week_8_sensitivity_analysis

October 23, 2023

[ ]:
```
import pandas as pd # standard
import numpy as np # standard
from sklearn.ensemble import RandomForestClassifier
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'])

# get location of cut off values
lower_column_index = df.columns.get_loc("T51")
upper_column_index = df.columns.get_loc("T83.1")
label_column_index = df.columns.get_loc("CancerType")

column_indices = np.arange(lower_column_index, upper_column_index)
column_indices = np.append(column_indices, 0)
column_indices = np.append(column_indices, 1)



column_indices = np.append(column_indices, label_column_index)

df = df.iloc[:, column_indices]
```

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

[ ]:
```
'''performance_metrics = pd.DataFrame(columns=['Weighted Accuracy', 'AUC',␣
 ↪'n_estimators', "max_depth", "max_features"])

# set number of bootstraps
total_bootstraps = 1000

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

# 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 for specified iterations
for i in range(total_bootstraps):

    # randomly select indices to use as train set
    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 indices not included in train_indices to use as test set
    test_indices = np.setdiff1d(all_indices, train_indices)

    # get test set using test indices
    test_set = df_tree.iloc[test_indices, :]

    for trees in [50, 100, 250, 500]:

        for depth in [round(num_rows/2), num_rows]:

            for features in ["sqrt", "log2", None]:


                # initialize random forest (default settings)
                clf = RandomForestClassifier(n_estimators=trees,␣
 ↪max_depth=depth, max_features=features, n_jobs= -1)
```

```
                # train forest
                clf = clf.fit(train_set.drop(drop_cols, axis = 1),␣
↪train_set['CancerType'])

                # 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 accuracy, auc to results df
                performance_metrics.loc[len(performance_metrics)] =␣
↪[balanced_acc, auc, trees, depth, features]

                performance_metrics.to_excel('sensitivity_analysis.xlsx',␣
↪index=False)

   print(i)'''
```

```
[ ]: 'performance_metrics = pd.DataFrame(columns=[\'Weighted Accuracy\', \'AUC\',
     \'n_estimators\', "max_depth", "max_features"])\n\n# set number of
     bootstraps\ntotal_bootstraps = 1000\n\n# length of df\nnum_rows =
     df_tree.shape[0]\n\n# create array of all indices in full data set\nall_indices
     = np.arange(num_rows)\n\n# columns to drop\ndrop_cols = [\'sample_id\',
     \'pub_id\', \'CancerType\']\n\n\n# loop for specified iterations\nfor i in
     range(total_bootstraps):\n    \n    # randomly select indices to use as train
     set\n    train_indices = np.random.choice(num_rows, num_rows, replace =
     True)\n\n    # get the train set using the indices\n    train_set =
     df_tree.iloc[train_indices, : ]\n\n    # get indices not included in
     train_indices to use as test set\n    test_indices = np.setdiff1d(all_indices,
     train_indices)\n\n    # get test set using test indices\n    test_set =
     df_tree.iloc[test_indices, :]\n\n    for trees in [50, 100, 250, 500]:\n
     \n        for depth in [round(num_rows/2), num_rows]:\n\n            for
     features in ["sqrt", "log2", None]:\n\n\n                # initialize random
     forest (default settings)\n                clf =
     RandomForestClassifier(n_estimators=trees, max_depth=depth,
```

```
max_features=features, n_jobs= -1)\n\n                # train forest\n
clf = clf.fit(train_set.drop(drop_cols, axis = 1),
train_set[\'CancerType\'])\n\n                # get probabilities\n
test_probabilities = clf.predict_proba(test_set.drop(drop_cols, axis = 1))\n\n
# test decision tree\n                test_predictions =
clf.predict(test_set.drop(drop_cols, axis = 1))\n\n                # calculate
weighted accuracy\n                balanced_acc =
balanced_accuracy_score(test_set[\'CancerType\'], test_predictions)\n\n
# calculate AUC\n                auc = roc_auc_score(test_set[\'CancerType\'] ==
\'Control\', test_probabilities[:, 1])\n\n                # append accuracy, auc
to results df\n                performance_metrics.loc[len(performance_metrics)]
= [balanced_acc, auc, trees, depth, features]\n\n
performance_metrics.to_excel(\'sensitivity_analysis.xlsx\', index=False)\n\n
print(i)'
```

[ ]:
```
sensitivity_analysis_df = pd.read_excel("sensitivity_analysis.xlsx")
```

[ ]:
```
boot_strap_number = np.repeat(np.arange(0, 1000), 24)
boot_strap_number = pd.Series(boot_strap_number)
result = pd.concat([boot_strap_number, sensitivity_analysis_df], axis=1)
result["max_features"] = result['max_features'].fillna('None')
```

We use sort_values() to sort the DataFrame by 'Value' in descending order. We then use groupby('Group') to group the sorted DataFrame by the 'Group' column. Finally, we use .head(1) to select the first row within each group, which corresponds to the row with the highest 'Value'.

