Linear Algebra for Chemists — Assignment 3

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Question 1. $\vec{w} = (-3, 4, 7, 1, 2, -9)$.

1. $\vec{x} = (9, 21, 3, 6, -4, 15)$.

$$\begin{aligned}\vec{w} \cdot \vec{x} &= (-3, 4, 7, 1, 2, -9) \cdot (9, 21, 3, 6, -4, 15)\\ &= -27 + 84 + 21 + 6 - 8 - 135\\ &= -59.\end{aligned}$$

2. $\vec{x} = (2, 0, 0, -13, -18, 6)$.

$$\begin{aligned}\vec{w} \cdot \vec{x} &= (-3, 4, 7, 1, 2, -9) \cdot (2, 0, 0, -13, -18, 6)\\ &= -6 - 13 - 36 - 54\\ &= -109.\end{aligned}$$

Question 2.

1.
$$A\,v = \begin{bmatrix} -1 & 0 & 1\\ 0 & 3 & 2\\ 9 & -2 & 6 \end{bmatrix} \begin{bmatrix} 4\\ -3\\ 2 \end{bmatrix} = \begin{bmatrix} -4+2\\ -9+4\\ 36+6+12 \end{bmatrix} = \begin{bmatrix} -2\\ -5\\ 54 \end{bmatrix}$$

2.
$$v^T v = [\,4 \quad -3 \quad 2\,] \begin{bmatrix} 4\\ -3\\ 2 \end{bmatrix} = 16 + 9 + 4 = 29$$

3.
$$v\,v^T = \begin{bmatrix} 4\\ -3\\ 2 \end{bmatrix} [\,4 \quad -3 \quad 2\,] = \begin{bmatrix} 4\cdot 4 & 4\cdot(-3) & 4\cdot 2\\ -3\cdot 4 & (-3)\cdot(-3) & (-3)\cdot 2\\ 2\cdot 4 & 2\cdot(-3) & 2\cdot 2 \end{bmatrix} = \begin{bmatrix} 16 & -12 & 8\\ -12 & 9 & -6\\ 8 & -6 & 4 \end{bmatrix}$$

4.
$$\begin{aligned} v^T A\,v = [\,4 \quad -3 \quad 2\,] \begin{bmatrix} -1 & 0 & 1\\ 0 & 3 & 2\\ 9 & -2 & 6 \end{bmatrix} \begin{bmatrix} 4\\ -3\\ 2 \end{bmatrix} &= [\,4 \quad -3 \quad 2\,] \begin{bmatrix} -2\\ -5\\ 54 \end{bmatrix}\\ &= -8 + 15 + 108 = 115 \end{aligned}$$

5.
$$\begin{aligned} A^T A &= \begin{bmatrix} -1 & 0 & 9\\ 0 & 3 & -2\\ 1 & 2 & 6 \end{bmatrix} \begin{bmatrix} -1 & 0 & 1\\ 0 & 3 & 2\\ 9 & -2 & 6 \end{bmatrix}\\ &= \begin{bmatrix} 1+81 & -18 & -1+54\\ -18 & 9+4 & 6-12\\ -1+54 & 6-12 & 1+4+36 \end{bmatrix} = \begin{bmatrix} 82 & -18 & 53\\ -18 & 13 & -6\\ 53 & -6 & 41 \end{bmatrix} \end{aligned}$$

6.

$$
\begin{aligned}
2AB &= 2\begin{bmatrix} -1 & 0 & 1 \\ 0 & 3 & 2 \\ 9 & -2 & 6 \end{bmatrix}\begin{bmatrix} 2 & 7 & -1 & 4 \\ 0 & 3 & 2 & 4 \\ 0 & 0 & 0 & 1 \end{bmatrix} \\
&= 2\begin{bmatrix} -2 & -7 & 1 & -4+1 \\ 0 & 9 & 6 & 12+2 \\ 18 & 63-6 & -9-4 & 36-8+6 \end{bmatrix} = \begin{bmatrix} -4 & -14 & 2 & -6 \\ 0 & 18 & 12 & 28 \\ 36 & 114 & -26 & 68 \end{bmatrix}
\end{aligned}
$$

