CS-466/566: Math for AI

Module 01: The Geometry of Data

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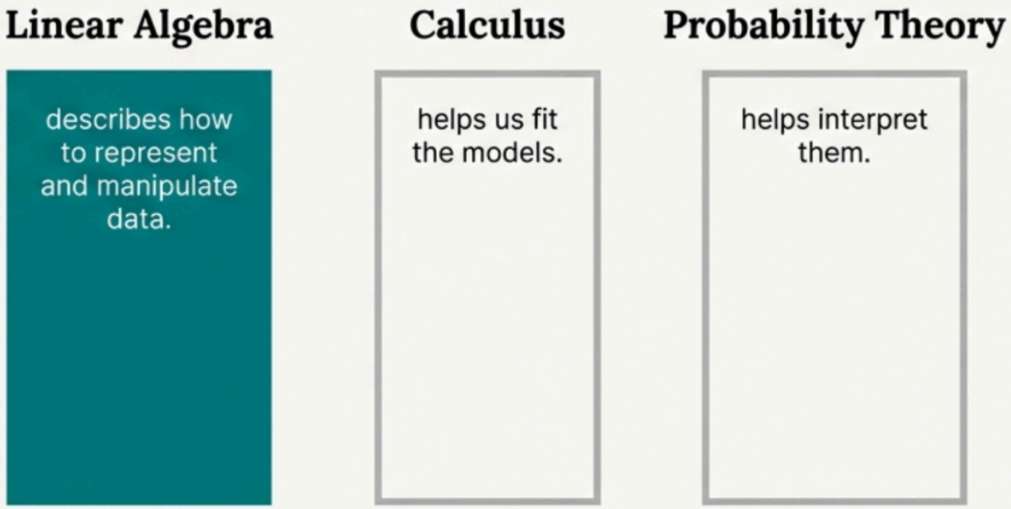
Mathematical Foundations of AI/ML

The Language of Data The mathematics of machine learning rests upon three pillars: linear algebra, calculus, and probability theory.



We will start at the beginning: representing and manipulating data.

The Iris Dataset

To guide our journey, we will use the famous Iris dataset. It contains measurements from three species of Iris flower.

Each data point (a **sample**) includes four measurements: sepal length, sepal width, petal length, and petal width.

- *Iris setosa*
- *Iris versicolor*
- *Iris virginica*

Each measurement type is a **feature**. The dataset contains 150 samples and 4 features.

Iris setosa *Iris versicolor* *Iris virginica*

Sepal L.	Sepal W.	Petal L.	Petal W.
5.1	3.5	1.4	0.2
4.9	3.0	1.4	0.2
4.7	3.2	1.3	0.2
4.6	3.1	1.5	0.2
4.8	3.6	1.4	0.2
5.0	3.6	1.4	0.2
...			

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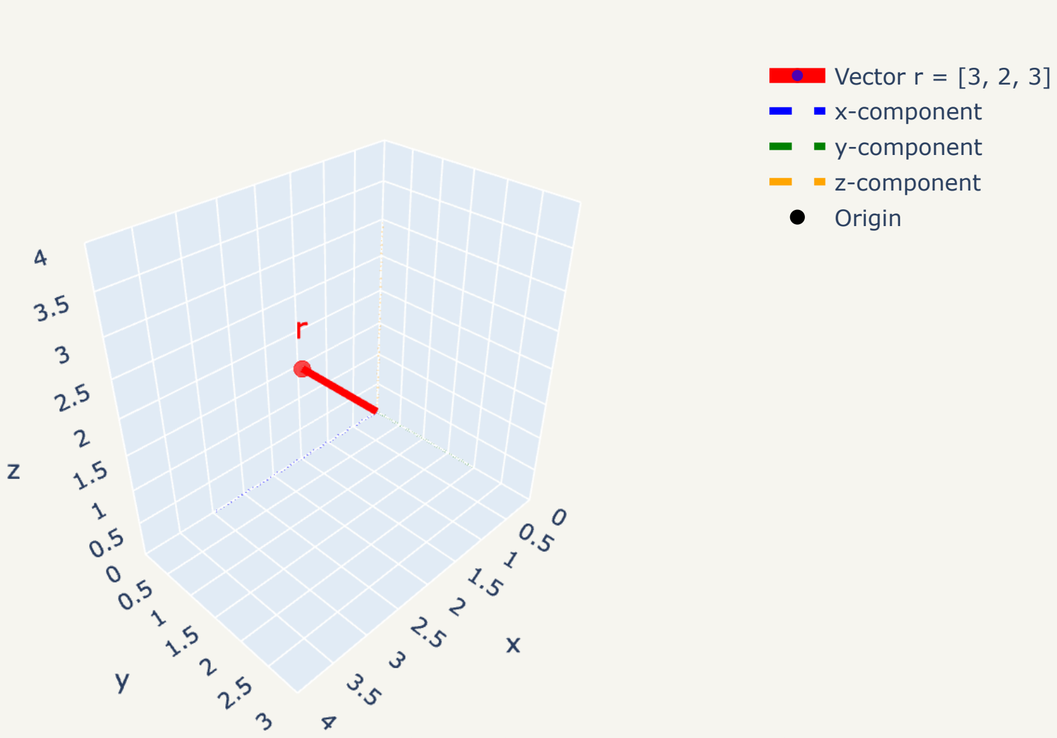
What is a Vector?

