CHEM1033 - Week 6 Lecture - Algebraic equations

Sections 2.5 and 2.8 of Steiner, "The Chemistry Maths Book", 2nd edition.
Chapters 10 and 11 of Monk and Munro, "Maths for Chemistry", 2nd edition.

1. Systems of linear equations

A system of linear equations is a collection of linear equations for the same variables. Its general form is:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots a_{1N}x_N = b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots a_{2N}x_N = b_2 \\ \ldots \\ a_{M1}x_1 + a_{M2}x_2 + \ldots a_{MN}x_N = b_M \end{cases} \quad (1)$$

in which x_k are variables, a_{nk} are coefficients and b_k are colloquially known as the "right hand side". Two most popular ways of solving systems of linear equations using pencil and paper are:

1. Substitution: a given variable is made the subject in one equation and all of its instances in all other equations are replaced by the resulting expression. The process is repeated until a numerical value is obtained for one of the variables and then reversed to obtain numerical values for all other variables. Example:

$$\begin{cases} x+2y=8 \\ x-y=-1 \end{cases} \Rightarrow \begin{cases} x=8-2y \\ x-y=-1 \end{cases} \Rightarrow \begin{cases} x=8-2y \\ 8-2y-y=-1 \end{cases}$$
$$\Rightarrow \begin{cases} x=8-2y \\ y=3 \end{cases} \Rightarrow \begin{cases} x=2 \\ y=3 \end{cases} \quad (2)$$

2. Elimination: sums and differences of linear equations, with any coefficients, are just as valid as the original equations. This may be used to eliminate some variables. For example, in the following system, consider the sum and the difference of the two equations:

$$\begin{cases} 2x+y=4 \\ 2x-y=0 \end{cases} \Rightarrow \begin{cases} 4x=4 & \text{(sum)} \\ 2y=4 & \text{(difference)} \end{cases} \Rightarrow \begin{cases} x=1 \\ y=2 \end{cases} \quad (3)$$

This technique is particularly useful for handling thermodynamic relations in chemistry, where the task of finding thermodynamic parameters of a composite process is often encountered. The reaction arrow is effectively an equal sign. For example:

$$\begin{array}{ll} \mathrm{H_2(g)+1/2\,O_2(g)\rightarrow H_2O(l)} & \Delta H = -286\ \text{kJ/mol} \\ \mathrm{H_2O(l)\rightarrow H_2O(g)} & \Delta H = 44\ \text{kJ/mol} \\ \mathrm{3O_2(g)+B_2H_6(g)\rightarrow B_2O_3(s)+3H_2O(g)} & \Delta H = -2035\ \text{kJ/mol} \\ \mathrm{2B(s)+3H_2(g)\rightarrow B_2H_6(g)} & \Delta H = 36\ \text{kJ/mol} \\ \mathrm{2B(s)+3/2\,O_2(g)\rightarrow B_2O_3(s)} & \Delta H = ? \end{array}$$

After a bit of looking, we can start with the fourth equation and subtract three copies of the first one to get rid of the hydrogen on the left hand side:

$$\mathrm{2B(s)-3/2\,O_2(g)\rightarrow B_2H_6(g)-3H_2O(l)} \qquad \Delta H = 894\ \text{kJ/mol}$$

Adding the third equation would allow us to cancel $\mathrm{B_2H_6(g)}$ on either side:

$$\mathrm{2B(s)+3/2\,O_2(g)\rightarrow B_2O_3(s)-3H_2O(l)+3H_2O}(g) \qquad \Delta H = -1141\ \text{kJ/mol}$$

After moving liquid water over to the left hand side, we get:

$$2\mathrm{B(s)}+3/2\,\mathrm{O_2(g)}+3\mathrm{H_2O(l)}\rightarrow \mathrm{B_2O_3(s)}+3\mathrm{H_2O}(g) \qquad \Delta H=-1141\ \mathrm{kJ/mol}$$

