MCL 732

AIR POLLUTION: SOURCES AND APPORTIONMENT

Assignment 1

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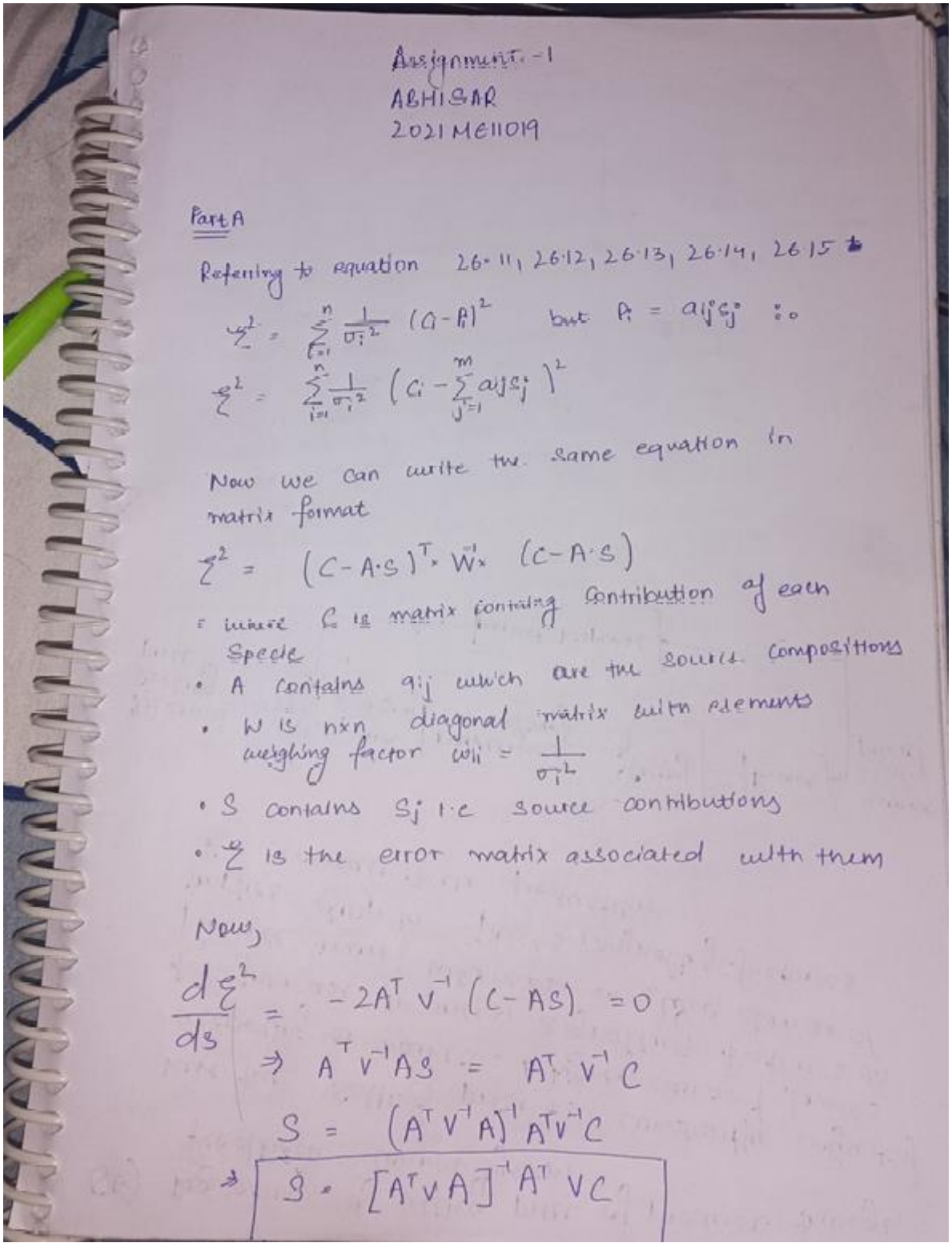
Made by:

ABHISAR 2021ME11019

A) Drive equation 26.16. Comment whether/how the derivation poses any constraint on the relationship between n and m.



