week_8_differencing_2

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'])

     # get location of cut off values
     lower_column_index = df.columns.get_loc("T50")
     upper_column_index = df.columns.get_loc("T85.1")
     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)
```

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[ ]: df_tree_dif1 = df_tree.select_dtypes(include=['number']).diff(axis = 1)
     non_numeric_columns = df_tree.select_dtypes(exclude=['number'])
     df_tree_dif1 = pd.concat( [df_tree_dif1, non_numeric_columns], axis=1)
     df_tree_dif1 = df_tree_dif1.iloc[:, 1:]
```

```
[ ]: df_long = pd.melt(df_tree_dif1, id_vars=['sample_id', 'pub_id', 'CancerType'],␣
      ↪var_name='temp', value_name='dsp' )
     df_long['temp'] = df_long['temp'].str.replace('T', '').astype(float)


     g = sns.FacetGrid(df_long, col="CancerType", col_wrap= 3, hue="sample_id",␣
      ↪palette = 'colorblind')
     g.map_dataframe(sns.lineplot, x="temp", y="dsp")
     g.set_axis_labels("Temperature (C)", "Specific Excess Heat Capacity")
     g.set_titles(col_template="{col_name}")
```

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[ ]: <seaborn.axisgrid.FacetGrid at 0x247aed0fd60>
```
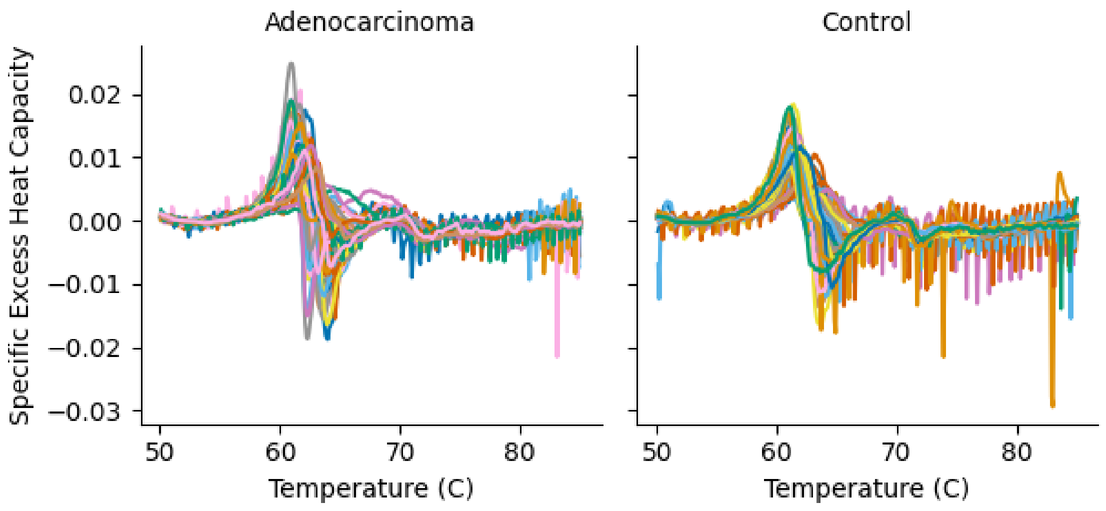
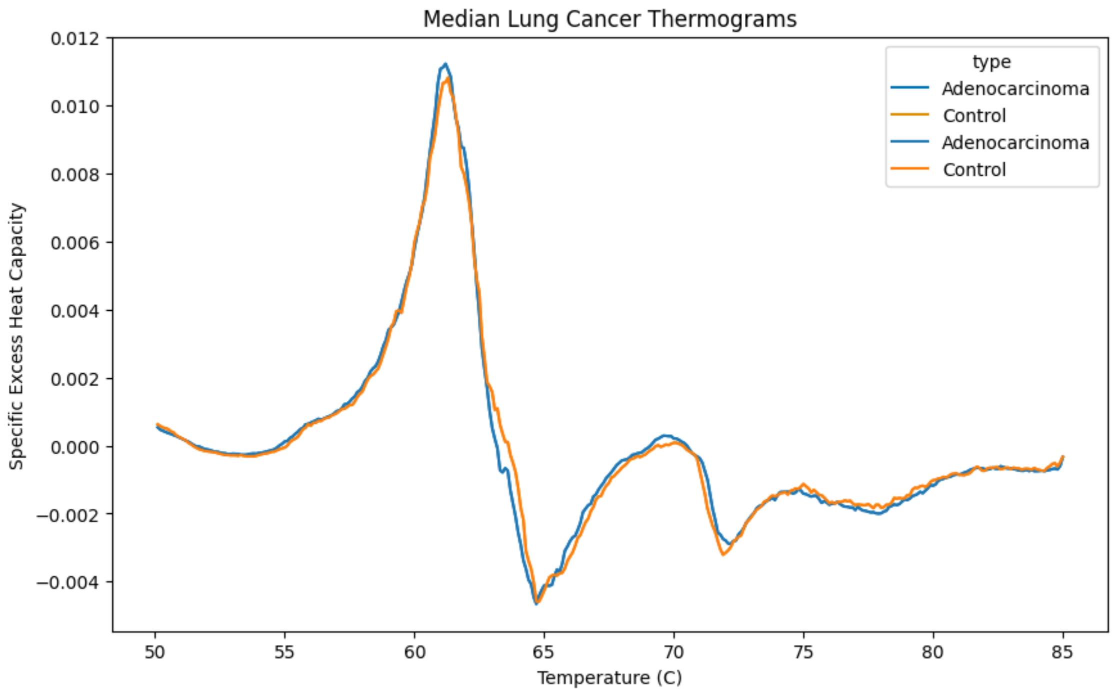