[ ]:
```
hyper_parameter_combinations = result.sort_values(by='Weighted Accuracy',␣
↪ascending=False).groupby(0).head(1)

hyper_parameter_combinations
```

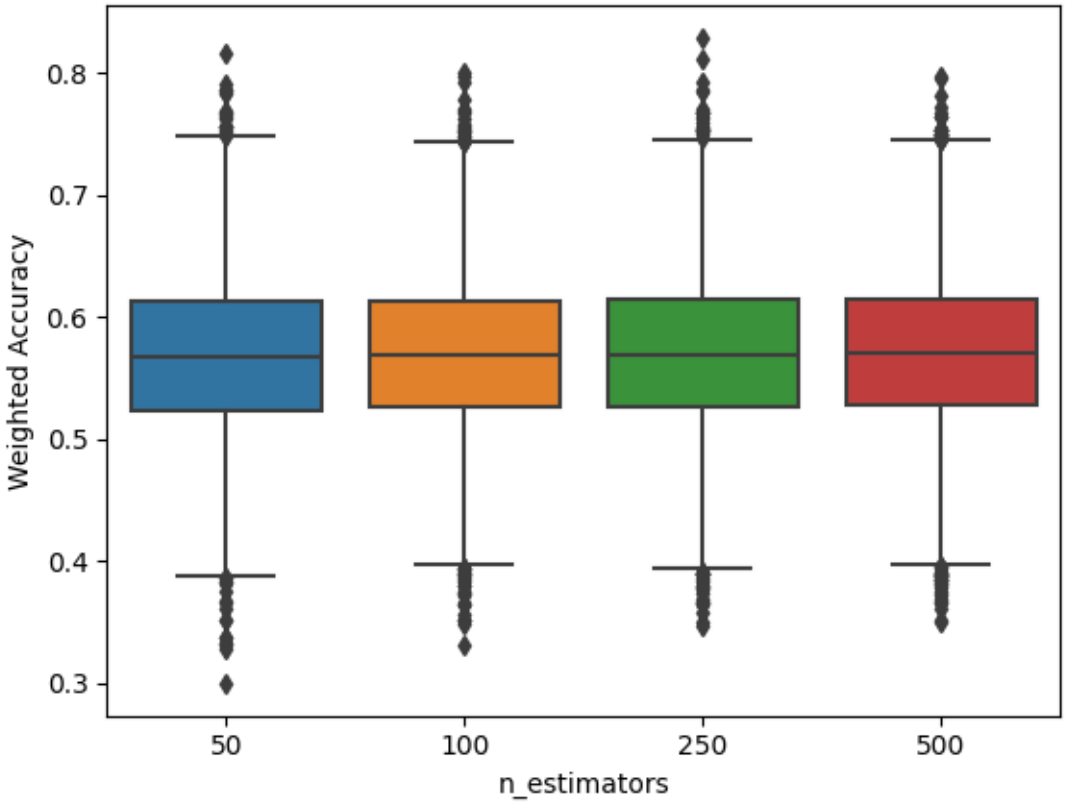
[ ]:

	0	Weighted Accuracy	AUC	n_estimators	max_depth	max_features
18495	770	0.829228	0.818555	250	123	sqrt
6888	287	0.815686	0.803922	50	62	sqrt
19377	807	0.800926	0.807870	100	123	sqrt
13340	555	0.798137	0.740683	500	62	None
20483	853	0.792735	0.727564	100	123	None
…	…	…	…	…	…	…
15727	655	0.476716	0.484069	100	62	log2
12723	530	0.453202	0.376847	50	123	sqrt
1178	49	0.452012	0.383127	50	62	None
17242	718	0.445701	0.418552	100	123	log2
23260	969	0.435185	0.420782	50	123	log2

[1000 rows x 6 columns]

