CHEM 3PC3 - Mathematical Tools for Chemical Problems

Alexandre de Camargo

November 6, 2026

Commutation between matrices

- When multiplying matrices the commutative law is usually broken.

$$AB \neq BA$$

Commutation between matrices

- When multiplying matrices the commutative law is usually broken.

$$AB \neq BA$$

- When two matrices commute $[A, B] = 0$.

Commutation between matrices

- When multiplying matrices the commutative law is usually broken.

$$AB \neq BA$$

- When two matrices commute $[A, B] = 0$.
- The $[$ symbol indicates:

$$[A, B] = AB - BA$$

Commutation between matrices

- When multiplying matrices the commutative law is usually broken.

$$AB \neq BA$$

- When two matrices commute $[A, B] = 0$.
- The $[$ symbol indicates:

$$[A, B] = AB - BA$$

- In quantum mechanics the position matrix P and the momentum matrix Q do not commute.

$$QP - PQ = I$$

- If we knew the position exactly, we could not also know the momentum exactly (Heinsenberg Principle).

Commutation between matrices

- When multiplying matrices the commutative law is usually broken.

$$AB \neq BA$$

- When two matrices commute $[A, B] = 0$.
- The $[$ symbol indicates:

$$[A, B] = AB - BA$$

- In quantum mechanics the position matrix P and the momentum matrix Q do not commute.

$$QP - PQ = I$$

- If we knew the position exactly, we could not also know the momentum exactly (Heinsenberg Principle).
- Moving to transposition of matrices now.

Transpose Matrix

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

Transpose Matrix

- 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

- 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 $(A^{\mathrm{T}})_{ij} = A_{ji}$.

- The transpose of A^{T} is A.

$$(A^{\mathrm{T}})^{\mathrm{T}} = A$$

Transpose Matrix

- The rules of transpose are very direct. We can transpose $A + B$ to get $(A + B)^{\mathrm{T}}$ or we can transpose A and B separately and then add $A^{\mathrm{T}} + B^{\mathrm{T}}$ and get the same result.

Transpose Matrix

- The rules of transpose are very direct. We can transpose $A + B$ to get $(A + B)^{\mathrm{T}}$ or we can transpose A and B separately and then add $A^{\mathrm{T}} + B^{\mathrm{T}}$ and get the same result.
- The serious questions are about the transpose of a product AB and an inverse A^{-1}.

Transpose Matrix

- The rules of transpose are very direct. We can transpose $A + B$ to get $(A + B)^{\mathrm{T}}$ or we can transpose A and B separately and then add $A^{\mathrm{T}} + B^{\mathrm{T}}$ and get the same result.
- The serious questions are about the transpose of a product AB and an inverse A^{-1}.
- For now it is sufficient to know that for a square matrix A the inverse is $A^{-1}A = AA^{-1} = I$, where I is the identity matrix.
- Example a 4x4 identity matrix is:

$$I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Transpose Matrix

- The rules of transpose are very direct. We can transpose $A + B$ to get $(A + B)^{\mathrm{T}}$ or we can transpose A and B separately and then add $A^{\mathrm{T}} + B^{\mathrm{T}}$ and get the same result.
- The serious questions are about the transpose of a product AB and an inverse A^{-1}.
- For now it is sufficient to know that for a square matrix A the inverse is $A^{-1}A = AA^{-1} = I$, where I is the identity matrix.
- Example a 4x4 identity matrix is:

$$I = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Multiplying any matrix by I leaves it unchanged:

$$\begin{bmatrix} 1 & 2 & 0 & 3 \\ 0 & 4 & 1 & 2 \\ 5 & 0 & 2 & 1 \\ 3 & 1 & 0 & 6 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 0 & 3 \\ 0 & 4 & 1 & 2 \\ 5 & 0 & 2 & 1 \\ 3 & 1 & 0 & 6 \end{bmatrix}$$

Transpose of a product

- The transpose of $(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^T$. How to prove this ?

Transpose of a product

- The transpose of $(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^{T}$. How to prove this ?
- We can start thinking of B as just a vector $\mathbf{x}$. So we need to calculate $(A\mathbf{x})^{\mathrm{T}}$.

Transpose of a product

- The transpose of $(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^T$. How to prove this ?
- We can start thinking of B as just a vector $\mathbf{x}$. So we need to calculate $(A\mathbf{x})^{\mathrm{T}}$.
- Take $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ and $\mathbf{x} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

Transpose of a product

- The transpose of $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{T}$. How to prove this ?
- We can start thinking of B as just a vector $\mathbf{x}$. So we need to calculate $(A\mathbf{x})^{\mathrm{T}}$.
- Take $A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ and $\mathbf{x} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$.

$$A\mathbf{x} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = \begin{bmatrix} 1(1)+2(2) \\ 3(1)+4(2) \end{bmatrix} = \begin{bmatrix} 5 \\ 11 \end{bmatrix}$$

$$(A\mathbf{x})^{\mathrm{T}} = \begin{bmatrix} 5 & 11 \end{bmatrix}$$

$$\mathbf{x}^{\mathrm{T}}A^{\mathrm{T}} = \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 1(1)+2(2) & 1(3)+2(4) \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 11 \end{bmatrix}$$

- So $(A\mathbf{x})^{\mathrm{T}} = \mathbf{x}^{\mathrm{T}}A^{\mathrm{T}}$.

