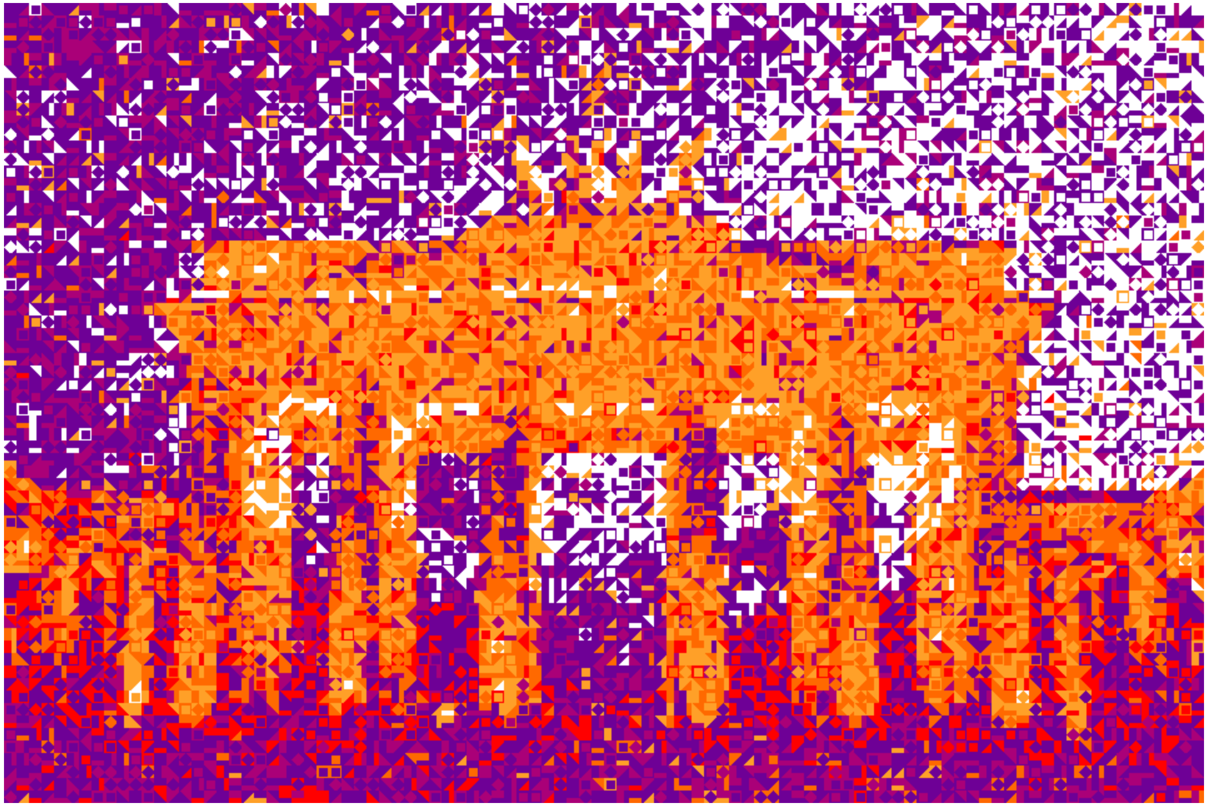
The Geometry of Data

Linear Algebra in Practice



Dr. Kristian Rother

Goal of this Workshop

1. introduce fundamentals
2. execute Python code for linear algebra
3. create plots and pictures

Your host: Dr. Kristian Rother

- PhD on 3D structures of molecules (HU Berlin)
- using Python since 1999
- freelance trainer since 2011

