CHEM 3PC3 - Mathematical Tools for Chemical Problems

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Linear Algebra

- The heart of linear algebra consists in two operations: We add vectors $\mathbf{v} + \mathbf{w}$ and we multiply then by numbers to get $c\mathbf{v}$ and $d\mathbf{w}$.
- Combining those two:

$$c\mathbf{v} + d\mathbf{w} = c\begin{bmatrix}1\\1\end{bmatrix} + d\begin{bmatrix}2\\3\end{bmatrix} = \begin{bmatrix}c+2d\\c+3d\end{bmatrix}$$

- We have a linear combination.
- Linear combinations are really important, and sometimes we want a particular one that reproduces a desired result.

Vectors and linear combination

1. $3\mathbf{v} + 5\mathbf{w}$ is a typical **linear combination** $c\mathbf{v} + d\mathbf{w}$ of the vectors $\mathbf{v}$ and $\mathbf{w}$.
2. For $\mathbf{v} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\mathbf{w} = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$ that combination is

$$3\begin{bmatrix} 1 \\ 1 \end{bmatrix} + 5\begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 3+10 \\ 3+15 \end{bmatrix} = \begin{bmatrix} 13 \\ 18 \end{bmatrix}.$$

3. The vector $\begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 3 \end{bmatrix}$ goes across to $x = 2$ and up to $y = 3$ in the xy plane.

Vectors and linear combination

Vector addition

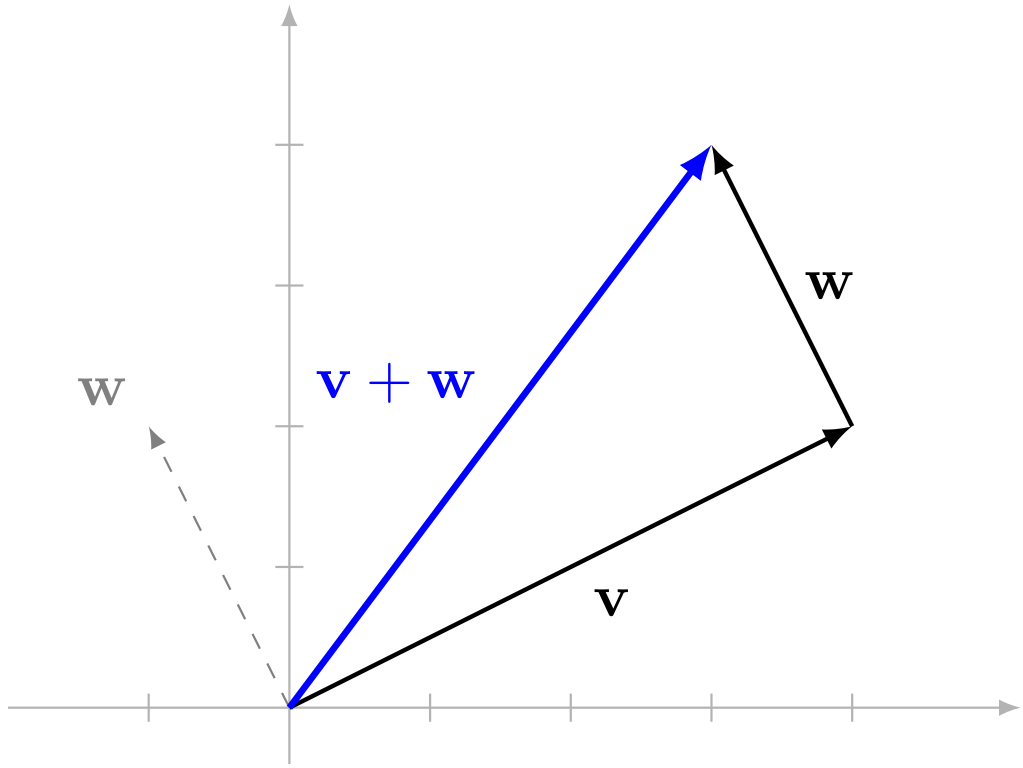
$$\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad \text{and} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \quad \text{add to} \quad \mathbf{v} + \mathbf{w} = \begin{bmatrix} v_1 + w_1 \\ v_2 + w_2 \end{bmatrix}$$

Scalar multiplication

$$2\mathbf{v} = \begin{bmatrix} 2v_1 \\ 2v_2 \end{bmatrix} = \mathbf{v} + \mathbf{v} \qquad -\mathbf{v} = \begin{bmatrix} -v_1 \\ -v_2 \end{bmatrix}$$