Transpose of a product

- The right answer $B^{\mathrm{T}}A^{\mathrm{T}}$ comes out a row at a time.

Transpose of a product

- The right answer $B^{\mathrm{T}}A^{\mathrm{T}}$ comes out a row at a time.
- If $B = [\,\mathbf{x}_1 \;\; \mathbf{x}_2\,]$ has two columns, apply the same idea to each column.

Transpose of a product

- The right answer $B^{\mathrm{T}}A^{\mathrm{T}}$ comes out a row at a time.
- If $B = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$ 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 $B^{\mathrm{T}}A^{\mathrm{T}}$:

$$\text{Transposing} \quad AB \quad = \quad \begin{bmatrix} A\mathbf{x}_1 & A\mathbf{x}_2 & \cdots \end{bmatrix}$$

$$\text{gives} \quad \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}}A^{\mathrm{T}} \\ \mathbf{x}_2^{\mathrm{T}}A^{\mathrm{T}} \\ \vdots \end{bmatrix} \qquad \text{which is } B^{\mathrm{T}}A^{\mathrm{T}}.$$

Transpose of a product

- The right answer $B^{\mathrm{T}}A^{\mathrm{T}}$ comes out a row at a time.
- If $B = \begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$ 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 $B^{\mathrm{T}}A^{\mathrm{T}}$:

$$\text{Transposing} \quad AB \quad = \quad \begin{bmatrix} A\mathbf{x}_1 & A\mathbf{x}_2 & \cdots \end{bmatrix}$$

$$\text{gives} \quad \begin{bmatrix} \mathbf{x}_1^{\mathrm{T}}A^{\mathrm{T}} \\ \mathbf{x}_2^{\mathrm{T}}A^{\mathrm{T}} \\ \vdots \end{bmatrix} \qquad \text{which is } B^{\mathrm{T}}A^{\mathrm{T}}.$$

- So, $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{T}$.

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 $A^{\mathrm{T}}A$.

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.

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.

- Given the example, now we can see how can we represent the dot product and the outer product using matrix representation.

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.
- $^{\mathrm{T}}$ is inside: *the dot product or inner product is* $\mathbf{x}^{\mathrm{T}}\mathbf{y}$
  $(1 \times n)(n \times 1)$

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.
- $^{\mathrm{T}}$ is inside: *the dot product or inner product is* $\mathbf{x}^{\mathrm{T}}\mathbf{y}$
  $(1 \times n)(n \times 1)$
- $^{\mathrm{T}}$ is outside: *the rank one product or outer product is* $\mathbf{x}\mathbf{y}^{\mathrm{T}}$
  $(n \times 1)(1 \times n)$

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.
- $^{\mathrm{T}}$ is inside: *the dot product or inner product is* $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ $(1 \times n)(n \times 1)$
- $^{\mathrm{T}}$ is outside: *the rank one product or outer product is* $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ $(n \times 1)(1 \times n)$
- $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ is a scalar.
- $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ is a matrix.

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.
- $^{\mathrm{T}}$ is inside: *the dot product or inner product is* $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ $(1 \times n)(n \times 1)$
- $^{\mathrm{T}}$ is outside: *the rank one product or outer product is* $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ $(n \times 1)(1 \times n)$
- $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ is a scalar.
- $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ is a matrix.
- Quantum mechanics would write those as $\langle x|y\rangle$ (inner) and $|x\rangle\langle y|$ (outer).

The meaning of inner products

- We know the dot product between $\mathbf{x}$ and $\mathbf{y}$. It is the sum $x_i y_i$.
- Now we have a better way to write $\mathbf{x} \cdot \mathbf{y}$, using the matrix notation.
- $^{\mathrm{T}}$ is inside: *the dot product or inner product is* $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ $(1 \times n)(n \times 1)$
- $^{\mathrm{T}}$ is outside: *the rank one product or outer product is* $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ $(n \times 1)(1 \times n)$
- $\mathbf{x}^{\mathrm{T}}\mathbf{y}$ is a scalar.
- $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ is a matrix.
- Quantum mechanics would write those as $\langle x|y\rangle$ (inner) and $|x\rangle\langle y|$ (outer).
- Maybe the universe is governed by linear algebra.

Examples

- Consider the two vectors $\mathbf{x} = (1, 2)$ and $\mathbf{y} = (3, 4)$.

$$\mathbf{x}^{\mathrm{T}}\mathbf{y} = \begin{bmatrix} 1 & 2 \end{bmatrix} \begin{bmatrix} 3 \\ 4 \end{bmatrix} = 1(3) + 2(4) = 11$$

$$\sum_{i=1}^{2} x_i y_i = x_1 y_1 + x_2 y_2 = 1(3) + 2(4) = 11$$

$$\mathbf{x}^{\mathrm{T}}\mathbf{y} = \sum_{i=1}^{n} x_i y_i$$

- If $\mathbf{x}^{\mathrm{T}}\mathbf{y} = 0$, then we say that the two vector are orthogonal.

