week_7_bootstrap_grid_search

October 12, 2023

[ ]:
```
import pandas as pd # standard
import numpy as np # standard
from sklearn import tree # package to make decision tree
from sklearn.metrics import accuracy_score # for accuracy calculation
from sklearn.metrics import balanced_accuracy_score
from sklearn.metrics import roc_auc_score

import matplotlib.pyplot as plt
import seaborn as sns

import thermogram_utilities

import warnings
warnings.filterwarnings("ignore")
```

[ ]:
```
df = pd.read_excel("/Users/avery/OneDrive/Documents/GitHub/
 ↪Clinical_TLB_2023-2024/lung_cancer_tlb.xlsx")

# replace NA with control
df['CancerType'] = np.where(df['CancerType'].isna(), 'Control',␣
 ↪df['CancerType'])

# keep only Control and Adenocarcinoma for analysis
df_tree = df[(df['CancerType'] == 'Control') | (df['CancerType'] ==␣
 ↪'Adenocarcinoma')]
df_tree = df_tree.reset_index(drop=True)
```

[ ]:
```
# length of df
num_rows = df_tree.shape[0]

# number of bootstraps
total_bootstraps = 15

# create results df
hyperparameter_tuning_df = pd.DataFrame(columns=["max_depth", "max_features",␣
 ↪'min_leaves', "balanced_accuracy", 'auc'])
```

```
best_combination_df = pd.DataFrame(columns=["max_depth", "max_features",␣
 ↪'min_leaves', "balanced_accuracy", 'auc'])

# create array of all indices in full data set
all_indices = np.arange(num_rows)

# columns to drop
drop_cols = ['sample_id', 'pub_id', 'CancerType']

# loop to bootstrap and validate many times
for i in range(total_bootstraps):

    hyperparameter_tuning_df = pd.DataFrame(columns=["max_depth",␣
 ↪"max_features", 'min_leaves', "balanced_accuracy", 'auc'])

    # sample indices with replacement of df
    train_indices = np.random.choice(num_rows, num_rows, replace = True)
    # get the train set using the indices
    train_set = df_tree.iloc[train_indices, : ]
    # get the indices not selected
    test_indices = np.setdiff1d(all_indices, train_indices)
    # use not selected indices as the train set
    test_set = df_tree.iloc[test_indices, : ]

    for depth in range(1, 16):
        for features in range(1, 452, 5):
            for leaves in range(1,6):

                # initialize decision tree
                clf = tree.DecisionTreeClassifier(max_depth= depth,␣
 ↪max_features=features, min_samples_leaf= leaves)

                # train and test tree
                clf = clf.fit( train_set.drop(drop_cols, axis = 1),␣
 ↪train_set['CancerType'])
                test_predictions = clf.predict(test_set.drop(drop_cols, axis =␣
 ↪1))

                # calculate balanced accuracy
                balanced_acc = balanced_accuracy_score(test_set['CancerType'],␣
 ↪test_predictions)

                # get probabilities
                test_probabilities = clf.predict_proba(test_set.drop(drop_cols,␣
 ↪axis = 1))
```

```
                # test decision tree
                test_predictions = clf.predict(test_set.drop(drop_cols, axis =␣
↪1))

                # calculate weighted accuracy
                balanced_acc = balanced_accuracy_score(test_set['CancerType'],␣
↪test_predictions)

                # calculate AUC
                auc = roc_auc_score(test_set['CancerType'] == 'Control',␣
↪test_probabilities[:, 1])

                # append to results df
                hyperparameter_tuning_df.loc[len(hyperparameter_tuning_df)] =␣
↪[depth, features, leaves, balanced_acc, auc]


    best_combination_df = pd.concat([best_combination_df,␣
↪hyperparameter_tuning_df.sort_values('balanced_accuracy', ascending=False).
↪head(1)])
```

```
C:\Users\avery\AppData\Local\Temp\ipykernel_14236\1892828419.py:61:
FutureWarning: The behavior of DataFrame concatenation with empty or all-NA
entries is deprecated. In a future version, this will no longer exclude empty or
all-NA columns when determining the result dtypes. To retain the old behavior,
exclude the relevant entries before the concat operation.
  best_combination_df = pd.concat([best_combination_df,
hyperparameter_tuning_df.sort_values('balanced_accuracy',
ascending=False).head(1)])
```

[ ]:
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best_combination_df.sort_values('balanced_accuracy', ascending=False).head(5)

#best_combination_df.to_excel("BSCV_Results.xlsx")
```

[ ]:

	max_depth	max_features	min_leaves	balanced_accuracy	auc
6041	14.0	126.0	2.0	0.826087	0.806238
3650	9.0	11.0	1.0	0.824405	0.824405
3686	9.0	46.0	2.0	0.820513	0.850427
1377	4.0	11.0	3.0	0.814935	0.852814
4572	11.0	21.0	3.0	0.808421	0.810526

[ ]:
```
best_combination_df.sort_values('balanced_accuracy', ascending=False).head(1)

max_depth = int(best_combination_df.sort_values('balanced_accuracy',␣
↪ascending=False).iloc[0, 0])
max_features = int(best_combination_df.sort_values('balanced_accuracy',␣
↪ascending=False).iloc[0, 1])
```