```
[ ]: median_difference = thermogram_utilities.median_curve(df_long,␣
      ↪"CancerType",'temp', 'dsp')

     plt.figure(figsize=(10, 6))  # Adjust the figure size if needed
     sns.lineplot(data=median_difference, x='temperature', y='median', hue='type',␣
      ↪palette='colorblind')
```

```
ax = plt.gca()

# Plot the lines with different colors for 'type'
sns.lineplot(data=median_difference, x='temperature', y='median', hue='type')

# Add ribbons for each 'type' with different colors
'''for _, row in median_df.iterrows():
    ax.fill_between([row['temperature']], row['lower_q'], row['upper_q'],␣
 ↪alpha=0.3, color='grey')'''

plt.xlabel('Temperature (C)')
plt.ylabel('Specific Excess Heat Capacity')
plt.title('Median Lung Cancer Thermograms')
```

```
[ ]: Text(0.5, 1.0, 'Median Lung Cancer Thermograms')
```

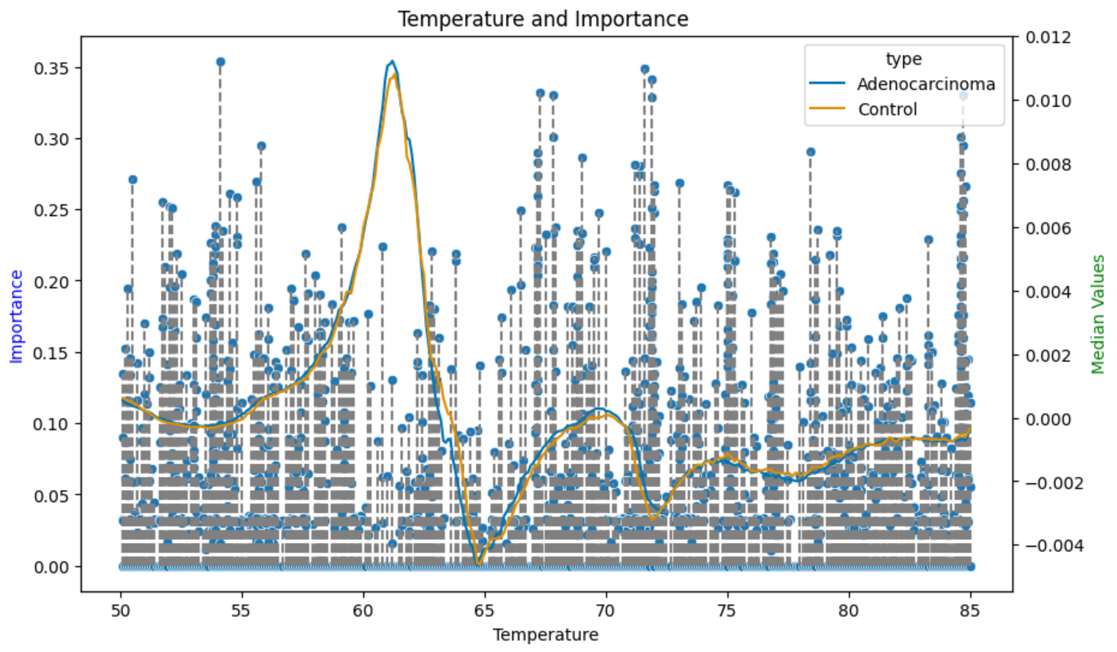


