CH5440 - Assignment 2

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In [1]:

```
# import libraries

import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns
```

In [2]:

```
# mean shift

def mean_shift(data):
    return pd.DataFrame(data-np.mean(data))
```

In [3]:

```
# get parameters for multi linear regression
# Calculating beta parameters from this (X_T.X)Beta=(X_T.y)
# inverse(X_T.X) = 1/S_uu and S_yu=(X_T.y)
# B0=y_mean-(X_mean.B_)

def multi_linear_reg(X,y):
    X_T=X.T
    S_uu=np.dot(X_T,X)
    S_uu=pd.DataFrame(np.linalg.pinv(S_uu)) # inversing the matrix S_uu
    S_yu=np.dot(X_T,y)
    B_=np.dot(S_uu,S_yu)

    B0=y.mean()-np.dot(X.mean().T,B_)

    B_=pd.DataFrame(B_.T)
    B_.columns=X.columns


    return B_,B0
```

OLS

In [4]:

```
'''
Defining Ordinary least squares
y=ax+b
from formulae, a= Syu/Suu and b=y_mean-a(x_mean)
'''
def getOLS(data,fea1, fea2):
```

```
    #x,y
    # calculating b

    x_mean=np.mean(data[fea1])
    y_mean=np.mean(data[fea2])

    # calculating numerator and denominator for a

    Syu= np.multiply(np.subtract(data[fea2],y_mean),np.subtract(data[fea1
],x_mean))
    Syu=np.sum(Syu)/len(data)
    numerator=Syu

    Suu= np.multiply(np.subtract(data[fea1],x_mean),np.subtract(data[fea1
],x_mean))
    Suu=np.sum(Suu)/len(data)
    denominator=Suu
    print('Syu:',Syu,'Suu:',Suu)
    a_OLS=numerator/denominator

    b_OLS=y_mean-a_OLS*x_mean

    print('Slope Parameter of OLS:',a_OLS)
    print('Offset Parameter of OLS:',b_OLS)
#     print(Syu,Suu,x_mean,y_mean)
    return a_OLS,b_OLS
```

Question 1

The following gases carbon dioxide (CO2), methane (CH4), nitrous oxide (N2O) and Ozone (O3) in the atmosphere are implicated in increasing global temperatures, and are known as greenhouse gases. The concentration of these gases in the atmosphere and corresponding global average temperatures obtained from the EPA website (https://www.epa.gov/climate-indicators/weather-climate) between the years 1984 to 2014 is given in the Excel file ghg-concentrations_1984-2014.xlsx (units for different variables are also given in Excel sheet).

In [5]:

```
# import data

data=pd.read_excel('ghg-concentrations_1984-2014.xlsx')
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 35 entries, 0 to 34
Data columns (total 7 columns):
 #   Column
Non-Null Count  Dtype
---  ------
--------------  -----
 0   Source: EPA's Climate Change Indicators in the United St
ates: www.epa.gov/climate-indicators  34 non-null     object
 1   Unnamed: 1
32 non-null     object
 2   Unnamed: 2
32 non-null     object

 3   Unnamed: 3
```

```
32 non-null      object
 4   Unnamed: 4
32 non-null      object
 5   Unnamed: 5
0 non-null      float64
 6   Unnamed: 6
32 non-null      object
dtypes: float64(1), object(6)
memory usage: 2.0+ KB
```

In [6]:

```python
data.head()
```

Out[6]:

	Source: EPA's Climate Change Indicators in the United States: www.epa.gov/climate-indicators	Unnamed: 1	Unnamed: 2	Unnamed: 3	Unnamed: 4	Unnamed: 5
0	Web update: April 2016	NaN	NaN	NaN	NaN	NaN
1	Temp is deviation from 1901-2000 average	NaN	NaN	NaN	NaN	NaN
2	NaN	NaN	NaN	NaN	NaN	NaN
3	Year	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)	NaN
4	1984	344.58	1655.843333	304.149167	282.07525	NaN

In [7]:

```python
# clean data

data=data[3:]
data.columns=data.iloc[0,:]
data=data[4:]
data.reset_index(drop=True, inplace=True)

# change data type to float
data=data.astype('float')
data.head()
```

Out[7]:

3	Year	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)	NaN	Temp (deg F)
0	1987.0	349.16	1693.105000	305.145455	279.769180	NaN	0.666
1	1988.0	351.56	1703.948333	306.035833	279.117045	NaN	0.666
2	1989.0	353.07	1717.980833	307.043333	283.993979	NaN	0.522
3	1990.0	354.35	1731.451667	308.169167	280.411319	NaN	0.774
4	1991.0	355.57	1740.968333	308.908333	282.554298	NaN	0.720

In [8]:

```
# drop nan column

data=data[[            'Year ',         'CO2 (ppm)',          'CH4 (ppb)',
            'N2O (ppb)O3 (', 'O3 (Dobson unit)',           'Temp (deg F)']]
data.head()
```

Out[8]:

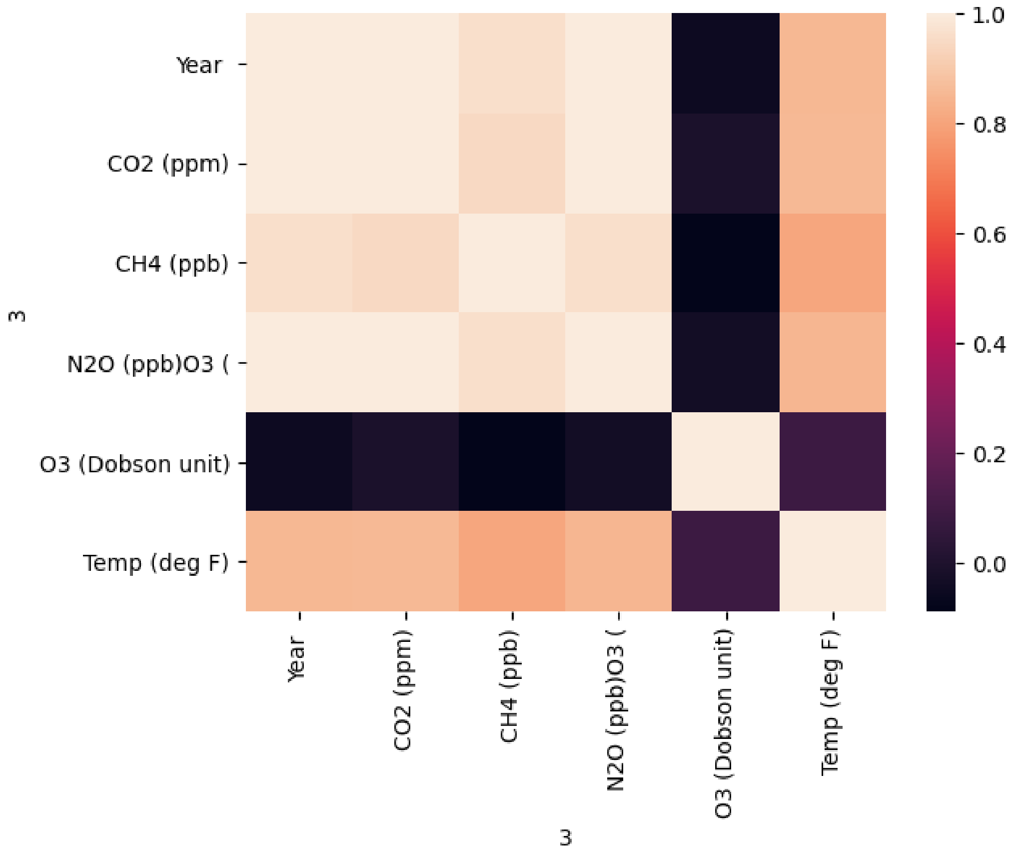
3	Year	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)	Temp (deg F)
0	1987.0	349.16	1693.105000	305.145455	279.769180	0.666
1	1988.0	351.56	1703.948333	306.035833	279.117045	0.666
2	1989.0	353.07	1717.980833	307.043333	283.993979	0.522
3	1990.0	354.35	1731.451667	308.169167	280.411319	0.774
4	1991.0	355.57	1740.968333	308.908333	282.554298	0.720