- Represents movement or direction in **physical space**, **data space**, or **parameter space**.
- In ML: list of attributes, e.g., a car's *[cost, emissions, top speed]*.



- **Vector r = [3, 2, 4]**: arrow from origin to point (3, 2, 4)
- **Components**: projections onto x, y, z axes (dashed lines)
- **Magnitude**:

$$|\mathbf{r}| = \sqrt{3^2 + 2^2 + 4^2} = \sqrt{29} \approx 5.39$$

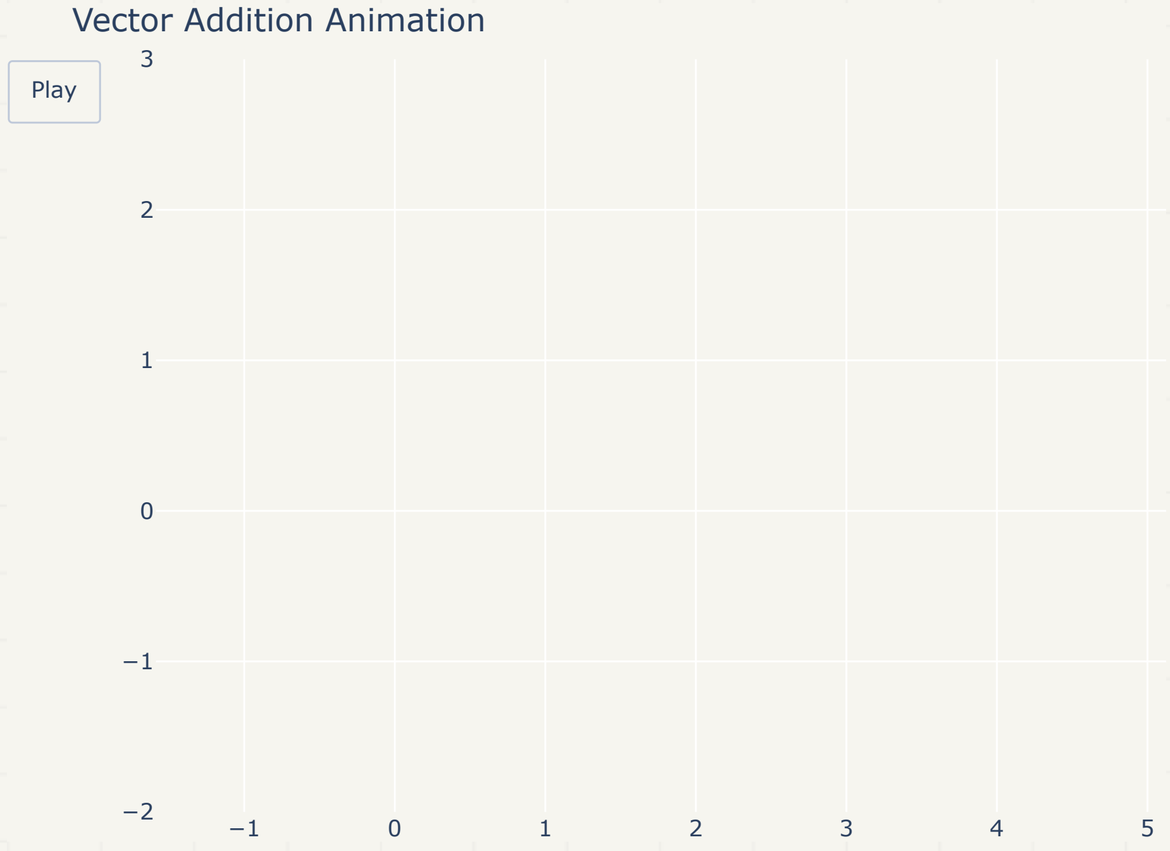
- **Direction**: determined by the ratios of components

Why Use Vectors?

- **Compact Representation**: Store multiple attributes (features) in a single mathematical object.
- **Efficient Computation**: Operations on vectors (addition, dot product) can be parallelized (SIMD).
- **Geometric Interpretation**: Allows us to visualize data relationships (distance, angle).
- **Basis for Matrix/Tensor**: Foundation for representing higher-dimensional data and transformations.

> **Tip**
>
> In AI, we treat everything (images, text, audio) as vectors to apply mathematical transformations!