7.

$$
AD = \begin{bmatrix} -1 & 0 & 1 \\ 0 & 3 & 2 \\ 9 & -2 & 6 \end{bmatrix}\begin{bmatrix} 4 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 2 \end{bmatrix} = \begin{bmatrix} (-1)\cdot 4 & 0 & 1\cdot 2 \\ 0 & 3\cdot(-3) & 2\cdot 2 \\ 9\cdot 4 & (-2)\cdot(-3) & 6\cdot 2 \end{bmatrix} = \begin{bmatrix} -4 & 0 & 2 \\ 0 & -9 & 4 \\ 36 & 6 & 12 \end{bmatrix}
$$

8.

$$
DA = \begin{bmatrix} 4 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 2 \end{bmatrix}\begin{bmatrix} -1 & 0 & 1 \\ 0 & 3 & 2 \\ 9 & -2 & 6 \end{bmatrix} = \begin{bmatrix} 4\cdot(-1) & 0 & 4\cdot 1 \\ 0 & (-3)\cdot(-3) & (-3)\cdot 2 \\ 2\cdot 9 & 2\cdot(-2) & 2\cdot 6 \end{bmatrix} = \begin{bmatrix} -4 & 0 & 4 \\ 0 & -9 & -6 \\ 18 & -4 & 12 \end{bmatrix}
$$

9.

$$
B^T A = \begin{bmatrix} 2 & 0 & 0 \\ 7 & 3 & 0 \\ -1 & 2 & 0 \\ 4 & 4 & 1 \end{bmatrix}\begin{bmatrix} -1 & 0 & 1 \\ 0 & 3 & 2 \\ 9 & -2 & 6 \end{bmatrix} = \begin{bmatrix} -2 & 0 & 2 \\ -7 & 9 & 7+6 \\ 1 & 6 & -1+4 \\ -4+9 & 12-2 & 4+8+6 \end{bmatrix} = \begin{bmatrix} -2 & 0 & 2 \\ -7 & 9 & 13 \\ 1 & 6 & 3 \\ 5 & 10 & 18 \end{bmatrix}
$$

10.

$$
\begin{aligned}
v^T B u &= \begin{bmatrix} 4 & -3 & 2 \end{bmatrix}\begin{bmatrix} 2 & 7 & -1 & 4 \\ 0 & 3 & 2 & 4 \\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 9 \\ 3 \\ -4 \\ -2 \end{bmatrix} \\
&= \begin{bmatrix} 4 & -3 & 2 \end{bmatrix}\begin{bmatrix} 18+21+4-8 \\ 9-8-8 \\ -2 \end{bmatrix} = \begin{bmatrix} 4 & -3 & 2 \end{bmatrix}\begin{bmatrix} 35 \\ -7 \\ -2 \end{bmatrix} \\
&= 140+21-4 = 157
\end{aligned}
$$

11.

$$
v^T D v = \begin{bmatrix} 4 & -3 & 2 \end{bmatrix}\begin{bmatrix} 4 & 0 & 0 \\ 0 & -3 & 0 \\ 0 & 0 & 2 \end{bmatrix}\begin{bmatrix} 4 \\ -3 \\ 2 \end{bmatrix} = \begin{bmatrix} 4 & -3 & 2 \end{bmatrix}\begin{bmatrix} 16 \\ 9 \\ 4 \end{bmatrix} = 64-27+8 = 45
$$