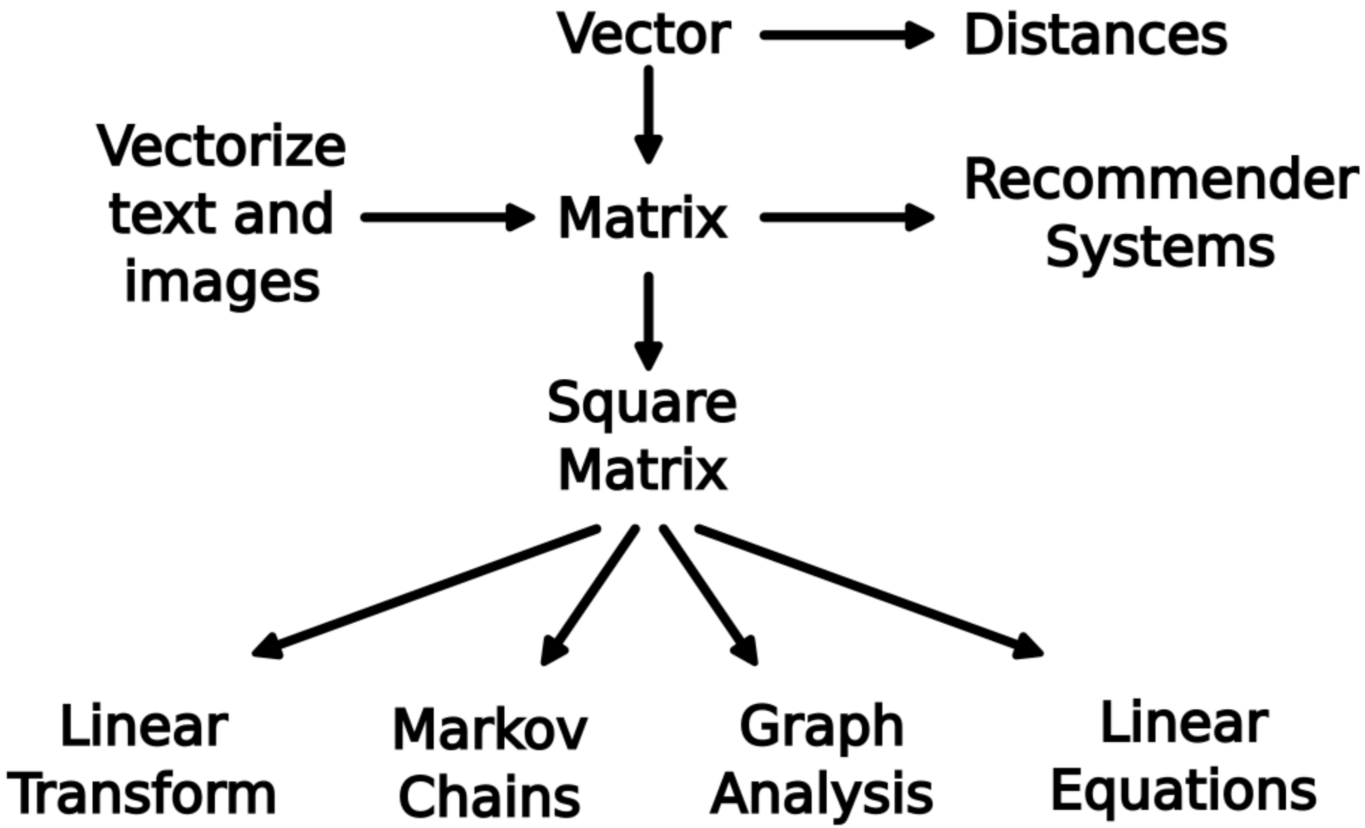
Exercises

- Python exercises on www.academis.eu/linear_algebra
- best executed on Google Colab
- used libraries: `numpy`, `pandas`, `seaborn`, `matplotlib`, `scikit-learn`

What is Linear Algebra?

- **Linear algebra is a set of shortcuts for common math operation on large datasets.**

Overview


Vector
Distances
Vectorize text and images
Matrix
Recommender Systems
Square Matrix
Linear Transform
Markov Chains
Graph Analysis
Linear Equations

Outline

1. Vectors
2. Matrices
3. Linear Transformations
4. Distances and Norms
5. Recommender Systems
6. Graph Analysis
7. Linear Equation Systems
8. Vectorizing images and text

1. Vectors

What is a vector?

