week_7_bootstrap_cv

October 16, 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)
```

Bootstrap Cross-Validation

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

# number of bootstraps
total_bootstraps = 500

# create results df
performance_metrics = pd.DataFrame(columns=['Weighted 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):

    # 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, : ]

    # train decision tree
    clf = tree.DecisionTreeClassifier()
    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]



'''
```

```
[ ]: "num_rows = df_tree.shape[0]\n\n# number of bootstraps\ntotal_bootstraps =
     500\n\n# create results df\nperformance_metrics =
     pd.DataFrame(columns=['Weighted Accuracy', 'AUC'])\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# loop to bootstrap
     and validate many times\nfor i in range(total_bootstraps):\n\n    # sample
     indices with replacement of df\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 the indices not
     selected\n    test_indices = np.setdiff1d(all_indices, train_indices)\n\n    #
     use not selected indices as the train set\n    test_set =
     df_tree.iloc[test_indices, : ]\n    \n    # train decision tree\n    clf =
     tree.DecisionTreeClassifier()\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]\n\n\n\n"
```

```
[ ]: 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})

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

     # number of bootstraps
     total_bootstraps = 100

     # create results df
     performance_metrics = pd.DataFrame(columns=['Weighted 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):

         # 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, : ]

    # train decision tree
    clf = tree.DecisionTreeClassifier()
    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]

    feature_importance_tree = clf.feature_importances_

    feature_importance[i] = feature_importance_tree
```

[ ]:

```
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)
```

[ ]:

```
feature_importance_long = pd.melt(feature_importance, id_vars=['Temperature'], var_name='Fold', value_name='Importance' )
feature_importance.iloc[:, 1:].mean(axis=1)

temps = temps.astype(float)
mean_feature_importance = pd.DataFrame({"Temperature":temps, "Mean Importance": feature_importance.iloc[:, 1:].mean(axis=1)
})
```

[ ]:

```
plt.figure(figsize=(10, 6))

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

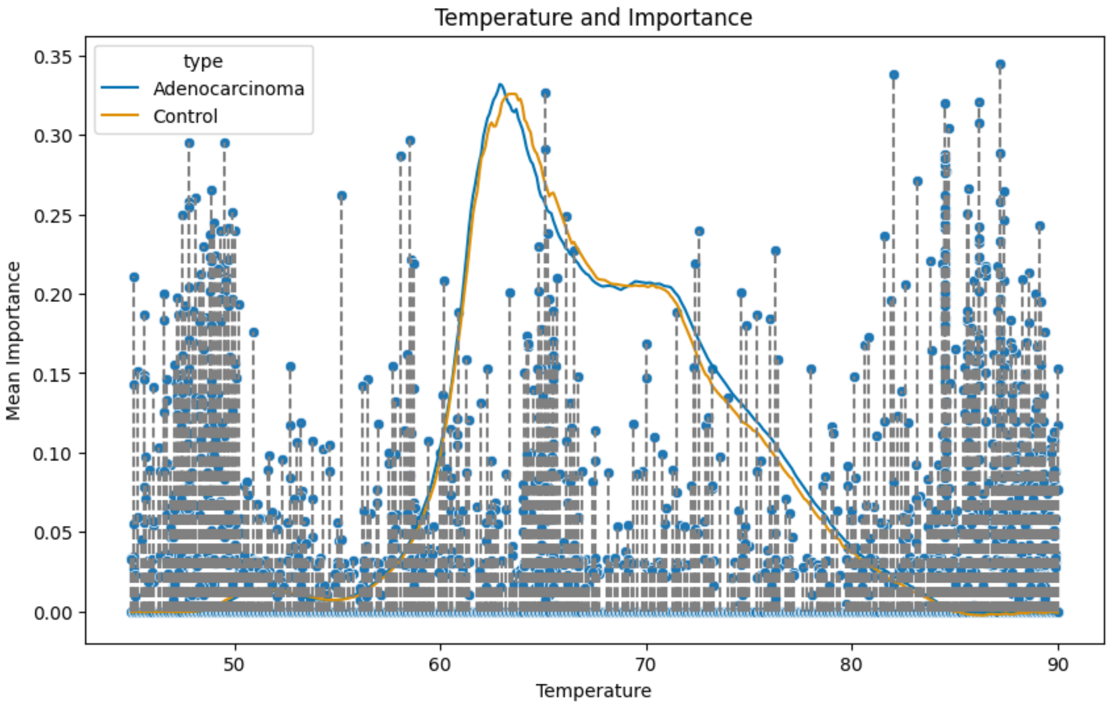
for index, row in feature_importance_long.iterrows():
    x_value = row['Temperature']
    y_value = row["Importance"]

    # 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')
plt.ylabel('Mean Importance')
plt.title('Temperature and Importance')
```