```
[ ]: temps = df_tree_dif1.drop(['CancerType', 'sample_id', 'pub_id'], axis = 1).
      ↪columns.str.replace('T', '')
     temps = temps.astype(float)
     feature_importance = pd.DataFrame({"Temperature":temps})

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

```python
# 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_dif1.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_dif1.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
```

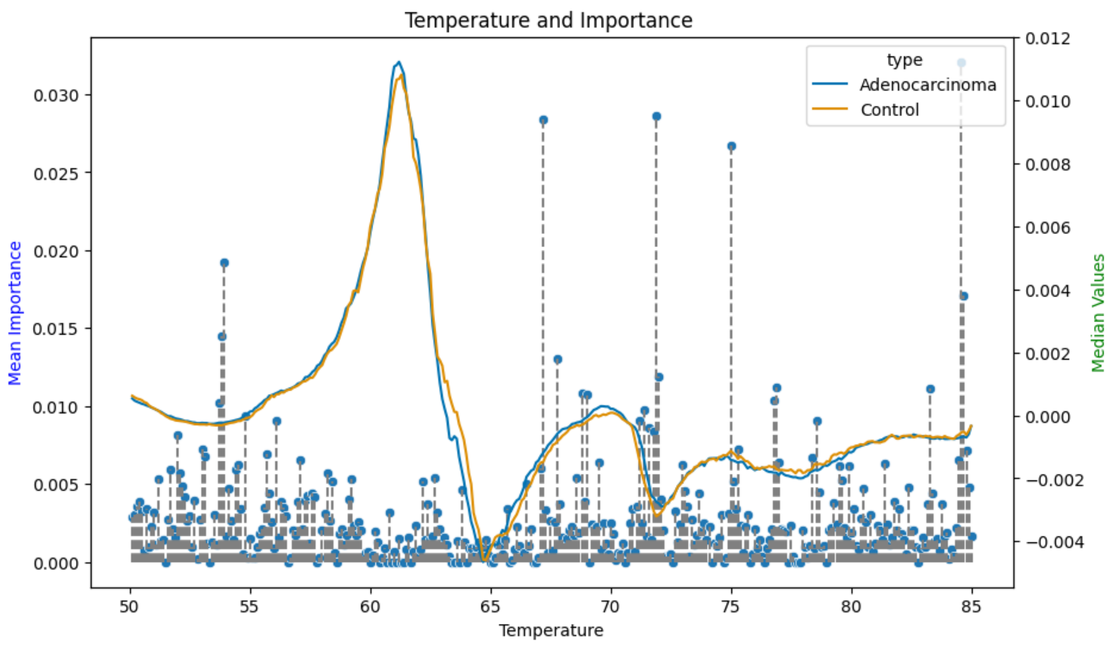
```
[ ]: feature_importance_long = pd.melt(feature_importance, id_vars=['Temperature'],␣
     ↪var_name='Fold', value_name='Importance' )
     feature_importance.iloc[:, 1:].mean(axis=1)

     temps = temps.astype(float)
     mean_feature_importance = pd.DataFrame({"Temperature":temps, "Mean Importance":␣
     ↪feature_importance.iloc[:, 1:].mean(axis=1)
     })
     # Create a figure with a specific size
     plt.figure(figsize=(10, 6))

     # Create a bar plot for "Importance"
     ax1 = sns.scatterplot(data=feature_importance_long, x='Temperature',␣
     ↪y='Importance')

     # Create a secondary y-axis
     ax2 = ax1.twinx()

     # Create a line plot for "Median" on the secondary y-axis
     #sns.lineplot(data=median_difference, x='temperature', y='median', hue='type',␣
     ↪palette='colorblind', ax=ax2)

     # Add vertical lines from the points to the x-axis for the bar plot
     for index, row in feature_importance_long.iterrows():
         x_value = row['Temperature']
         y_value = row['Importance']
         ax1.plot([x_value, x_value], [0, y_value], color='gray', linestyle='--')


     sns.lineplot(data=median_difference, x='temperature', y='median', hue='type',␣
     ↪palette='colorblind', ax=ax2)

     # Set labels for both y-axes
     ax1.set_ylabel('Importance', color='blue')
     ax2.set_ylabel('Median Values', color='green')

     # Add a legend
     #lines, labels = ax1.get_legend_handles_labels()
     #lines2, labels2 = ax2.get_legend_handles_labels()
     #ax1.legend(lines + lines2, labels + labels2, loc='upper left')

     # Add labels and title
```

```
plt.xlabel('Temperature')
plt.title('Temperature and Importance ')

# Show the plot
plt.show()
```



