CHEM 3PC3 - Mathematical Tools for Chemical Problems

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November 18, 2026

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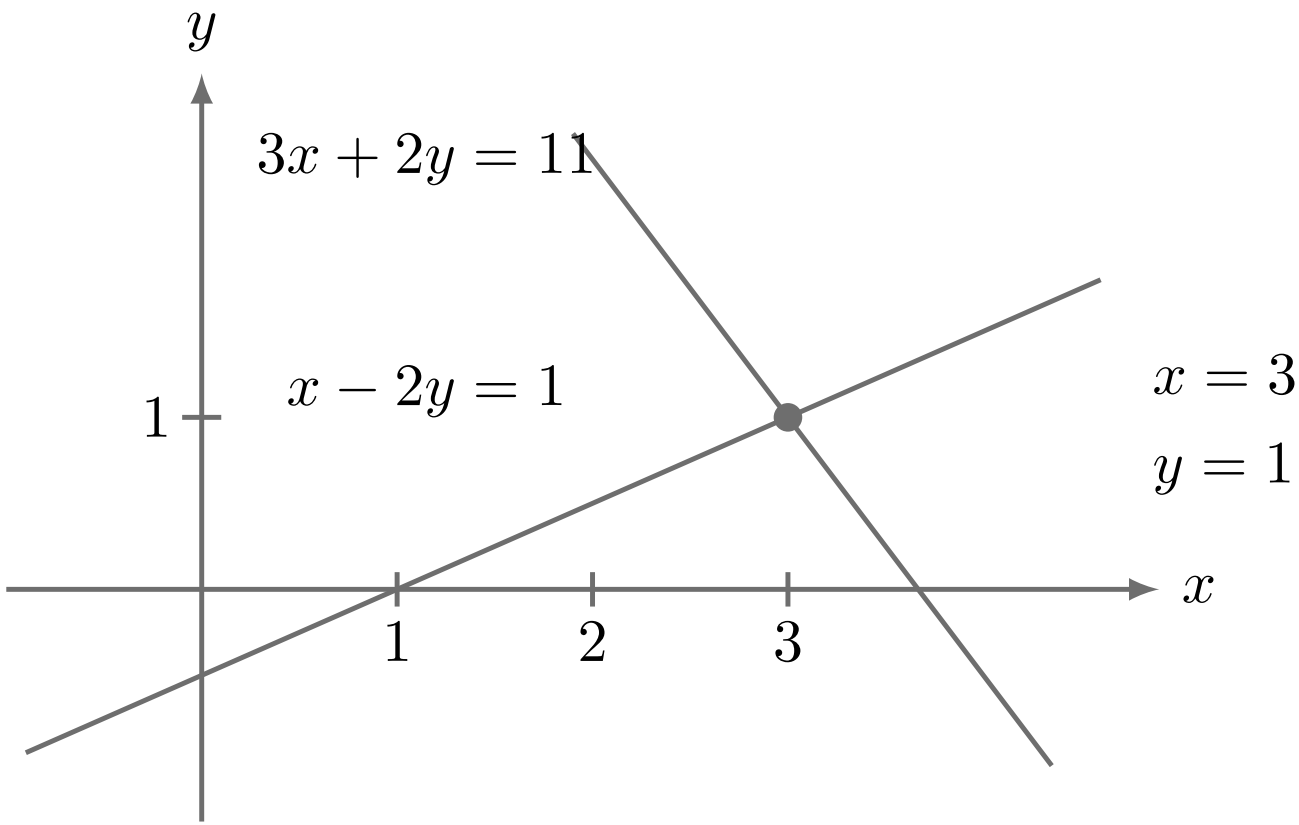
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- The two equations represent lines in the xy plane.
- If we plot the graph of the two we can see the solution at (3,1) where the lines meet.

Two lines meet at a point



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- We are multiplying the first vector by x and the second by y, and adding.
- With the right choice $x = 3$ and $y = 1$ this produces $\mathbf{b}$.

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- So we have a linear combination:

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- To solve this system we can use elimination.

Elimination

- We can multiply equation 1 by 3 and subtract to eliminate $3x$.

Before	$x - 2y = 1$	**After**	$x - 2y = 1$	(*multiply equation* 1 *by* 3)
	$3x + 2y = 11$		$8y = 8$	(*subtract to eliminate* $3x$)

- Elimination produces an upper triangular system - this is the goal.
- Then you solve the system from the bottom upwards.