Data is cleaned

In [9]:

```
# checking correlation between variables

print(data.drop(['Year '],axis=1).corr())
sns.heatmap(data.corr())
plt.show()
```

```
3                  CO2 (ppm)  CH4 (ppb)  N2O (ppb)O3 (  O3 (Do
bson unit)  \
3
CO2 (ppm)           1.000000   0.946248       0.997231
-0.010862
CH4 (ppb)           0.946248   1.000000       0.964379
-0.088517
N2O (ppb)O3 (       0.997231   0.964379       1.000000
-0.036824
O3 (Dobson unit)   -0.010862  -0.088517      -0.036824
1.000000
Temp (deg F)        0.855976   0.807377       0.847564
0.083734

3                  Temp (deg F)
3
CO2 (ppm)              0.855976
CH4 (ppb)              0.807377
N2O (ppb)O3 (          0.847564
O3 (Dobson unit)       0.083734
Temp (deg F)           1.000000
```



part (a)

Develop a multilinear regression model between global temperature (deviations) and concentrations of greenhouse gases using OLS. Is the global temperature positively correlated with increase in the concentration of these gases?

In [10]:

```
# mean shift the data
# assuming offset parameter is non zero

data_ms=pd.concat([mean_shift(data.drop(['Temp (deg F)'],axis=1)),data[['T
emp (deg F)']]],axis=1)
data_ms.head()
```

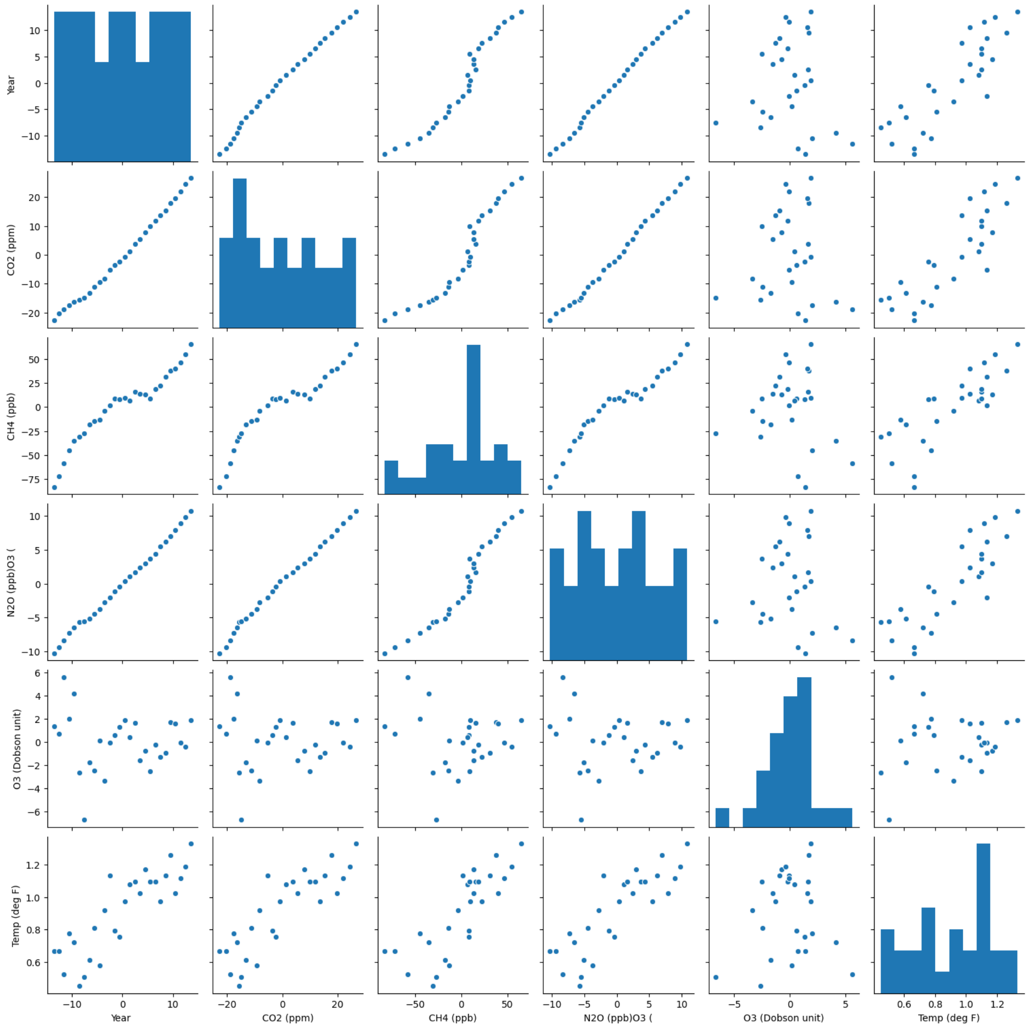
Out[10]:

3	Year	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)	Temp (deg F)
0	-13.5	-22.768571	-83.156429	-10.274282	1.355069	0.666
1	-12.5	-20.368571	-72.313096	-9.383903	0.702934	0.666
2	-11.5	-18.858571	-58.280596	-8.376403	5.579868	0.522
3	-10.5	-17.578571	-44.809762	-7.250570	1.997208	0.774
4	-9.5	-16.358571	-35.293096	-6.511403	4.140187	0.720

In [11]:

```
# Data Visualization
```

```
sns.pairplot(data_ms)
plt.show()
```



Observations from data visualization

The Year, CO2, CH4, N2O are highly correlated. There is no significaant linear relationship is observed between O3 and Temp. Temperature is linearly realted with the year, CO2, CH4, N2O.