Assignment - 1
ABHISAR
2021ME11019

Part A

Referring to equation 26.11, 26.12, 26.13, 26.14, 26.15 &

$$\chi^2 = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} (C_i - P_i)^2 \quad \text{but } P_i = a_{ij} s_j \therefore$$

$$\chi^2 = \sum_{i=1}^{n} \frac{1}{\sigma_i^2} \left(C_i - \sum_{j=1}^{m} a_{ij} s_j\right)^2$$

Now we can write the same equation in matrix format

$$\chi^2 = (C - A \cdot S)^T \times W \times (C - A \cdot S)$$

- where C is matrix containing contribution of each specie
- A contains a_{ij} which are the source compositions
- W is nxn diagonal matrix with elements weighing factor $w_{ii} = \frac{1}{\sigma_i^2}$
- S contains s_j i.e source contributions
- χ is the error matrix associated with them

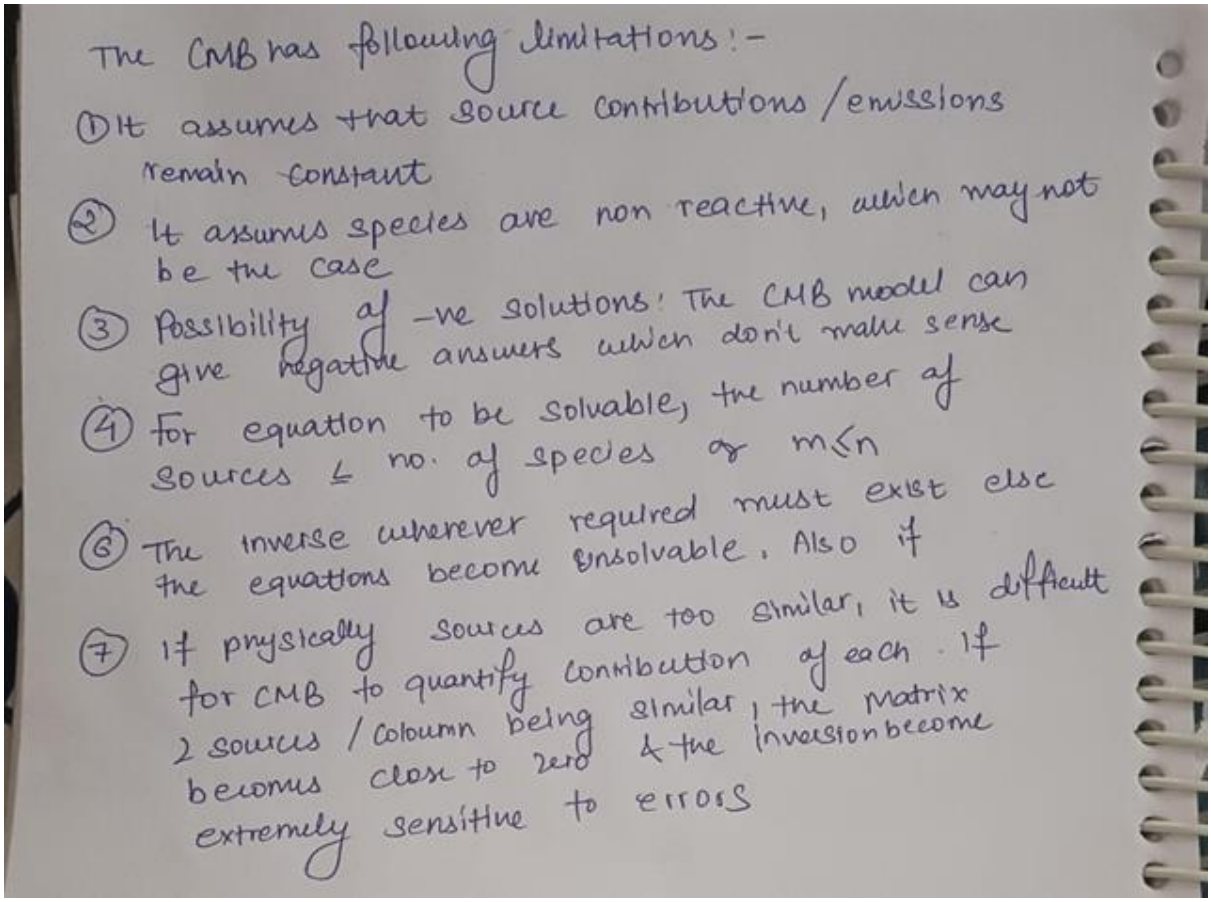
Now,

$$\frac{d\chi^2}{ds} = -2A^T V^{-1} (C - AS) = 0$$

$$\Rightarrow A^T V^{-1} A S = A^T V^{-1} C$$

$$S = (A^T V^{-1} A)^{-1} A^T V^{-1} C$$

$$\Rightarrow \boxed{S = [A^T V A]^{-1} A^T V C}$$



B) Calculate the source contributions g_j using Equation 26.16 and tabulate the deviations with the values given in table 26.3.

SOURCE	$PM_{2.5}$ (Observed)	$PM_{2.5}$ (Calculated)	Deviations
Geologic	2.26	1.37	0.89
Motor Vehicles	9.24	8.62	0.62
Vegetative Burning	5.92	7.01	-1.09
Primary Crude Oil	0.25	0.33	-0.08
$(NH_4)_2SO_4$ - Secondary	3.48	3.16	0.32
NH_4NO_3 - Secondary	12.35	14.09	-1.74
Sea salt (NaCl - $NaNO_3$)	0.45	-2.09	2.54
OC - Secondary	0.36	0.379	-0.019

Table – calculated source contributions for PM2.5

SOURCE	PM_{10} (Observed)	PM_{10} (Calculated)	Deviations
Geologic	31.78	12.83	18.95
Motor Vehicles	6.8	5.89	0.91
Vegetative Burning	5.1	19.2	-14.1
Primary Crude Oil	0.29	0.54	-0.25
$(NH_4)_2SO_4$ - Secondary	3.58	3.47	0.11
