Theoretical Methods Problem Sheet 1

Matrices, Determinants and Linear Equations

Evaluating determinants

Calculate the following matrix determinants:

1. $\begin{vmatrix} 1 & 8 \\ 6 & 2 \end{vmatrix}$ 2. $\begin{vmatrix} 2 & 3 \\ 4 & 1 \end{vmatrix}$ 3. $\begin{vmatrix} 3 & 2 \\ 1 & 6 \end{vmatrix}$

4. $\begin{vmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{vmatrix}$ 5. $\begin{vmatrix} 1 & 1 & 0 \\ 2 & 3 & 2 \\ 3 & 2 & 3 \end{vmatrix}$ 6. $\begin{vmatrix} 2 & 2 & 0 \\ 2 & 3 & 2 \\ 3 & 2 & 3 \end{vmatrix}$

Explain why the answers to questions 5. And 6. are related.

Solutions:

1. $\begin{vmatrix} 1 & 8 \\ 6 & 2 \end{vmatrix} = (1\times 2)-(8\times 6) = -46$

2. $\begin{vmatrix} 2 & 3 \\ 4 & 1 \end{vmatrix} = (2\times 1)-(3\times 4) = -10$

3. $\begin{vmatrix} 3 & 2 \\ 1 & 6 \end{vmatrix} = (3\times 6)-(2\times 1) = 16$

4. $\begin{vmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{vmatrix} = 1\times \begin{vmatrix} 1 & 1 \\ 1 & 1 \end{vmatrix} - 1 \begin{vmatrix} 1 & 1 \\ 0 & 1 \end{vmatrix} = 1\times 1 = -1$

   Note: Chose to expand from the first row but could have used any row or column.
   Note: Determinant zero when two rows or columns are the same (see ex. 5 too) – compare with Pauli exclusion principle and Slater determinants.

5. $\begin{vmatrix} 1 & 1 & 0 \\ 2 & 3 & 2 \\ 3 & 2 & 3 \end{vmatrix} = 1\times \begin{vmatrix} 3 & 2 \\ 2 & 3 \end{vmatrix} - 1\times \begin{vmatrix} 2 & 2 \\ 3 & 3 \end{vmatrix} = 1\times(9-4)-0 = 5$

6. $\begin{vmatrix} 2 & 2 & 0 \\ 2 & 3 & 2 \\ 3 & 2 & 3 \end{vmatrix} = 10$

   First row is simply twice that in ex. 5 so determinant must be 2x5=10.

Solving Systems of Linear Equations

Solve for x and y in the following sets of equations using the method of determinants

1. $\begin{aligned} 2x + y &= 4 \\ x + 2y &= 6 \end{aligned}$

2. $\begin{aligned} x + 3y &= 1 \\ 2x + 3y &= 2 \\ 3x + 4y &= 3 \end{aligned}$

Solutions
From the lectures, for the equations;

$$a_{11}x + a_{12}y = b_1$$
$$a_{21}x + a_{22}y = b_2$$

$$x = \frac{\begin{vmatrix} b_1 & b_2 \\ a_{12} & a_{22} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}} \qquad y = \frac{\begin{vmatrix} b_2 & b_1 \\ a_{21} & a_{11} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}}$$

1. $$x = \frac{(4\times 2)-(6\times 1)}{(2\times 2)-(1\times 1)} = \frac{2}{3}$$
   $$y = \frac{(6\times 2)-(4\times 1)}{3} = \frac{8}{3}$$
   Plug back in and check.

2. Three equations in two unknowns ? Take the first two equations and solve as in 1. to get x=1, y=0 – this also satisfies the third equations. Is the solution unique ? As it happens – yes; the first equation reduces to y=1/3(1-x) the second to 2/3(1-x) and the third to ¾(1-x) so, as it happens, all lines cross at the point x=1, y=0.