Geometric Representation

Vector addition (head to tail)



$$\mathbf{v} + \mathbf{w} = \begin{bmatrix} 4 \\ 2 \end{bmatrix} + \begin{bmatrix} -1 \\ 2 \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$$

Lengths and Dot Products

1. The "dot product" of $\mathbf{v} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ and $\mathbf{w} = \begin{bmatrix} 4 \\ 5 \end{bmatrix}$ is $\mathbf{v} \cdot \mathbf{w} = (1)(4) + (2)(5) = 4 + 10 = \mathbf{14}$.
2. $\mathbf{v} = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}$ and $\mathbf{w} = \begin{bmatrix} 4 \\ -4 \\ 4 \end{bmatrix}$ are perpendicular because $\mathbf{v} \cdot \mathbf{w}$ is zero:

$$(1)(4) + (3)(-4) + (2)(4) = \mathbf{0}.$$

3. The length squared of $\mathbf{v} = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}$ is $\mathbf{v} \cdot \mathbf{v} = 1 + 9 + 4 = 14$.
4. Then $\mathbf{u} = \frac{\mathbf{v}}{\|\mathbf{v}\|} = \frac{\mathbf{v}}{\sqrt{14}} = \frac{1}{\sqrt{14}} \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}$ has length $\|\mathbf{u}\| = 1$.
5. The angle θ between $\mathbf{v}$ and $\mathbf{w}$ has $\cos\theta = \frac{\mathbf{v} \cdot \mathbf{w}}{\|\mathbf{v}\| \, \|\mathbf{w}\|}$.

Cross Product

DEFINITION The *cross product* of $\mathbf{u} = (u_1, u_2, u_3)$ and $\mathbf{v} = (v_1, v_2, v_3)$ is a vector

$$\mathbf{u}\times\mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} = (u_2v_3 - u_3v_2)\,\mathbf{i} + (u_3v_1 - u_1v_3)\,\mathbf{j} + (u_1v_2 - u_2v_1)\,\mathbf{k}. \tag{1}$$

This vector $\mathbf{u} \times \mathbf{v}$ *is perpendicular to* $\mathbf{u}$ *and* $\mathbf{v}$. The cross product $\mathbf{v} \times \mathbf{u}$ is $-(\mathbf{u} \times \mathbf{v})$.

Cross Product

Property 1 $\mathbf{v} \times \mathbf{u}$ reverses rows 2 and 3 in the determinant so it equals $-(\mathbf{u} \times \mathbf{v})$.

Property 2 The cross product $\mathbf{u} \times \mathbf{v}$ is perpendicular to $\mathbf{u}$ (and also to $\mathbf{v}$).

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$$\mathbf{u}\cdot(\mathbf{u}\times\mathbf{v}) = u_1(u_2v_3-u_3v_2)+u_2(u_3v_1-u_1v_3)+u_3(u_1v_2-u_2v_1) = 0.$$

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Property 3 The cross product of any vector with itself (two equal rows) is $\mathbf{u} \times \mathbf{u} = \mathbf{0}$.

When $\mathbf{u}$ and $\mathbf{v}$ are parallel, the cross product is zero. When $\mathbf{u}$ and $\mathbf{v}$ are perpendicular, the dot product is zero. One involves $\sin\theta$ and the other involves $\cos\theta$:

$$\|\mathbf{u} \times \mathbf{v}\| = \|\mathbf{u}\|\,\|\mathbf{v}\|\,|\sin\theta| \qquad \text{and} \qquad |\mathbf{u} \cdot \mathbf{v}| = \|\mathbf{u}\|\,\|\mathbf{v}\|\,|\cos\theta|.$$

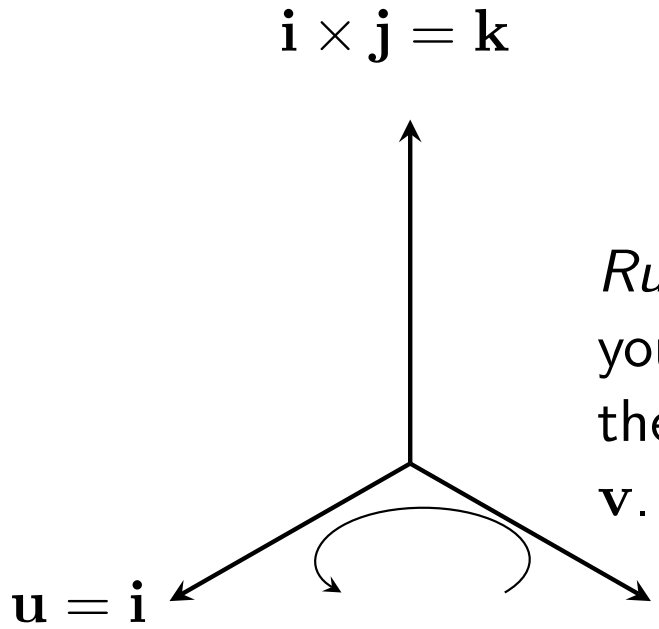
Examples

Example 1 Draw the cross product of $\mathbf{i} = (1, 0, 0)$ and $\mathbf{j} = (0, 1, 0)$ (it obeys the *right hand rule*)