What remains is to subtract three copies of the second equation to get rid of the water:

$$2\mathrm{B(s)}+3/2\,\mathrm{O_2(g)}\rightarrow \mathrm{B_2O_3(s)} \qquad \Delta H=-1273\ \mathrm{kJ/mol}$$

Note that modern computers use very different methods and routinely handle systems, including chemical systems, with thousands of equations (google BICGSTAB to find out more). Not all systems of linear equations have a unique solution. In general, three situations are possible:

1. The system has no solutions. This often happens when the number of equations M is greater than the number of variables N. Example:

$$\begin{cases} x+y=3 \\ x+2y=3 \\ 2x+y=3 \end{cases} \tag{4}$$

2. The system has exactly one solution. This situation requires that $N=M$ and that all equations in the system are linearly independent. Example:

$$\begin{cases} x+y=2 \\ x-y=0 \end{cases} \tag{5}$$

3. The system has infinitely many solutions. This is always the case when $N>M$. Example:

$$\{x-y=0 \tag{6}$$

We will look at these situations in more detail when we look at vectors and matrices later in the course – they require matrix arithmetic for a rigorous consideration.

2. Quadratic and higher order equations

You have likely seen the general solutions to quadratic equations already. Here's the derivation:

$$\begin{gathered} ax^2+bx+c=0 \quad\Rightarrow\quad x^2+\frac{b}{a}x+\frac{c}{a}=0 \quad\Rightarrow\quad x^2+\frac{b}{a}x=-\frac{c}{a} \\ x^2+\frac{b}{a}x+\left(\frac{b}{2a}\right)^2=-\frac{c}{a}+\left(\frac{b}{2a}\right)^2 \quad\Rightarrow\quad \left(x+\frac{b}{2a}\right)^2=\frac{b^2}{4a^2}-\frac{c}{a}=\frac{b^2-4ac}{4a^2} \\ x+\frac{b}{2a}=\pm\sqrt{\frac{b^2-4ac}{4a^2}}=\pm\frac{\sqrt{b^2-4ac}}{2a} \quad\Rightarrow\quad x=\frac{-b\pm\sqrt{b^2-4ac}}{2a} \end{gathered} \tag{7}$$

The quantity b^2-4ac under the square root is called the *discriminant*. We will eventually encounter situations when the discriminant is negative and square roots of negative numbers consequently make an appearance. Those are known as complex numbers, they will be considered later in this course.

Many equations may be reduced to quadratic equations by a variable substitution, for example:

$$\cos^2(x)+2\cos(x)+1=0 \quad\Rightarrow\quad \begin{cases} y^2+2y+1=0 \\ y=\cos(x) \end{cases} \tag{8}$$

In these cases first the quadratic equation is solved and then the substitution equation for each of the two solutions. Example:

$$x^4 - 4x^2 + 3 = 0 \quad \Rightarrow \quad \begin{cases} y = x^2 \\ y^2 - 4y + 3 = 0 \end{cases} \quad \Rightarrow \quad \left[\begin{array}{l} x^2 = 3 \\ x^2 = 1 \end{array} \right. \quad \Rightarrow \quad \left[\begin{array}{l} x = \pm\sqrt{3} \\ x = \pm 1 \end{array} \right. \tag{9}$$

More complicated expressions, which look broadly similar to Equation (7), exist for cubic and quartic equations, but quintic and higher order equations are not in general soluble using basic arithmetic operations and roots. This non-trivial fact was proven by Niels Abel in 1823.