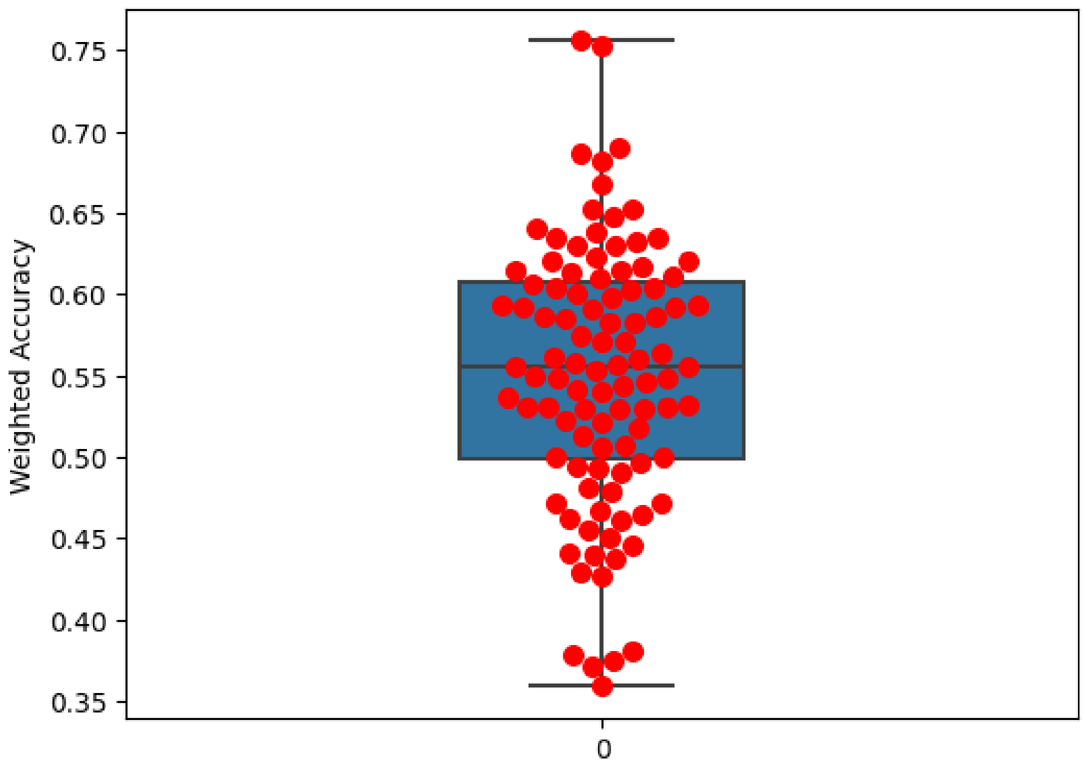
[ ]:
```
feature_importance_long = pd.melt(feature_importance, id_vars=['Temperature'],␣
 ↪var_name='Fold', value_name='Importance' )
feature_importance.iloc[:, 1:].mean(axis=1)

temps = temps.astype(float)
mean_feature_importance = pd.DataFrame({"Temperature":temps, "Mean Importance":␣
 ↪feature_importance.iloc[:, 1:].mean(axis=1)
})
# Create a figure with a specific size
plt.figure(figsize=(10, 6))

# Create a bar plot for "Importance"
ax1 = sns.scatterplot(data=mean_feature_importance, x='Temperature', y='Mean␣
 ↪Importance')

# Create a secondary y-axis
ax2 = ax1.twinx()

# Create a line plot for "Median" on the secondary y-axis
```

```
#sns.lineplot(data=median_difference, x='temperature', y='median', hue='type',␣
↪palette='colorblind', ax=ax2)

# Add vertical lines from the points to the x-axis for the bar plot
for index, row in mean_feature_importance.iterrows():
    x_value = row['Temperature']
    y_value = row['Mean Importance']
    ax1.plot([x_value, x_value], [0, y_value], color='gray', linestyle='--')


sns.lineplot(data=median_difference, x='temperature', y='median', hue='type',␣
↪palette='colorblind', ax=ax2)

# Set labels for both y-axes
ax1.set_ylabel('Mean Importance', color='blue')
ax2.set_ylabel('Median Values', color='green')

# Add a legend
#lines, labels = ax1.get_legend_handles_labels()
#lines2, labels2 = ax2.get_legend_handles_labels()
#ax1.legend(lines + lines2, labels + labels2, loc='upper left')

# Add labels and title
plt.xlabel('Temperature')
plt.title('Temperature and Importance ')

# Show the plot
plt.show()
```



```
[ ]: 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