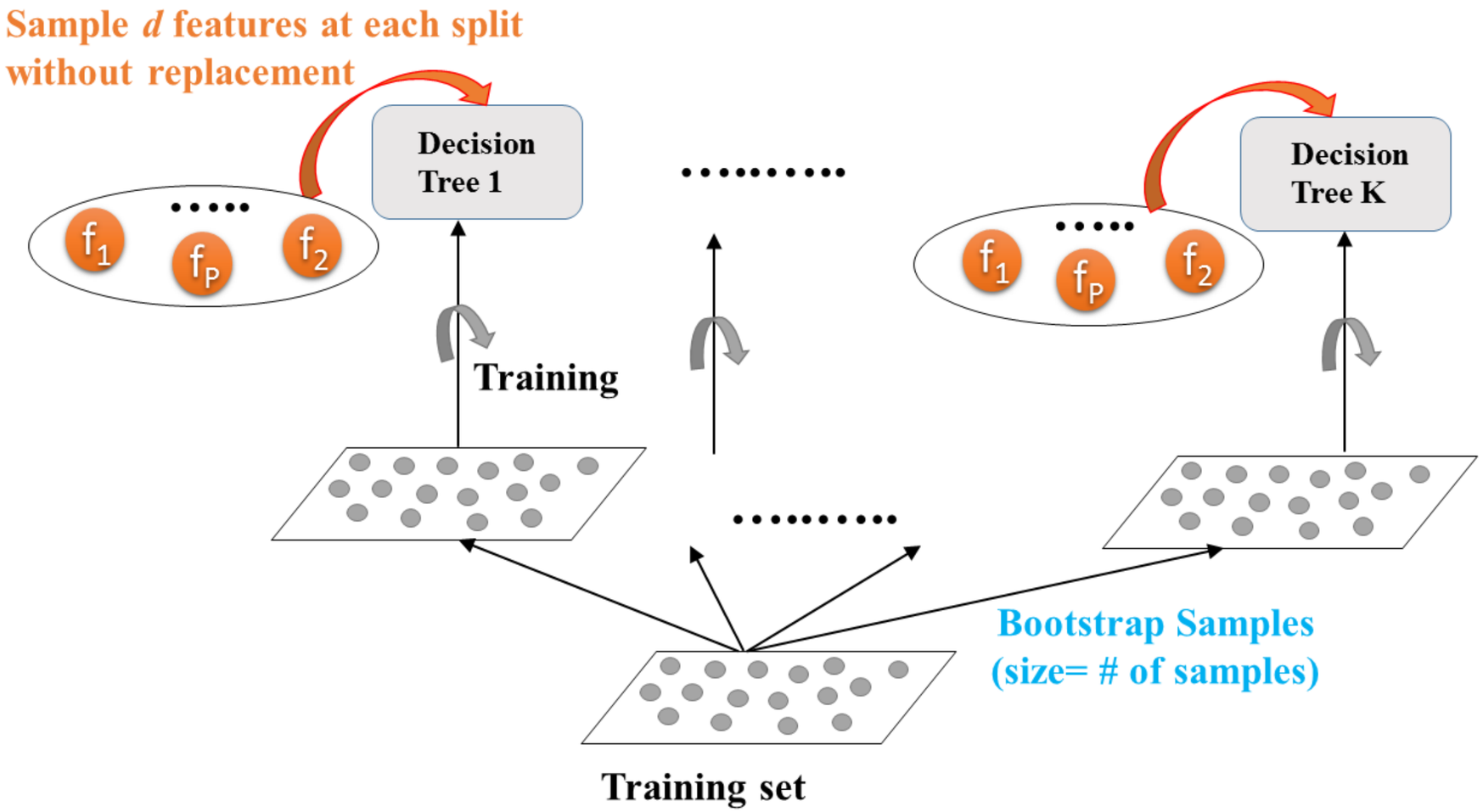
Bagging

- Base estimator: Decision Tree, Logistic Regression, Neural Net, ...
- Each estimator is trained on a distinct bootstrap sample of the training set
- Estimators use all features for training and prediction