Examples

- The outer product $\mathbf{x}\mathbf{y}^{\mathrm{T}}$:

$$\mathbf{x}\mathbf{y}^{\mathrm{T}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \begin{bmatrix} 3 & 4 \end{bmatrix} = \begin{bmatrix} 1(3) & 1(4) \\ 2(3) & 2(4) \end{bmatrix} = \begin{bmatrix} 3 & 4 \\ 6 & 8 \end{bmatrix}$$

- This is **not** the cross product. The outer product $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ is a matrix; the cross product $\mathbf{x} \times \mathbf{y}$ is a vector:

$$\mathbf{x} \times \mathbf{y} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 1 & 2 & 0 \\ 3 & 4 & 0 \end{vmatrix} = \big(1(4) - 2(3)\big)\,\mathbf{k} = -2\,\mathbf{k}$$

- Now, what happens if we take the transpose of the inverse of a matrix ?

Transpose of inverse

- The transpose of A^{-1} is $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$.

Transpose of inverse

- The transpose of A^{-1} is $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$.
- The easy way is to believe this is true and then see in an example.

Transpose of inverse

- The transpose of A^{-1} is $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$.
- The easy way is to belive this is true and then see in an example.
- The inverse of $A = \left[\begin{smallmatrix} 1 & 0 \\ 6 & 1 \end{smallmatrix}\right]$ is $A^{-1} = \left[\begin{smallmatrix} 1 & 0 \\ -6 & 1 \end{smallmatrix}\right]$. The transpose is $A^{\mathrm{T}} = \left[\begin{smallmatrix} 1 & 6 \\ 0 & 1 \end{smallmatrix}\right]$.

$$(A^{-1})^{\mathrm{T}} \quad \textit{and} \quad (A^{\mathrm{T}})^{-1} \quad \textit{are both equal to} \quad \begin{bmatrix} 1 & -6 \\ 0 & 1 \end{bmatrix}.$$

Transpose of inverse

- The transpose of A^{-1} is $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$.
- The easy way is to belive this is true and then see in an example.
- The inverse of $A = \left[\begin{smallmatrix} 1 & 0 \\ 6 & 1 \end{smallmatrix}\right]$ is $A^{-1} = \left[\begin{smallmatrix} 1 & 0 \\ -6 & 1 \end{smallmatrix}\right]$. The transpose is $A^{\mathrm{T}} = \left[\begin{smallmatrix} 1 & 6 \\ 0 & 1 \end{smallmatrix}\right]$.

$$(A^{-1})^{\mathrm{T}} \quad \textit{and} \quad (A^{\mathrm{T}})^{-1} \quad \textit{are both equal to} \quad \begin{bmatrix} 1 & -6 \\ 0 & 1 \end{bmatrix}.$$

- We can invert the transpose or transpose the inverse.

Transpose of inverse

- The transpose of A^{-1} is $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$.
- The easy way is to believe this is true and then see in an example.
- The inverse of $A = \left[\begin{smallmatrix} 1 & 0 \\ 6 & 1 \end{smallmatrix}\right]$ is $A^{-1} = \left[\begin{smallmatrix} 1 & 0 \\ -6 & 1 \end{smallmatrix}\right]$. The transpose is $A^{\mathrm{T}} = \left[\begin{smallmatrix} 1 & 6 \\ 0 & 1 \end{smallmatrix}\right]$.

$$(A^{-1})^{\mathrm{T}} \quad \textit{and} \quad (A^{\mathrm{T}})^{-1} \quad \textit{are both equal to} \quad \begin{bmatrix} 1 & -6 \\ 0 & 1 \end{bmatrix}.$$

- We can invert the transpose or transpose the inverse.
- How can we find the inverse of a 2x2 matrix ?

Inverse of a 2x2 matrix

- For a 2×2 matrix A if its determinant is different than zero, than the matrix is invertible.

Inverse of a 2x2 matrix

- For a 2×2 matrix A if its determinant is different than zero, than the matrix is invertible.
- The determinant of a 2×2 matrices,

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc,$$

- and for a 3×3 matrix is,

$$\det \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = a(ei - fh) - b(di - fg) + c(dh - eg)$$

Inverse of a 2x2 matrix

- For a 2×2 matrix A if its determinant is different than zero, than the matrix is invertible.
- The determinant of a 2×2 matrices,

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc,$$

- and for a 3×3 matrix is,

$$\det \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = a(ei - fh) - b(di - fg) + c(dh - eg)$$

- Does this expression ring a bell ?

Inverse of a 2x2 matrix

- For a 2×2 matrix A if its determinant is different than zero, than the matrix is invertible.
- The determinant of a 2×2 matrices,

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc,$$

- and for a 3×3 matrix is,

$$\det \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = a(ei - fh) - b(di - fg) + c(dh - eg)$$

- Does this expression ring a bell ?
- For 4×4 and larger matrices there are more advanced techniques that we will see later.