[ ]:

```
Text(0.5, 1.0, 'Temperature and Importance')
```



[ ]:

```
plt.figure(figsize=(10, 6))

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

for index, row in mean_feature_importance.iterrows():
    x_value = row['Temperature']
    y_value = row["Mean 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')
plt.ylabel('Mean Importance')
plt.title('Temperature and Importance')
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Text(0.5, 1.0, 'Temperature and Importance')
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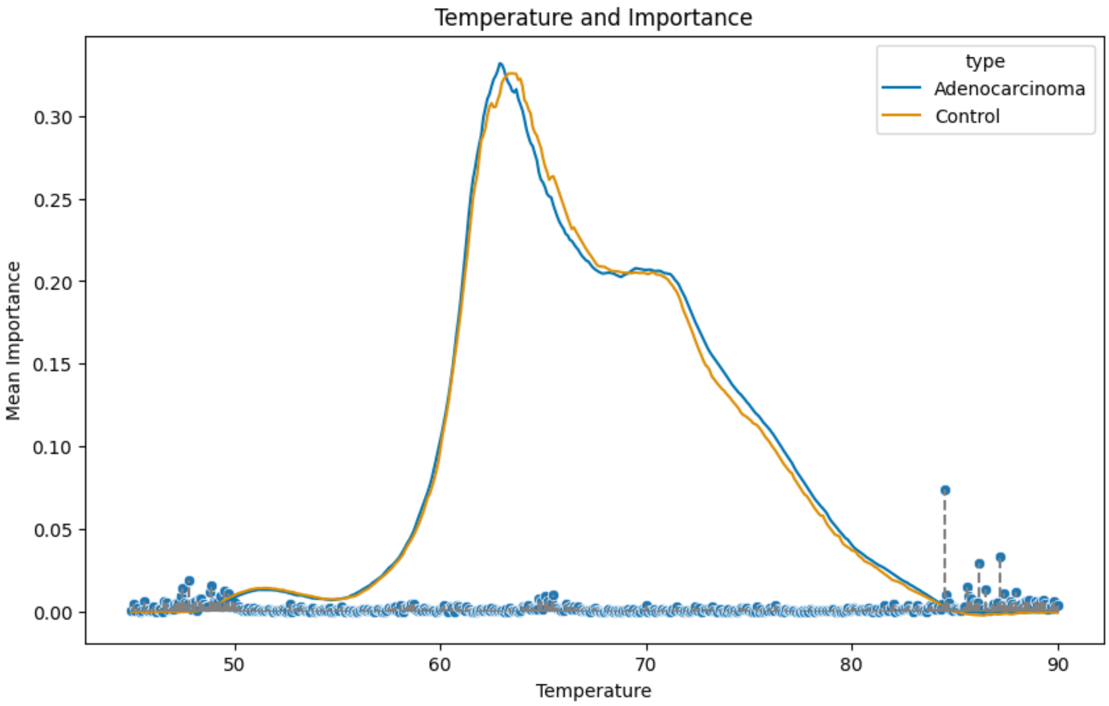
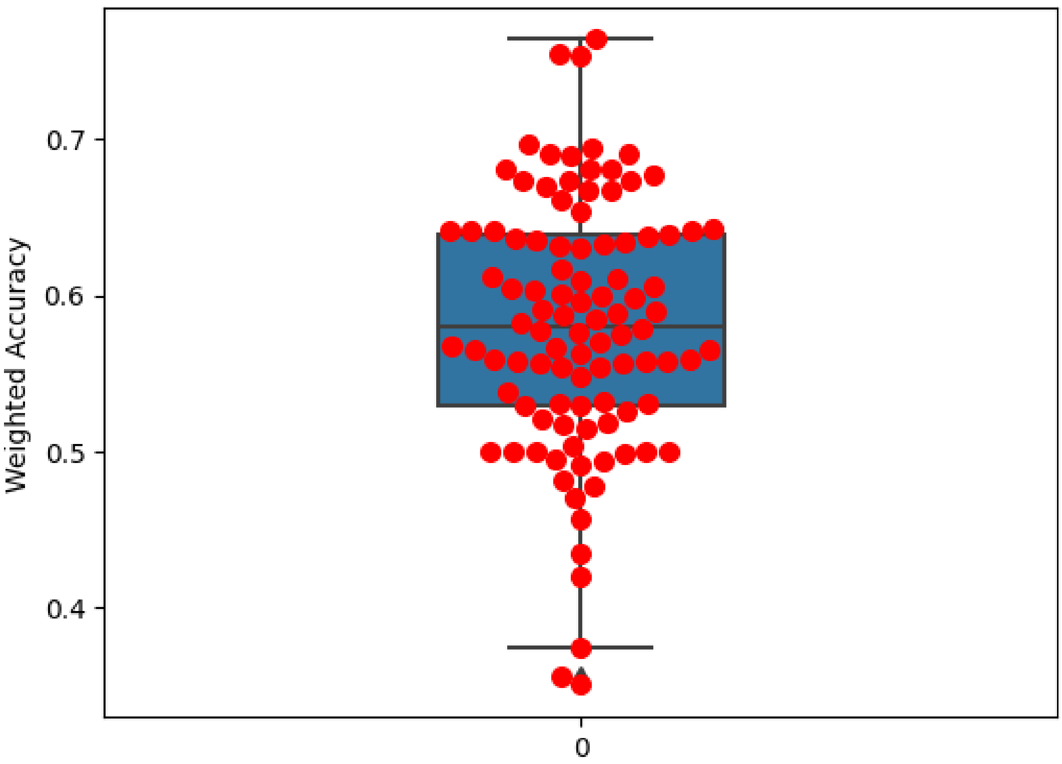


```
[ ]: sns.boxplot(data=performance_metrics['Weighted Accuracy'], width=0.3)

     # Add points to the boxplot using the swarmplot function
     sns.swarmplot(data=performance_metrics['Weighted Accuracy'], color='red',␣
      ↪size=8)
```

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


Weighted Accuracy
0.7
0.6
0.5
0.4
0