Elimination: a 4×4 system

- Solve

$$\begin{cases} 2x_1 + 4x_2 - 2x_3 + 2x_4 = 14 \\ 4x_1 + 9x_2 - 3x_3 + 7x_4 = 34 \\ -2x_1 - 3x_2 + 6x_3 + 2x_4 = -9 \\ 2x_1 + 6x_2 + 3x_3 + 11x_4 = 29 \end{cases}$$

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- Same idea, one more round: equation 1 removes x_1 from equations 2, 3, 4. Then equation 2 removes x_2 from 3 and 4. Then equation 3 removes x_3 from 4.

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- Same idea, one more round: equation 1 removes x_1 from equations 2, 3, 4. Then equation 2 removes x_2 from 3 and 4. Then equation 3 removes x_3 from 4.
- What is left is a triangular system that we solve from the bottom up.

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$$\begin{aligned} \text{eq } 2 - 2(\text{eq } 1): &\quad x_2 + x_3 + 3x_4 = 6 \\ \text{eq } 3 + (\text{eq } 1): &\quad x_2 + 4x_3 + 4x_4 = 5 \\ \text{eq } 4 - (\text{eq } 1): &\quad 2x_2 + 5x_3 + 9x_4 = 15 \end{aligned}$$

Step 2: eliminate x_2

- The system is now

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$$\text{eq } 3 - (\text{eq } 2): \qquad 3x_3 + x_4 = -1$$

$$\text{eq } 4 - 2(\text{eq } 2): \qquad 3x_3 + 3x_4 = 3$$

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$$\begin{aligned} (3x_3 + 3x_4) - (3x_3 + x_4) &= 3 - (-1) \\ 2x_4 &= 4 \end{aligned}$$

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- Now solve from the bottom up — **back substitution**.

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- From the fourth equation:

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$$3x_3 + 2 = -1 \qquad \Longrightarrow \qquad x_3 = -1$$
- Put $x_3 = -1$ and $x_4 = 2$ into the second equation:
$$x_2 - 1 + 6 = 6 \qquad \Longrightarrow \qquad x_2 = 1$$

Back substitution

- Finally the first equation:

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- The solution is $(x_1, x_2, x_3, x_4) = (2, 1, -1, 2)$.

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$$\begin{aligned}
2(2) + 4(1) - 2(-1) + 2(2) &= 4 + 4 + 2 + 4 = 14 \quad \checkmark \\
4(2) + 9(1) - 3(-1) + 7(2) &= 8 + 9 + 3 + 14 = 34 \quad \checkmark \\
-2(2) - 3(1) + 6(-1) + 2(2) &= -4 - 3 - 6 + 4 = -9 \quad \checkmark \\
2(2) + 6(1) + 3(-1) + 11(2) &= 4 + 6 - 3 + 22 = 29 \quad \checkmark
\end{aligned}$$

The matrix form $A\mathbf{x} = \mathbf{b}$

- The coefficients go into A, the unknowns into $\mathbf{x}$, the right hand sides into $\mathbf{b}$:

$$A = \begin{bmatrix} 2 & 4 & -2 & 2 \\ 4 & 9 & -3 & 7 \\ -2 & -3 & 6 & 2 \\ 2 & 6 & 3 & 11 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 14 \\ 34 \\ -9 \\ 29 \end{bmatrix}$$

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- $A\mathbf{x}$ is the combination of the columns of A using 2, 1, -1, 2:

$$2\begin{bmatrix} 2 \\ 4 \\ -2 \\ 2 \end{bmatrix} + 1\begin{bmatrix} 4 \\ 9 \\ -3 \\ 6 \end{bmatrix} - 1\begin{bmatrix} -2 \\ -3 \\ 6 \\ 3 \end{bmatrix} + 2\begin{bmatrix} 2 \\ 7 \\ 2 \\ 11 \end{bmatrix} = \begin{bmatrix} 14 \\ 34 \\ -9 \\ 29 \end{bmatrix} = \mathbf{b}$$

What elimination did to A

- Elimination turned A into an upper triangular matrix U, and $\mathbf{b}$ into a new right hand side $\mathbf{c}$:

$$U = \begin{bmatrix} 2 & 4 & -2 & 2 \\ 0 & 1 & 1 & 3 \\ 0 & 0 & 3 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix} \qquad \mathbf{c} = \begin{bmatrix} 14 \\ 6 \\ -1 \\ 4 \end{bmatrix}$$

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- A 4×4 needs six multipliers instead of three. For $n \times n$ it is about $n^3/3$ operations — this is why we let the computer do it.