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$$\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{vmatrix} = \mathbf{k}$$



Rule $\mathbf{u} \times \mathbf{v}$ points along your right thumb when the fingers curl from $\mathbf{u}$ to $\mathbf{v}$.

Examples

Thus $\mathbf{i} \times \mathbf{j} = \mathbf{k}$. The right hand rule also gives $\mathbf{j} \times \mathbf{k} = \mathbf{i}$ and $\mathbf{k} \times \mathbf{i} = \mathbf{j}$. Note the cyclic order. In the opposite order (anti-cyclic) the thumb is reversed and the cross product goes the other way: $\mathbf{k} \times \mathbf{j} = -\mathbf{i}$ and $\mathbf{i} \times \mathbf{k} = -\mathbf{j}$ and $\mathbf{j} \times \mathbf{i} = -\mathbf{k}$. You see the three plus signs and three minus signs from a 3 by 3 determinant.

Examples

Example 2 $\mathbf{u} = (3, 2, 0)$ and $\mathbf{v} = (1, 4, 0)$ are in the xy plane, $\mathbf{u} \times \mathbf{v}$ goes up the z axis:

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$$\mathbf{u}\times\mathbf{v} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 3 & 2 & 0 \\ 1 & 4 & 0 \end{vmatrix} = 10\mathbf{k}. \qquad \text{The cross product is } \mathbf{u}\times\mathbf{v} = (0, 0, 10).$$

The length of $\mathbf{u} \times \mathbf{v}$ *equals the area of the parallelogram with sides* $\mathbf{u}$ *and* $\mathbf{v}$*.* This will be important: In this example the area is 10.

Example 3 The cross product of $\mathbf{u} = (1, 1, 1)$ and $\mathbf{v} = (1, 1, 2)$ is $(1, -1, 0)$:

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$$\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 1 & 1 \\ 1 & 1 & 2 \end{vmatrix} = \mathbf{i}\begin{vmatrix} 1 & 1 \\ 1 & 2 \end{vmatrix} - \mathbf{j}\begin{vmatrix} 1 & 1 \\ 1 & 2 \end{vmatrix} + \mathbf{k}\begin{vmatrix} 1 & 1 \\ 1 & 1 \end{vmatrix} = \mathbf{i} - \mathbf{j}.$$

This vector $(1, -1, 0)$ is perpendicular to $(1, 1, 1)$ and $(1, 1, 2)$ as predicted. Area $= \sqrt{2}$.

Important Remarks

- The dot product is a scalar.
- The cross product is a vector.
- If the vectors are perpendicular then the dot product is zero.
- The cross product $\mathbf{u} \times \mathbf{v}$ is perpendicular to $\mathbf{u}$ and $\mathbf{v}$. Notice $\mathbf{i} \times \mathbf{j} = \mathbf{k}$.

Matrices

1. $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$ is a 3 by 2 matrix: $m = 3$ rows and $n = 2$ columns.
2. $A\mathbf{x} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ is a **combination of the columns**

$$A\mathbf{x} = x_1 \begin{bmatrix} 1 \\ 3 \\ 5 \end{bmatrix} + x_2 \begin{bmatrix} 2 \\ 4 \\ 6 \end{bmatrix}.$$

3. The 3 components of $A\mathbf{x}$ are dot products of the 3 rows of A with the vector $\mathbf{x}$:

Row at a time
$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix} \begin{bmatrix} 7 \\ 8 \end{bmatrix} = \begin{bmatrix} 1 \cdot 7 + 2 \cdot 8 \\ 3 \cdot 7 + 4 \cdot 8 \\ 5 \cdot 7 + 6 \cdot 8 \end{bmatrix} = \begin{bmatrix} 23 \\ 53 \\ 83 \end{bmatrix}.$$

Matrices

1. Equations in matrix form $A\mathbf{x} = \mathbf{b}$:

$$\begin{bmatrix} 2 & 5 \\ 3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad \text{replaces} \quad \begin{aligned} 2x_1 + 5x_2 &= b_1 \\ 3x_1 + 7x_2 &= b_2 \end{aligned}$$

2. The solution to $A\mathbf{x} = \mathbf{b}$ can be written as $\mathbf{x} = A^{-1}\mathbf{b}$. But some matrices don't allow A^{-1}.