Inverse of a 2x2 matrix

- A 2 by 2 matrix is invertible if and only if $ad - bc$ is not zero:

2 by 2 Inverse: $$A^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

Take $A = \begin{bmatrix} 5 & 2 \\ -7 & -3 \end{bmatrix}$, so $a = 5$, $b = 2$, $c = -7$, $d = -3$.

Inverse of a 2x2 matrix

- A 2 by 2 matrix is invertible if and only if $ad - bc$ is not zero:

  2 by 2 Inverse: $$A^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

  Take $A = \begin{bmatrix} 5 & 2 \\ -7 & -3 \end{bmatrix}$, so $a = 5$, $b = 2$, $c = -7$, $d = -3$.

- Determinant:

$$ad - bc = (5)(-3) - (2)(-7) = -15 + 14 = -1$$

- It is not zero, so A is invertible. Swap a and d, change the sign of b and c, and divide by the determinant:

$$A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{-1} \begin{bmatrix} -3 & -2 \\ 7 & 5 \end{bmatrix}$$

$$= \begin{bmatrix} 3 & 2 \\ -7 & -5 \end{bmatrix}$$

Inverse of a 2x2 matrix

- A 2 by 2 matrix is invertible if and only if $ad - bc$ is not zero:

  2 by 2 Inverse: $$A^{-1} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

  Take $A = \begin{bmatrix} 5 & 2 \\ -7 & -3 \end{bmatrix}$, so $a = 5$, $b = 2$, $c = -7$, $d = -3$.

- Determinant:

$$ad - bc = (5)(-3) - (2)(-7) = -15 + 14 = -1$$

- It is not zero, so A is invertible. Swap a and d, change the sign of b and c, and divide by the determinant:

$$A^{-1} = \frac{1}{ad-bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{-1} \begin{bmatrix} -3 & -2 \\ 7 & 5 \end{bmatrix}$$

$$= \begin{bmatrix} 3 & 2 \\ -7 & -5 \end{bmatrix}$$

- Check if $AA^{-1} = I$.

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.
- But if the product AB has an inverse, if and only if the two factors A and B are separately invertible.

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.
- But if the product AB has an inverse, if and only if the two factors A and B are separately invertible.
- It is important to point that A^{-1} and B^{-1} come in reverse order.
- The inverse of the product AB is

$$(AB)^{-1} = B^{-1}A^{-1}$$

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.
- But if the product AB has an inverse, if and only if the two factors A and B are separately invertible.
- It is important to point that A^{-1} and B^{-1} come in reverse order.
- The inverse of the product AB is

$$(AB)^{-1} = B^{-1}A^{-1}$$

- To see why the order is reversed, multiply AB times $B^{-1}A^{-1}$:

$$(AB)(B^{-1}A^{-1}) = AIA^{-1} = AA^{-1} = I$$

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.
- But if the product AB has an inverse, if and only if the two factors A and B are separately invertible.
- It is important to point that A^{-1} and B^{-1} come in reverse order.
- The inverse of the product AB is

$$(AB)^{-1} = B^{-1}A^{-1}$$

- To see why the order is reversed, multiply AB times $B^{-1}A^{-1}$:

$$(AB)(B^{-1}A^{-1}) = AIA^{-1} = AA^{-1} = I$$

- Inverses come in reverse order. If you put socks on and then shoes, the first to be taken off are the ?

The inverse of a product AB

- It is hard to say if the sum of two matrices is invertible.
- But if the product AB has an inverse, if and only if the two factors A and B are separately invertible.
- It is important to point that A^{-1} and B^{-1} come in reverse order.
- The inverse of the product AB is

$$(AB)^{-1} = B^{-1}A^{-1}$$

- To see why the order is reversed, multiply AB times $B^{-1}A^{-1}$:

$$(AB)(B^{-1}A^{-1}) = AIA^{-1} = AA^{-1} = I$$

- Inverses come in reverse order. If you put socks on and then shoes, the first to be taken off are the ?
- The next step is to study symmetric matrices, which are very important.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.
- **Symmetric matrices**

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} = S^{\mathrm{T}} \quad \text{and} \quad D = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} = D^{\mathrm{T}}.$$

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.
- **Symmetric matrices**

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} = S^{\mathrm{T}} \quad \text{and} \quad D = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} = D^{\mathrm{T}}.$$

- The inverse of a symmetric matrix is also symmetric.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.
- **Symmetric matrices**

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} = S^{\mathrm{T}} \quad \text{and} \quad D = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} = D^{\mathrm{T}}.$$

- The inverse of a symmetric matrix is also symmetric.
- Given a symmetric matrix S the transpose of S^{-1} is $(S^{-1})^{\mathrm{T}} = (S^{\mathrm{T}})^{-1} = S^{-1}$.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.
- **Symmetric matrices**

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} = S^{\mathrm{T}} \quad \text{and} \quad D = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} = D^{\mathrm{T}}.$$

- The inverse of a symmetric matrix is also symmetric.
- Given a symmetric matrix S the transpose of S^{-1} is $(S^{-1})^{\mathrm{T}} = (S^{\mathrm{T}})^{-1} = S^{-1}$.
- That says that S^{-1} is symmetric when S is invertible.

