CIS 635 Knowledge Discovery & Data Mining

Introduction to Linear Algebra

Outline

- Concept of Vectors and Vector operations
- Proximity vs Distance Metric
- k-NN, our first ML model

Basic Math - Concept of Vectors, and Vector Operations

We are aware of Scalars: A person's

Height (1.72m)

We are aware of Scalars: A person's

Height (1.72m) Weight (72kg)

We are aware of Scalars: A person's

Height (1.72m) Weight (72kg) Salary (100K)

We are aware of Scalars: A person's

Height (1.72m) Weight (72kg) Salary (100K)

• • • •

A closed form definition of a person through some features

[Height (1.72m), Weight (72kg), Salary (100K)]

A closed form definition of a person through some features

no explicit unit mentions

[1.72, 72, 100]

A closed form definition of a person through some features

- no explicit unit mentions

[1.72, 72, 100]

Is a vectoried representation of a person through some attributes: <u>height</u>, <u>weight</u>, <u>salary</u>

A closed form definition of a person through some features

- no explicit unit mentions

[1.72, 72, 100], [1.65, 70, 120], [1.81, 110, 90],

•••

[1.45, 65, 130],

And here we are talking about a number of people through same features: <u>height, weight, salary</u>

Formal definition of Vectors

Formal definition of Vectors

1. Vectors

We begin by defining a mathematical abstraction known as a **vector space**. In linear algebra the fundamental concepts relate to the n-tuples and their algebraic properties.

Definition: An ordered *n*-tuple is considered as a sequence of *n* terms (a_1, a_2, \dots, a_n) , where *n* is a positive integer.

We see that an ordered *n*-tuple has terms whereas a set has members.

Example: A sequence (5) is called an ordered 1-tuple. A 2-tuple, for example (3, 6) (where 6 appears after 3) is called an ordered pair, and 3-tuple is called an ordered triple. A sequence (9, 3, 4, 4, 1) is called an ordered 5-tuple.

Let us denote the set of all ordered 1-tuples of real numbers by \mathbb{R} . We will write for example $(3.5) \in \mathbb{R}$.

X = [1.78, 72, 100]

$$\mathbf{x} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

We are aware of Scalars: A person's height, weight, salary

Physics vector: velocity (scalar value + direction)

Algebraic vector (in general): Common representation of an entity (1 to n dimension):

- A person's (height, weight, salary), say [1.78, 72, 100]: once defined, we have to follow it.

$$\mathbf{x} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Vector operation rules

```
1. \mathbf{x} + \mathbf{y} \in \mathbb{R}^{n}

2. \alpha \cdot \mathbf{x} \in \mathbb{R}^{n}

3. \mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x} \in \mathbb{R}^{n} (commutativity)

4. \alpha \cdot (\mathbf{x} + \mathbf{y}) = \alpha \cdot \mathbf{x} + \alpha \cdot \mathbf{y} (distributivity)

5. (\alpha + \beta) \cdot \mathbf{x} = \alpha \cdot \mathbf{x} + \beta \cdot \mathbf{x} (distributivity)

6. (\mathbf{x} + \mathbf{y}) + \mathbf{z} = \mathbf{x} + (\mathbf{y} + \mathbf{z}) (associativity)

7. (\alpha \beta) \cdot \mathbf{x} = \alpha \cdot (\beta \cdot \mathbf{x}) (associativity)
```

Vector Operation

1.1.2. Vector Addition

Addition of vectors is defined:

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_n + y_n \end{bmatrix}$$

Example:

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix} 2 \\ 6 \\ -5 \end{bmatrix} + \begin{bmatrix} 0 \\ 3 \\ 4 \end{bmatrix} = \begin{bmatrix} 2 \\ 9 \\ -1 \end{bmatrix}$$

Vector Operation

1.1.4. Zero Vector

The **zero** vector **sometimes denoted 0** is a vector having all elements equal to zero, e.g., the 2-dimensional **0** vector:

$$\mathbf{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{A.7}$$

Vector Operation

1.1.9. Inner Product

The inner or dot product of two vectors x and y of the same dimension is a scalar defined by:

$$\mathbf{x}^T \cdot \mathbf{y} = (\mathbf{x}, \mathbf{y}) = x_1 y_1 + x_2 y_2 + \dots + x_n y_n = \sum_{i=1}^n x_i y_i$$
 (A.11)

Note that the inner product of vector \mathbf{x} and \mathbf{y} requires that a transposed vector \mathbf{x} be multiplied by the \mathbf{y} vector. Sometimes the inner product is denoted simply by juxtaposition of the vectors x and y, for example, as $\langle \mathbf{x}, \mathbf{y} \rangle$ or (\mathbf{x}, \mathbf{y}) .