- **a geometric entity** with a direction and length, in an n-dimensional coordinate system.
- **a feature vector**: a data point consisting of n numerical features.
- in both cases, vectors are arrays of n real numbers

Vector notation

Example: we were fruit shopping and store the amount of each type:

$$\vec{fruit} = \begin{pmatrix} 3 \text{🍎} \\ 2 \text{🍌} \\ 1 \text{🍒} \end{pmatrix}$$

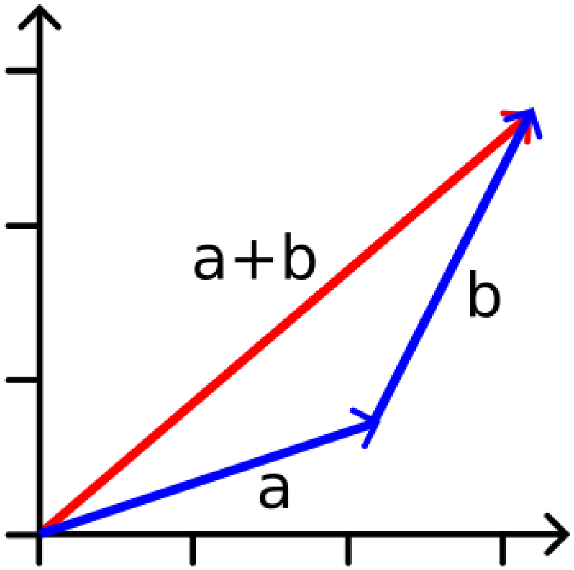
$$a_i \in \mathbb{R}$$

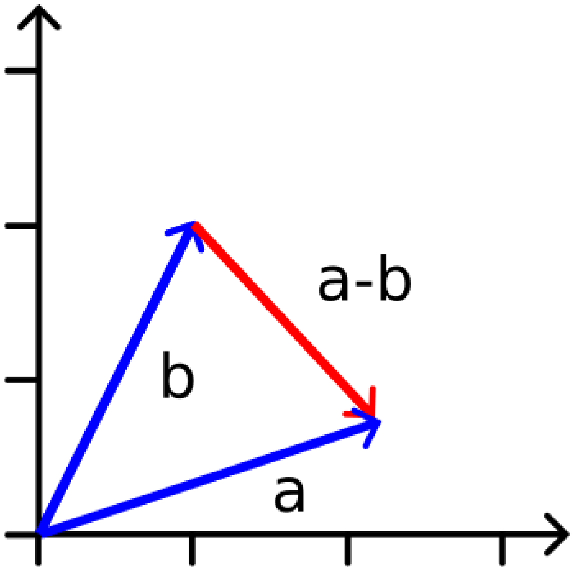
Conventions

- lowercase letters
- often written with an arrow on top (not always)
- can have any number of dimensions

Adding and subtracting vectors

$$\vec{c} = \vec{a} + \vec{b} = \begin{pmatrix} a_1 - b_1 \\ a_2 - b_2 \end{pmatrix} = \begin{pmatrix} 3\,\text{🍎} + 4\,\text{🍎} \\ 2\,\text{🍌} + 5\,\text{🍌} \\ 1\,\text{🍒} + 6\,\text{🍒} \end{pmatrix}$$





There are 4 ways to multiply vectors

1. scalar multiplication
2. component-wise product
3. dot product
4. cross product

(even more types of products exist, but not in this workshop)

Scalar multiplications

$$3\vec{a} = \begin{pmatrix} 3a_1 \\ 3a_2 \\ 3a_3 \end{pmatrix}$$

- result is a vector of the same size
- multiply each item with the same number
- makes the vector longer or shorter (scaling)

Component-wise Product

$$\vec{a} \circ \vec{b} = \begin{pmatrix} a_1 b_1 \\ a_2 b_2 \\ a_3 b_3 \end{pmatrix}$$