Symmetric Matrices

- For a symmetric matrix, transposing A to A^{T} produces no change.
- Then $A = A^{\mathrm{T}}$.
- **Symmetric matrices**

$$S = \begin{bmatrix} 1 & 2 \\ 2 & 5 \end{bmatrix} = S^{\mathrm{T}} \quad \text{and} \quad D = \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} = D^{\mathrm{T}}.$$

- The inverse of a symmetric matrix is also symmetric.
- Given a symmetric matrix S the transpose of S^{-1} is $(S^{-1})^{\mathrm{T}} = (S^{\mathrm{T}})^{-1} = S^{-1}$.
- That says that S^{-1} is symmetric when S is invertible.
- What happens when we multiply symmetric matrices ?

Symmetric Products

- Choose any matrix A, probably rectangular. Multiply A^{T} times A.

Symmetric Products

- Choose any matrix A, probably rectangular. Multiply A^{T} times A.
- Then the product $S = A^{\mathrm{T}}A$ is automatically a square symmetric matrix.

Symmetric Products

- Choose any matrix A, probably rectangular. Multiply A^{T} times A.
- Then the product $S = A^{\mathrm{T}}A$ is automatically a square symmetric matrix.
- **Example** Multiply $A = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$ and $A^{\mathrm{T}} = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$ in both orders.

Symmetric Products

- Choose any matrix A, probably rectangular. Multiply A^{T} times A.
- Then the product $S = A^{\mathrm{T}}A$ is automatically a square symmetric matrix.
- **Example** Multiply $A = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$ and $A^{\mathrm{T}} = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$ in both orders.
- You see that both are symmetric but different.

Symmetric Products

- Choose any matrix A, probably rectangular. Multiply A^{T} times A.
- Then the product $S = A^{\mathrm{T}}A$ is automatically a square symmetric matrix.
- **Example** Multiply $A = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix}$ and $A^{\mathrm{T}} = \begin{bmatrix} -1 & 0 \\ 1 & -1 \\ 0 & 1 \end{bmatrix}$ in both orders.
- You see that both are symmetric but different.
- With the understanding of symmetric matrices we need to see its complex correspondent, which is a kind of matrix very important in quantum mechanics. But first we need to recap complex numbers.

Real versus Complex

$$\mathbf{R} = \text{line of all real numbers } -\infty < x < \infty \quad \leftrightarrow \quad \mathbf{C} = \text{plane of all complex numbers } z = x + iy$$

$$|x| = \text{absolute value of } x \quad \leftrightarrow \quad |z| = \sqrt{x^2 + y^2} = r = \text{absolute value (or modulus) of } z$$

The **complex conjugate** of $z = x + iy$ is $\overline{z} = \boldsymbol{x - iy}$

$$|z|^2 = x^2 + y^2 = z\overline{z} \qquad \text{and} \qquad \frac{1}{z} = \frac{\overline{z}}{|z|^2}$$

Complex numbers

- **A complex number** (say $3 + 2i$) **is a real number** (3) **plus an imaginary number** ($2i$)
- Addition keeps the real and imaginary parts separate
- Multiplication uses $i^2 = -1$
- **Add:** $(3 + 2i) + (3 + 2i) = 6 + 4i$
- **Multiply:** $(3 + 2i)(1 - i) = 3 + 2i - 3i - 2i^2 = 5 - i$
- **The complex conjugate:** of $3 + 2i$ is $3 - 2i$.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$
- A matrix is said to be Hermitian if it is equal to its transpose conjugate $\overline{S}^{\,\mathrm{T}}$.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$
- A matrix is said to be Hermitian if it is equal to its transpose conjugate $\overline{S}^{\,\mathrm{T}}$.
- If it is equal to minus its transpose conjugate $S = -S^{\mathrm{H}}$ that it is said to be antiHermitian.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$
- A matrix is said to be Hermitian if it is equal to its transpose conjugate $\overline{S}^{\,\mathrm{T}}$.
- If it is equal to minus its transpose conjugate $S = -S^{\mathrm{H}}$ that it is said to be antiHermitian.
- Every *real symmetric matrix* is Hermitian, because taking the conjugate of real matrices have no effect.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$
- A matrix is said to be Hermitian if it is equal to its transpose conjugate $\overline{S}^{\,\mathrm{T}}$.
- If it is equal to minus its transpose conjugate $S = -S^{\mathrm{H}}$ that it is said to be antiHermitian.
- Every *real symmetric matrix* is Hermitian, because taking the conjugate of real matrices have no effect.
- There are some neat feature of the Hermitian matrices that are really important in quantum mechanics, that we are going to see in the future.