Matrices

This section starts with three vectors $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$. I will combine them using *matrices*.

Three vectors $\mathbf{u} = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$ $\mathbf{v} = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}$ $\mathbf{w} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$.

Their linear combinations in three-dimensional space are $x_1\mathbf{u} + x_2\mathbf{v} + x_3\mathbf{w}$:

Combination of the vectors

$$x_1 \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} + x_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 - x_1 \\ x_3 - x_2 \end{bmatrix}.$$

Now something important: Rewrite that combination using a matrix. The vectors $\mathbf{u}$, $\mathbf{v}$, $\mathbf{w}$ go into the columns of the matrix A.

Matrices

$$A\mathbf{x} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 - x_1 \\ x_3 - x_2 \end{bmatrix}. \qquad (2)$$

The numbers x_1, x_2, x_3 are the components of a vector $\mathbf{x}$. The matrix A times the vector $\mathbf{x}$ is the **same** as the combination $x_1\mathbf{u} + x_2\mathbf{v} + x_3\mathbf{w}$ of the three columns.

Combination of the vectors

$$x_1 \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix} + x_2 \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix} + x_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 - x_1 \\ x_3 - x_2 \end{bmatrix}.$$

Matrices

- At first, the numbers x_1, x_2, x_3 were multiplying the vectors. Now the matrix is multiplying those numbers. The matrix A acts on the vector $\mathbf{x}$. The output $A\mathbf{x}$ is a combination $\mathbf{b}$ of the columns of A.
- To see that action, I will write b_1, b_2, b_3 for the components of $A\mathbf{x}$:

$$A\mathbf{x} = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 \\ x_2 - x_1 \\ x_3 - x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} = \mathbf{b}. \quad (3)$$

Matrix Multiplication

The big question is: **How do we multiply two matrices?** When the first matrix is E, we know what to expect for EA.

$$EA = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ -2 & -3 & 7 \end{bmatrix} \tag{4}$$

Associative law is true $A(BC) = (AB)C$

Commutative law is false Often $AB \neq BA$

Matrix Multiplication

Multiply these matrices in the orders EF and FE:

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \qquad F = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 4 & 1 \end{bmatrix}.$$

EF step by step

Each entry $(EF)_{ij}$ is row i of E dotted with column j of F:

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 0 & 1 \end{bmatrix} \qquad F = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 4 & 1 \end{bmatrix}$$

$$\text{row } 1 = (1,0,0): \qquad \begin{aligned} (1,1) &= 1(1) + 0(0) + 0(0) = 1 \\ (1,2) &= 1(0) + 0(1) + 0(4) = 0 \\ (1,3) &= 1(0) + 0(0) + 0(1) = 0 \end{aligned}$$

EF step by step

$$\text{row } 2 = (2,1,0): \qquad (2,1) = 2(1) + 1(0) + 0(0) = 2$$
$$(2,2) = 2(0) + 1(1) + 0(4) = 1$$
$$(2,3) = 2(0) + 1(0) + 0(1) = 0$$

$$\text{row } 3 = (3,0,1): \qquad (3,1) = 3(1) + 0(0) + 1(0) = 3$$
$$(3,2) = 3(0) + 0(1) + 1(4) = 4$$
$$(3,3) = 3(0) + 0(0) + 1(1) = 1$$

$$EF = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 4 & 1 \end{bmatrix}$$

FE step by step

Now row i of F dotted with column j of E:

$$\text{row } 1 = (1,0,0): \quad (1,1) = 1(1)+0(2)+0(3) = 1$$
$$(1,2) = 1(0)+0(1)+0(0) = 0$$
$$(1,3) = 1(0)+0(0)+0(1) = 0$$

$$\text{row } 2 = (0,1,0): \quad (2,1) = 0(1)+1(2)+0(3) = 2$$
$$(2,2) = 0(0)+1(1)+0(0) = 1$$
$$(2,3) = 0(0)+1(0)+0(1) = 0$$

FE step by step

$$\text{row } 3 = (0,4,1): \qquad \begin{aligned}(3,1) &= 0(1)+4(2)+1(3) = 11\\ (3,2) &= 0(0)+4(1)+1(0) = 4\\ (3,3) &= 0(0)+4(0)+1(1) = 1\end{aligned}$$

$$FE = \begin{bmatrix}1 & 0 & 0\\ 2 & 1 & 0\\ 11 & 4 & 1\end{bmatrix} \neq \begin{bmatrix}1 & 0 & 0\\ 2 & 1 & 0\\ 3 & 4 & 1\end{bmatrix} = EF$$

Transpose Matrix

1 The transposes of $A\mathbf{x}$ and AB and A^{-1} are $\mathbf{x}^{\mathrm{T}}A^{\mathrm{T}}$ and $B^{\mathrm{T}}A^{\mathrm{T}}$ and $(A^{\mathrm{T}})^{-1}$.