Example:

$$bill = \vec{fruit} \circ \vec{prices} = \begin{pmatrix} 3\text{🍎} \\ 2\text{🍌} \\ 1\text{🍒} \end{pmatrix} \cdot \begin{pmatrix} 2€ \\ 1€ \\ 3€ \end{pmatrix} = \begin{pmatrix} 3\text{🍎} \cdot 2€ \\ 2\text{🍌} \cdot 1€ \\ 1\text{🍒} \cdot 3€ \end{pmatrix} = \begin{pmatrix} 6\text{🍎}€ \\ 2\text{🍌}€ \\ 3\text{🍒}€ \end{pmatrix}$$

- result is a vector of the same size
- multiply each item with the corresponding position
- also called Hadamard or Schur product

Dot Product (inner product)

$$\vec{a} \cdot \vec{b} = \sum_i a_i b_i$$

Example:

$$bill = \vec{fruit} \cdot \vec{prices} = \begin{pmatrix} 3\text{🍎} \\ 2\text{🍌} \\ 1\text{🍒} \end{pmatrix} \cdot \begin{pmatrix} 2€ \\ 1€ \\ 3€ \end{pmatrix} = \begin{pmatrix} 3\text{🍎} \cdot 2€ \\ 2\text{🍌} \cdot 1€ \\ 1\text{🍒} \cdot 3€ \end{pmatrix} = 11€$$

- result is a scalar
- sum of the component-wise product
- geometrically a projection
- 0 if the vectors are *orthogonal*

Cross Product (outer product)

$$\vec{a} \times \vec{b} = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix}$$

- calculates an orthogonal vector
- non-commutative ($\vec{a} \times \vec{b} \neq \vec{b} \times \vec{a}$)
- 0 if vectors a and b are colinear
- works for > 3 dimensions but more complicated

Special vectors

Null vector

$$\vec{0} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Special vectors

Null vector

$$\vec{0} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Unit vector

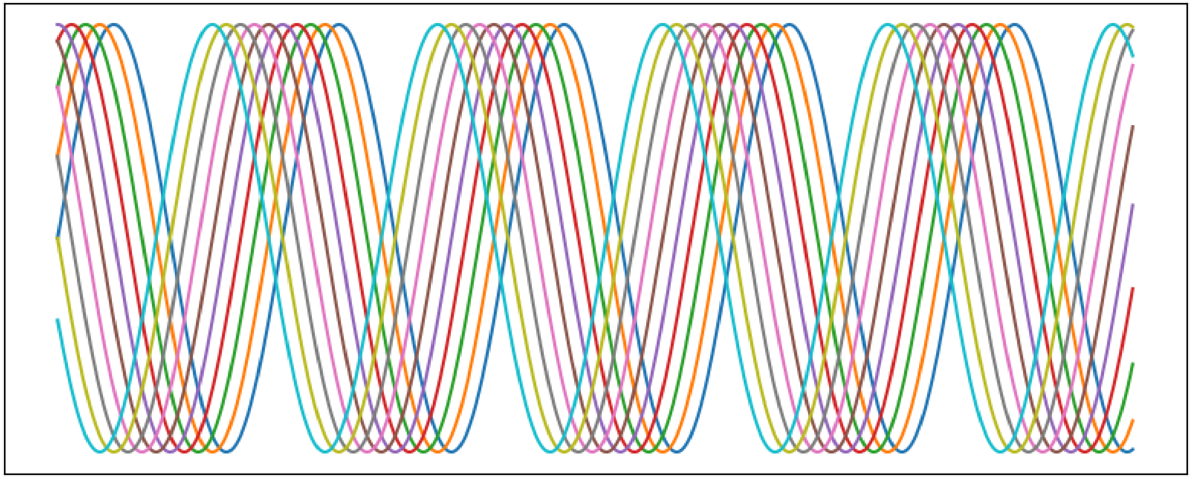
$$\vec{u} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \vec{v} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- length 1, aligned with axes
- define a corrdinate system