Hermitian Matrices

- Among complex matrices, the special class contains the **Hermitian Matrices:** $S = S^{\mathrm{H}}$.
- Example: $S = \begin{bmatrix} 2 & 3-3i \\ 3+3i & 5 \end{bmatrix} = S^{\mathrm{H}}$
- A matrix is said to be Hermitian if it is equal to its transpose conjugate $\overline{S}^{\,\mathrm{T}}$.
- If it is equal to minus its transpose conjugate $S = -S^{\mathrm{H}}$ that it is said to be antiHermitian.
- Every *real symmetric matrix* is Hermitian, because taking the conjugate of real matrices have no effect.
- There are some neat feature of the Hermitian matrices that are really important in quantum mechanics, that we are going to see in the future.
- Let's take a look of all the important identities we learnt today.

Useful and important identities

- $c(dA) = (cd)A$
- $A(BC) = (AB)C$
- $A(B + C) = AB + AC$
- $AB \neq BA$, multiplication of matrices is not commutative
- $AI = IA = A$

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

Useful and important identities

Transpose

- $(A^{\mathrm{T}})_{ij} = A_{ji}$
- $(A^{\mathrm{T}})^{\mathrm{T}} = A$
- $(A + B)^{\mathrm{T}} = A^{\mathrm{T}} + B^{\mathrm{T}}$
- $(AB)^{\mathrm{T}} = B^{\mathrm{T}} A^{\mathrm{T}}$
- $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$

Inverse

- $A^{-1}A = AA^{-1} = I$
- $(AB)^{-1} = B^{-1}A^{-1}$

Hermitian

- $S = S^{\mathrm{H}}$, with $S^{\mathrm{H}} = \overline{S}^{\,\mathrm{T}}$
- Real symmetric $\Rightarrow$ Hermitian

Symmetric

- $S = S^{\mathrm{T}}$
- $(S^{-1})^{\mathrm{T}} = S^{-1}$
- $A^{\mathrm{T}}A$ and AA^{T} are symmetric for any A

Inner and outer products

- $\mathbf{x}^{\mathrm{T}}\mathbf{y} = \sum_{i=1}^{n} x_i y_i$ (scalar)
- $\mathbf{x}\mathbf{y}^{\mathrm{T}}$ (matrix)
- $\mathbf{x}^{\mathrm{T}}\mathbf{y} = 0 \iff \mathbf{x} \perp \mathbf{y}$

Linear equations

- The central problem of linear algebra is to solve a system of equations.

Linear equations

- The central problem of linear algebra is to solve a system of equations.
- Those equations are linear, which means that we don't see x times y.

Linear equations

- The central problem of linear algebra is to solve a system of equations.
- Those equations are linear, which means that we don't see x times y.
- Our first system, with two equations and two unknowns.

$$\begin{cases} x - 2y = 1 \\ 3x + 2y = 11 \end{cases}$$

Linear equations

- The central problem of linear algebra is to solve a system of equations.
- Those equations are linear, which means that we don't see x times y.
- Our first system, with two equations and two unknowns.

$$\begin{cases} x - 2y = 1 \\ 3x + 2y = 11 \end{cases}$$

- The two equations represent lines in the xy plane.

