Tyler Hancock

MATH 2270 – Professor Grant Gustafson

Semester Project

April 11, 2018

Application of Linear Algebra to the Beer-Lambert Law

The Beer-Lambert Law (sometimes referred to simply as Beer's Law) is a tool that is often used in analytical chemistry to solve for various aspects of a chemical mixture most notably the concentration of a particular species within a solution. The Beer-Lambert Law is derived from relationship between absorbance and transmittance of light.

- $A = \log(1/T)$
- $A = -\log(T)$

Where "A" is equal to the absorbance and "T" is equal to the transmittance.

This expression gives the true absorbance value of the species, in order to relate the measured absorbance with the true absorbance the solution has to be adequately diluted.

From this relationship and other derivations from the area and opaqueness of the surface that the light is being transmitted upon, he final and most useful equation becomes:

- $A = \varepsilon bc$

Where "A" is equal to the absorbance of the solution at a specific wavelength, "ε" equals the molar absorptivity in units of $M^{-1}cm^{-1}$ at the same wavelength, "b" is equal to the path length in centimeters, and "c" equals the concentration expressed in terms of molarity M (mols/L). A more accurate representation:

- $A_\lambda = \varepsilon_\lambda bc$

In order to use this expression, the sample must be measured using an absorbance spectrometer. During this process a sample is placed into a cell (cuvette) and the cell is then placed into the instrument which is set at a particular wavelength, at which the sample absorbs light. The instrument then reads out the absorbance of the solution. The path length (b) is the measurement of the length the light has to travel through the sample cell. The molar absorptivity (ε) is often determined through a least squares analysis, in which standard solutions of the sample at known concentrations are measured and plotted as a function of absorbance vs. concentration and the molar absorptivity is thus determined from the slope of the line. From this data the only quantity that is still unknown is the concentration of the sample which can now be determined through algebraic manipulation.

Anyhow that is the basic concept of the Beer-Lambert Law. Now for the purpose of this project which involves the use of linear algebra to solve these equations. It is likely that there are multiple components of a given mixture, which means that the equation is going to have to be solved multiple times and this is possible due to the fact that absorbance at a particular wavelength is additive.

- $A = \varepsilon_1 bc_1 + \varepsilon_2 bc_2 + \ldots$

This expression becomes even more valuable when the absorbance is measured at multiple different wavelengths. For example:

- $A^{\lambda 1} = \varepsilon_1^{\lambda 1} bc_1 + \varepsilon_2^{\lambda 1} bc_2$
- $A^{\lambda 2} = \varepsilon_1^{\lambda 2} bc_1 + \varepsilon_2^{\lambda 2} bc_2$

In this example there are two equations and two unknowns.

- If $\varepsilon_1^{\lambda 1} b = k_{11}$ and $\varepsilon_1^{\lambda 2} b = k_{21}$ etc.
- Then $A_1 = k_{11}c_1 + k_{12}c_2$ and $A_2 = k_{21}c_1 + k_{22}c_2$

These equations can then be put into matrix form in order to solve for the concentration of each species at each wavelength by multiplying the molar absorptivity (ε) by the path length (b).

$$\begin{bmatrix} A \\ A \end{bmatrix} = \begin{bmatrix} k_{1,1} & k_{1,2} \\ k_{2,1} & k_{2,2} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

Example 1: Find c_1 and c_2.

$A_1 = 0.2$
$\lambda = 600$ nm

$A_2 = 0.16$
$\lambda = 680$ nm

$K_{1,1} = 3500\ M^{-1}$ $K_{1,2} = 2800\ M^{-1}$

$K_{2,1} = 6400\ M^{-1}$ $K_{2,2} = 482\ M^{-1}$

Put into equation above and multiply both sides by the left inverse of K. The right side of the equation will yield the identity matrix which will allow for c_1 and c_2 to be determined. The inverse of K is:

By $\begin{bmatrix} -\frac{241}{8116500} & \frac{2}{11595} \\ \frac{32}{81165} & -\frac{1}{4638} \end{bmatrix}$ multiplying by the inverse the concentration (in Molarity M) is determined as:

$$\begin{bmatrix} 0.00002165958233228608 5 \\ 0.0000443540935132138 3 \end{bmatrix}$$

Example 2: Find c_1, c_2, and c_3.

$A_1 = 1.505$ $\lambda = 450$ nm

$A_2 = 0.73$ $\lambda = 500$ nm

$A_3 = 1.233$ $\lambda = 415$ nm

$K_{1,1} = 3438\ M^{-1}$	$K_{1,2} = 6237\ M^{-1}$	$K_{1,3} = 237\ M^{-1}$
$K_{2,1} = 1123\ M^{-1}$	$K_{2,2} = 448\ M^{-1}$	$K_{2,3} = 8874\ M^{-1}$
$K_{3,1} = 1434\ M^{-1}$	$K_{3,2} = 9600\ M^{-1}$	$K_{3,3} = 1002\ M^{-1}$

The inverse of K =

$$\begin{bmatrix} \frac{14123584}{36098143491} & \frac{220793}{12032714497} & -\frac{9206827}{36098143491} \\ -\frac{101755}{1899902289} & -\frac{9079}{633300763} & \frac{530573}{3799804578} \\ -\frac{1689728}{36098143491} & \frac{1336719}{12032714497} & \frac{607103}{24065428994} \end{bmatrix}$$

and thus c_1, c_2, and c3 (in Molarity M), respectively, are:

$$\begin{bmatrix} 0.0002877575380459612 \\ 0.00008109573339221341 \\ 0.00004175314358966351 4 \end{bmatrix}$$

Linear algebra allows for these equations to be computed rather easily, especially with the aid of mathematical software such as maple (which was used for this project). These equations can be solved in the traditional fashion via two-equations-two-unknowns, 3-equations-three-unknowns, etc. Though linear algebra simplifies the matter. This project shows that linear algebra has applications within many different fields and different aspects of said fields; chemistry is just one example. This particular application is not present within any of the course material for this class.