BIOINFORMATICS MODELING AND SIMULATION

SECB 4313

ASSIGNMENT 3

Lecturer:

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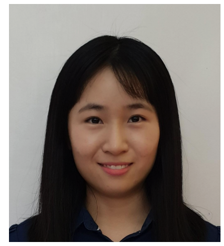
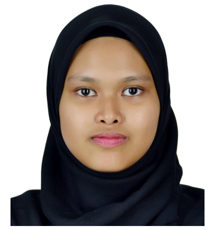
1. Profile

Profile Picture				
Name	Chang Min Xuan	Hanis Rafiqah	Lee Jia Yee	Nik Syahdina
GitHub Link	https://github.com/ChangMinXuan	https://github.com/hanisrafiqah	https://github.com/jiayee00	https://github.com/NikSyahdina

2. Summary from Assignment 2

The selected FOUR hyperparameters are number of trees (n_estimators), maximum depth (max_depth), minimum samples split (min_samples_split) and maximum leaf nodes (max_leaf_nodes). The combination of hyperparameters that generate the most improved result is 100 for n_estimators, max_depth which is 20, 10 for the min_sample_split and max_leaf_nodes value is 10.

3. Grid Search and Random Search

3.1 Grid Search

Table 3.1.1 Best cross-validation score, test set accuracy, and best parameters for Random forest using Grid Search as the hyperparameter tuning techniques.

Best cross-validation score	0.8304
Test set accuracy	0.8852
Best parameters found	
n_estimators	100
min_samples_split	2
max_leaf_nodes	10
max_depth	20

Table 3.1.2 Classification report for Random Forest using Grid Search as the hyperparameter tuning techniques.

Class	Precision	Recall	F1-Score	Support
0	0.86	0.89	0.88	28
1	0.91	0.88	0.89	33

3.2 Random Search

Table 3.2.1 Best cross-validation score, test set accuracy, and best parameters for Random forest using Random Search as the hyperparameter tuning techniques.

Best cross-validation score	0.8264
Test set accuracy	0.8852
Best parameters found	
n_estimators	100
min_samples_split	10
max_leaf_nodes	10
max_depth	20

Table 3.2.2 Classification report for Random Forest using Random Search as the hyperparameter tuning techniques.

Class	Precision	Recall	F1-Score	Support
0	0.89	0.86	0.88	29
1	0.88	0.91	0.89	32

4. Discussion and Comparison

The grid search achieved a slightly higher accuracy (0.8688524590163934) compared to the random search (0.8524590163934426).

a) Effort to get the results:

- **Grid Search:**
  - Requires more effort to set up and tune.
  - Requires specifying a grid of hyperparameters to search over.
  - Can be computationally expensive, especially with a large grid.
- **Random Search:**
  - Requires less effort to set up and tune.
  - Only requires specifying a range of values for each hyperparameter.
  - Can be less computationally expensive than grid search.

b) Computational time:

- **Grid Search:**
  - Typically takes longer than random search, as it evaluates every combination of hyperparameters in the grid.
- **Random Search:**
  - Typically takes less time than grid search, as it only evaluates a random sample of hyperparameter combinations.

5. Hyperparameter Optimization/Tuning

Hyperparameter optimization/tuning is vital due to several main reasons. First of all, it is undeniable that it can improve model accuracy. As shown above, there are two automated search methods, which are grid search and random search. Grid search involves specifying a set of values for each hyperparameter and training the model for all possible combinations. Therefore, it guarantees the best combination within the specified range of parameters. On the other hand, random search samples a fixed number of hyperparameter combinations and is more efficient than grid search.

Secondly, hyperparameter optimization is crucial to prevent overfitting and underfitting. Since it can help in balancing the complexity of the model, it avoids scenarios of having a model which is too complex to perform well in training data but poorly on unseen data. Meanwhile, it can also prevent from failing to capture the underlying patterns of data due to too simple of hyperparameters in the model. By doing so, it enhances generalization, which means the model is not only accurate on the training data but also performs well on validation and test datasets.