Example: The inner product of two vectors $\mathbf{x} = \begin{bmatrix} 4 \\ 1 \\ 7 \end{bmatrix}$ and $\mathbf{y} = \begin{bmatrix} 0 \\ 2 \\ -3 \end{bmatrix}$

$$\mathbf{x}^{T}\mathbf{y} = \begin{bmatrix} 4 \ 1 \ 7 \end{bmatrix}^{T} \begin{bmatrix} 0 \\ 2 \\ -3 \end{bmatrix} = 4 \cdot 0 + 1 \cdot 2 + 7 \cdot (-3) = 19$$

Vector Operation

1.1.10. Orthogonal Vectors

Two vectors \mathbf{x} and \mathbf{y} are said to be **orthogonal** if their inner product is equal to zero

$$\mathbf{x}^T \mathbf{y} = 0 \tag{A.12}$$

here 0 is a scalar.

Example: Two vectors $\mathbf{x} = \begin{bmatrix} 4 \\ 0 \end{bmatrix}$ and $\mathbf{y} = \begin{bmatrix} 0 \\ 2 \end{bmatrix}$ and are orthogonal, since their inner product is equal to zero

$$\mathbf{x}^T \cdot \mathbf{y} = \begin{bmatrix} 4 \\ 0 \end{bmatrix}^T = \begin{bmatrix} 0 \ 2 \end{bmatrix} = 4 \cdot 0 + 0 \cdot 2 = 0$$

Vector Operation

1.1.11. Vector Norm

The magnitude of a vector may be measure in different ways. One method, called the vector **norm**, is a function from \mathbb{R}^n into \mathbb{R} for \mathbf{x} an element of \mathbb{R}^n . It is denoted $||\mathbf{x}||$ and satisfies the following conditions:

- 1. $||\mathbf{x}|| \ge 0$, and the equality holds if and only if $\mathbf{x} = \mathbf{0}$
- 2. $||\alpha \mathbf{x}|| = |\alpha| \cdot ||\mathbf{x}||$, where $|\alpha|$ is the absolute value of scalar α

and is defined as:

$$||\mathbf{x}|| = \sqrt{\mathbf{x}^T \mathbf{x}} = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$
 (A.13)

Example: For the vector $\mathbf{x} = \begin{bmatrix} 4 \\ 3 \end{bmatrix}$ the norm is

$$||\mathbf{x}|| = \sqrt{\mathbf{x}^T \mathbf{x}} = \sqrt{4^2 + 3^2} = 5$$

Break!

- Let's we are give two data points: one, the **blue**, and the other is the **green** circle.

- Let's we are give two data points: one, the **blue**, and the other is the **green** circle.
- Now lets, we are given a new circle, and we are given the task to label it with either blue or green.

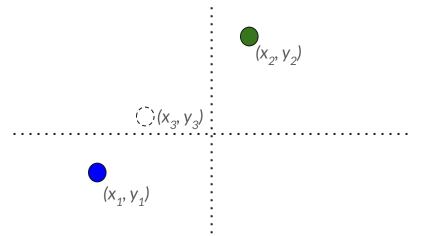
- Let's we are give two data points: one, the **blue**, and the other is the **green** circle.
- Now lets, we are given a new circle, and we are given the task to label it with either blue or green.

 Visually, it looks to be closer to the blue, dot; but how do we quantify it?

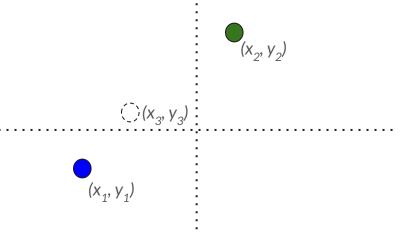
- Let's we are give two data points: one, the **blue**, and the other is the **green** circle.
- Now lets, we are given a new circle, and we are given the task to label it with either blue or green.

- Visually, it looks to be closer to the blue, dot; but how do we quantify it?
- We can use a proximity or distance metric.