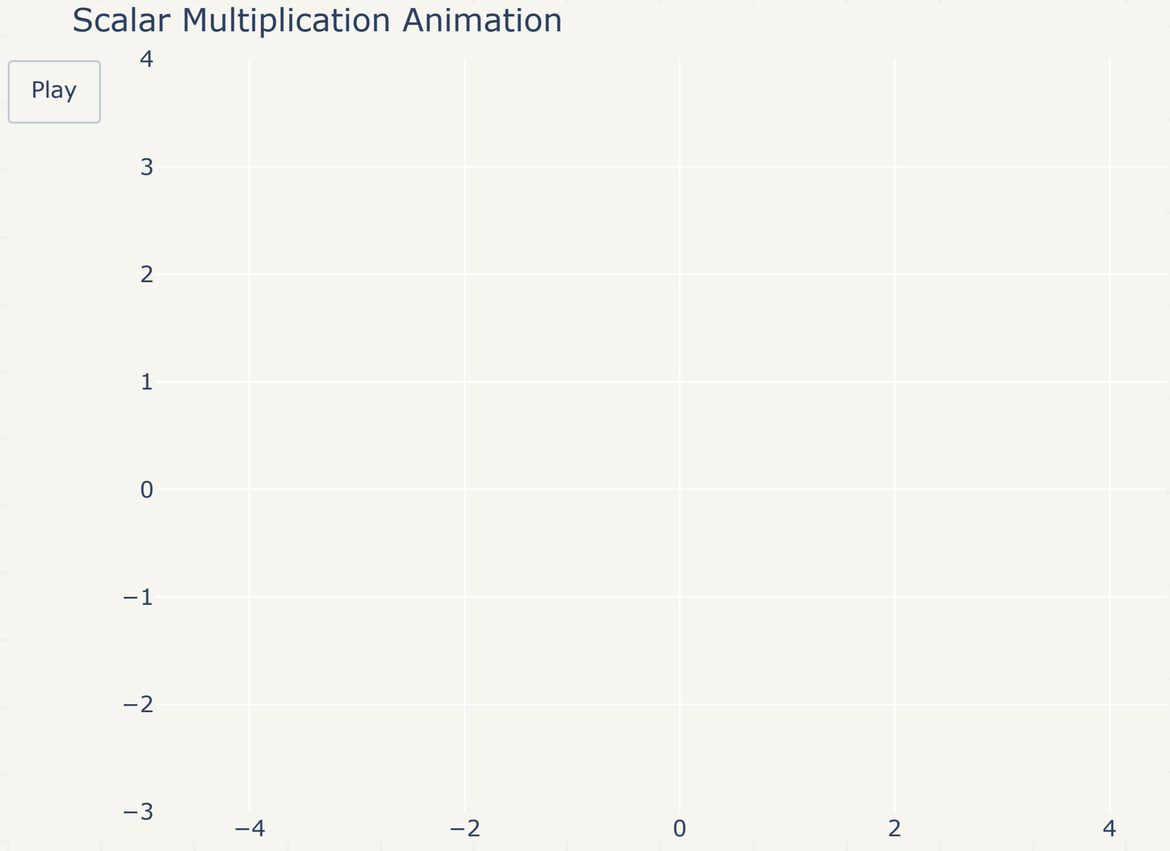
Vector Operations (Addition)



Vector Addition Animation

- **Addition**: $(r + s = s + r)$, commutative & associative
- **Parallelogram Rule**: tip-to-tail method
- **r = [3, 2]** (red vector)
- **s = [1, -1]** (blue vector)
- **r + s = [4, 1]** (green vector)
- Dashed lines show parallelogram construction

Vector Operations (Scalar Multiplication)



Scalar Multiplication Animation

- **Scalar Multiplication**: scales length, preserves/reverses direction
- **Original vector v = [3, 2]** (blue)
- **0.5v**: half length, same direction (orange)
- **1.5v**: 1.5× length, same direction (green)
- **-v**: same length, opposite direction (red)
- All vectors are collinear (same line)

The Rules of the Game

The intuitive operations we performed follow a consistent set of rules. These rules define the **structure** that our vectors live in.

Vector Addition ($+ : V \times V \to V$)

- $x + y = y + x$ (Commutativity)
- $(x + y) + z = x + (y + z)$ (Associativity)
- Existence of a **null vector** ($x + 0 = x$)
- Existence of an **additive inverse** ($x + (-x) = 0$)

Scalar Multiplication ($\cdot : \mathbb{F} \times V \to V$)

- $a(bx) = (ab)x$ (Associativity)
- $a(x + y) = ax + ay$ (Distributivity)
- $(a + b)x = ax + bx$ (Distributivity)
- $1x = x$ (Identity element)

A Vector Space Defined

This collection of objects and rules forms a **vector space**. It is a mathematical structure $(V, \mathbb{F}, +, \cdot)$ where:

- V is a **set of vectors** (like our Iris data points).
- $\mathbb{F}$ is a **field of scalars** (for us, the real numbers $\mathbb{R}$).
- $+$ is the **vector addition** operation.
- $\cdot$ is the **scalar multiplication** operation.

Key Insight: Our Iris dataset, represented as tuples in $\mathbb{R}^4$, forms a vector space. This is the structure that guarantees our scaling operations are mathematically sound. The definition is not arbitrary; it's formalised in hindsight to capture our geometric intuition.

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Vector Space Requirements

Let V be a set of vectors and $\mathbb{F}$ a field of scalars. V is a vector space over $\mathbb{F}$ if:

1. **Closure under addition** $u, v \in V \implies u + v \in V$
2. **Additive identity** $\exists 0 \in V$ such that $v + 0 = v$
3. **Additive inverse** $\forall v \in V, \exists (-v) \in V$ such that $v + (-v) = 0$
4. **Closure under scalar multiplication** $a \in \mathbb{F}, v \in V \implies av \in V$
5. **Distributivity over vector addition** $a(u + v) = au + av$
6. **Distributivity over scalar addition** $(a + b)v = av + bv$
7. **Scalar identity** $1v = v$

$(V, \mathbb{F}, +, \cdot)$ is a vector space over $\mathbb{F}$ if it satisfies the above properties.

