week_8_differencing

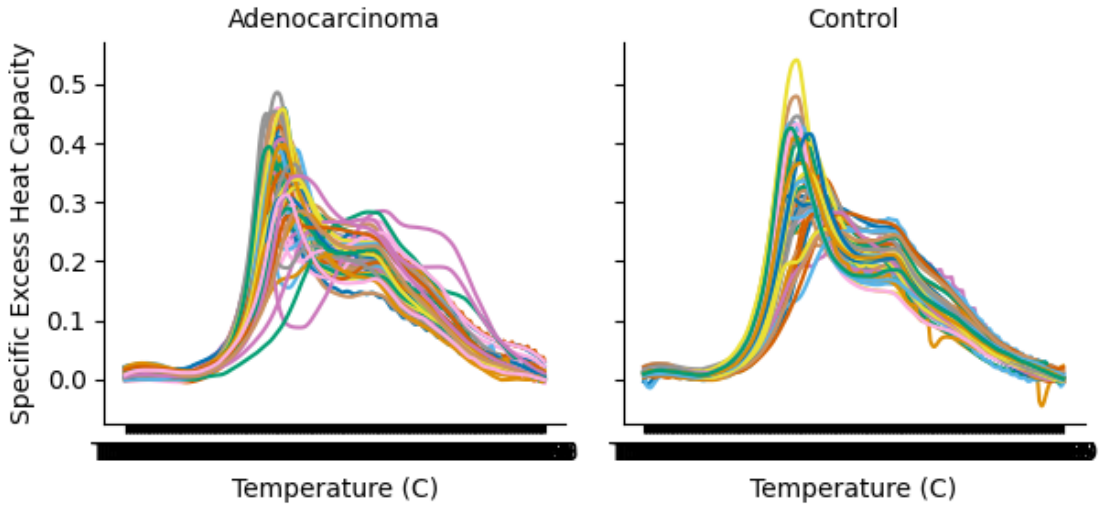
October 16, 2023

[ ]:
```
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)
```

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

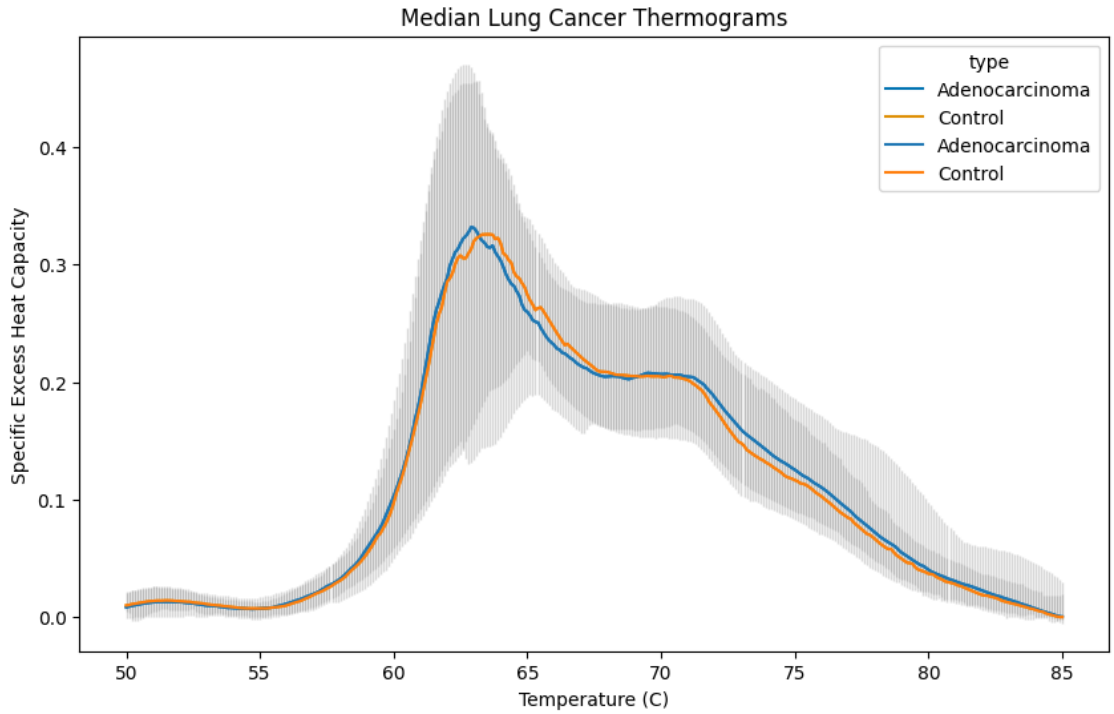
[ ]:
```
<seaborn.axisgrid.FacetGrid at 0x1c92521f9d0>
```