12. Calculate via Gauss-Seidel method.

$$
[D \mid I] = \left[\begin{array}{ccc|ccc} 4 & 0 & 0 & 1 & 0 & 0 \\ 0 & -3 & 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 0 & 0 & 1 \end{array}\right] \xrightarrow[R_3 \to \frac{1}{2}R_3]{\substack{R_1 \to \frac{1}{4}R_1 \\ R_2 \to -\frac{1}{3}R_2}} \left[\begin{array}{ccc|ccc} 1 & 0 & 0 & \frac{1}{4} & 0 & 0 \\ 0 & 1 & 0 & 0 & -\frac{1}{3} & 0 \\ 0 & 0 & 1 & 0 & 0 & \frac{1}{2} \end{array}\right] = [I \mid D^{-1}].
$$

$$
D^{-1} = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & -\frac{1}{3} & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix}
$$

Question 3.

a) By definition, for square $n \times n$ matrices A, B, we have

$$(A\,B)^T_{ji} = (A\,B)_{ij} = \sum_{k=1}^{n} A_{ik}\,B_{kj}\,.$$

On the other hand,

$$(B^T A^T)_{ji} = \sum_{k=1}^{n} B^T_{jk}\,A^T_{ki}\,.$$

Using $B^T_{jk} = B_{kj}$ and $A^T_{ki} = A_{ik}$,

$$\sum_{k=1}^{n} B^T_{jk}\,A^T_{ki}, = \sum_{k=1}^{n} B_{kj}\,A_{ik} = \sum_{k=1}^{n} A_{ik}\,B_{kj} = (A\,B)_{ij}\,.$$

By transitivity, we get that each element in $(A\,B)^T$ equals each element in $B^T A^T$. We can conclude then that $(A\,B)^T = B^T A^T$.

b) Matrix A is symmetric if $A = A^T$. Let $B \equiv A\,A^T$.

$$B^T = (A\,A^T)^T = (A^T A)\,.$$

Since $A = A^T$, we can write

$$B^T = (A\,A^T) \equiv B\,.$$

B is symmetric. Let $C \equiv (A + A^T)$.

$$C^T = (A + A^T)^T = (A^T + A)\,.$$

Because matrix addition is commutative, we have

$$C^T = (A + A^T) \equiv C\,.$$

C is symmetric.

c) A is invertible. Therefore, there exists A^{-1} such that

$$A\,A^{-1} = I, \qquad A^{-1}\,A = I\,.$$

Transpose both sides of the expression:

$$(A\,A^{-1})^T = I^T = I = (A^{-1})^T A^T\,.$$

Since A is symmetric,

$$(A^{-1})^T A^T = (A^{-1})^T A = I\,.$$

Multiply on the right by A^{-1},

$$(A^{-1})^T A\,A^{-1} = (A^{-1})^T = A^{-1}\,.$$

We thus proved that if A is invertible and symmetric then also its inverse is symmetric.

d) Let A, B be symmetric matrices, i.e. $A^T = A$, $B^T = B$. The matrix $A\,B$ is symmetric if and only if

$$(A\,B)^T = A\,B.$$

By definition,

$$(A\,B)^T = B^T A^T.$$

Applying symmetry, we get

$$B^T A^T = B\,A.$$

Comining the above equations, we get

$$(A\,B)^T = A\,B = B\,A,$$

so $A\,B = B\,A$. Conversely, if $A\,B = B\,A$, then

$$(A\,B)^T = (B\,A)^T = A^T B^T = A\,B,$$

so $A\,B$ is symmetric.

Question 4. Let there be two matrices A, B such that

$$A\,A^{-1} = I, \quad A^{-1}A = I, \quad B\,B^{-1} = I, \quad B^{-1}B = I$$

The product $A\,B$ is invertible if and only if there is a matrix C such that

$$(A\,B)\,C = C\,(A\,B) = I.$$

We show that $C = B^{-1}A^{-1}$.

$$A\,B\,B^{-1}A^{-1} = A\,I\,A^{-1} = A\,A^{-1} = I,$$

and

$$B^{-1}A^{-1}A\,B = B^{-1}I\,B = B^{-1}B = I.$$

We thus proved that $A\,B$ is invertible, and the matrix C satisfies: $C = (A\,B)^{-1} = B^{-1}A^{-1}$.