Vectors Terminology

What is this notation? $(\mathbb{Z}_2^3, \mathbb{Z}_2, +, \cdot)$

- $\mathbb{Z}_2$: The set of scalars $\{0, 1\}$.
- $\mathbb{Z}_2^3$: **Vectors of length 3 where entries are from $\mathbb{Z}_2$.**

  Example: $(1, 0, 1) \in \mathbb{Z}_2^3$.
- $+$: Component-wise addition modulo 2.
- $\cdot$: Scalar multiplication modulo 2.

Check Your Understanding 2

Let's warm up with "Binary Arithmetic" (where $1 + 1 = 0$).

1. In $\mathbb{Z}_2$, what is $1 + 1 + 1$?

   Answer: 1 (since $1 + 1 = 0$, then $0 + 1 = 1$)

2. In $\mathbb{Z}_2^3$, compute $\mathbf{u} + \mathbf{v}$ for $\mathbf{u} = (1, 0, 1)$ and $\mathbf{v} = (1, 1, 0)$.

   Answer: (0, 1, 1)

3. Is the vector $(2, 0)$ in $\mathbb{Z}_2^2$?

   Answer: No (Elements must be 0 or 1)

Exercise

Show that $(\mathbb{Z}_2^2, \mathbb{Z}_2, +, \cdot)$ is a vector space.

Proof Sketch: Check the 7 requirements for vectors $\mathbf{u} = (u_1, u_2) \in \mathbb{Z}_2^2$:

1. **Closure (+):** $(u_1 + v_1, u_2 + v_2) \in \mathbb{Z}_2^2$ since sums are mod 2.
2. **Add. Identity:** $\mathbf{0} = (0, 0)$ exists ($\mathbf{u} + \mathbf{0} = \mathbf{u}$).
3. **Add. Inverse:** $-\mathbf{u} = \mathbf{u}$ (since $1 + 1 = 0 \implies -1 = 1$).
4. **Closure ($\cdot$):** $c(u_1, u_2) = (cu_1, cu_2) \in \mathbb{Z}_2^2$ for $c \in \{0, 1\}$.
5. **Distributivity (Vector):** $c(\mathbf{u} + \mathbf{v}) = c\mathbf{u} + c\mathbf{v}$.
6. **Distributivity (Scalar):** $(a + b)\mathbf{u} = a\mathbf{u} + b\mathbf{u}$.
7. **Scalar Identity:** $1 \cdot \mathbf{u} = \mathbf{u}$.

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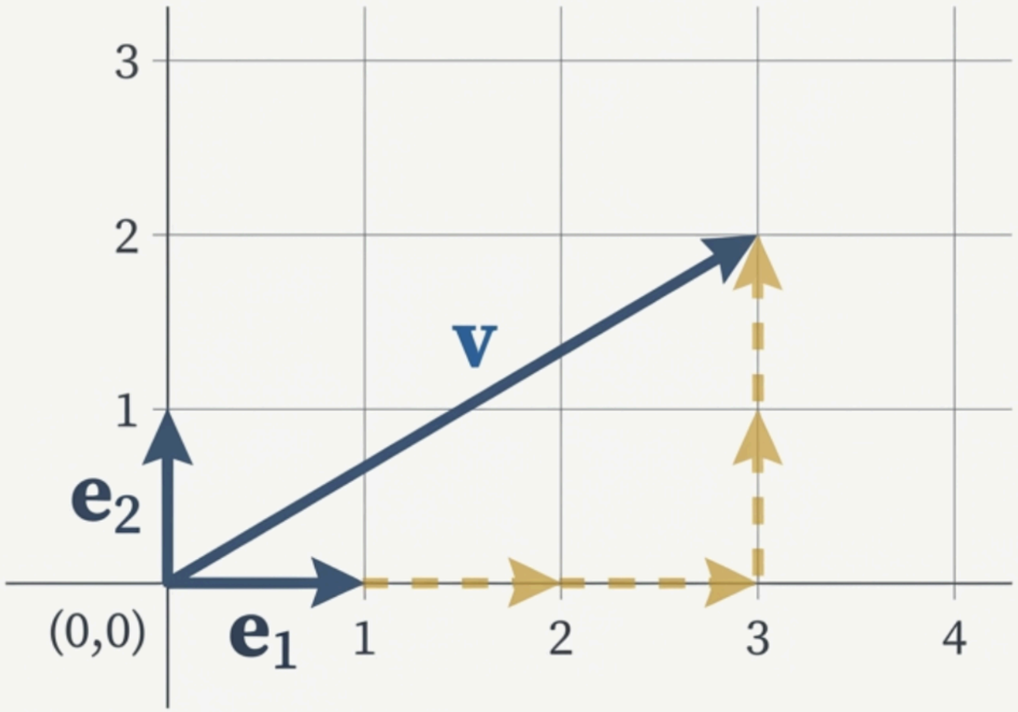
Basis Vectors & Coordinates



$$\mathbf{v} = (3, 2) = 3\mathbf{e}_1 + 2\mathbf{e}_2$$

We represent the vector $\mathbf{v}$ with the coordinate pair $(3, 2)$.

