Phthalates and Plasticizers Metabolites - Urine in file PHTHTE_J

April 13, 2023

0.0.1 Phthalates and Plasticizers Metabolites - Urine in file PHTHTE J

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Gets rid of all rows that contain NA values and outputs the cleaned data to "Clean PHTHTE_J.xlsx"

[11]:
```
import os
import numpy as np
import pandas as pd
from scipy import stats
import seaborn as sns
import statsmodels.api as sm
import matplotlib.pyplot as plt
%matplotlib inline

result_dir = '~/Environmental Health Project - Part 2/result'
data_dir = '~/Environmental Health Project - Part 2/data'
in_file_name = 'PHTHTE_J.xlsx'
out_file_name = 'Clean PHTHTE_J.xlsx'

in_file_full_name = os.path.join(data_dir, in_file_name)
out_file_full_name = os.path.join(result_dir, out_file_name)

data_in = pd.read_excel(in_file_full_name)
data = data_in.drop(['Unnamed: 0'], axis = 1)
data_no_na = data.dropna()
data_no_na.to_excel(out_file_full_name)
```

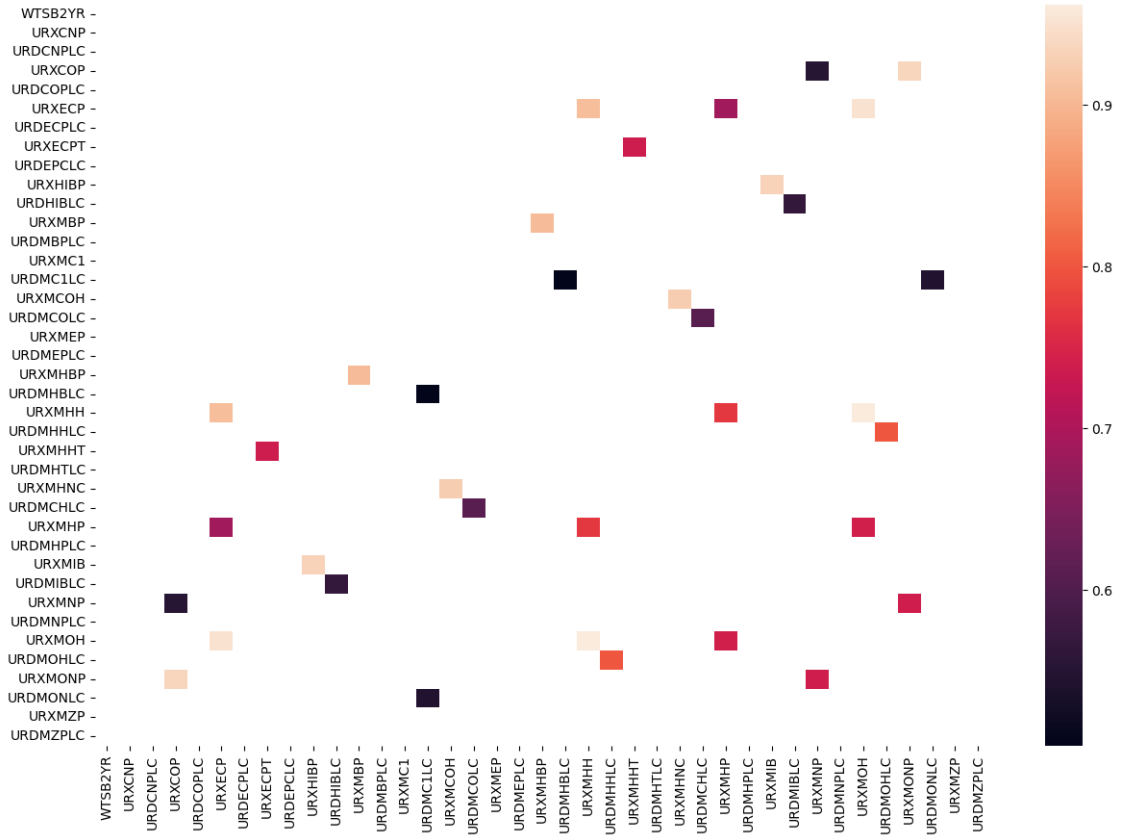
```
C:\Users\kecoc\anaconda3\lib\site-packages\openpyxl\styles\stylesheet.py:226:
UserWarning: Workbook contains no default style, apply openpyxl's default
  warn("Workbook contains no default style, apply openpyxl's default")
```