Question 5.

1.

$$A = \begin{bmatrix} 1 & -1 & 0 \\ -3 & 4 & 6 \\ 4 & -5 & -6 \end{bmatrix} \xrightarrow[R_3 \to R_3 - 4R_1]{R_2 \to R_2 + 3R_1} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & 6 \\ 0 & -1 & -6 \end{bmatrix} \xrightarrow{R_3 \to R_3 + R_2} \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & 6 \\ 0 & 0 & 0 \end{bmatrix}$$

$\mathrm{rank}(A) = 2$, as it's row-echelon form has 2 non-zero rows.

2.

$$A = \begin{bmatrix} 1 & 2 & 5 \\ -1 & 6 & 6 \\ 4 & -5 & -6 \end{bmatrix} \xrightarrow[R_3 \to R_3 - 4R_1]{R_2 \to R_2 + R_1} \begin{bmatrix} 1 & 2 & 5 \\ 0 & 8 & 11 \\ 0 & -13 & -26 \end{bmatrix} \xrightarrow{R_3 \to R_3 + \frac{13}{8}R_2} \begin{bmatrix} 1 & 2 & 5 \\ 0 & 8 & 11 \\ 0 & 0 & -\frac{65}{8} \end{bmatrix}$$

$\operatorname{rank}(A) = 3$, as it's row-echelon form has 3 non-zero rows.

3.

$$A = \begin{bmatrix} 1 & 4 & -3 & 2 \\ 1 & 2 & -1 & 0 \\ -1 & 1 & 0 & -1 \\ 2 & -2 & 7 & 0 \\ 0 & 1 & 3 & 5 \end{bmatrix} \xrightarrow[R_3 \to R_3 + R_1]{\substack{R_2 \to R_2 + R_3 \\ R_4 \to R_4 + 2R_3}} \begin{bmatrix} 1 & 4 & -3 & 2 \\ 0 & 3 & -1 & -1 \\ 0 & 5 & -3 & 1 \\ 0 & 0 & 7 & -2 \\ 0 & 1 & 3 & 5 \end{bmatrix} \xrightarrow[R_2 \leftrightarrow R_5]{\substack{R_2 \to R_2 - 3R_5 \\ R_3 \to R_3 - 5R_5}}$$

$$\begin{bmatrix} 1 & 4 & -3 & 2 \\ 0 & 1 & 3 & 5 \\ 0 & 0 & -18 & -24 \\ 0 & 0 & 7 & -2 \\ 0 & 0 & -10 & -16 \end{bmatrix} \xrightarrow{R_3 \to R_3/(-18)} \begin{bmatrix} 1 & 4 & -3 & 2 \\ 0 & 1 & 3 & 5 \\ 0 & 0 & 1 & \frac{4}{3} \\ 0 & 0 & 7 & -2 \\ 0 & 0 & -10 & -16 \end{bmatrix} \xrightarrow[R_5 \to R_5 + 10R_3]{R_4 \to R_4 - 7R_3}$$

$$\begin{bmatrix} 1 & 4 & -3 & 2 \\ 0 & 1 & 3 & 5 \\ 0 & 0 & 1 & \frac{4}{3} \\ 0 & 0 & 0 & -\frac{34}{3} \\ 0 & 0 & 0 & -\frac{14}{3} \end{bmatrix} \xrightarrow{R_5 \to R_5 - \frac{34}{14} R_4} \begin{bmatrix} 1 & 4 & -3 & 2 \\ 0 & 1 & 3 & 5 \\ 0 & 0 & 1 & \frac{4}{3} \\ 0 & 0 & 0 & -\frac{34}{3} \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$\operatorname{rank}(A) = 4$, as it's row-echelon form has 4 non-zero rows.