This is shorthand for saying we take **3 steps** along the first axis and **2 steps** along the second.

These “steps” are defined by a special set of vectors: $\mathbf{e}_1$ and $\mathbf{e}_2$.

Defining the Basis

The **basis vectors** are the fundamental reference directions we agree upon.

For 2D space ($\mathbb{R}^2$), we typically use:

- $\mathbf{e}_1 = (1, 0)$: "One step East"
- $\mathbf{e}_2 = (0, 1)$: "One step North"

Every other vector is just a weighted sum of these two.

Think of it like a recipe:

If $\mathbf{e}_1$ is "Cups of Flour" and $\mathbf{e}_2$ is "Cups of Sugar"…

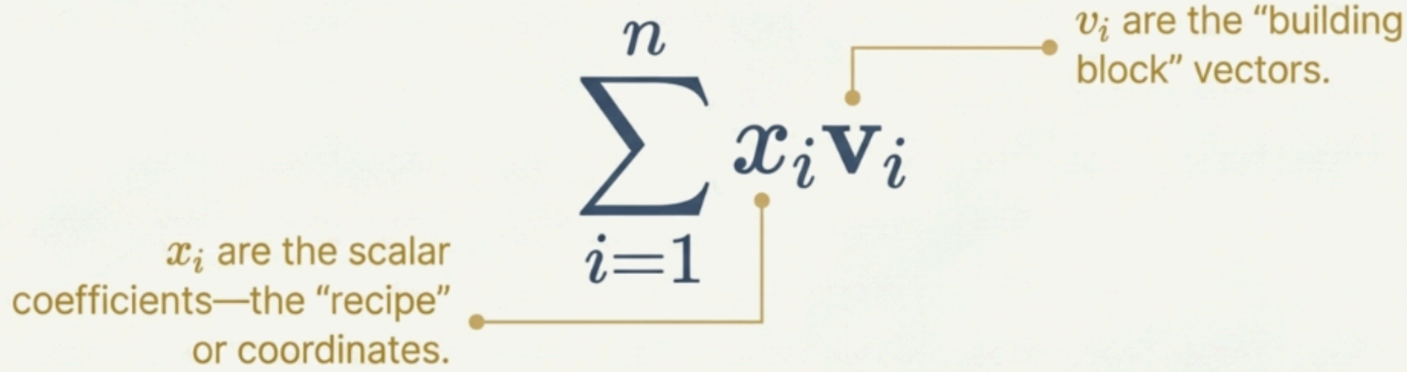
Then the vector $\mathbf{v} = (3, 2)$ is the mix:

$$3 \times \text{Flour} + 2 \times \text{Sugar}$$

Linear Combinations

Coordinates are simply the instructions - the **recipe** - for building a vector using a pre-agreed set of “building block” vectors.

This recipe is called a **linear combination**.



The same vector can have **different coordinates** if we change the building blocks.

Our mission is to understand what makes a **good** set of building blocks.

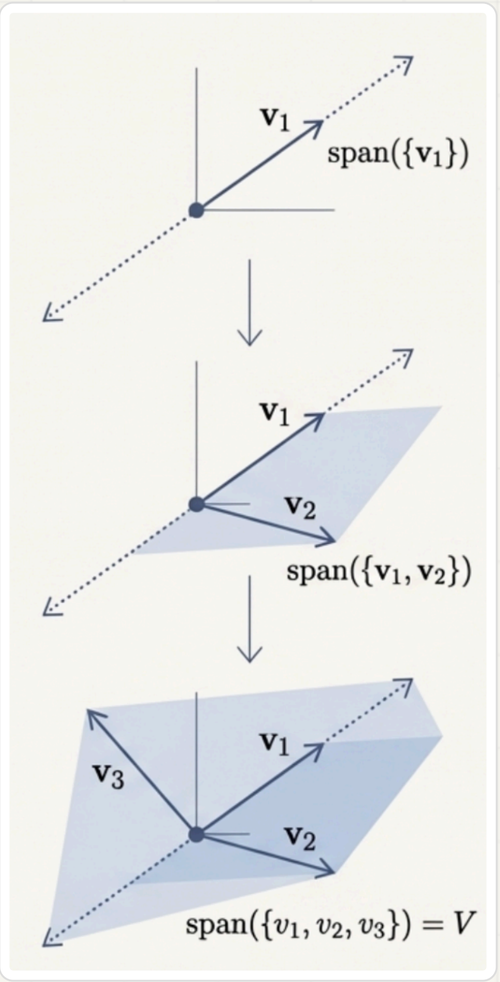
Check Your Understanding 1

- **If we choose a *different* set of basis vectors to describe the same physical arrow $\mathbf{v}$:**
  - ☐ The vector $\mathbf{v}$ changes direction.
  - ☐ The physical arrow $\mathbf{v}$ remains unchanged, but its coordinates change.
  - ☐ The coordinates remain the same, but the arrow shifts.
- **Suppose our new basis vectors are twice as long ($\mathbf{u}_1 = 2\mathbf{e}_1$, $\mathbf{u}_2 = 2\mathbf{e}_2$). To build the same vector $\mathbf{v}$ that was $(4, 6)$ before, what are the new coordinates?**
  - ☐ $(8, 12)$
  - ☐ $(2, 3)$
  - ☐ $(4, 6)$
  - ☐ $(2, 2)$

The Span

For a set of vectors $S = \{\mathbf{u}, \mathbf{v}\}$, its **span** is the set of all possible linear combinations of those vectors.