[ ]:
```
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)

plt.figure(figsize=(10, 6))  # Adjust the figure size if needed
```

```
sns.lineplot(data=median_df, x='temperature', y='median', hue='type',␣
 ↪palette='colorblind')
ax = plt.gca()

# Plot the lines with different colors for 'type'
sns.lineplot(data=median_df, 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')
```

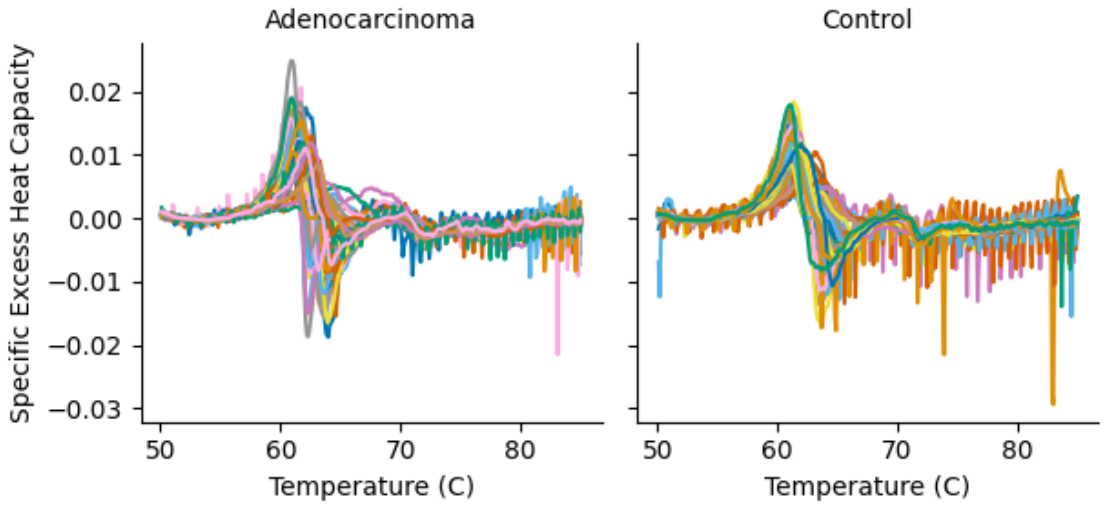
[ ]:
```
Text(0.5, 1.0, 'Median Lung Cancer Thermograms')
```



[ ]:
```
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}")
```

[ ]:
```
<seaborn.axisgrid.FacetGrid at 0x1c95c063130>
```



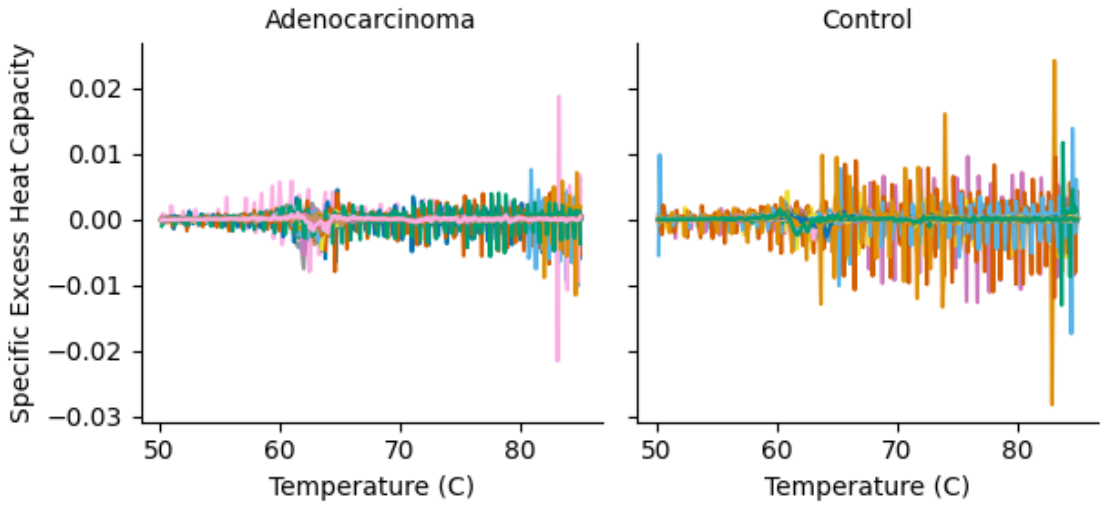
[ ]:
```
df_tree_dif1 = df_tree.select_dtypes(include=['number']).diff(axis = 1)
df_tree_dif2 = df_tree_dif1.diff(axis = 1)
non_numeric_columns = df_tree.select_dtypes(exclude=['number'])
df_tree_dif2 = pd.concat( [df_tree_dif2, non_numeric_columns], axis=1)
df_tree_dif2 = df_tree_dif2.iloc[:, 2:]

#df_tree_dif2
```