NH_4NO_3 - Secondary	10.39	13.76	-3.37
Sea salt (NaCl - $NaNO_3$)	0.96	-0.67	1.63
OC - Secondary	0.07	-0.69	0.76

Table – calculated source contributions for PM10

C) Calculate the source contributions g_j using Equation 26.17 and tabulate the deviations with the values given in table 26.3

PM 2.5							
SOURCE	Observation	Iteration 1		Iteration 5		Iteration 10	
		Calculated	Deviation	Calculated	Deviation	Calculated	Deviation
Geologic	2.26	1.39	0.87	2.06	0.2	2.06	0.2
Motor Vehicles	9.24	10.1	-0.86	10.53	-1.29	10.53	-1.29
Vegetative Burning	5.92	6.97	-1.05	6.92	-1	6.92	-1
Primary Crude Oil	0.25	0.32	-0.07	0.32	-0.07	0.32	-0.07
$(NH_4)_2SO_4$ - Secondary	3.48	3.09	0.39	3.07	0.41	3.07	0.41
NH_4NO_3 - Secondary	12.35	14.17	-1.82	14.19	-1.84	14.19	-1.84
Seasalt (NaCl - $NaNO_3$)	0.45	-2.17	2.62	-2.19	2.64	-2.19	2.64
OC - Secondary	0.36	-0.35	0.71	-0.54	0.9	-0.54	0.9

Table – calculated source contributions for PM2.5 after accounting for error in measurements for different source profiles

PM 10							
SOURCE	Observation	Iteration 1		Iteration 5		Iteration 10	
		Calculated	Deviation	Calculated	Deviation	Calculated	Deviation
Geologic	31.78	12.75	19.03	12.72	19.06	12.72	19.06
Motor Vehicles	6.8	6.42	0.38	6.51	0.29	6.52	0.28
Vegetative Burning	5.1	19.37	-14.27	19.34	-14.24	19.34	-14.24
Primary Crude Oil	0.29	0.56	-0.27	0.56	-0.27	0.56	-0.27
(NH4)2SO4 - Secondary	3.58	3.43	0.15	3.43	0.15	3.43	0.15
NH4NO3 - Secondary	10.39	13.79	-3.4	13.8	-3.41	13.8	-3.41
Seasalt (NaCl - NaNO3)	0.96	-0.71	1.67	-0.72	1.68	-0.72	1.68
OC - Secondary	0.07	-1.02	1.09	-1.05	1.12	-1.05	1.12

Table – calculated source contributions for PM10 after accounting for error in measurements for different source profiles