If $\text{span}(S) = V$, we say S is a **generating set** for the vector space V.



Linear Independence: Is this a Basis?

Consider the set $S = \{v_1, v_2, v_3\}$ where:

$$v_1 = (1, 0), \quad v_2 = (0, 1), \quad v_3 = (1, 1)$$

Question: Is S a basis for $\mathbb{R}^2$?

Answer: No.

Why? Because it contains **redundant** information (violates independence). For example, the vector $(2, 1)$ has multiple recipes:

$$(2, 1) = 2v_1 + v_2$$

$$(2, 1) = v_1 + v_3$$

Defining the Basis

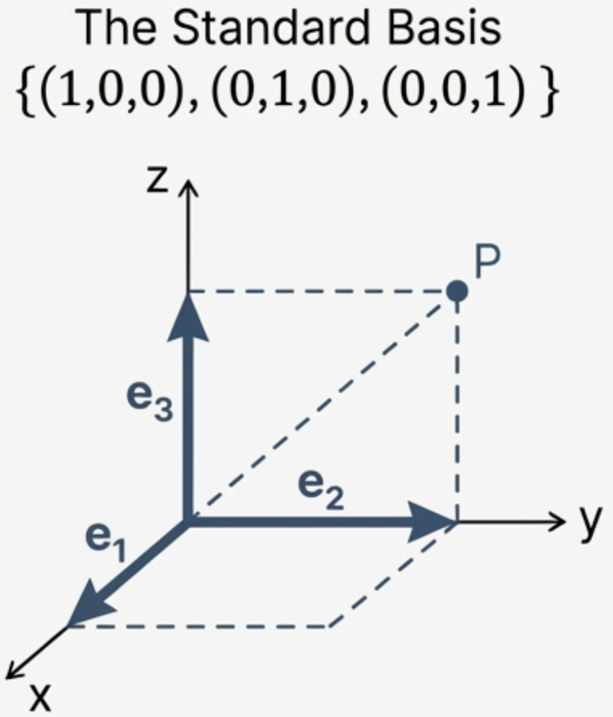
The ideal ‘skeleton’ for a vector space must have maximum reach and zero redundancy. This perfect set is called a **basis**.

Definition 4. (Basis)

Let V be a vector space and S be a subset of its vectors. S is a **basis** of V if:

(a) S **is linearly independent.** (Efficiency)

(b) $\text{span}(S) = V$. (Reach)



How to Check if a Set is a Basis?

The "Goldilocks" Test: Compare vector count (k) to dimension (n).

$k < n$	$k = n$	$k > n$
Too Few	Just Right?	Too Many
Cannot span space	Check Determinant $\neq 0$	Must be dependent

Or test manually for linear independence!

A Basis Hits the Sweet Spot

A basis is perfectly balanced. It contains the exact amount of information needed to describe the entire space, no more and no less.

Property 1: Maximal Linear Independence

Adding any **other** vector from the space to a basis will make the set linearly dependent.

*A basis is a **maximal** linearly independent set.*

Property 2: Minimal Generating Set

Removing any **single** vector from a basis means it can no longer span the entire space.

*A basis is a **minimal** generating set.*

Every vector in a basis is essential.

Exercise.

Are the following vector sets linearly independent?

1. $S_1 = \{(1,0,0),(1,1,0),(1,1,1)\} \subseteq \mathbb{R}^3$

   Yes. (determinant $\neq 0$)

2. $S_2 = \{(1,1,1),(1,2,4),(1,3,9)\} \subseteq \mathbb{R}^3$

   Yes. (determinant $\neq 0$)

3. $S_3 = \{(1,1,1),(1,1,-1),(1,-1,-1)\} \subseteq \mathbb{R}^3$

   Yes. (determinant $\neq 0$)

4. $S_4 = \{(\pi,e),(-42,13/6),(\pi^3,-2)\} \subseteq \mathbb{R}^2$

   No. (3 vectors in $\mathbb{R}^2 \rightarrow$ too many!)