[ ]:
```
             T50.2    T50.3    T50.4    T50.5    T50.6    T50.7    T50.8  \
0   -2.200000e-04 -0.00002  0.00025  0.00032 -0.00035 -0.00017 -0.00031
1   -1.400000e-04  0.00023  0.00005 -0.00052  0.00034 -0.00021 -0.00002
2   -2.600000e-04  0.00006 -0.00021  0.00003  0.00006 -0.00019  0.00007
3    1.700000e-04  0.00028 -0.00038 -0.00007 -0.00017 -0.00047  0.00024
4   -1.000000e-04 -0.00061 -0.00040  0.00054  0.00023 -0.00039  0.00016
..            …        …        …        …        …        …        …
118  1.600000e-04 -0.00016 -0.00021 -0.00001 -0.00017 -0.00009 -0.00006
```

```
119  1.000000e-05  0.00010  0.00001 -0.00003 -0.00007 -0.00002 -0.00006
120 -1.000000e-05  0.00002 -0.00010 -0.00010 -0.00006 -0.00003  0.00002
121  2.900000e-04 -0.00045 -0.00034 -0.00020 -0.00008 -0.00011 -0.00001
122  1.734723e-18 -0.00005 -0.00007 -0.00004 -0.00004 -0.00004 -0.00001

       T50.9           T51    T51.1  …     T84.4         T84.5  \
0    0.00012 -1.400000e-04 -0.00032  …  0.000080  2.100000e-04
1   -0.00020  1.400000e-04 -0.00020  … -0.000070  6.000000e-05
2   -0.00040 -8.000000e-05 -0.00014  … -0.000062  1.090000e-04
3   -0.00018  1.100000e-04  0.00019  … -0.000740  3.800000e-04
4   -0.00026 -4.100000e-04  0.00010  … -0.000670 -5.400000e-04
..       …           …      …  …       …            …
118 -0.00006 -4.000000e-05 -0.00009  …  0.000140  4.336809e-19
119 -0.00001 -6.000000e-05 -0.00008  …  0.000080  7.000000e-05
120 -0.00008 -1.000000e-04 -0.00009  …  0.000150  1.500000e-04
121 -0.00011 -1.734723e-18  0.00006  … -0.000080 -1.300000e-04
122 -0.00009 -1.200000e-04 -0.00004  …  0.000160  1.600000e-04

            T84.6     T84.7     T84.8         T84.9       T85  sample_id  \
0   -6.100000e-05  0.000269  0.000072  6.280000e-04  0.000193     C67801
1    1.300000e-04  0.000220  0.000259  6.000000e-05  0.000573     C67901
2   -4.220000e-04  0.000920  0.000580 -4.336809e-19  0.000050     C55701
3   -2.600000e-04  0.000180  0.000480 -3.000000e-04  0.000460     C67201
4    1.381000e-03  0.001220  0.000022  2.713000e-04  0.000096     L15701
..            …       …       …           …       …        …
118  1.700000e-04  0.000050  0.000330  1.550000e-04  0.000556         44
119  5.000000e-05  0.000200  0.000089  1.050000e-04  0.000501         45
120  1.700000e-04  0.000000 -0.000150 -5.000000e-05  0.000090         46
121 -8.673617e-19  0.000190  0.000080  5.000000e-05  0.000150         47
122  3.000000e-05 -0.000160  0.000020  2.000000e-05 -0.000090         48

     pub_id      CancerType
0       L14  Adenocarcinoma
1       L15  Adenocarcinoma
2        L4  Adenocarcinoma
3       L13  Adenocarcinoma
4       L83  Adenocarcinoma
..      …              …
118     C39         Control
119     C40         Control
120     C41         Control
121     C42         Control
122     C43         Control

[123 rows x 352 columns]
```

[ ]:
```
df_long = pd.melt(df_tree_dif2, 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}")
```