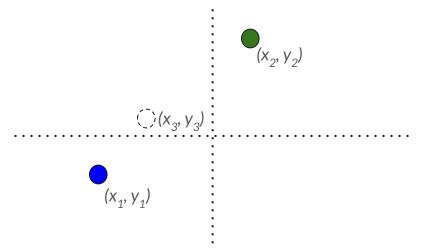
- We can use a proximity or distance metric.
- These three points are depicted on a 2D plane; right?



- We can use a proximity or distance metric.
- These three points are depicted on a 2D plane; right?
- We can use the **Cartesian coordinate system** to quantify the location, and measure their distance; more specifically the Euclidean distance that we learned in our high-school math.



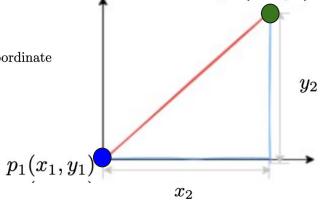
- We can use a proximity or distance metric.
- These three points are depicted on a 2D plane; right?
- We can use the **Cartesian coordinate system** to quantify the location, and measure their distance; more specifically the Euclidean distance that we learned in our high-school math.
- The Euclidean distance is also known as L2 distance in the DS community



L2 (or Euclidean) distance: The L2 distance between point $p_1(x_1,y_1)$ and $p_2(x_2,y_2)$ is:

$$\sqrt{(x_2-x_1)^2+(y_2-y_1)^2}$$
 = $\sqrt{x_2^2+y_2^2}$ given that $p_1(x_1,y_1)=(0,0)$, the origin of the coordinate

I.e. **L2 distance** is the **diagonal** side of a triangle at the right, also known as **Euclidean distance**



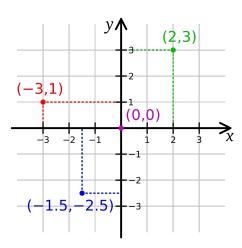
 $p_2(x_2, y_2)$

• L2 (or Euclidean) distance:



- L2 distance between vectors [2, 3] and [0, 0]?

- L2 distance between vectors [2, 3] and [-3, 1]?



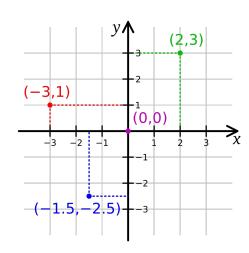
• L2 (or Euclidean) distance:

- L2 distance between vectors [2, 3] and [0, 0] is:

$$\sqrt{(2-0)^2 + (3-0)^2} = \sqrt{13} = 3.61$$

- L2 distance between vectors [2, 3] and [-3, 1] is:

$$\sqrt{(2 - (-3)^2 + (3 - 1)^2} = \sqrt{29} = 5.39$$



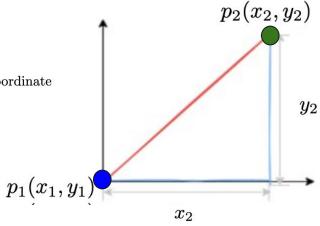
- We have other distance metrics, such as
- L1 distance

L1 distance: The L1 distance between point $\,p_1(x_1,y_1)\,$ and $\,p_2(x_2,y_2)\,$ is :

$$|x_2 - x_1| + |y_2 - y_1|$$

$$=x_2+y_2$$
 given that $p_1(x_1,y_1)=(0,0)$, the origin of the coordinate

I.e. L1 distance is the summation of the **horizontal** and the **vertical** sides of a triangle at the right.

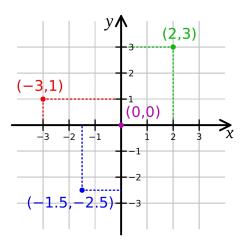


• L1 distance



- L1 distance between vectors [2, 3] and [0, 0]?

- L1 distance between vectors [2, 3] and [-3, 1]?