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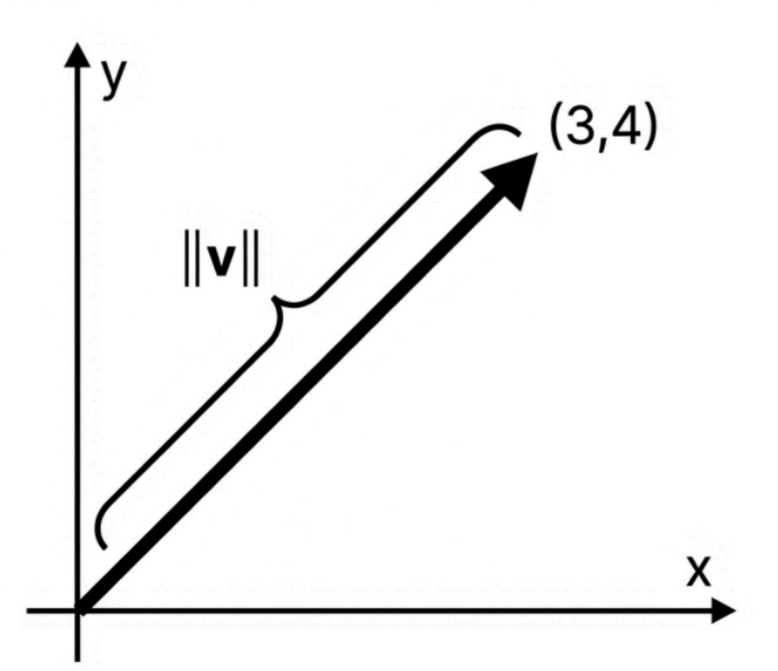
The Definition of Magnitude



Definition: In vector space, a **Norm** is the function that assigns a strictly positive length or size to a vector.

Common Norms

L^2 **(Euclidean)** – Most common in ML

$$\|\mathbf{v}\|_2 = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}$$

Squaring penalises outliers

Returns to original scale

L^1 **(Manhattan)** – Used in regularization

$$\|\mathbf{v}\|_1 = |v_1| + |v_2| + \cdots + |v_n|$$

Magnitude regardless of direction

Accumulation of components

L^∞ **(Max)** – Largest component

$$\|\mathbf{v}\|_\infty = \max(|v_1|, |v_2|, \ldots, |v_n|)$$

Discards all information except the single greatest dimension

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Dot Product: Definition

The **dot product** (or inner product) of two vectors $\mathbf{u}$ and $\mathbf{v}$ is:

$$\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + \cdots + u_n v_n = \sum_{i=1}^{n} u_i v_i$$

Element-wise multiply → Sum all products

Example:

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix} = \begin{bmatrix} 1 \times 4 \\ 2 \times 5 \\ 3 \times 6 \end{bmatrix} = \begin{bmatrix} 4 \\ 10 \\ 18 \end{bmatrix} \rightarrow 4 + 10 + 18 = 32$$

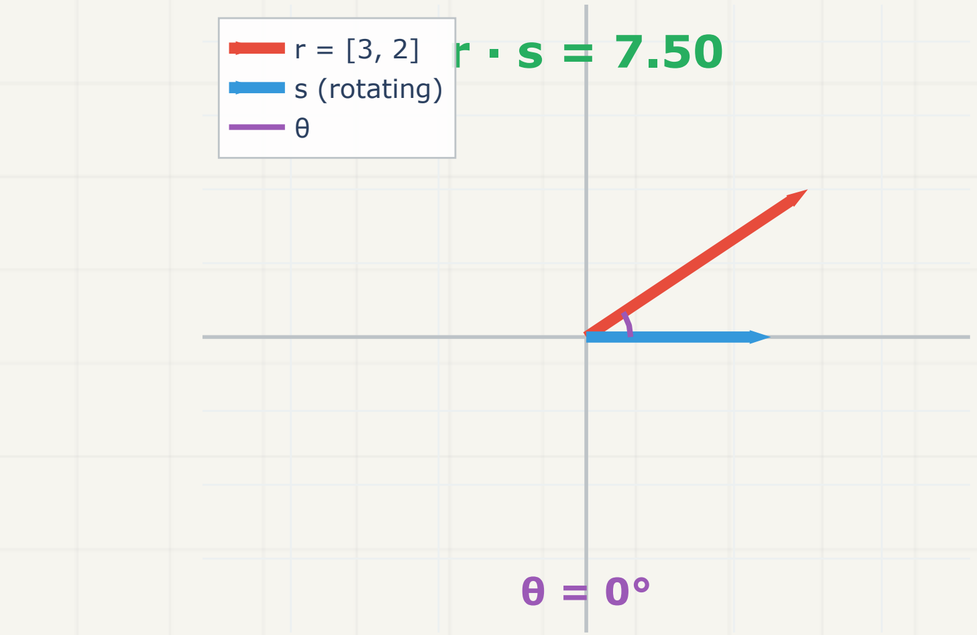
Dot Product: Geometric Interpretation

The dot product relates to the **angle** θ between vectors:

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos(\theta)$$

- If $\mathbf{u} \cdot \mathbf{v} > 0$: Angle is **acute** ($\theta < 90°$)
- If $\mathbf{u} \cdot \mathbf{v} = 0$: Vectors are **orthogonal** ($\theta = 90°$)
- If $\mathbf{u} \cdot \mathbf{v} < 0$: Angle is **obtuse** ($\theta > 90°$)

Dot Product: Interactive Visualization



▶ Play ⏸ Pause

Angle: 0°

0° 41° 82° 123° 165° 206° 247° 288° 329°

Dot Product is maximum when vectors are in the same direction and minimum when they are in opposite directions.

