2. Balancing a chemical reaction

Let's consider the problem of balancing a chemical reaction. Suppose that we need to find the smallest positive integers a, b, c, and d that balance the reaction

$$a\mathrm{NO_2} + b\mathrm{H_2O} \longrightarrow c\mathrm{HNO_2} + d\mathrm{HNO_3}.$$

The constraint that the number of nitrogen atoms on the left and right hand sides of the reaction must be equal says that

$$a = c + d,$$

which can be rewritten as $a - c - d = 0$. Similarly, there is a constraint on the number of oxygen and hydrogen atoms on both sides of the equation. These equations constitute a linear system

$$\begin{aligned} a \quad\;\; - c - \; d &= 0 \qquad\qquad (\text{nitrogen}) \\ 2a + b - 2c - 3d &= 0 \qquad\qquad (\text{oxygen}) \\ 2b - \; c - \; d &= 0 \qquad\qquad (\text{hydrogen}). \end{aligned}$$

This linear system in matrix form $\mathbf{Ax} = \mathbf{b}$ is

$$\underbrace{\begin{pmatrix} 1 & 0 & -1 & -1 \\ 2 & 1 & -2 & -3 \\ 0 & 2 & -1 & -1 \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}}_{\mathbf{x}} = \underbrace{\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}}_{\mathbf{b}},$$

which can be represented by the augmented matrix

$$\left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 2 & 1 & -2 & -3 & 0 \\ 0 & 2 & -1 & -1 & 0 \end{array}\right).$$

Definition 2.1 A linear system is **homogeneous** if the right hand sides (the constants in the vector $\mathbf{b}$) are all zero, and **inhomogeneous** otherwise. So a linear system is homogeneous if and only if the zero vector is a solution.

To solve a homogeneous system, we use elimination to put the augmented matrix in row echelon form. The leftmost pivot in each subsequent column is denoted in blue as we move through the steps of the algorithm. (The augmented column is all zeros, so it contains no extra information. It would be OK to leave this column off, but we will keep it in order to have a uniform approach for both homogeneous and inhomogeneous systems.)

$$\mathbf{A} = \left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 2 & 1 & -2 & -3 & 0 \\ 0 & 2 & -1 & -1 & 0 \end{array}\right) \longrightarrow \left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 2 & -1 & -1 & 0 \end{array}\right) \longrightarrow \left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 & 0 \end{array}\right)$$

Let $\mathbf{U}$ be the row echelon form of $\mathbf{A}$ that we just found. Then solving the system $\mathbf{Ux} = \mathbf{0}$ is equivalent to solving $\mathbf{Ax} = \mathbf{0}$. The system $\mathbf{Ux} = \mathbf{0}$ written as a system of equations is

$$\begin{aligned} a \quad - c - d &= 0 \\ b \quad - d &= 0 \\ - c + d &= 0. \end{aligned}$$

Recall that in back-substitution we solve for the variables in reverse order. If a variable corresponds to a pivot column, then some equation expresses it in terms of later variables. Recall that the variables, corresponding to non-pivot columns, are called free variables. And each free variable requires a new parameter. In this case, our free variable is d; its value can be any real number. So we rename this variable to be a parameter $d = t$.

We solve the system for c, b, and a in terms of the free parameter t by plugging in the found values at each step:

$$\begin{aligned} d &= t \\ c &= d = t \\ b &= d = t \\ a &= c + d = 2t. \end{aligned}$$

Written as vectors, the solutions to the system have the form

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = t \begin{pmatrix} 2 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \qquad \text{where } t \text{ is any real number.}$$

In other words, the solutions are exactly the scalar multiples of the vector $\begin{pmatrix} 2 \\ 1 \\ 1 \\ 1 \end{pmatrix}$. In particular, there are infinitely many of them.

But the problem was to find the *smallest* positive integers a, b, c, and d that balance the reaction.The smallest such integers occur when $t = 1$, so the balanced chemical reaction is

$$\mathbf{2NO_2 + H_2O \longrightarrow HNO_2 + HNO_3.}$$

Note: We solved the system by converting the matrix to row echelon form. Let's now solve it again, by going further to find the **reduced** row echelon form. Once the matrix is in this form, each row expresses a pivot variable directly in terms of free variables, so we can write down the solution immediately.

Find the reduced row echelon form

1/1 point (graded)
Find $\mathtt{rref}(\mathbf{A})$ for the matrix in the example above.

$$\mathbf{A} = \left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 2 & 1 & -2 & -3 & 0 \\ 0 & 2 & -1 & -1 & 0 \end{array}\right)$$

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

- $\left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 & 0 \end{array}\right)$

- $\left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \end{array}\right)$

$$\left(\begin{array}{cccc|c} 1 & 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \end{array}\right)$$

$$\left(\begin{array}{cccc|c} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{array}\right)$$

Solution:

We start with the row echelon form found above, and perform the steps of the algorithm to reduce the matrix to reduced echelon form. The leftmost pivot in each subsequent column is denoted in blue as we move through the steps of the algorithm.

$$\left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 1 & 0 \end{array}\right) \longrightarrow \left(\begin{array}{cccc|c} 1 & 0 & -1 & -1 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \end{array}\right) \longrightarrow \left(\begin{array}{cccc|c} 1 & 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -1 & 0 \end{array}\right) = \mathbf{rref}(\mathbf{A}).$$

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Using reduced row echelon form

Let $\mathbf{R}$ be the reduced row echelon form $\mathbf{rref}(\mathbf{A})$. Then the solutions to $\mathbf{Ax} = \mathbf{0}$ are the same as the solutions to $\mathbf{Rx} = \mathbf{0}$, which is the system

$$\begin{aligned} a \qquad - 2d &= 0 \\ b \quad - d &= 0 \\ c - d &= 0. \end{aligned}$$

The **pivot variables** are a , b , and c . The only **free variable** is d . We set the free variable d equal to a parameter, say t. For each pivot variable, there is an equation expressing it in terms of d , so we can immediately write down the general solution in terms of t:

$$\begin{aligned} d &= t \\ a &= 2t \end{aligned}$$

$$b = t$$
$$c = t.$$

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