Furthermore, training efficiency is another main reason to carry out hyperparameter optimization. This can be shown clearly as it optimizes the training process in terms of time and resources, leading to a more efficient model. For instance, a properly tuned Random Forest might require fewer trees to achieve the same or better accuracy, saving computational time and resources.

APPENDIX

Python codes of Grid Search and Random search
Code link:
https://colab.research.google.com/drive/1SU-WU59EkYYMmQ4xNUH1M4m47XUzuZKt?usp=sharing

```
[ ] import numpy as np
    import pandas as pd
    from sklearn.model_selection import train_test_split, GridSearchCV
    from itertools import product
    from sklearn.ensemble import RandomForestClassifier
    from sklearn.metrics import accuracy_score, classification_report
```

```
[ ] df = pd.read_csv('/content/heart.csv')
    df
```

	age	sex	cp	trestbps	chol	fbs	restecg	thalach	exang	oldpeak	slope	ca	thal	target
0	63	1	3	145	233	1	0	150	0	2.3	0	0	1	1
1	37	1	2	130	250	0	1	187	0	3.5	0	0	2	1
2	41	0	1	130	204	0	0	172	0	1.4	2	0	2	1
3	56	1	1	120	236	0	1	178	0	0.8	2	0	2	1
4	57	0	0	120	354	0	1	163	1	0.6	2	0	2	1
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
298	57	0	0	140	241	0	1	123	1	0.2	1	0	3	0
299	45	1	3	110	264	0	1	132	0	1.2	1	0	3	0
300	68	1	0	144	193	1	1	141	0	3.4	1	2	3	0
301	57	1	0	130	131	0	1	115	1	1.2	1	1	3	0
302	57	0	1	130	236	0	0	174	0	0.0	1	1	2	0

303 rows × 14 columns

```
[ ] df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 303 entries, 0 to 302
Data columns (total 14 columns):
 #   Column    Non-Null Count  Dtype  
---  ------    --------------  -----  
 0   age       303 non-null    int64  
 1   sex       303 non-null    int64  
 2   cp        303 non-null    int64  
 3   trestbps  303 non-null    int64  
 4   chol      303 non-null    int64  
 5   fbs       303 non-null    int64  
 6   restecg   303 non-null    int64  
 7   thalach   303 non-null    int64  
 8   exang     303 non-null    int64  
 9   oldpeak   303 non-null    float64
 10  slope     303 non-null    int64  
 11  ca        303 non-null    int64  
 12  thal      303 non-null    int64  
 13  target    303 non-null    int64  
dtypes: float64(1), int64(13)
memory usage: 33.3 KB
```

```
[ ] df.shape
```

```
(303, 14)
```

```
[ ] df.columns
```

```
Index(['age', 'sex', 'cp', 'trestbps', 'chol', 'fbs', 'restecg', 'thalach',
       'exang', 'oldpeak', 'slope', 'ca', 'thal', 'target'],
      dtype='object')
```

```
[ ] null_values = df.isnull().sum()
    print("Null values in each column:\n", null_values)
```

```
Null values in each column:
 age         0
sex         0
cp          0
trestbps    0
chol        0
fbs         0
restecg     0
thalach     0
exang       0
oldpeak     0
slope       0
ca          0
thal        0
target      0
dtype: int64
```

```
[ ] X = df.drop("target", axis=1)
    y = df["target"].apply(lambda x: 1 if x > 0 else 0)  # Binarize the target
```

```
[ ] X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)
```