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NumPy: Creating Vectors

```
1 import numpy as np
2
3 #> Create vectors
4 v = np.array([3, 2, 4])
5 u = np.array([1, -1, 2])
6
7 print(f"v = {v}") #> formatted string literal
8 print(f"u = {u}")
9 print(f"Shape: {v.shape}")
```

```
v = [3 2 4]
u = [ 1 -1  2]
Shape: (3,)
```

NumPy: Vector Operations

```python
import numpy as np
v = np.array([3, 2, 4])
u = np.array([1, -1, 2])

#> Vector addition
print(f"v + u = {v + u}")

#> Scalar multiplication
print(f"2 * v = {2 * v}")

#> Magnitude (norm)
print(f"|v| = {np.linalg.norm(v):.4f}")
```

```
v + u = [4 1 6]
2 * v = [6 4 8]
|v| = 5.3852
```

NumPy: Linear Independence Check

```
#> Check if vectors are linearly independent
#> by computing the determinant of the matrix they form
S = np.array([
    [1, 0, 0],
    [1, 1, 0],
    [1, 1, 1]
])

det = np.linalg.det(S)
print(f"Matrix:\n{S}")
print(f"Determinant = {det:.1f}")
print(f"Linearly Independent? {'Yes' if det != 0 else 'No'}")
```

```
Matrix:
[[1 0 0]
 [1 1 0]
 [1 1 1]]
Determinant = 1.0
Linearly Independent? Yes
```

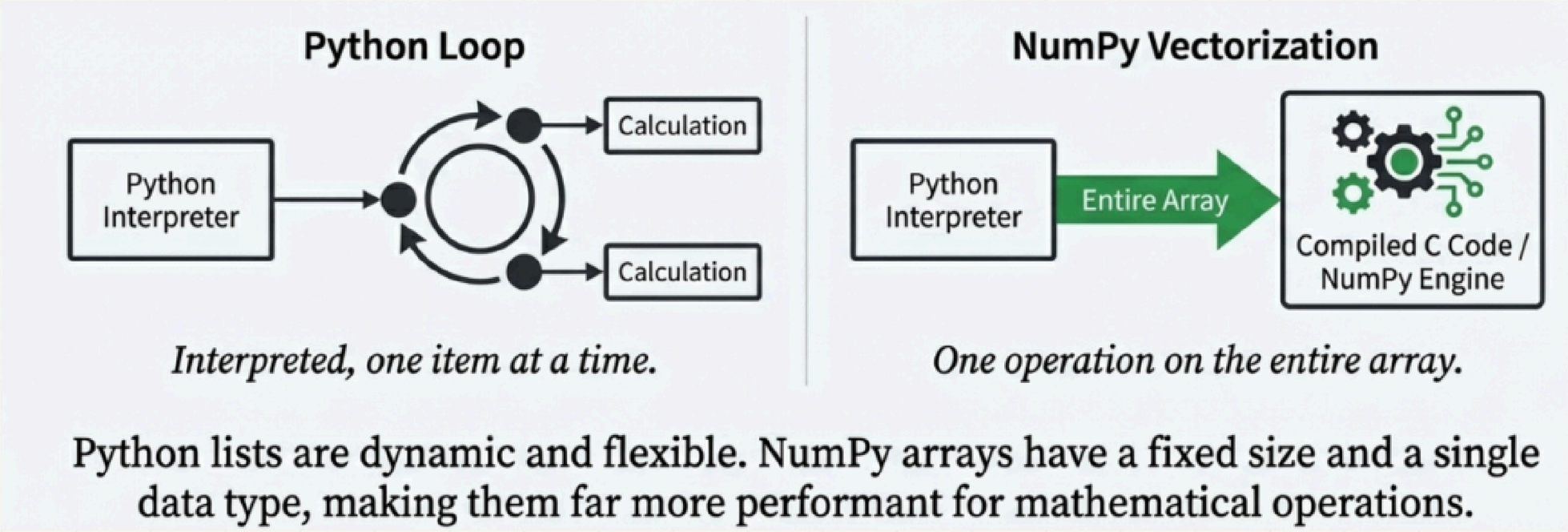
Why Vectorize? Speed Comparison

```python
import time

n = 1_000_000
a = np.random.rand(n)
b = np.random.rand(n)
#> For loop approach
start = time.time()
result_loop = 0
for i in range(n):
    result_loop += a[i] * b[i]
loop_time = time.time() - start
#> Vectorized approach
start = time.time()
result_vec = np.dot(a, b)
vec_time = time.time() - start

print(f"For loop: {loop_time:.4f}s")
print(f"Vectorized: {vec_time:.6f}s")
```

```
For loop: 0.1737s
Vectorized: 0.000190s
Speedup: 915x faster!
```

Vectorization: Visual Comparison

- Vectorization is the process of converting a loop-based algorithm into a vector-based algorithm.
- GPUs are designed to perform vectorized operations.



Exercise: Standard vs Vectorized

Write two Python functions to compute the **Euclidean distance** between two vectors:

1. `euclidean_loop(a, b)` — using a **for loop**
2. `euclidean_vectorized(a, b)` — using **NumPy operations only**
3. Compare their speed on vectors of size 1,000,000

$$d(\mathbf{a}, \mathbf{b}) = \sqrt{\sum_{i=1}^{n} (a_i - b_i)^2}$$

Thank You!