```
min_leaves = int(best_combination_df.sort_values('balanced_accuracy',␣
 ↪ascending=False).iloc[0, 2])
print(max_depth, max_features, min_leaves)

clf = tree.DecisionTreeClassifier(max_depth= max_depth,␣
 ↪max_features=max_features, min_samples_leaf= min_leaves)

# train and test tree
clf = clf.fit( df_tree.drop(drop_cols, axis = 1), df_tree['CancerType'])

feature_importance1 = clf.feature_importances_

temps = df_tree.drop(['CancerType', 'sample_id', 'pub_id'], axis = 1).columns.
 ↪str.replace('T', '')
temps = temps.astype(float)
feature_importance = pd.DataFrame({"Temperature":temps, "Importance":␣
 ↪feature_importance1})
```

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14 126 2
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[ ]:
```
df_long = pd.melt(df_tree, id_vars=['sample_id', 'pub_id', 'CancerType'],␣
 ↪var_name='temp', value_name='dsp' )

median_df = thermogram_utilities.median_curve(df_long, 'CancerType', 'temp',␣
 ↪'dsp')

median_df['temperature'] = median_df['temperature'].str.replace('T', '').
 ↪astype(float)
```

[ ]:
```
# pivot variable importance df to long
plt.figure(figsize=(10, 6))

# create a bar plot
sns.scatterplot(data=feature_importance, x='Temperature', y='Importance')
p = sns.lineplot(data=median_df, x='temperature', y='median', hue='type',␣
 ↪palette='colorblind')

for index, row in feature_importance.iterrows():
    x_value = row['Temperature']
    y_value = row['Importance']

    # Add a vertical line from the point to the x-axis
    plt.plot([x_value, x_value], [0, y_value], color='gray', linestyle='--')


# add labels and title
plt.xlabel('Temperature')
```

```python
plt.ylabel('Importance')
plt.title('Temperature and Importance')
```

```
c:\Users\avery\AppData\Local\Programs\Python\Python310\lib\site-
packages\seaborn\_oldcore.py:1498: FutureWarning: is_categorical_dtype is
deprecated and will be removed in a future version. Use isinstance(dtype,
CategoricalDtype) instead
  if pd.api.types.is_categorical_dtype(vector):
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packages\seaborn\_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
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packages\seaborn\_oldcore.py:1119: FutureWarning: use_inf_as_na option is
deprecated and will be removed in a future version. Convert inf values to NaN
before operating instead.
  with pd.option_context('mode.use_inf_as_na', True):
```
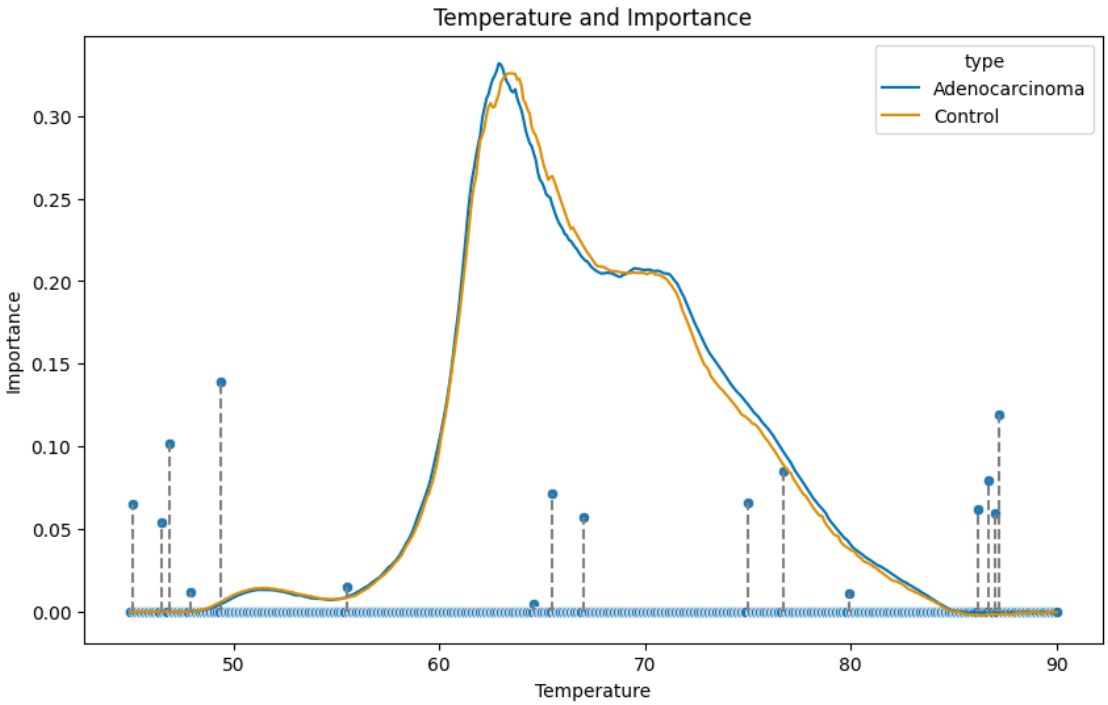

[ ]: Text(0.5, 1.0, 'Temperature and Importance')



[ ]:
```
df_tree.shape
```

[ ]: (123, 454)