The **"transpose"** of A, which is denoted by A^{T}. *The columns of A^{T} are the rows of A.*

When A is an m by n matrix, the transpose is n by m:

Transpose If $A = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 0 & 4 \end{bmatrix}$ then $A^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 2 & 0 \\ 3 & 4 \end{bmatrix}$.

You can write the rows of A into the columns of A^{T}. Or you can write the columns of A into the rows of A^{T}:

Exchange rows and columns $(A^{\mathrm{T}})_{ij} = A_{ji}$.

Transpose Matrix

If $B = [\,\mathbf{x}_1 \;\; \mathbf{x}_2\,]$ has two columns, apply the same idea to each column. The columns of AB are $A\mathbf{x}_1$ and $A\mathbf{x}_2$. Their transposes appear correctly in the rows of $B^{\mathrm{T}}A^{\mathrm{T}}$:

$$\text{Transposing } \; AB = \begin{bmatrix} A\mathbf{x}_1 & A\mathbf{x}_2 & \cdots \end{bmatrix} \quad \text{gives} \quad \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}}A^{\mathrm{T}} \\ \mathbf{x}_2^{\mathrm{T}}A^{\mathrm{T}} \\ \vdots \end{bmatrix}$$

which is $\mathrm{B}^{\mathrm{T}}A^{\mathrm{T}}$.

Transpose Matrix

The right answer $B^{\mathrm{T}}A^{\mathrm{T}}$ comes out a row at a time. Here are numbers in $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{\mathrm{T}}$:

$$AB = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 5 & 0 \\ 4 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 0 \\ 9 & 1 \end{bmatrix}$$

$$B^{\mathrm{T}}A^{\mathrm{T}} = \begin{bmatrix} 5 & 4 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 9 \\ 0 & 1 \end{bmatrix}$$

Transpose Matrix

Verify that $(AB)^{\mathrm{T}}$ equals $B^{\mathrm{T}}A^{\mathrm{T}}$ but those are different from $A^{\mathrm{T}}B^{\mathrm{T}}$:

$$A = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} \qquad B = \begin{bmatrix} 1 & 3 \\ 0 & 1 \end{bmatrix} \qquad AB = \begin{bmatrix} 1 & 3 \\ 2 & 7 \end{bmatrix}.$$

Show also that AA^{T} is different from $A^{\mathrm{T}}A$. But both of those matrices are symmetric.

Step 1: AB and its transpose

$$AB = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1(1)+0(0) & 1(3)+0(1) \\ 2(1)+1(0) & 2(3)+1(1) \end{bmatrix} = \begin{bmatrix} 1 & 3 \\ 2 & 7 \end{bmatrix}$$

$$(AB)^{\mathrm{T}} = \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

Step 2: $B^{\mathrm{T}}A^{\mathrm{T}}$ gives the same answer

Flip each matrix first:

$$A^{\mathrm{T}} = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \qquad B^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix}$$

$$B^{\mathrm{T}}A^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1(1)+0(0) & 1(2)+0(1) \\ 3(1)+1(0) & 3(2)+1(1) \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

This is exactly $(AB)^{\mathrm{T}}$.

Step 3: the wrong order $A^{\mathrm{T}}B^{\mathrm{T}}$

$$A^{\mathrm{T}}B^{\mathrm{T}} = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 1(1)+2(3) & 1(0)+2(1) \\ 0(1)+1(3) & 0(0)+1(1) \end{bmatrix} = \begin{bmatrix} 7 & 2 \\ 3 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 7 & 2 \\ 3 & 1 \end{bmatrix} \neq \begin{bmatrix} 1 & 2 \\ 3 & 7 \end{bmatrix}$$

so the order matters: $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{\mathrm{T}}$.

Step 4: AA^{T} against $A^{\mathrm{T}}A$

$$AA^{\mathrm{T}} = \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix}$$

$$A^{\mathrm{T}}A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 2 & 1 \end{bmatrix} = \begin{bmatrix} 5 & 2 \\ 2 & 1 \end{bmatrix}$$

They are different, but each one equals its own transpose: both are symmetric.