D) Part 1 : Change the % contribution of EC to 21% (from 15.89%) and OC to 38% (from 44.60%) in vegetative burning source. Change the % contribution of EC to 42% (from 54.15%) and OC to 58% (from 49.81%) in motor vehicles source. Evaluate the source contributions g_j using Equation 26.16 and tabulate the deviations with your answers in part B)

D1 – PM2.5				
SOURCE	$PM_{2.5}$ (Observed)	$PM_{2.5}$ (Part B)	$PM_{2.5}$ (Part D1)	Deviation (B – D1)
Geologic	2.26	1.37	1.37	0
Motor Vehicles	9.24	8.62	8.71	-0.09
Vegetative Burning	5.92	7.01	7.1	-0.09
Primary Crude Oil	0.25	0.33	0.33	0
$(NH_4)_2SO_4$ - Secondary	3.48	3.16	3.15	0.01
NH_4NO_3 - Secondary	12.35	14.09	14.09	0
Seasalt (NaCl - $NaNO_3$)	0.45	-2.09	-2.09	0
OC - Secondary	0.36	0.379	0.045	0.334

Table – calculated source contributions for PM2.5 after accounting for changes made to A matrix in part D (1) of the assignment

D1 – PM10				
SOURCE	PM_{10}(Observed)	PM_{10}(Part B)	PM_{10}(Part D1)	Deviation (B – D1)
Geologic	31.78	12.83	12.84	-0.01
Motor Vehicles	6.8	5.89	5.85	0.04
Vegetative Burning	5.1	19.2	19	0.2
Primary Crude Oil	0.29	0.54	0.54	0
$(NH_4)_2SO_4$ - Secondary	3.58	3.47	3.47	0
NH_4NO_3 - Secondary	10.39	13.76	13.75	0.01
Seasalt (NaCl - $NaNO_3$)	0.96	-0.67	-0.67	0
OC - Secondary	0.07	-0.69	0.17	-0.86

Table – calculated source contributions for PM10 after accounting for changes made to A matrix in part D (1) of the assignment

Part 2: Change the % contribution of Si to 16% (from 23.2%) and Ca to 10% (from 2.98%) in paved road dust source. Change the % contribution of Si to 12% (from 6.5%) and Ca to 20% (from 29.52%) in limestone source. Evaluate the source contributions g_j using Equation 26.16 and tabulate the deviations with your answers in part B)

D2 – PM2.5				
SOURCE	$PM_{2.5}$ (0bserved)	$PM_{2.5}$ (Part B)	$PM_{2.5}$ (Part D2)	Deviation (B – D2)
Geologic	2.26	1.37	0.987	0.383
Motor Vehicles	9.24	8.62	8.78	-0.16
Vegetative Burning	5.92	7.01	7	0.01
Primary Crude Oil	0.25	0.33	0.33	0
$(NH_4)_2SO_4$ - Secondary	3.48	3.16	3.17	-0.01
NH_4NO_3 - Secondary	12.35	14.09	14.08	0.01
Seasalt (NaCl - $NaNO_3$)	0.45	-2.09	-2.07	-0.02
OC - Secondary	0.36	0.379	0.29	0.089

Table – calculated source contributions for PM2.5 after accounting for changes made to A matrix in part D (2) of the assignment

D2-PM10				
SOURCE	PM_{10}(Observed)	PM_{10}(Part B)	PM_{10}(Part D2)	Deviation (B – D2)
Geologic	31.78	12.83	10.32	2.51
Motor Vehicles	6.8	5.89	6.26	-0.37
Vegetative Burning	5.1	19.2	19.51	-0.31
Primary Crude Oil	0.29	0.54	0.55	-0.01
$(NH_4)_2SO_4$ - Secondary	3.58	3.47	3.53	-0.06
NH_4NO_3 - Secondary	10.39	13.76	13.68	0.08
Seasalt (NaCl - $NaNO_3$)	0.96	-0.67	-0.59	-0.08
OC - Secondary	0.07	-0.69	-0.92	0.23

Table – calculated source contributions for PM10 after accounting for changes made to A matrix in part D (2) of the assignment

Appendix

This zipped file contains the following files :