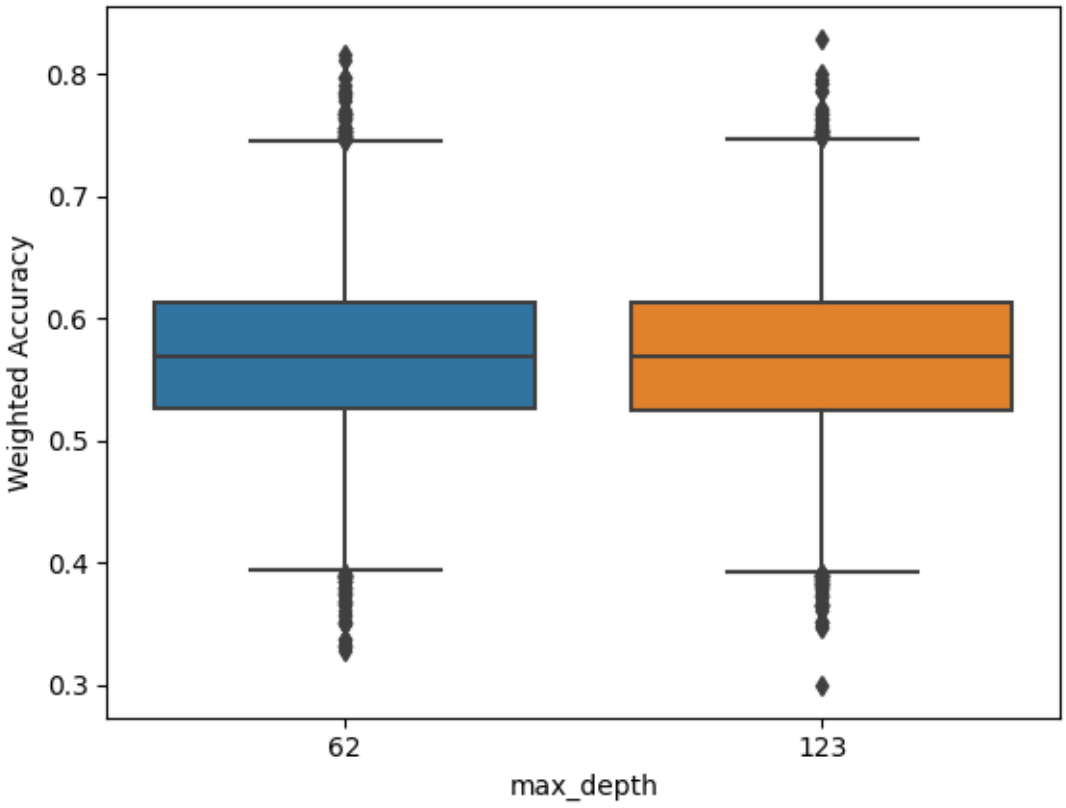
[ ]:
```
sns.boxplot(data=result, x='n_estimators', y='Weighted Accuracy')
```

[ ]: <Axes: xlabel='n_estimators', ylabel='Weighted Accuracy'>



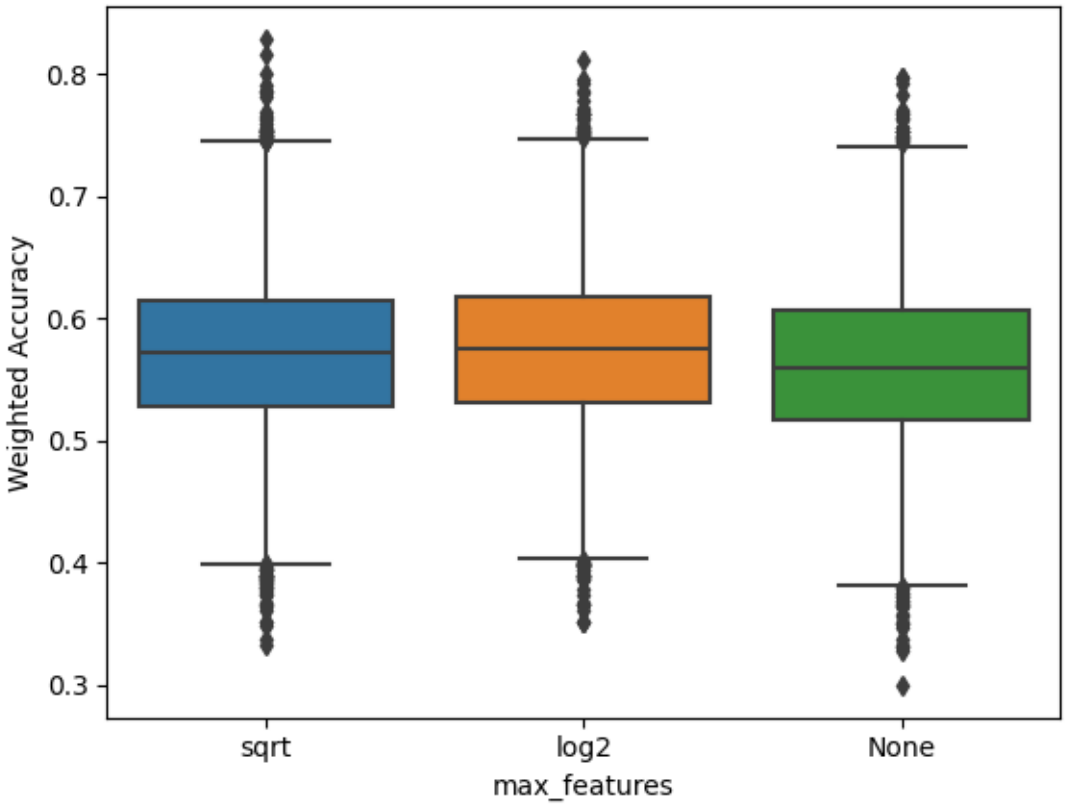
[ ]:
```
sns.boxplot(data=result, x='max_depth', y='Weighted Accuracy')
```

[ ]: <Axes: xlabel='max_depth', ylabel='Weighted Accuracy'>



[ ]:
```
sns.boxplot(data=result, x='max_features', y='Weighted Accuracy')
```

[ ]:
```
<Axes: xlabel='max_features', ylabel='Weighted Accuracy'>
```



[ ]:
```
hyper_parameter_combinations['n_estimators'].value_counts()
```

[ ]:
```
n_estimators
50     404
100    292
250    181
500    123
Name: count, dtype: int64
```