In [12]:

```
X=data_ms.drop(['Temp (deg F)'],axis=1)
y=data_ms[['Temp (deg F)']]
```

In [13]:

```
# multi linear regression model: y=B0+B_.X
# Here B_params is transpose of B_ matrix
# B_params = [B_1,B_2, B_3, B_4, B_5] where Temp=B0+B_1*Year+B_2*CO2+B_3*C
H4+B_4*N2O+B_5*O3

print('*Considering all the independent features*')
B_params,B0=multi_linear_reg(X,y)
print(B0)
B_params
```

```
*Considering all the independent features*
```

```
3
Temp (deg F)    0.909643
dtype: float64
```

Out[13]:

3	Year	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)
0	0.081275	0.038324	0.003039	-0.184811	0.012921

In [14]:

```
print('*Considering only concentration of gases*')
B_params,B0=multi_linear_reg(X.drop(['Year '],axis=1),y)
print(B0)
B_params
```

```
*Considering only concentration of gases*
3
Temp (deg F)    0.909643
dtype: float64
```

Out[14]:

3	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)
0	0.061097	0.004851	-0.142275	0.006065

Part (a) - Solution

The global temperature positively correlated with increase in the concentration of CO2,CH4 and,O3 gases and negatively correlated with increase in the concentration of O3.

Part (b)

Estimate the error variance in temperature measurements and confidence intervals (CIs) for all regression coefficients. Based on residual analysis, remove samples suspected of being outliers (one at a time) until there are no outliers.

In [15]:

```
# sigma^2=((y-y_hat)^2)/N-p-1

X_g=X.drop(['Year '],axis=1)
estimated_y=np.dot(X_g,B_params.T)+B0[0]
error=np.subtract(y,estimated_y)
sq_error=sum(error.values**2)
error_variance=sq_error/(len(y)-4-1)
print('Error variance in temperature measurements is',error_variance[0])
```

```
Error variance in temperature measurements is 0.0180093679401
48225
```

Confidence intervals for regression coefficients

CI= [B-t.*s.e(B),B+t.*s.e(B)]

where s.e(B_j)=sigma.*root(C_jj), C=inverse(X_T.*X)

alpha=0.05 and t value at (n-p-1,alpha/2) i.e, t value at 0.025 and 23 df

T-table: https://www.sjsu.edu/faculty/gerstman/StatPrimer/t-table.pdf

from t table, t value with 23 df and 95% CI is 2.069

In [16]:

```
from math import sqrt

t=2.069
sigma=np.sqrt(error_variance)

X_g=X.drop(['Year '],axis=1)
C=np.linalg.pinv(np.dot(X_g.T,X_g))
C=np.sqrt(C)
CI=[] # confidence intervals

for i in range(len(X_g.columns)):
    SE=sigma*sqrt(C[i][i])
    CI.append([B_params.iloc[0][i]-t*SE[0],B_params.iloc[0][i]+t*SE[0]])
    print('The confidence intervals of regression coefficient of',X_g.colu
mns[i],'is:',CI[-1])
```

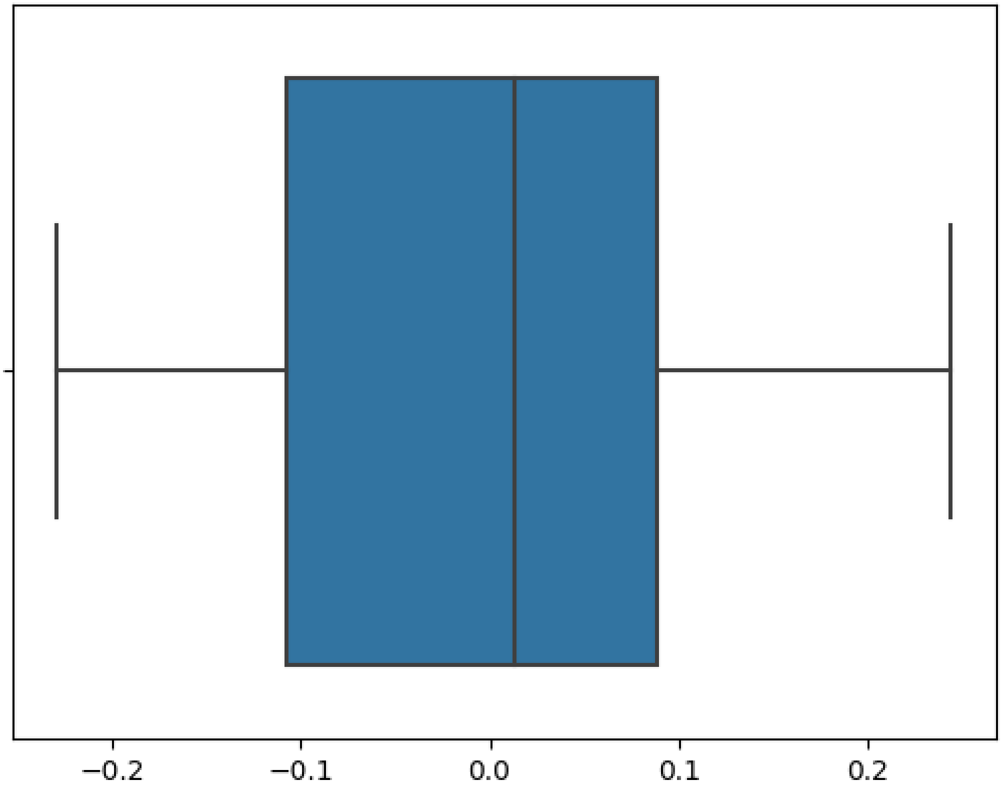
```
The confidence intervals of regression coefficient of CO2 (pp
m) is: [-0.08924042354184919, 0.21143373464652654]
The confidence intervals of regression coefficient of CH4 (pp
b) is: [-0.04504964282753206, 0.05475126797992809]
The confidence intervals of regression coefficient of N2O (pp
b)O3 ( is: [-0.40115091704658107, 0.11660034956863613]
The confidence intervals of regression coefficient of O3 (Dob
son unit) is: [-0.07536079353081503, 0.08749143949119355]
```

```
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launche
r.py:8: RuntimeWarning: invalid value encountered in sqrt
```

Zero is present in all the confidence intervals of regression coefficients, which means they are insignificant. As the independent variables observed to be depended, Let's see if the confidence intervals change when some of the independent variables are dropped.

