Balancing Chemical Equations with Matrices

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1 Introduction

Balancing chemical equations can be seen as an algebraic problem, therefore reducing the trial and error processes required to obtain solutions for the coefficients of each compound. We are trying to find the coefficients for each compound in the equation that enable it to be valid. Linear algebra greatly simplifies this problem by allowing for efficient reduction and solving of large systems of equations where there are many coefficients to be found.

One can also solve such a problem computationally with a programming language. Here is a working chemical equation balancer written in Java.

2 Example and Solution

Take, for example, the reaction of ammonia (NH_3) and oxygen (O_2) to produce nitrogen (N_2) and water (H_2O) represented by the following unbalanced equation:

$$\mathrm{NH_3} + \mathrm{O_2} \longrightarrow \mathrm{N_2} + \mathrm{H_2O}$$

As the 4 coefficients for each reactant or product are unknown, we can then make the objective to solve for some $w,\ x,\ y,\ z\ \in \mathbb{R}$ in the following modified formula:

$$w\mathrm{NH_3} + x\mathrm{O_2} \longrightarrow y\mathrm{N_2} + z\mathrm{H_2O}$$

Now, we must consider the number of unique atoms in this equation. There are 3: Na, O, and H. Using this fact, we can write a system of 3 equations with 4 unknowns. For each equation, we consider a single atom and the number of that atom in each term of the chemical equation in terms of the coefficients $w,\ x,\ y,\ z$:

$$\begin{cases} \mathrm{Na} : w + 0x = 2y + 0z \\ \mathrm{O} : 0w + 2x = 0y + z \\ \mathrm{H} : 3w + 0x = 0y + 2z \end{cases}$$

We can then rewrite this a more formal system:

$$\begin{cases} w + 0x - 2y - 0z = 0 \\ 0w + 2x - 0y - z = 0 \\ 3w + 0x - 0y - 2z = 0 \end{cases}$$

Now, we can involve linear algebra through the introduction of matrices. This system can be written as the product of a matrix and a column vector in the form $A\vec{x} = \vec{b}$, where $\vec{b}$ is our solution vector that contains the numerical solution for $w,\ x,\ y,\ z$. Here is the matrix-vector equation for this system:

$$\begin{bmatrix} 1 & 0 & -2 & 0 \\ 0 & 2 & 0 & -1 \\ 3 & 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

This can be rewritten as the following augmented matrix, suitable for row-reduction. Once row reduction (Gauss-Jordan elimination) is completed, the resulting augmented matrix will indicate the solutions for our linear system. The following notation will use R_n for row n of the augmented matrix.

$$\left[\begin{array}{cccc|c} 1 & 0 & -2 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 \\ 3 & 0 & 0 & -2 & 0 \end{array}\right]$$

Subtracting $3R_1$ from R_3:

$$\left[\begin{array}{cccc|c} 1 & 0 & -2 & 0 & 0 \\ 0 & 2 & 0 & -1 & 0 \\ 0 & 0 & 6 & -2 & 0 \end{array}\right]$$

Dividing R_2 by 2 and R_3 by 6:

$$\left[\begin{array}{cccc|c} 1 & 0 & -2 & 0 & 0 \\ 0 & 1 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 & -\frac{1}{3} & 0 \end{array}\right]$$

Lastly, adding $2R_3$ to R_1:

$$\left[\begin{array}{cccc|c} 1 & 0 & 0 & -\frac{2}{3} & 0 \\ 0 & 1 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 1 & -\frac{1}{3} & 0 \end{array}\right]$$

We now have the following relations:

$$w = \frac{2}{3}z$$
$$x = \frac{1}{2}z$$
$$y = \frac{1}{3}z$$

Therefore, z is considered a free variable and can be parameterized with some $t = z \in \mathbb{R}$. Then, we can write the solution vector in the following form:

$$\begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{2}{3}t \\ \frac{1}{2}t \\ \frac{1}{3}t \\ t \end{bmatrix} = t \begin{bmatrix} \frac{2}{3} \\ \frac{1}{2} \\ \frac{1}{3} \\ 1 \end{bmatrix}$$

Now, finding a unique solution vector $\vec{b}$ is a matter of finding t such that all entries in $\vec{b}$, or $w,\ x,\ y,\ z$ are positive integers in order to satisfy the requirements for a balanced chemical equation. Note that there are infinite solutions where $t \in \mathbb{R}$ but we want to put constraints such that we get a valid balanced equation. Mathematically, these are $t > 0$ and $t\vec{b} \in Z$. We then find that $t = 6$ satisfies this condition. Thus,

$$\boxed{\vec{b} = \begin{bmatrix} 4 \\ 3 \\ 2 \\ 6 \end{bmatrix} = \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix}}$$

We can finally conclude that the balanced equation is the following, which should prove valid with use of the brute-force technique:

$$\boxed{4\mathrm{NH}_3 + 3\mathrm{O}_2 \longrightarrow 2\mathrm{N}_2 + 6\mathrm{H}_2\mathrm{O}}$$

3 Conclusions

Clearly, the use of matrices involves a more mathematical approach to this problem, but is a more computationally efficient way to balance chemical equations. The advantages to this method become more apparent when programming is used to find solutions, as well as when large and complicated reactions are provided with n terms. As for simple reactions such as this, either method can be used since one can intuitively visualize the solution beforehand.