Spectroscopic Analysis

The use of the Beer Lambert law in spectroscopic analysis was mentioned in the lectures and the table of data included below was presented. Set up and solve the 4x4 system of equations needed to determine the concentrations in this system

	p-xylene	*m*-xylene	*o*-xylene	ethyl-benzene	A_{total}
λ	εl	εl	εl	εl	
12.5	1.502	0.0514	0	0.0408	0.1013
13.0	0.0261	1.1516	0	0.0820	0.09943
13.4	0.0342	0.0355	2.532	0.2933	0.2194
14.3	0.0340	0.0684	0	0.3470	0.03396

Solution:

This is four simultaneous equations as discussed in the lectures.

$$A_{total}(\lambda_1) = l\varepsilon_1(\lambda_1)c_1 + l\varepsilon_2(\lambda_1)c_2 + l\varepsilon_3(\lambda_1)c_3 + l\varepsilon_4(\lambda_1)c_4$$
$$A_{total}(\lambda_2) = l\varepsilon_1(\lambda_2)c_1 + l\varepsilon_2(\lambda_2)c_2 + l\varepsilon_3(\lambda_2)c_3 + l\varepsilon_4(\lambda_2)c_4$$
$$A_{total}(\lambda_3) = l\varepsilon_1(\lambda_3)c_1 + l\varepsilon_2(\lambda_3)c_2 + l\varepsilon_3(\lambda_3)c_3 + l\varepsilon_4(\lambda_3)c_4$$
$$A_{total}(\lambda_4) = l\varepsilon_1(\lambda_4)c_1 + l\varepsilon_2(\lambda_4)c_2 + l\varepsilon_3(\lambda_4)c_3 + l\varepsilon_4(\lambda_4)c_4$$

Or

$$\begin{pmatrix} l\varepsilon_1(\lambda_1) & l\varepsilon_2(\lambda_1) & l\varepsilon_3(\lambda_1) & l\varepsilon_4(\lambda_1) \\ l\varepsilon_1(\lambda_2) & l\varepsilon_2(\lambda_2) & l\varepsilon_3(\lambda_2) & l\varepsilon_4(\lambda_2) \\ l\varepsilon_1(\lambda_3) & l\varepsilon_2(\lambda_3) & l\varepsilon_3(\lambda_3) & l\varepsilon_4(\lambda_3) \\ l\varepsilon_1(\lambda_4) & l\varepsilon_2(\lambda_4) & l\varepsilon_3(\lambda_4) & l\varepsilon_4(\lambda_4) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} A_{total}(\lambda_1) \\ A_{total}(\lambda_2) \\ A_{total}(\lambda_3) \\ A_{total}(\lambda_4) \end{pmatrix}$$

In general, for a 4x4 problem

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

the solutions may be written as;

$$c_1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} & a_{14} \\ b_2 & a_{22} & a_{23} & a_{24} \\ b_3 & a_{32} & a_{33} & a_{34} \\ b_4 & a_{42} & a_{43} & a_{44} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix}} \qquad c_2 = \frac{\begin{vmatrix} a_{11} & b_1 & a_{13} & a_{14} \\ a_{21} & b_2 & a_{23} & a_{24} \\ a_{31} & b_3 & a_{33} & a_{34} \\ a_{41} & b_4 & a_{43} & a_{44} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix}}$$

etc.

ie: in the numerator determinant the right hand side vector simply replaces the column of data for the coefficient you want.

In this case the coefficients are therefore determined as;

$$c_1 = \frac{\begin{vmatrix} 0.1013 & 0.0514 & 0 & 0.0408 \\ 0.09943 & 1.1516 & 0 & 0.0820 \\ 0.2194 & 0.0355 & 2.532 & 0.2933 \\ 0.03396 & 0.0684 & 0 & 0.3470 \end{vmatrix}}{\begin{vmatrix} 1.502 & 0.0514 & 0 & 0.0408 \\ 0.0261 & 1.1516 & 0 & 0.0820 \\ 0.0342 & 0.0355 & 2.532 & 0.2933 \\ 0.0340 & 0.0684 & 0 & 0.3470 \end{vmatrix}} = \frac{0.094}{1.494} = 0.063$$

$$c_2 = \frac{\begin{vmatrix} 1.502 & 0.1013 & 0 & 0.0408 \\ 0.0261 & 0.09943 & 0 & 0.0820 \\ 0.0342 & 0.2194 & 2.532 & 0.2933 \\ 0.0340 & 0.03396 & 0 & 0.3470 \end{vmatrix}}{\begin{vmatrix} 1.502 & 0.0514 & 0 & 0.0408 \\ 0.0261 & 1.1516 & 0 & 0.0820 \\ 0.0342 & 0.0355 & 2.532 & 0.2933 \\ 0.0340 & 0.0684 & 0 & 0.3470 \end{vmatrix}} = \frac{0.119}{1.494} = 0.08$$

etc. to obtain c_3=0.076 and c_4 = 0.076

Thus from this data we deduce that the molar concentrations of p-, m-, o- xylene and ethylbenzene are 0.063, 0.08, 0.076 and 0.076 respectively.