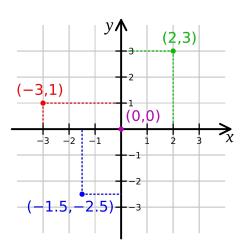
• L1 distance

- L1 distance between vectors [2, 3] and [0, 0] is:

$$|2-0| + |3-0| = 5$$

- L1 distance between vectors [2, 3] and [-3, 1] is:

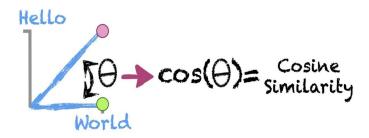
$$|2 - (-3)| + |3 - 1| = 5 + 2 = 7$$



Another unique Distance metric

- We have other distance metrics, such as
- L1 distance, and
- Cosine distance

Cosine similarity



Cosine similarity between vectors: a & b is:

$$\cos \theta = \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \|\vec{b}\|}$$
$$\|\vec{a}\| = \sqrt{a_1^2 + a_2^2 + a_3^2 + \dots + a_n^2}$$
$$\|\vec{b}\| = \sqrt{b_1^2 + b_2^2 + b_3^2 + \dots + b_n^2}$$

Cosine distance = 1 - Cosine similarity

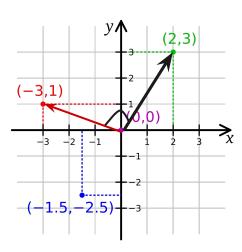
Cosine distance between vectors: a & b is:

$$1 - \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \|\vec{b}\|}$$
$$\|\vec{a}\| = \sqrt{a_1^2 + a_2^2 + a_3^2 + \dots + a_n^2}$$
$$\|\vec{b}\| = \sqrt{b_1^2 + b_2^2 + b_3^2 + \dots + b_n^2}$$

Let's practice

- Cosine similarity between vectors [2, 3] and [-3, 1]?

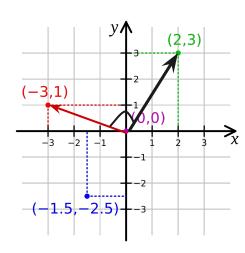
- Cosine distance?



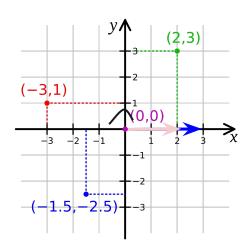
- Cosine similarity between vectors [2, 3] and [-3, 1] is:

$$\frac{-3}{\sqrt{13}\sqrt{10}} = -0.26$$

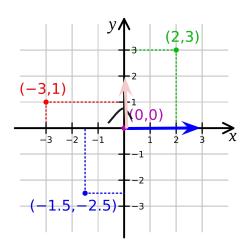
- Cosine distance = 1 - (-0.26) = 1.26



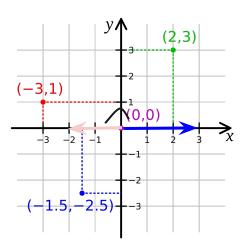
- Cosine similarity range: (-1, +1)
- Two <u>proportional vectors</u> [3, 0] and [2, 0] (same direction) have a Cosine similarity: 1,
- And Cosine distance = 1 1 = 0



- Cosine similarity range: (-1, +1)
- Two orthogonal vectors [3, 0] and [0, 2] have a Cosine similarity: 0,
- And Cosine distance = 1 0 = 1



- Cosine similarity range: (-1, +1)
- Two opposite vectors, [3, 0], [-2, 0], have a Cosine similarity: -1,
- And Cosine distance = 1 (-1) = 2
- Cosine distance range is: (0, 2)

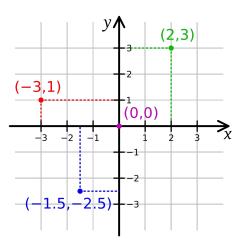


Our first ML Model

- k-NN

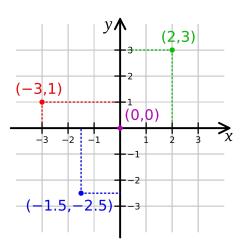
k-NN model

- k-nearest neighbors (k-NN)
 - Supervised learning



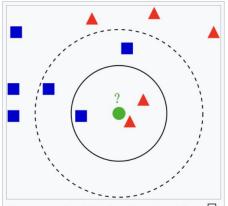
k-NN model

- k-nearest neighbors (k-NN)
 - Supervised learning
 - Non parametric



k-NN model

- k-nearest neighbors (k-NN)
 - Supervised learning
 - Non parametric (distance based method)
 - Both for Classification and Regression solutions



Example of k-NN classification. The test sample (green dot) should be classified either to blue squares or to red triangles. If k = 3 (solid line circle) it is assigned to the red triangles because there are 2 triangles and only 1 square inside the inner circle. If k = 5 (dashed line circle) it is assigned to the blue squares (3 squares vs. 2 triangles inside the outer circle).