3. Factorisation of polynomials

A *polynomial* is a function of the following general form:

$$p(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \ldots a_N x^N = \sum_{k=0}^{N} a_k x^k \tag{10}$$

where the capital sigma stands for a sum over the index k from $k = 0$ to $k = N$. It may be demonstrated (we will not prove this fact here) that any polynomial can be written as:

$$p(x) = (x - b_0)(x - b_1)\ldots(x - b_N) = \prod_{k=0}^{N} (x - b_k) \tag{11}$$

where b_k are solutions of $p(x) = 0$ and the capital pi stands for a product over the index k from $k = 0$ to $k = N$. The procedure of expressing a polynomial in this form is called *factorisation*. To factorise a polynomial $p(x)$, we must solve the corresponding $p(x) = 0$ equation and put the roots into Equation (11). As an example, let us write the polynomial from Equation (9) in a factorised form:

$$x^4 - 4x^2 + 3 = \left(x - \sqrt{3}\right)\left(x + \sqrt{3}\right)(x - 1)(x + 1) \tag{12}$$

Another example for a quadratic polynomial:

$$p(x) = x^2 - 5x + 6 \quad \Rightarrow \quad x^2 - 5x + 6 = 0 \quad \Rightarrow \quad \left[\begin{array}{l} x = 2 \\ x = 3 \end{array} \right. \quad \Rightarrow \quad p(x) = (x - 2)(x - 3)$$

The difference between the curly bracket (system of equations) and the square bracket (set of equations) is that equations in a system must hold *simultaneously*, whereas equations in a set are different instances of a particular problem or solution that are independent from each other.

4. Geometric meaning of equation systems

Every equation in a system containing two variables

$$\begin{cases} a_{11} x + a_{12} y = b_1 \\ a_{21} x + a_{22} y = b_2 \end{cases} \quad \Rightarrow \quad \begin{cases} y = -\dfrac{a_{11}}{a_{12}} x + \dfrac{b_1}{a_{12}} \\ y = -\dfrac{a_{21}}{a_{22}} x + \dfrac{b_2}{a_{22}} \end{cases} \tag{13}$$

may be viewed as an equation for a straight line. If these lines intersect, there is one point where both equations are true and that point is the solution. If the lines are parallel, they never intersect and there are therefore no solutions. If the two lines coincide, there are infinitely many solutions. The same applies to linear systems with three or more variables: in that case we are dealing with planes in 3D space or hyperplanes in spaces of a higher dimension.

Week 7 workshop exercises

Monk and Munro, 2nd edition: self-tests 7.6, 10.4; problems 7.8, 7.10, 10.6, 10.8, 10.9.

Steiner, 2nd edition: Section 2.9 (36-39, 66-73).

Extra difficulty exercises for the brave

1. Derive the conversion formula from the Celsius scale (°C) to the Fahrenheit scale (°F), given that 0°C corresponds to 32°F and 100°C corresponds to 212°F.

2. Solve the following systems of equations:

   (a) $\begin{cases} xy = 10 \\ x + y = 7 \end{cases}$; (b) $\begin{cases} xy = 6 \\ x^2 + y^2 = 13 \end{cases}$;

3. Solve the following systems of equations:

   (a) $\begin{cases} x - 2y + 3z = 7 \\ 2x + y + z = 4 \\ -3x + 2y - 2z = -10 \end{cases}$; (b) $\begin{cases} 2x - 4y + 5z = -33 \\ 4x - y = -5 \\ -2x + 2y - 3z = 19 \end{cases}$; (c) $\begin{cases} 3x + 5y + 7z = 34 \\ -x - y + 2z = 3 \\ 2x - y - z = -3 \end{cases}$

4. Solve the following equations (real roots only) by reducing them to quadratic equations:

   (a) $x^4 + 2x^2 - 3 = 0$

   (b) $2\cos^2(x) + \cos(x) - 1 = 0$

   (c) $x^{-6} - 9x^{-3} + 8 = 0$

   (d) $x - 9\sqrt{x} + 14 = 0$

5. Way back, in the era when computer games were still intellectually sophisticated, the following problem was offered by a genie in *Baldur's Gate 2*:

   A princess is as old as the prince will be when the princess is twice as old as the prince was when the princess' age was half the sum of their current ages. Which of the following could be true?

   (a) princess is 30, prince is 20

   (b) princess is 30, prince is 40

   (c) princess is 40, prince is 30

   (d) princess is 20, prince is 30

   (e) they are both the same age

   This is a surprisingly difficult question. Find the system of equations that it leads to and solve that system.