In [17]:

```
# Outlier detection by using IQR (Inter Quartile Range) i.e, [Q1 - 1.5 * I
QR, Q3 + 1.5 * IQR]

sns.boxplot(error)
plt.show()
```



No Outliers are found

In [18]:

```
print('Squared error is',sq_error[0])
```

```
Squared error is 0.41421546262340914
```

part (b) - solution

Error variance in temperature measurements is 0.018009367940148225

Confidence Intervals

The confidence intervals of regression coefficient of CO2 (ppm) is: [-0.08924042354184919, 0.21143373464652654]

The confidence intervals of regression coefficient of CH4 (ppb) is: [-0.04504964282753206, 0.05475126797992809]

The confidence intervals of regression coefficient of N2O (ppb)O3 (is: [-0.40115091704658107, 0.11660034956863613]

The confidence intervals of regression coefficient of O3 (Dobson unit) is: [-0.07536079353081503, 0.08749143949119355]

Outliers

No Outliers are found

Part (c)

Improve the regression model obtained in step (b) by dropping unimportant (insignificant) variables (one at a time)

In [19]:

```
data.drop(['Year '],axis=1).corr()
```

Out[19]:

3 3	CO2 (ppm)	CH4 (ppb)	N2O (ppb)O3 (	O3 (Dobson unit)	Temp (deg F)
CO2 (ppm)	1.000000	0.946248	0.997231	-0.010862	0.855976
CH4 (ppb)	0.946248	1.000000	0.964379	-0.088517	0.807377
N2O (ppb)O3 (	0.997231	0.964379	1.000000	-0.036824	0.847564
O3 (Dobson unit)	-0.010862	-0.088517	-0.036824	1.000000	0.083734
Temp (deg F)	0.855976	0.807377	0.847564	0.083734	1.000000

From correlation, the order of importance of features is O3, CH4, N2O,CO2

On another note, as CO2 and N2O are highly correlated and N2O is less correlated to Temperature compared to CO2, first we can drop N2O. secondly, CO2 and CH4 are also highly correlated and CO2 is more correlated to Temperature, secondly CH4 can be droped. Thirdly O3, followed by CO2 would be the second considered order. i.e, N2O, CH4, O3, CO2

In [20]:

```
# first order

X_g.columns=['CO2','CH4','N2O','O3']
imp_fea=['O3','CH4','N2O','CO2']
X_new=X_g.copy()
B_params_new=B_params.copy()
print('Squared Error with features',X_new.columns,'is',sq_error[0])
for fea in imp_fea:
    if fea !='CO2':
        X_new=X_new.drop([fea],axis=1)
        B_params_new,B0_new=multi_linear_reg(X_new,y)
        estimated_y_new=np.dot(X_new,B_params_new.T)+B0_new[0]
        error_new=np.subtract(y,estimated_y_new)
        sq_error_new=sum(error_new.values**2)
        print('Squared Error with features',X_new.columns,'is',sq_error_ne
w[0])
```

```
Squared Error with features Index(['CO2', 'CH4', 'N2O', 'O
3'], dtype='object') is 0.41421546262340914
Squared Error with features Index(['CO2', 'CH4', 'N2O'], dtyp
e='object') is 0.4191893034146299
Squared Error with features Index(['CO2', 'N2O'], dtype='obje
ct') is 0.44489450495014565
Squared Error with features Index(['CO2'], dtype='object') is
```

```
0.45615533152560056
```

In [21]:

```
# second order

X_g.columns=['CO2','CH4','N2O','O3']
imp_fea=['N2O','CH4','O3','CO2']
X_new=X_g.copy()
B_params_new=B_params.copy()
print('Squared Error with features',X_new.columns,'is',sq_error[0])
for fea in imp_fea:
    if fea !='CO2':
        X_new=X_new.drop([fea],axis=1)
        B_params_new,B0_new=multi_linear_reg(X_new,y)
        estimated_y_new=np.dot(X_new,B_params_new.T)+B0_new[0]
        error_new=np.subtract(y,estimated_y_new)
        sq_error_new=sum(error_new.values**2)
        print('Squared Error with features',X_new.columns,'is',sq_error_ne
w[0])
```

```
Squared Error with features Index(['CO2', 'CH4', 'N2O', 'O
3'], dtype='object') is 0.41421546262340914
Squared Error with features Index(['CO2', 'CH4', 'O3'], dtype
='object') is 0.44100302085122467
Squared Error with features Index(['CO2', 'O3'], dtype='objec
t') is 0.4413842859911566
Squared Error with features Index(['CO2'], dtype='object') is
0.45615533152560056
```

Part (c) - Solution

The models with [CO2,CH4,N20,O3] and ['CO2', 'CH4', 'N2O'] are performing nearly same as the squared error values are very near. As the second model has low features, considering the model complexity, model with ['CO2', 'CH4', 'N2O'] as features is considered as improved regreddion model. If we further consider squared error of 0.456 is not indifferent from 0.414, we can consider only CO2 as independent feature and predict the temparatures. The error values are close and the consideration of model depends on the error tolerance. For this case, I am considering model with CO2, CH4, NO2 as optimal model.

Part (d)

The effect of different gases on the global temperature is expressed in terms of CO2 equivalents or global warming potential (GWP). Is it possible to make any inference regarding GWP of the gases from the regression coefficients? Compare the GWP obtained from regression coefficients to the values obtained over a 20 year time horizon: CO2 (1), CH4 (86), N2O (289)

In [22]:

```
# Reference values: CO2 (1), CH4 (86), N2O (289)
# As the the GWP value is in terms of CO2,
# lets divide the regression coefficients of CH4 and N2O with regression c
oefficient of CO2.

# OLS
```

```
CO2_OLS=0.061097
CH4_OLS=0.004851
N2O_OLS=0.142275

CO2_OLS_GWP=(CO2_OLS/CO2_OLS)
CH4_OLS_GWP=(CH4_OLS/CO2_OLS)*1000 #convert ppb to ppm
N2O_OLS_GWP=(N2O_OLS/CO2_OLS)*1000 #convert ppb to ppm

print('GWP obtained from OLS regression coefficents: CO2(',CO2_OLS_GWP,
'),','CH4(',CH4_OLS_GWP,'),','N2O(',N2O_OLS_GWP,')' )
# # TLS

# CO2_TLS=
# CH4_TLS=
# N2O_TLS=

# CO2_TLS_GWP=CO2_TLS/CO2_TLS
# CH4_TLS_GWP=CH4_TLS/CO2_TLS
# N2O_TLS_GWP=N2O_TLS/CO2_TLS

# print('GWP obtained from TLS regression coefficents: CO2(',CO2_TLS_GW
P,')','CH4(',CH4_TLS_GWP,')','N2O(',N2O_TLS,')' )
```

```
GWP obtained from OLS regression coefficents: CO2( 1.0 ), CH4
( 79.39833379707679 ), N2O( 2328.674075650196 )
```

Part (d) - Solution

GWP values of CO2 and CH4 are close to obtained GWP values. Where GWP value of N20 is almost 10 times of the obtained N2O GWP. From the results, the affect of N2O on global temperature has increased rapidly.