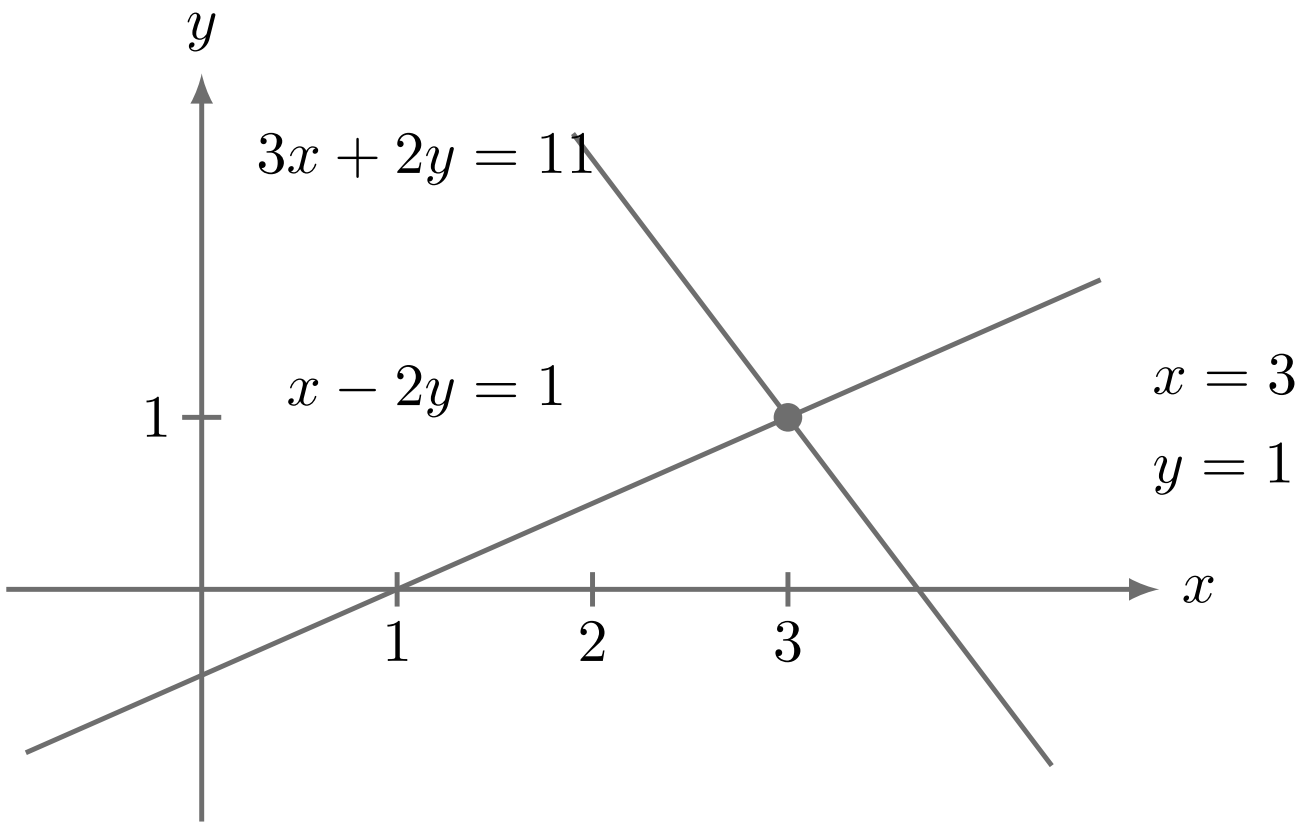
Linear equations

- The central problem of linear algebra is to solve a system of equations.
- Those equations are linear, which means that we don't see x times y.
- Our first system, with two equations and two unknowns.

$$\begin{cases} x - 2y = 1 \\ 3x + 2y = 11 \end{cases}$$

- 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



Linear equations

- We want to recognize the same linear system as a "vector equation".

Linear equations

- We want to recognize the same linear system as a "vector equation".
- Instead of numbers we need to see vectors. Separating the original system.

$$x \begin{bmatrix} 1 \\ 3 \end{bmatrix} + y \begin{bmatrix} -2 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 11 \end{bmatrix} = \mathbf{b}.$$

Linear equations

- We want to recognize the same linear system as a "vector equation".
- Instead of numbers we need to see vectors. Separating the original system.

$$x \begin{bmatrix} 1 \\ 3 \end{bmatrix} + y \begin{bmatrix} -2 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 11 \end{bmatrix} = \mathbf{b}.$$

- The problem is to find the combination of those vectors that equals the vector in the right.

Linear equations

- We want to recognize the same linear system as a "vector equation".
- Instead of numbers we need to see vectors. Separating the original system.

$$x \begin{bmatrix} 1 \\ 3 \end{bmatrix} + y \begin{bmatrix} -2 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 11 \end{bmatrix} = \mathbf{b}.$$

- The problem is to find the combination of those vectors that equals the vector in the right.
- We are multiplying the first vector by x and the second by y, and adding.

Linear equations

- We want to recognize the same linear system as a "vector equation".
- Instead of numbers we need to see vectors. Separating the original system.

$$x \begin{bmatrix} 1 \\ 3 \end{bmatrix} + y \begin{bmatrix} -2 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 11 \end{bmatrix} = \mathbf{b}.$$

- The problem is to find the combination of those vectors that equals the vector in the right.
- 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 $\mathbf{b}$.

Linear equations

- So we have a linear combination:

$$3\begin{bmatrix}1\\3\end{bmatrix} + 1\begin{bmatrix}-2\\2\end{bmatrix} = \begin{bmatrix}1\\11\end{bmatrix}.$$

Linear equations

- So we have a linear combination:

$$3\begin{bmatrix}1\\3\end{bmatrix}+1\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

- Looking at the original system again:

$$x\begin{bmatrix}1\\3\end{bmatrix}+y\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}=\mathbf{b}.$$

Linear equations

- So we have a linear combination:

$$3\begin{bmatrix}1\\3\end{bmatrix}+1\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

- Looking at the original system again:

$$x\begin{bmatrix}1\\3\end{bmatrix}+y\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}=\mathbf{b}.$$

- The coefficient matrix on the left side of the equations is the 2 by 2 matrix A:

$$A=\begin{bmatrix}1&-2\\3&2\end{bmatrix}.$$

Linear equations

- So we have a linear combination:

$$3\begin{bmatrix}1\\3\end{bmatrix}+1\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

- Looking at the original system again:

$$x\begin{bmatrix}1\\3\end{bmatrix}+y\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}=\mathbf{b}.$$

- The coefficient matrix on the left side of the equations is the 2 by 2 matrix A:

$$A=\begin{bmatrix}1&-2\\3&2\end{bmatrix}.$$

- Matrix equation $A\mathbf{x}=\mathbf{b}$:

$$\begin{bmatrix}1&-2\\3&2\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

Linear equations

- So we have a linear combination:

$$3\begin{bmatrix}1\\3\end{bmatrix}+1\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

- Looking at the original system again:

$$x\begin{bmatrix}1\\3\end{bmatrix}+y\begin{bmatrix}-2\\2\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}=\mathbf{b}.$$

