

13.1: The Solutions of Simultaneous Linear Equations

The concept of determinants has its origin in the solution of simultaneous linear equations. In physical chemistry, they are an important tool in quantum mechanics

Suppose you want to solve the following system of two equations with two unknowns (x and y):

$$a_1x + b_1y = c_1$$

$$a_2x + b_2y = c_2$$

In order to find y , we could use the following general procedure: we multiply the first equation by a_2 and the second by a_1 , and subtract one line from the other to cancel the term in x :

$$a_1x + b_1y = c_1 \xrightarrow{\times a_2} a_1a_2x + b_1a_2y = c_1a_2$$

$$a_2x + b_2y = c_2 \xrightarrow{\times a_1} a_1a_2x + b_2a_1y = c_2a_1$$

$$\left. \begin{array}{l} a_1a_2x + b_1a_2y = c_1a_2 \\ a_1a_2x + b_2a_1y = c_2a_1 \end{array} \right\} \rightarrow (b_2a_1 - b_1a_2)y = a_1c_2 - a_2c_1 \rightarrow y = \frac{a_1c_2 - a_2c_1}{b_2a_1 - b_1a_2}$$

We can follow the same strategy to find x : we multiply the first equation by b_2 and the second by b_1 , and subtract one line from the other to cancel the term in y :

$$a_1x + b_1y = c_1 \xrightarrow{\times b_2} a_1b_2x + b_1b_2y = c_1b_2$$

$$a_2x + b_2y = c_2 \xrightarrow{\times b_1} b_1a_2x + b_2b_1y = c_2b_1$$

$$\left. \begin{array}{l} a_1b_2x + b_1b_2y = c_1b_2 \\ b_1a_2x + b_2b_1y = c_2b_1 \end{array} \right\} \rightarrow (b_2a_1 - b_1a_2)x = b_2c_1 - b_1c_2 \rightarrow x = \frac{b_2c_1 - b_1c_2}{b_2a_1 - b_1a_2}$$

We define a 2×2 determinant as:

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - cb$$

The determinant, which is denoted with two parallel bars, is a number. For example,

$$\begin{vmatrix} 3 & -1 \\ 1/2 & 2 \end{vmatrix} = 3 \times 2 - (-1) \times 1/2 = 13/2$$

Let's look at the expressions we obtained for x and y , and write them in terms of determinants:

$$x = \frac{b_2c_1 - b_1c_2}{b_2a_1 - b_1a_2} = \frac{\begin{vmatrix} c_1 & b_1 \\ c_2 & b_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

$$y = \frac{a_1c_2 - a_2c_1}{b_2a_1 - b_1a_2} = \frac{\begin{vmatrix} a_1 & c_1 \\ a_2 & c_2 \end{vmatrix}}{\begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix}}$$

Let's look at our equations, and see how these determinants are constructed from the coefficients.

$$a_1x + b_1y = c_1$$

$$a_2x + b_2y = c_2$$

The determinant in the denominator of both x and y is the determinant of the coefficients on the left-side of the equal sign:

$$\left. \begin{array}{l} a_1x + b_1y = c_1 \\ a_2x + b_2y = c_2 \end{array} \right\} \left| \begin{array}{l} a_1 \quad b_1 \\ a_2 \quad b_2 \end{array} \right|$$

The numerator in the expression of y is built by replacing the coefficients in the y -column with the coefficients on the right side of the equation:

$$\left. \begin{array}{l} a_1x + b_1y = c_1 \\ a_2x + b_2y = c_2 \end{array} \right\} \left| \begin{array}{l} a_1 \quad c_1 \\ a_2 \quad c_2 \end{array} \right|$$

The numerator in the expression of x is built by replacing the coefficients in the x -column with the coefficients on the right side of the equation:

$$\left. \begin{array}{l} a_1x + b_1y = c_1 \\ a_2x + b_2y = c_2 \end{array} \right\} \left| \begin{array}{l} c_1 \quad b_1 \\ c_2 \quad b_2 \end{array} \right|$$

We can extend this idea to n equations with n unknowns $(x_1, x_2, x_3, \dots, x_n)$.

$$\begin{array}{cccccc} a_{11}x_1 & + & a_{12}x_2 & + & \cdots & + & a_{1n}x_n & = & b_1 \\ a_{21}x_1 & + & a_{22}x_2 & + & \cdots & + & a_{2n}x_n & = & b_2 \\ \vdots & & \vdots & & \ddots & & \vdots & & \vdots \\ a_{n1}x_1 & + & a_{n2}x_2 & + & \cdots & + & a_{nn}x_n & = & b_n \end{array}$$

Note that we use two subscripts to identify the coefficients. The first refers to the row, and the second to the column. Let's define the determinant D as the determinant of the coefficients of the equation (the ones on the left side of the equal sign):

$$D = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix}$$

and let's define the determinant D_k as the one obtained from D by replacement of the k th column of D by the column with elements b_1, b_2, \dots, b_n . For example, D_2 is

$$D_2 = \begin{vmatrix} a_{11} & b_1 & \cdots & a_{1n} \\ a_{21} & b_2 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & b_n & \cdots & a_{nn} \end{vmatrix}$$

The unknowns of the system of equations are calculated as:

$$x_1 = \frac{D_1}{D}, x_2 = \frac{D_2}{D}, \dots, x_n = \frac{D_n}{D}$$

For example, let's say we want to find x, y and z in the following system of equations:

$$\begin{array}{l} 2x + 3y + 8z = 0 \\ x - \frac{1}{2}y - 3z = \frac{1}{2} \\ -x - y - z = \frac{1}{2} \end{array}$$

We can calculate the unknowns as;

$$x = \frac{D_1}{D}, y = \frac{D_2}{D}, z = \frac{D_3}{D}$$

where

$$D = \begin{vmatrix} 2 & 3 & 8 \\ 1 & -1/2 & -3 \\ -1 & -1 & -1 \end{vmatrix}$$

$$D_1 = \begin{vmatrix} 0 & 3 & 8 \\ 1/2 & -1/2 & -3 \\ 1/2 & -1 & -1 \end{vmatrix}$$

$$D_2 = \begin{vmatrix} 2 & 0 & 8 \\ 1 & 1/2 & -3 \\ -1 & 1/2 & -1 \end{vmatrix}$$

$$D_3 = \begin{vmatrix} 2 & 3 & 0 \\ 1 & -1/2 & 1/2 \\ -1 & -1 & 1/2 \end{vmatrix}$$

In order to do this, we need to learn how to solve 3×3 determinants, or in general, $n \times n$ determinants.

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