Question 2

Consider the problem of developing a correlation between saturated pressure (Psat) and saturated temperature T (boiling point). For pure components, the Antoine equation given below generally fits the data well

$ln(P\_sat) = A - B/(T + C)$

For n-hexane, the values of the constants are A = 14.0568, B = 2825.42, and C = 230.44 where Psat is given in kPa and T in deg C. Using this correlation a data set consisting of 100 samples have been generated in the temperature range 10 - 70 deg C . Gaussian measurements errors to both the true temperature and saturated pressures with standard deviations of 0.18 deg C and 2 kPa , respectively, have been added to generate the measurements (available in vpdata.mat)

In [23]:

```
import scipy.io
data_mat = scipy.io.loadmat('vpdata.mat')
```

In [24]:

```
# Data prepocessing, in .mat file, the data is in a dictionary.
```

```
# Therefore, converting the data in dictionary format to dataframe

temp=[]
psat=[]

for i in range(len(data_mat['temp'])):
    temp.append(data_mat['temp'][i][0])
    psat.append(data_mat['psat'][i][0])
data=pd.concat([pd.DataFrame(temp),pd.DataFrame(psat)],axis=1)
data.columns=['temp','psat']
data.head()
```

Out[24]:

	temp	psat
0	37.114450	29.315594
1	32.986367	28.547205
2	57.152844	66.982238
3	31.646108	24.656088
4	41.677937	39.074630

Part (a)

The Classius-Clapeyron equation is a theoretically derived model between Psat and T and is given by

$ln(P\_sat) = A' - B'/T$

Assuming that temperature measurements are noise-free and pressure measurements are noisy, use linear regression to obtain estimates of parameters A’ and B’.

In [25]:

```
# Assume X=1/T and y=ln(p), the the model equation becomes y=a*X+b

X=np.divide(1,data.temp)
y=np.log(data.psat)   # Assuming error in psat are normal
data_new=pd.concat([pd.DataFrame(X),pd.DataFrame(y)],axis=1)
data_new.columns=['X','y']
```

In [26]:

```
# mean shift the data

# data_new=mean_shift(data_new)
# data_new
```

In [27]:

```
# fit OLS as X is assumed to be noise free

a_OLS,b_OLS=getOLS(data_new,'X','y')
```

```
Syu: -0.008916949173671578 Suu: 0.00023530071083357592
```

```
Slope Parameter of OLS: -37.895972103451825
Offset Parameter of OLS: 4.760732187067934
```

In [28]:

```
A=b_OLS
B=-a_OLS
print('Parameter estimate of A is',A,'and of B is',B)
```

```
Parameter estimate of A is 4.760732187067934 and of B is 37.8
95972103451825
```

part (a) - solution

Parameter estimate of A = 4.761

Parameter estimate of B = 37.896

Part (b)

Assuming that temperature measurements are noise-free and pressure measurements are noisy, use nonlinear regression to obtain estimates of parameters A, B and C

In [29]:

```
# Assume X=1/T and y=ln(p), the the model equation becomes y=a*X+b

X=data.temp
y=np.log(data.psat)   # Assuming error in psat are normal
data_new2=pd.concat([pd.DataFrame(X),pd.DataFrame(y)],axis=1)
data_new2.columns=['X','y']
data_new2.head()
```

Out[29]:

	X	y
0	37.114450	3.378120
1	32.986367	3.351559
2	57.152844	4.204427
3	31.646108	3.205024
4	41.677937	3.665473

In [30]:

```
# mean shift

# data_new2=mean_shift(data_new2)
# data_new2.head()
```

In [31]:

```
X=data_new2.X
```

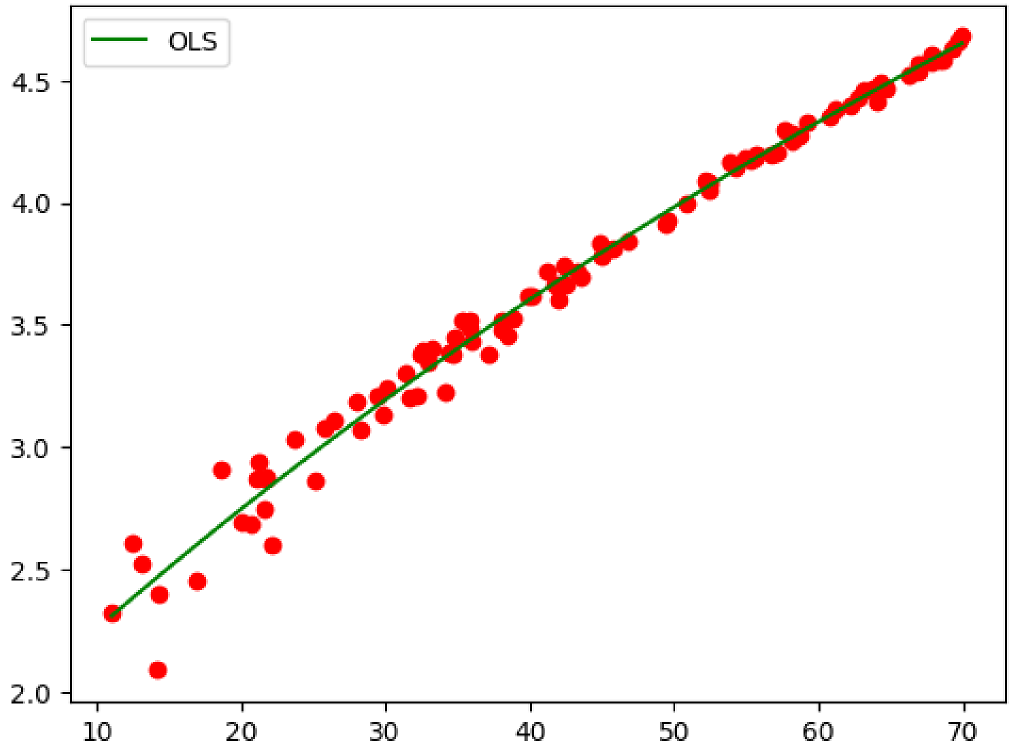
```
y=data_new2.y
```

In [32]:

```
def objective(X,A,B,C):
    return A-(B/(X+C))
```

In [33]:

```
#  we have to use scipy.odr which uses orthogonal distance. fit_type=2 ind
icates OLS

from scipy.odr import ODR, Model, RealData

def function(beta,X):
    A,B,C=beta[0],beta[1],beta[2]
    return A-(B/(X+C))

model = Model(function)
data_real=scipy.odr.Data(X,y)

odr = ODR(data_real, model,beta0=[1.,1.,1.])

xn = np.linspace(min(X),max(X),100)
plt.plot(X,y,'ro')
odr.set_job(fit_type=2)
output = odr.run()
yn = function(output.beta, xn)
plt.plot(xn,yn,'g-',label='OLS')
plt.legend(loc=0)
plt.show()
output.pprint()
```




```
Beta: [   13.08128121 2281.88178669  200.7819102 ]
Beta Std Error: [   1.69718814 820.44997012  43.29743098]
Beta Covariance: [[4.79604228e+02 2.31718998e+05 1.22079985e+
```

```
04]
 [2.31718998e+05 1.12079771e+08 5.91144144e+06]
 [1.22079985e+04 5.91144144e+06 3.12138461e+05]]
Residual Variance: 0.006005884446867539
Inverse Condition #: 8.970632610496292e-06
Reason(s) for Halting:
  Sum of squares convergence
```