- PM2.5.ipynb and PM10.ipynb – These are jupyter source files, coded in python to run the code for assignment 1. Kindly Import these files in google colab or anything which supports jupyter notebooks. These files contain calculations of A,W,V,C and S

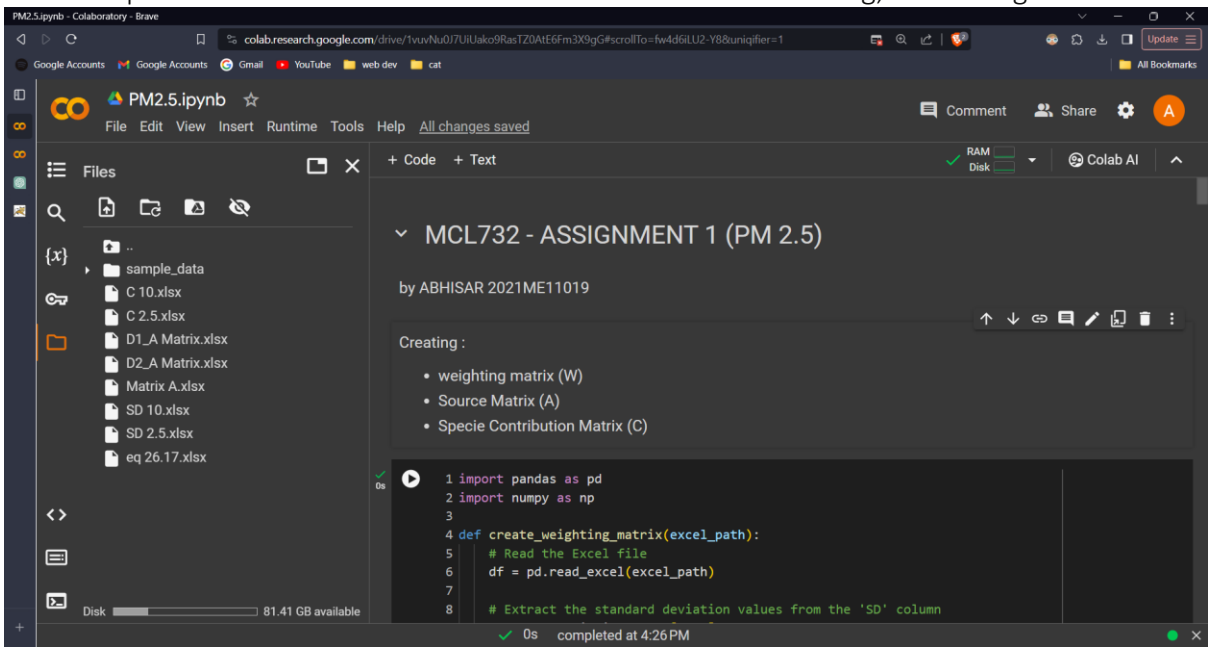
matrices. It also contains the code required for answering part b,c and d of the assignment.

Excel Files –

- C 2.5.xlsx and C 10.xlsx – these excel contain the contribution of each specie (c_i) for PM2.5 and PM10 respectively.
- Matrix A.xlsx – This file contains the source compositions. It is used for generating the A matrix (a_{ij})
- SD 2.5.xlsx and SD.xlsx – This file contains standard deviations for generating diagonal matrix W and V (w_{ii} and v_{ii} particularly for σ_{ii})
- Eq 26.17.xlsx - This file contains all values required to form V matrix particularly σ_{aij}.
- D1_A Matrix.xlsx and D2_A Matrix.xlsx – These file contain the changes made to Matrix A.xlsx to answer D part of the assignment, part 1 and part 2 respectively.

- PM2.5.pdf and PM10.pdf – These file are simply a pdf file of the code provided, with answer of each part of the assignment printed for PM2.5 and PM10 respectively.

Please import all the excels with same name in colab before running, something like this :



Incase the code does not run : Colab file links -
PM2.5 :
https://colab.research.google.com/drive/1vuvNu0J7UiUako9RasTZ0AtE6Fm3X9gG#scrollTo=fw4d6iLU2-Y8&uniqifier=1

PM10 :
https://colab.research.google.com/drive/11QHqpmHGsAbSw_GHAU7mJi8Y2C-iPA2_#scrollTo=fw4d6iLU2-Y8