Computes the pearson correlation coefficient between every pair of variables and exports coefficients that are greater than 0.5 and less than 0.999 to a CSV file

[14]:
```
in_file_name = 'Clean PHTHTE_J.xlsx'
out_file_name = "PHTHTE_J_J_Filtered_Pearson_Correlation_Coefficient.csv"
```

```
in_file_full_name = os.path.join(result_dir, in_file_name)
out_file_full_name = os.path.join(result_dir, out_file_name)

data_in = pd.read_excel(in_file_full_name)
data = data_in.drop(['Unnamed: 0', 'SEQN'], axis = 1) #Drops the index column␣
 ↪and the seqn label column.

column_points = data.columns #Gets the labels for the final data frame
length = len(column_points) #Gets the amount of labels of the dataframe for the␣
 ↪column and index so the final dataframe can be shaped correctly
values = [] #Creates an empty list that the pearson correlation coefficients␣
 ↪will be stored in

for h in column_points: #Calculates the pearson correlation coefficient for␣
 ↪every pair of columns
    for k in column_points:
        res = stats.pearsonr(data[h], data[k])
        values.append(res.statistic) #Stores the pearson correlation␣
 ↪coefficient for each pair of columns in the values list

reshaped_values = np.array(values).reshape(length,length) #Creates a reshaped␣
 ↪numpy array using the values list
matrix = pd.DataFrame(reshaped_values, index = column_points, columns =␣
 ↪column_points) #Creates a dataframe of the pearson correlation coefficient␣
 ↪with the variables as the index and column
filtered_matrix = matrix[(matrix > 0.50) & (matrix < 0.999)] #Filters the␣
 ↪matrix to only show the values greater than 0.50 and less than 0.999

plt.figure(figsize=(15,10))
print("Heatmap of the filtered pearson correlation coefficient values")
print(sns.heatmap(filtered_matrix)) #Creates a heatmap of the filtered values
filtered_matrix.to_csv(out_file_full_name) #Outputs the filtered matrix to a␣
 ↪csv file
```

```
Heatmap of the filtered pearson correlation coefficient values
AxesSubplot(0.125,0.11;0.62x0.77)
```