In [34]:

```
print('Parameter Estimate of A is', 13.08)
print('Parameter Estimate of B is', 2281.88)
print('Parameter Estimate of C is',  200.78)
```

```
Parameter Estimate of A is 13.08
Parameter Estimate of B is 2281.88
Parameter Estimate of C is 200.78
```

Part (b) - solution

Parameter Estimate of A = 13.08

Parameter Estimate of B = 2281.88

Parameter Estimate of C = 200.78

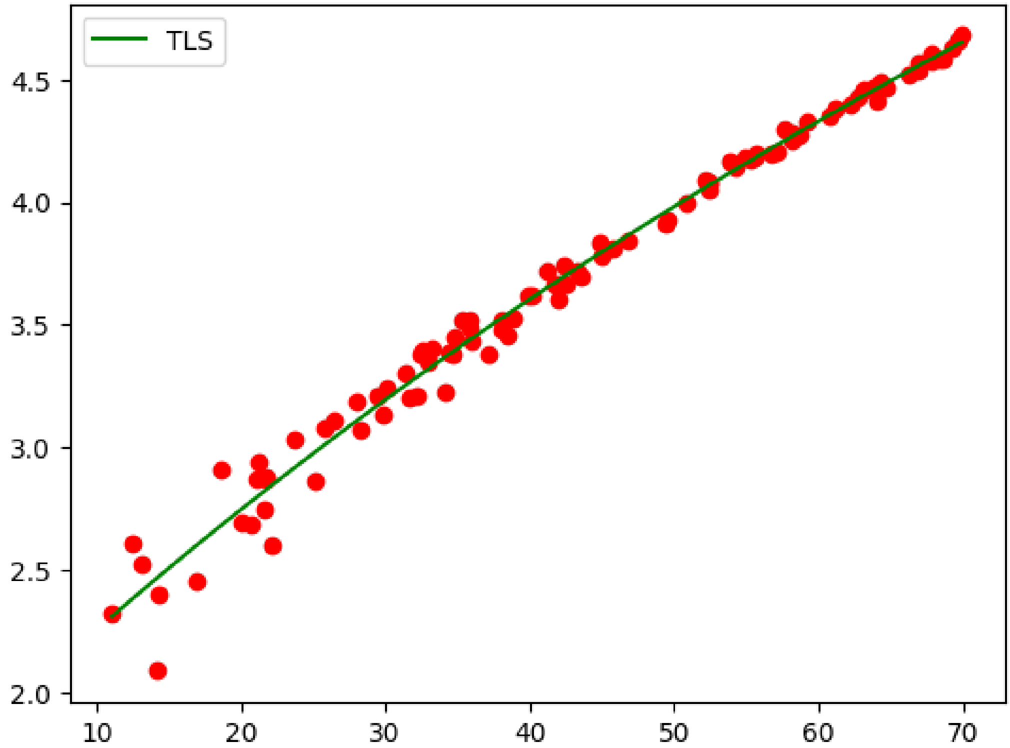
Part (c)

Assuming both pressures and temperature measurements are noisy apply weighted total least squares obtain estimates of parameters A, B, and C. Use the inverse of standard deviation of errors as weights to set up the nonlinear optimization problem.

In [35]:

```
#  For considering error in independent variable, we have to use scipy.odr which uses orthogonal distance. fit_type=0 indicates TLS

from scipy.odr import ODR, Model, RealData

def function(beta,X):
    A,B,C=beta[0],beta[1],beta[2]
    return A-(B/(X+C))

model = Model(function)
data_real=scipy.odr.Data(X,y)

odr = ODR(data_real, model,beta0=[1.,1.,1.])

xn = np.linspace(min(X),max(X),100)
plt.plot(X,y,'ro')
odr.set_job(fit_type=0)
output = odr.run()
yn = function(output.beta, xn)
plt.plot(xn,yn,'g-',label='TLS')
plt.legend(loc=0)
```

```
plt.show()
output.pprint()
```




```
Beta: [  13.0707509   2276.71854583  200.50555396]
Beta Std Error: [  1.6929195   817.4548417    43.18763611]
Beta Covariance: [[4.78207655e+02 2.30780953e+05 1.21721357e+
04]
 [2.30780953e+05 1.11499122e+08 5.88738834e+06]
 [1.21721357e+04 5.88738834e+06 3.11216614e+05]]
Residual Variance: 0.005993163057415993
Inverse Condition #: 9.000367963318945e-06
Reason(s) for Halting:
  Sum of squares convergence
```

In [36]:

```
print('Parameter Estimate of A is', 13.07)
print('Parameter Estimate of B is', 2276.72)
print('Parameter Estimate of C is', 200.50)
```

```
Parameter Estimate of A is 13.07
Parameter Estimate of B is 2276.72
Parameter Estimate of C is 200.5
```

Part (c) - solution

Parameter Estimate of A = 13.07

Parameter Estimate of B = 2276.72

Parameter Estimate of C = 200.5

Part (d)

For the models obtained in (a), (b), and (c) report the maximum error in predicting the saturated pressures using the identified model for the sample data.

In [37]:

```
model_A=[4.760732187067934,37.895972103451825]
model_B=[  13.08128121, 2281.88178669,  200.7819102 ]
model_C=[13.0707509, 2276.71854583, 200.50555396]
```

In [38]:

```
estimated_y_A=model_A[0]-np.multiply(model_A[1],np.divide(1,data.temp))
estimated_y_B=model_B[0]-np.divide(model_B[1],np.add(data_new2.X,model_B[2
]))
estimated_y_C=model_C[0]-np.divide(model_C[1],np.add(data_new2.X,model_B[2
]))
```

In [39]:

```
error_A=np.sum(np.sqrt(np.subtract(y,estimated_y_A)))
error_B=np.sum(np.sqrt(np.subtract(y,estimated_y_B)))
error_C=np.sum(np.sqrt(np.subtract(y,estimated_y_C)))
```

```
C:\Users\himas\AppData\Roaming\Python\Python37\site-packages
\pandas\core\arraylike.py:358: RuntimeWarning: invalid value
encountered in sqrt
  result = getattr(ufunc, method)(*inputs, **kwargs)
```

In [40]:

```
error_A,error_B,error_C
```

Out[40]:

```
(21.299279834631026, 10.206109879235179, 8.192712142960858)
```

Part (d) - Solution

Maximum Squared error is produced by model from part (a) and it is equal to 21.299

Question 3

A zoologist obtained measurements of the mass (in grams), the snout-vent length (SVL) and hind limb span (HLS) in mm of 25 lizards. The mean and covariance matrix of the data about the mean are given by

X.T=[9, 68, 123] and S=[[7,21,34],[21,64,102],[34,102,186]]

Part (a)

The largest eigenvalue of the above covariance matrix is 250.4. Determine the normalized eigenvector corresponding to this eigenvalue. Also determine the remaining eigenvalues and corresponding mutually orthogonal eigenvectors