- The coefficient matrix on the left side of the equations is the 2 by 2 matrix A:

$$A=\begin{bmatrix}1&-2\\3&2\end{bmatrix}.$$

- Matrix equation $A\mathbf{x}=\mathbf{b}$:

$$\begin{bmatrix}1&-2\\3&2\end{bmatrix}\begin{bmatrix}x\\y\end{bmatrix}=\begin{bmatrix}1\\11\end{bmatrix}.$$

- 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 3×3 system

- Solve

$$\begin{cases} 2x + 4y - 2z = 2 \\ 4x + 9y - 3z = 8 \\ -2x - 3y + 7z = 10 \end{cases}$$

- The idea: use the first equation to remove x from the other two, then use the second to remove y from the third.
- What is left is a triangular system that we solve from the bottom up.

Step 1: eliminate x

- The first pivot is the coefficient 2 in equation 1.

Step 1: eliminate x

- The first pivot is the coefficient 2 in equation 1.
- Multipliers: $\ell_{21} = \dfrac{4}{2} = 2$ and $\ell_{31} = \dfrac{-2}{2} = -1$.

Step 1: eliminate x

- The first pivot is the coefficient 2 in equation 1.
- Multipliers: $\ell_{21} = \dfrac{4}{2} = 2$ and $\ell_{31} = \dfrac{-2}{2} = -1$.
- Subtract ℓ_{21} times equation 1 from equation 2:

$$\begin{aligned} (4x + 9y - 3z) - 2(2x + 4y - 2z) &= 8 - 2(2) \\ y + z &= 4 \end{aligned}$$

Step 1: eliminate x

- The first pivot is the coefficient 2 in equation 1.
- Multipliers: $\ell_{21} = \dfrac{4}{2} = 2$ and $\ell_{31} = \dfrac{-2}{2} = -1$.
- Subtract ℓ_{21} times equation 1 from equation 2:

$$\begin{aligned} (4x + 9y - 3z) - 2(2x + 4y - 2z) &= 8 - 2(2) \\ y + z &= 4 \end{aligned}$$

- Subtract ℓ_{31} times equation 1 from equation 3 (that is, add equation 1):

$$\begin{aligned} (-2x - 3y + 7z) + (2x + 4y - 2z) &= 10 + 2 \\ y + 5z &= 12 \end{aligned}$$

Step 2: eliminate y

- The system is now

$$\begin{cases} 2x + 4y - 2z = 2 \\ y + z = 4 \\ y + 5z = 12 \end{cases}$$

Step 2: eliminate y

- The system is now

$$\begin{cases} 2x + 4y - 2z = 2 \\ y + z = 4 \\ y + 5z = 12 \end{cases}$$

- The second pivot is the coefficient 1 of y. The multiplier is $\ell_{32} = \dfrac{1}{1} = 1$.

Step 2: eliminate y

- The system is now

$$\begin{cases} 2x + 4y - 2z = 2 \\ y + z = 4 \\ y + 5z = 12 \end{cases}$$

- The second pivot is the coefficient 1 of y. The multiplier is $\ell_{32} = \dfrac{1}{1} = 1$.
- Subtract equation 3 from equation 2:

$$\begin{aligned} (y + 5z) - (y + z) &= 12 - 4 \\ 4z &= 8 \end{aligned}$$

The triangular system

- Three pivots: 2, 1 and 4. None of them is zero, so the system has exactly one solution.

$$\begin{cases} 2x + 4y - 2z = 2 \\ y + z = 4 \\ 4z = 8 \end{cases}$$

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

Back substitution

- From the third equation:

$$4z = 8 \qquad \Longrightarrow \qquad z = 2$$

- Put $z = 2$ into the second equation:

$$y + 2 = 4 \qquad \Longrightarrow \qquad y = 2$$

- Put $y = 2$ and $z = 2$ into the first equation:

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

- The solution is $(x, y, z) = (-1, 2, 2)$.

Check

- Put $(-1, 2, 2)$ back into the original three equations:

$$\begin{aligned} 2(-1) + 4(2) - 2(2) &= -2 + 8 - 4 = 2 \quad \checkmark \\ 4(-1) + 9(2) - 3(2) &= -4 + 18 - 6 = 8 \quad \checkmark \\ -2(-1) - 3(2) + 7(2) &= 2 - 6 + 14 = 10 \quad \checkmark \end{aligned}$$

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

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

$$A = \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix}$$

- The whole system is one matrix equation:

$$A\mathbf{x} = (-\mathbf{1}) \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} + \mathbf{2} \begin{bmatrix} 4 \\ 9 \\ -3 \end{bmatrix} + \mathbf{2} \begin{bmatrix} -2 \\ -3 \\ 7 \end{bmatrix} \quad \text{equals} \quad \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} = \mathbf{b}.$$

What elimination did to A

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

$$U = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \qquad \mathbf{c} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

- The pivots 2, 1, 4 sit on the diagonal of U.
- $U\mathbf{x} = \mathbf{c}$ has the same solution as $A\mathbf{x} = \mathbf{b}$, but it is easy to solve by back substitution.