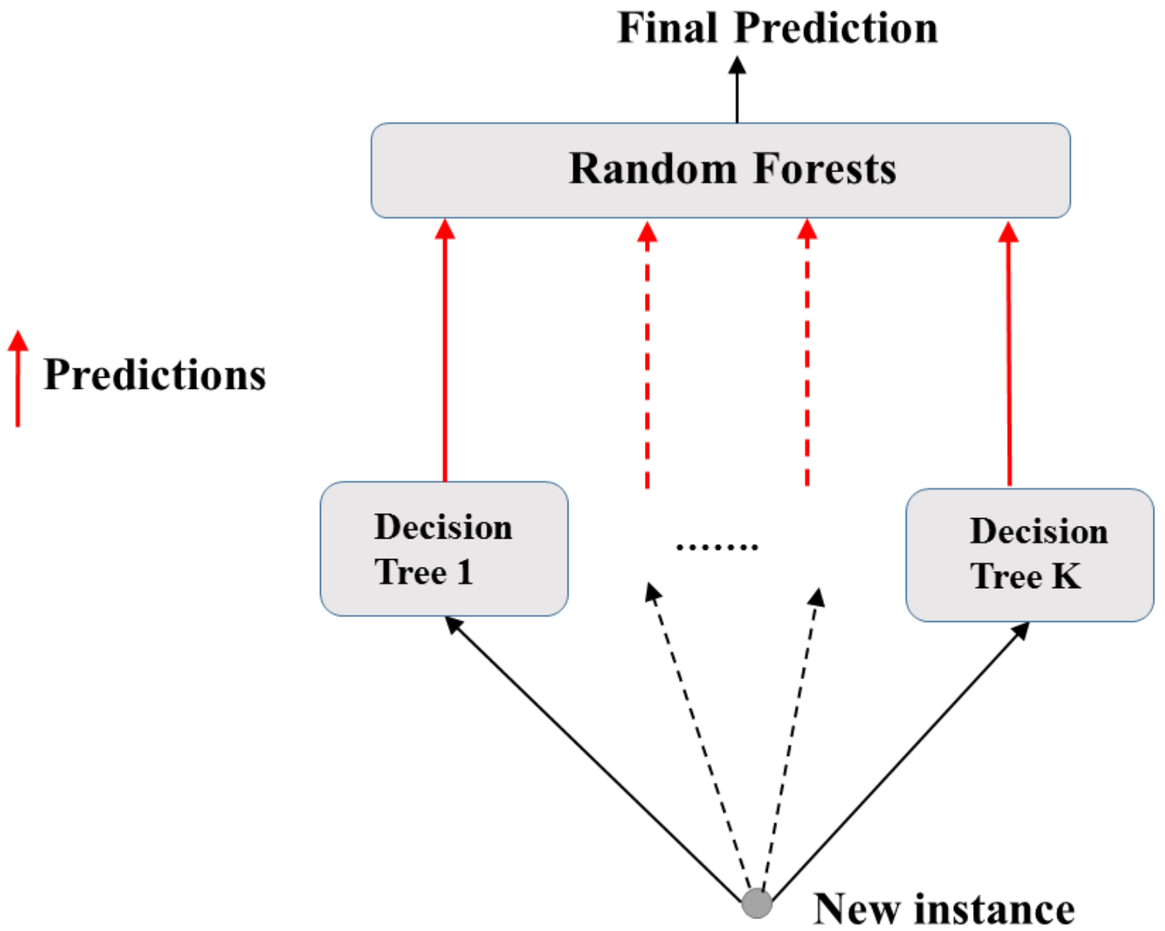
Further Diversity with Random Forests

- Base estimator: Decision Tree
- Each estimator is trained on a different bootstrap sample having the same size as the training set
- RF introduces further randomization in the training of individual trees
- d features are sampled at each node without replacement
  ($d < \text{total number of features}$)

Random Forests: Training



Random Forests: Prediction



Random Forests: Classification & Regression

Classification:

- Aggregates predictions by majority voting
- `RandomForestClassifier` in scikit-learn

Regression:

- Aggregates predictions through averaging
- `RandomForestRegressor` in scikit-learn

Random Forests Regressor in sklearn (auto dataset)

```
# Basic imports
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error as MSE
# Set seed for reproducibility
SEED = 1

# Split dataset into 70% train and 30% test
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    test_size=0.3,
                                                    random_state=SEED)
```

```
# Instantiate a random forests regressor 'rf' 400 estimators
rf = RandomForestRegressor(n_estimators=400,
                                    min_samples_leaf=0.12,
                                    random_state=SEED)
# Fit 'rf' to the training set
rf.fit(X_train, y_train)
# Predict the test set labels 'y_pred'
y_pred = rf.predict(X_test)
```

```
# Evaluate the test set RMSE
rmse_test = MSE(y_test, y_pred)**(1/2)

# Print the test set RMSE
print('Test set RMSE of rf: {:.2f}'.format(rmse_test))
```

```
Test set RMSE of rf: 3.98
```

Feature Importance

Tree-based methods: enable measuring the importance of each feature in prediction.