In [41]:

```
from numpy.linalg import eig

S=[[7,21,34],[21,64,102],[34,102,186]]
X_bar=[[9], [68], [123]]
W,V=eig(S)    # eigen vectors are already normalized
print('Eigen values:', W)
print('Eigen vectors', V)
```

```
Eigen values: [2.50400915e+02 8.95711992e-02 6.50951385e+00]
Eigen vectors [[ 0.16191025  0.95890336 -0.23300092]
 [ 0.48767833 -0.28302089 -0.8258747 ]
 [ 0.85787815 -0.02008808  0.51346037]]
```

In [42]:

```
# eigen vector correspondng to 250.4 is p (done by hand calculations)
p=[0.188733383465708, 0.5684703912682,1]
magnitude_V0=np.linalg.norm(p)
print(magnitude_V0)
norm_V0=np.divide(p,magnitude_V0)
print('The normalized eigenvector corresponding to this eigenvalue 250.4 i
s',norm_V0)
```

```
1.1656667087049515
The normalized eigenvector corresponding to this eigenvalue 2
50.4 is [0.16191025 0.48767833 0.85787815]
```

In [43]:

```
for i in range(len(W)):
    print('The Eigen vector corressponding to',W[i],'is [',V[0][i],',',V[1
][i],',',V[2][i],']')
```

```
The Eigen vector corressponding to 250.40091494719053 is [ 0.
16191024591874054 , 0.48767832779557313 , 0.857878150359972 ]
The Eigen vector corressponding to 0.08957119921388516 is [
0.9589033550947192 , -0.2830208909424421 , -0.020088078012520
532 ]
The Eigen vector corressponding to 6.509513853595643 is [ -0.
23300091814115964 , -0.8258747022936713 , 0.5134603667827891
]
```

Part (a) - Solutions

The normalized eigenvector corresponding to this eigenvalue 250.4 is [0.16191025, 0.48767833, 0.85787815]

The Eigen vector corressponding to 250.40091494719053 is [0.1619 , 0.4876 , 0.8578]

The Eigen vector corressponding to 0.08957119921388516 is [0.959 , -0.2830 , -0.020]

The Eigen vector corressponding to 6.509513853595643 is [-0.233 , -0.8258 , 0.5134]

Part (b)

How many principal components should be retained, if at least 95% of the variance in the data has to be captured?

In [44]:

```
eigen_values=[2.50400915e+02, 6.50951385e+00,8.95711992e-02] #in order
for i in range(len(W)):
    print('Percentage of variance captured by',len(eigen_values[:i+1]),' p
ricical components is',sum(eigen_values[:i+1])/sum(eigen_values))
```

```
Percentage of variance captured by 1  pricical components is
0.9743226262726199
Percentage of variance captured by 2  pricical components is
0.9996514739331406
Percentage of variance captured by 3  pricical components is
1.0
```

part (b) - Solution

One Principal component should be retained to capture at least 95% of the variance in the data

Part (c)

Assuming that there are two linear relationships among the three variables, determine one possible set of these linear relations.

In [89]:

```
# The two linear relationships are PCs of two smallest eigen values
# Linear Relationship: V_T.(X-X_bar)

from sympy import *

V2=[ 0.959 , -0.2830 , -0.020]
V3=[ -0.233 , -0.8258 , 0.5134 ]
var('x1,x2,x3')
X=[[x1], [x2], [x3]]
X_=np.subtract(X,X_bar)
lin_rel_1= np.sum(np.dot(V2,X_))
print('Linear Relationship 1:',lin_rel_1,'= 0')

lin_rel_2= np.sum(np.dot(V3,X_))
print('Linear Relationship 2:',lin_rel_2,'= 0')
```

```
Linear Relationship 1: 0.959*x1 - 0.283*x2 - 0.02*x3 + 13.073
= 0
Linear Relationship 2: -0.233*x1 - 0.8258*x2 + 0.5134*x3 - 4.
8968 = 0
```

Part (c) - Solution

Assuming two linear relationships, The two relationships are

0.959*x1 - 0.283*x2 - 0.02*x3 + 13.073 = 0

-0.233*x1* - *0.8258*x2 + 0.5134*x3 - 4.8968 = 0

Part (d)

Using the PCA model, determine the scores for a female lizard with the following measurements: mass = 10.1 gms, SVL = 73mm and HLS = 135.5mm.

In [93]:

```
# X=[[10.1],[73],[135.5]]
X_=[[1.1],[5],[6.5]]     # X-X_bar
V1=np.array([ 0.1619 , 0.4876 , 0.8578])
V2=[ 0.959 , -0.2830 , -0.020]
V3=[ -0.233 , -0.8258 , 0.5134 ]
score1=np.dot(V1,X_)
print( 'score from V1:',score1)

score2=np.dot(V2,X_)
print( 'score from V2:',score2)

score3=np.dot(V3,X_)
print( 'score from V3:',score3)

print('Therefore scores for female lizard are', score1,score2,score3)
```

```
score from V1: [8.19179]
score from V2: [-0.4901]
score from V3: [-1.0482]
Therefore scores for female lizard are [8.19179] [-0.4901] [-
1.0482]
```

Part (d) - Solution

Therefore scores for female lizard are 8.19179, -0.4901, -1.0482

Part (e)

Using the PCA model, estimate the mass of a lizard whose measured SVL is 73mm

In [94]:

```
# in the two linear equations, substitue 73 in x2 and solve

# The solution is hand solved and the answer is 10.66 gms
```

Part (f)

Using the PCA model, estimate the mass of a lizard whose measured SVL is 73mm and measured HLS is 135.5 mm.

In [95]:

```
# The solution is hand solved!
```

MM17B113

3) $\bar{x} = \begin{bmatrix} 9 \\ 68 \\ 129 \end{bmatrix}$ $S = \begin{bmatrix} 7 & 21 & 34 \\ 21 & 64 & 102 \\ 34 & 102 & 186 \end{bmatrix}$

a) Largest eigen value = 250.4

$$|S-\lambda I| = \begin{bmatrix} 7-\lambda & 21 & 34 \\ 21 & 64-\lambda & 102 \\ 34 & 102 & 186-\lambda \end{bmatrix}$$

$\Rightarrow -\lambda^3 + 257\lambda^2 - 1653\lambda + 146 = 0$

$\lambda_1 + \lambda_2 + \lambda_3 = 257$

$\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_1\lambda_3 = 1653$

$\lambda_1\lambda_2\lambda_3 = 146$

$\Rightarrow \lambda_2 + \lambda_3 = 6.6$ and $\lambda_2\lambda_3 = 0.58$

$\Rightarrow \lambda_2 = 0.089$ and $\lambda_3 = 6.509$

Eigen vector corresponding to 250.4

$$\begin{bmatrix} 7 & 21 & 34 \\ 21 & 64 & 102 \\ 34 & 102 & 186 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 250.4 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$\Rightarrow 7x_1 + 21x_2 + 34x_3 = 250.4x_1 \rightarrow (1)$

$\Rightarrow 21x_1 + 64x_2 + 102x_3 = 250.4x_2 \rightarrow (2)$

$\Rightarrow 34x_1 + 102x_2 + 186x_3 = 250.4x_3 \rightarrow (3)$

Solving eq(1), eq(2), eq(3)