[ ]:
```
<seaborn.axisgrid.FacetGrid at 0x1c95ef2bbe0>
```



[ ]:
```
df_tree_dif1 = df_tree.select_dtypes(include=['number']).diff(axis = 1)
df_tree_dif2 = df_tree_dif1.diff(axis = 1)
df_tree_dif3 = df_tree_dif2.diff(axis = 1)
non_numeric_columns = df_tree.select_dtypes(exclude=['number'])
df_tree_dif3 = pd.concat( [df_tree_dif3, non_numeric_columns], axis=1)
df_tree_dif3 = df_tree_dif3.iloc[:, 3:]

#df_tree_dif3
```

[ ]:

	T50.3	T50.4	T50.5	T50.6	T50.7	T50.8	\
0	0.00020	0.00027	7.000000e-05	-6.700000e-04	1.800000e-04	-0.00014	
1	0.00037	-0.00018	-5.700000e-04	8.600000e-04	-5.500000e-04	0.00019	
2	0.00032	-0.00027	2.400000e-04	3.000000e-05	-2.500000e-04	0.00026	
3	0.00011	-0.00066	3.100000e-04	-1.000000e-04	-3.000000e-04	0.00071	
4	-0.00051	0.00021	9.400000e-04	-3.100000e-04	-6.200000e-04	0.00055	
..	…	…	…	…	…	…	

```
118 -0.00032 -0.00005  2.000000e-04 -1.600000e-04  8.000000e-05  0.00003
119  0.00009 -0.00009 -4.000000e-05 -4.000000e-05  5.000000e-05 -0.00004
120  0.00003 -0.00012 -1.734723e-18  4.000000e-05  3.000000e-05  0.00005
121 -0.00074  0.00011  1.400000e-04  1.200000e-04 -3.000000e-05  0.00010
122 -0.00005 -0.00002  3.000000e-05 -1.734723e-18 -1.734723e-18  0.00003

            T50.9      T51    T51.1    T51.2  …     T84.4         T84.5  \
0    4.300000e-04 -0.00026 -0.00018  0.00003  …  0.000910  1.300000e-04
1   -1.800000e-04  0.00034 -0.00034  0.00057  …  0.000440  1.300000e-04
2   -4.700000e-04  0.00032 -0.00006  0.00075  … -0.000177  1.710000e-04
3   -4.200000e-04  0.00029  0.00008 -0.00033  … -0.001170  1.120000e-03
4   -4.200000e-04 -0.00015  0.00051  0.00020  … -0.000220  1.300000e-04
..            …      …       …       …  …       …            …
118  1.734723e-18  0.00002 -0.00005  0.00002  …  0.000290 -1.400000e-04
119  5.000000e-05 -0.00005 -0.00002  0.00004  …  0.000100 -1.000000e-05
120 -1.000000e-04 -0.00002  0.00001  0.00002  …  0.000190  8.673617e-19
121 -1.000000e-04  0.00011  0.00006 -0.00004  … -0.000030 -5.000000e-05
122 -8.000000e-05 -0.00003  0.00008 -0.00008  …  0.000080  0.000000e+00

        T84.6     T84.7     T84.8         T84.9       T85  sample_id  pub_id  \
0   -0.000271  0.000330 -0.000197  5.560000e-04 -0.000435     C67801     L14
1    0.000070  0.000090  0.000039 -1.990000e-04  0.000513     C67901     L15
2   -0.000531  0.001342 -0.000340 -5.800000e-04  0.000050     C55701      L4
3   -0.000640  0.000440  0.000300 -7.800000e-04  0.000760     C67201     L13
4    0.001921 -0.000161 -0.001199  2.497000e-04 -0.000176     L15701     L83
..        …       …         …            …         …          …
118  0.000170 -0.000120  0.000280 -1.750000e-04  0.000401         44     C39
119 -0.000020  0.000150 -0.000111  1.600000e-05  0.000396         45     C40
120  0.000020 -0.000170 -0.000150  1.000000e-04  0.000140         46     C41
121  0.000130  0.000190 -0.000110 -3.000000e-05  0.000100         47     C42
122 -0.000130 -0.000190  0.000180 -4.336809e-19 -0.000110         48     C43

         CancerType
0    Adenocarcinoma
1    Adenocarcinoma
2    Adenocarcinoma
3    Adenocarcinoma
4    Adenocarcinoma
..              …
118         Control
119         Control
120         Control
121         Control
122         Control

[123 rows x 351 columns]
```

[ ]:
```
df_long = pd.melt(df_tree_dif3, 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}")
```

[ ]:
```
<seaborn.axisgrid.FacetGrid at 0x1c95f0e06d0>
```