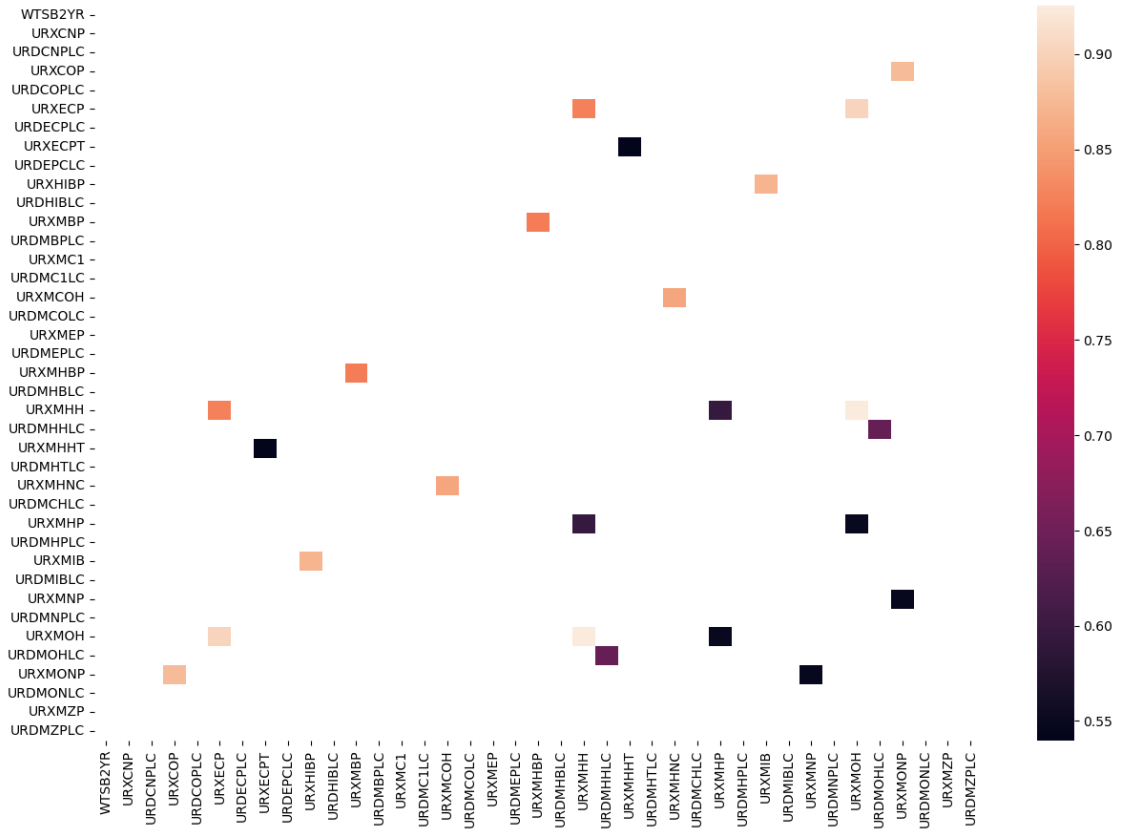


Computes the p-values for the F statistic as well as the R^2 values for each pair of variables and exports the R2 values that are greater than 0.5 and less than 0.999 to a CSV file

[16]:
```
out_file_name = "PHTHTE_J_J_Filtered_R^2_values.csv"
out_file_full_name = os.path.join(result_dir, out_file_name)

P_values = [] #Creates an empty list that the P-values of the F statistic will␣
 ↪be stored in
R_squared_values = [] #Creates an empty list that the R^2 values will be stored␣
 ↪in

for h in column_points: #Calculates the pvalue of the f-statistic and r^2 value␣
 ↪for each pair of variables
    for k in column_points:
        X2 = sm.add_constant(data[h])
        est = sm.OLS(data[k],X2)
        est2 = est.fit()
        P_values.append(est2.f_pvalue) #Appends the pvalue of the f-statistic␣
 ↪to the p_values list
```

```
        R_squared_values.append(est2.rsquared) #Appends the r^2 value to the␣
 ↪R_squared_values list

reshaped_p_values = np.array(P_values).reshape(length,length) #Reshapes the␣
 ↪P_value list into a numpy array of the correct shape
p_value_matrix = pd.DataFrame(reshaped_p_values, index = column_points, columns␣
 ↪= column_points) #Creates a dataframe of the P_values array with the␣
 ↪variable names as the columns and indexs

reshaped_R_squared_values = np.array(R_squared_values).reshape(length,length)␣
 ↪#Reshapes the R_squared_values list into a numpy array of the correct shape
R_squared_values_matrix = pd.DataFrame(reshaped_R_squared_values, index =␣
 ↪column_points, columns = column_points) #Creates a dataframe of the␣
 ↪R_squared_values array with the variable names as the columns and indexs

filtered_matrix = R_squared_values_matrix[(R_squared_values_matrix > 0.50) &␣
 ↪(R_squared_values_matrix < 0.999)] #Filters the R_squared_values matrix to␣
 ↪only show values greater than 0.50 and less than 0.999

plt.figure(figsize=(15,10))
print("HeatMap of filtered R^2 values")
print(sns.heatmap(filtered_matrix))
filtered_matrix.to_csv(out_file_full_name) #Outputs the filtered matrix to a␣
 ↪csv file
```

```
HeatMap of filtered R^2 values
AxesSubplot(0.125,0.11;0.62x0.77)
```



The data indicates that there are multiple positively correlated relationships between variables in the PHTHTE_J file. The highly correlated pairs of variables are:

URXMONP:URXCOP - PCR value - 0.93684

URXMHH:URXECP - PCR value - 0.90760

URXMOH:URXECP - PCR value - 0.94982

URXMIB:URXHIBP - PCR value- 0.87054

URDMEPLC:URXMBP - PCR value- 0.82099

URXMHNC:URXMCOH - PCR value- 0.85714

URXMBP:URXMHBP - PCR value- 0.82099

URXMOH:URXMHH - PCR value- 0.92554

The highest value belongs to URXMOH and URXMHH, URXMOH is MEOH phthalate and URXMHH is MHHT phthalate. This makes sense as the structure for URXMOH is Mono-(2-ethyl-5-oxohexyl) phthalate and the structure for URXMHH is Mono-(2-ethyl-5-hydroxyhexyl) phthalate. These are two very similar structures. The other highly related values also make sense as they are all phthalates, with many of them having similar structures.