$x_1 = 0.1887$
$x_2 = 0.5685$
$x_3 = 1$

$V_1 = \begin{bmatrix} 0.1887 \\ 0.5685 \\ 1 \end{bmatrix}$

normalizing V_1

$L = \sqrt{1.887^2 + 0.5685^2 + 1^2} = 1.1656$

$$V_1 = \begin{bmatrix} 0.1887/1.1656 \\ 0.5685/1.1656 \\ 1/1.1656 \end{bmatrix} = \begin{bmatrix} 0.162 \\ 0.487 \\ 0.857 \end{bmatrix}$$

$\leftarrow$ normalized eigen vector corresponding to eigen value: 250.4

Ily for x_2 and x_3

$$\begin{bmatrix} 7 & 21 & 34 \\ 21 & 64 & 102 \\ 34 & 102 & 186 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 0.089 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$7x_1 + 21x_2 + 34x_3 = 0.089x_1$$
$$21x_1 + 64x_2 + 102x_3 = 0.089x_2$$
$$34x_1 + 102x_2 + 186x_3 = 0.089x_3$$

solving above 3 equations

$$V_2 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -47.735 \\ 14.0889 \\ 1 \end{bmatrix}$$

normalizing V_2

$$L = \sqrt{-47.735^2 + 14.0889^2 + 1}$$

normalized V_2 = $\begin{bmatrix} 0.959 \\ -0.283 \\ -0.020 \end{bmatrix}$ ← normalized eigen vector corresponding to eigen value 0.089.

$$\begin{bmatrix} 7 & 21 & 34 \\ 21 & 64 & 102 \\ 34 & 102 & 186 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = 6.509 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$7x_1 + 21x_2 + 34x_3 = 6.509x_1$$
$$21x_1 + 64x_2 + 102x_3 = 6.509x_2$$
$$34x_1 + 102x_2 + 186x_3 = 6.509x_3$$

solving above 3 equations

$$V_3 = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -0.454 \\ -1.608 \\ 1 \end{bmatrix}$$

normalizing V_3

$$L = \sqrt{-0.454^2 + (-1.608)^2 + 1^2}$$

normalized V_3 = $\begin{bmatrix} -0.233 \\ -0.825 \\ 0.513 \end{bmatrix}$ ← normalized eigen vector corresponding to eigen value 6.509

b) $\lambda_1 = 250.4$ $\quad \lambda_2 = 0.089$ $\quad \lambda_3 = 6.509$

in order its $250.4, 6.509, 0.089$

% of variance captured by 1 PC $= \frac{\lambda_1 \times 100}{\lambda_1+\lambda_2+\lambda_3} = \frac{250.4 \times 100}{257}$

$= 0.974 \times 100$

$= 97.4\%$

Therefore, ~~at~~ one principal component should be retained to capture atleast 95% of variance in data.

(c) transformed variables are $z_i = v_i^T(x)$

for two possible linear relationships, consider 2 smallest eigenvalues

$z_2 = v_2^T(x - \bar{x})$ $\qquad z_3 = v_3^T(x-\bar{x})$ $\qquad \begin{bmatrix} 0.233 \\ -0.825 \\ 0.513 \end{bmatrix}^T$

$z_2 = 0$ and $z_3 = 0$

$$\begin{bmatrix} 0.959 \\ -0.283 \\ -0.020 \end{bmatrix}^T \begin{bmatrix} x_1 - 9 \\ x_2 - 68 \\ x_3 - 129 \end{bmatrix} = 0 \quad \text{and} \quad \begin{bmatrix} -0.454 \\ -1.608 \\ 1 \end{bmatrix}^T \begin{bmatrix} x_1 - 9 \\ x_2 - 68 \\ x_3 - 129 \end{bmatrix} = 0$$

$\Rightarrow 0.233 z_1 + 0.826 z_2 - 0.513 z_3 + 7.983 = 0$ and

$\Rightarrow 0.958 z_1 \mp 0.283 z_2 - 0.020 z_3 + 13.20 = 0$

are two possible linear relationships

(d) Projecting data onto largest eigen vector, given $x = \begin{bmatrix} 10.1 \\ 73 \\ 135.5 \end{bmatrix}$

$$\text{score} = v_1^T (x - \bar{x})$$

$$= \begin{bmatrix} 0.162 \\ 0.487 \\ 0.857 \end{bmatrix}^T \begin{bmatrix} 10.1 - 9 \\ 73 - 68 \\ 135.5 - 129 \end{bmatrix}$$

$$= \begin{bmatrix} 0.162 & 0.487 & 0.857 \end{bmatrix} \begin{bmatrix} 1.1 \\ 5 \\ 6.5 \end{bmatrix}$$

$\boxed{\text{score} = 8.1837}$ → when considering only one eigen vector

when all three are considered, the scores are

$8.1837, -0.4901, -1.0482$

(e) SVL = 73 mm (z_2)

from two linear relationships from part (c)

$$0.233 z_1 + 0.826 z_2 - 0.513 z_3 + 7.983 = 0$$
$$0.958 z_1 - 0.283 z_2 - 0.02 z_3 + 13.20 = 0$$

replace z_2 by 73 and solve

$$\Rightarrow 0.2330 z_1 + 0.826(73) - 0.513 z_3 + 7.983 = 0$$
$$\Rightarrow 0.2330 z_1 - 0.0513 z_3 = -68.224 \rightarrow (1)$$

$$\Rightarrow 0.958 z_1 - 0.283(73) - 0.02(z_3) + 13.20 = 0$$
$$\Rightarrow 0.958 z_1 - 0.02 z_3 = 7.452 \rightarrow (2)$$

From eq (1) & (2)

$$z_1 = 10.66 \qquad z_2 = 138.01$$

that is, $\boxed{\text{mass} = 10.66 \text{ gms}}$

(f) SVL = 73 mm (z_2)
HLS = 135.5mm (z_3)

find z_1

As both z_2 and z_3 are given, one linear relationship is sufficient to estimate mass (z_1), so lets eliminate z_1 from two equations

$$\Rightarrow 3.681 z_2 - 2.093 z_3 + 19.646 = 0$$

using TLS

$$\min_{\hat{z}} (z - \hat{z})^T (z - \hat{z})$$

s.t $A\hat{z} = b \rightarrow$ this from above equation

$A = [3.681, -2.093]$

$b = -19.646$

$$\Rightarrow \hat{z} = z - A(AA^T)^{-1}(Az - b)$$ → we get this by substituting linear relationship in objective function

$$\min \frac{1}{2}(z - \hat{z})^T (z - \hat{z}) + \lambda (A\hat{z} - b)$$

$$\Rightarrow \hat{z} = [75.97, 140.43]$$

these values are close to given values

From linear relationships;

$$0.233 z_1 + 0.826(75.97) - 0.513(140.43) + 7.983 = 0$$

$$\boxed{Z_1 = 11.12 \text{ grams}}$$