Hyperparameters: n_estimators, max_depth, min_samples_split, and max_leaf_nodes.

```
[ ] # Define hyperparameters and their values
    hyperparameters = {
        'n_estimators': [100, 500],
        'max_depth': [10, 20],
        'min_samples_split': [2, 10],
        'max_leaf_nodes': [10, 20]
    }
```

```
[ ] # Hyperparater Optimazation using GridSearch
    model = RandomForestClassifier()
    model_gs = GridSearchCV(estimator=model, param_grid=hyperparameters)
    model_gs.fit(X_train, y_train)
```

```
▸ GridSearchCV
▸ estimator: RandomForestClassifier
  ▸ RandomForestClassifier
```

```
[ ] # Get the best parameters
    model_gs.best_params_
```

```
{'max_depth': 20,
 'max_leaf_nodes': 10,
 'min_samples_split': 2,
 'n_estimators': 100}
```

```
[ ] # Get the best score
    model_gs.best_score_
```

```
0.8304421768707482
```

Grid Search

```
[ ] # Random Forest with Grid Search
    y_pred_gs = model_gs.predict(X_test)

    print("\nRandom Forest Grid Search Performance:")
    print("Accuracy:", accuracy_score(y_pred_gs, y_test))
    print("\nClassification Report:")
    print(classification_report(y_pred_gs, y_test))
```

```
Random Forest Grid Search Performance:
Accuracy: 0.8852459016393442

Classification Report:
              precision    recall  f1-score   support

           0       0.86      0.89      0.88        28
           1       0.91      0.88      0.89        33

    accuracy                           0.89        61
   macro avg       0.88      0.89      0.88        61
weighted avg       0.89      0.89      0.89        61
```

Random Search

```
[ ] from sklearn.metrics import classification_report
    from sklearn.model_selection import train_test_split
    import pandas as pd
    from sklearn.ensemble import RandomForestClassifier
    from sklearn.model_selection import RandomizedSearchCV
```

```
[ ] # Initialize the RandomForestClassifier
    rf = RandomForestClassifier()

    # Initialize RandomizedSearchCV
    random_search = RandomizedSearchCV(
        estimator=rf,
        param_distributions=hyperparameters,
        n_iter=100,  # Number of parameter settings that are sampled
        cv=5,  # 5-fold cross-validation
        verbose=2,
        random_state=42,
        n_jobs=-1  # Use all available cores
    )

    # Fit RandomizedSearchCV to the data
    random_search.fit(X_train, y_train)
```

```
Fitting 5 folds for each of 16 candidates, totalling 80 fits
/usr/local/lib/python3.10/dist-packages/sklearn/model_selection/_search.py:30
  warnings.warn(
```

```
▸        RandomizedSearchCV
▸ estimator: RandomForestClassifier
      ▸ RandomForestClassifier
```

```python
from sklearn.metrics import precision_score, recall_score, f1_score, confusion_matrix, accuracy_score

# Print the best parameters and the corresponding score
print(f"Best parameters found: {random_search.best_params_}")
print(f"Best cross-validation score: {random_search.best_score_}")

# Predict with the best estimator
best_rf = random_search.best_estimator_
y_pred = best_rf.predict(X_test)

# Evaluate the model
accuracy = accuracy_score(y_test, y_pred)
print(f"Test set accuracy: {accuracy}")

# Calculate and print precision, recall, f1 score, and support
precision = precision_score(y_test, y_pred, average=None)
recall = recall_score(y_test, y_pred, average=None)
f1 = f1_score(y_test, y_pred, average=None)
cm = confusion_matrix(y_test, y_pred)

# Calculate support from confusion matrix
support = cm.sum(axis=1)

# Print the classification report manually
print("\nClassification Report:")
print(f"{'Class':<10}{'Precision':<10}{'Recall':<10}{'F1-Score':<10}{'Support':<10}")
for i in range(len(precision)):
    print(f"{i:<10}{precision[i]:<10.2f}{recall[i]:<10.2f}{f1[i]:<10.2f}{support[i]:<10}")
```

```
Best parameters found: {'n_estimators': 100, 'min_samples_split': 10, 'max_leaf_nodes': 10, 'max_depth': 10}
Best cross-validation score: 0.8263605442176871
Test set accuracy: 0.8852459016393442

Classification Report:
Class     Precision Recall    F1-Score  Support
0         0.89      0.86      0.88      29
1         0.88      0.91      0.89      32
```