In `sklearn` :

- how much the tree nodes use a particular feature (weighted average) to reduce impurity
- accessed using the attribute `feature_importance_`

Feature Importance in sklearn

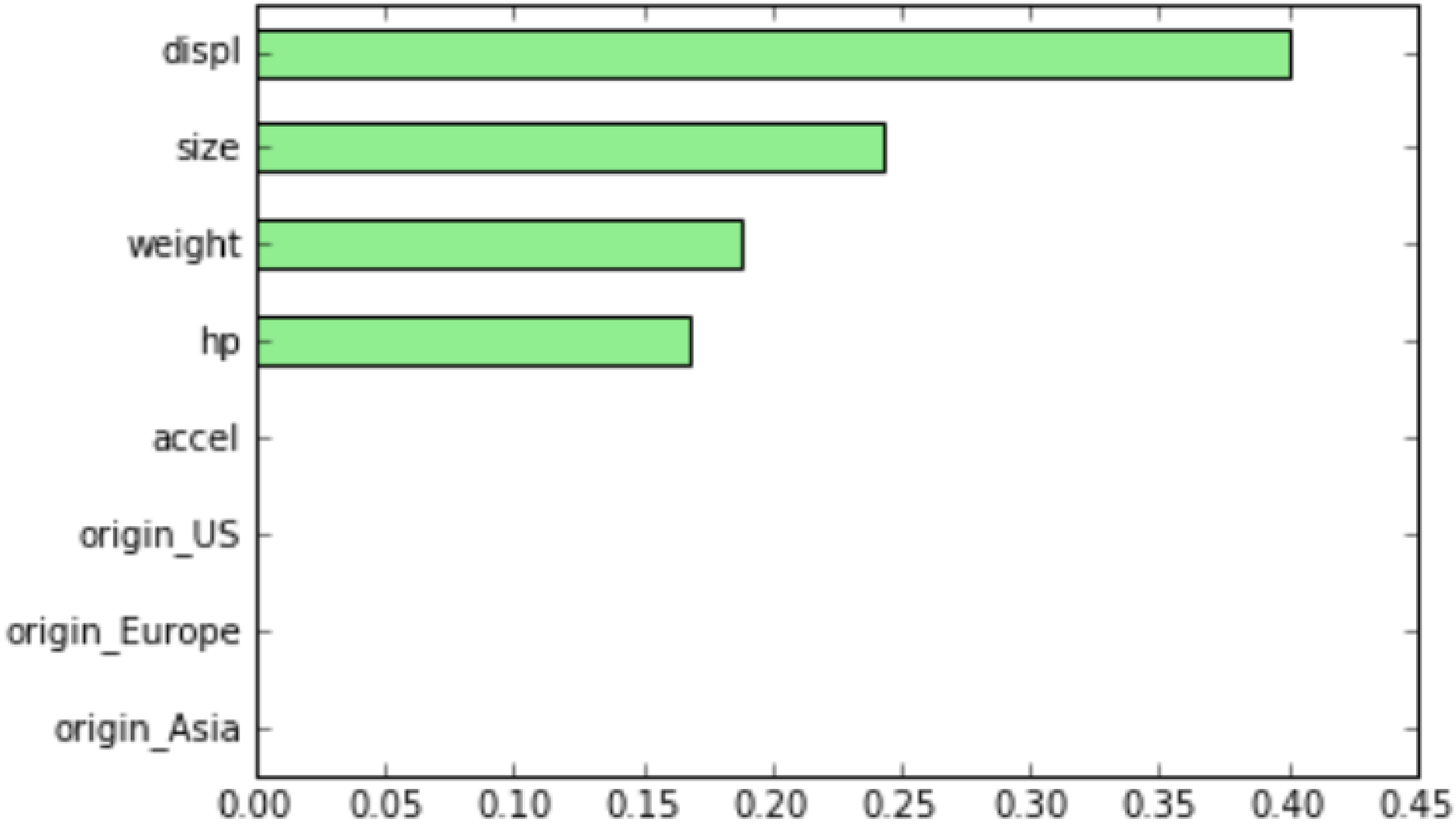
```
import pandas as pd
import matplotlib.pyplot as plt

# Create a pd.Series of features importances
importances_rf = pd.Series(rf.feature_importances_, index = X.columns)

# Sort importances_rf
sorted_importances_rf = importances_rf.sort_values()

# Make a horizontal bar plot
sorted_importances_rf.plot(kind='barh', color='lightgreen'); plt.show()
```

Feature Importance in sklearn



Let's practice!

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