Takeaways

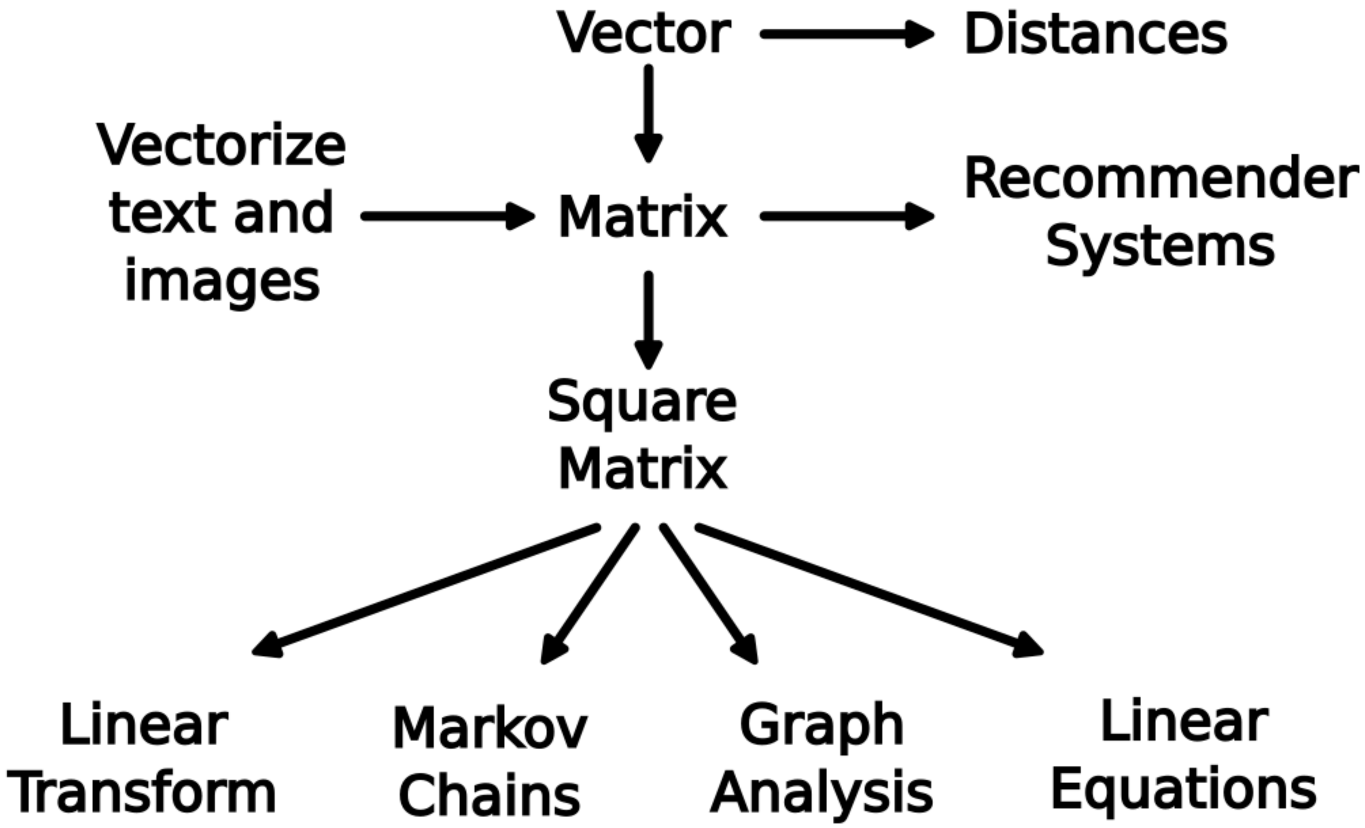
- Linear algebra is a set of shortcuts for common math operation on large datasets.
- **Vectors are arrays of numbers that represent geometrical entities or just data.**
- **there are four ways to multiply vectors**.

Exercises:



- Go to **www.academis.eu/linear_algebra**.
- download and open the first Python notebeook on Colab.
- run the code examples on **Vectors**.

Overview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2. Matrices

What is a matrix?

$$D = \begin{pmatrix} d_{11} & d_{12} \\ d_{21} & d_{22} \\ d_{31} & d_{32} \end{pmatrix} = \begin{pmatrix} 3\text{🍎} & 6\text{🍎} \\ 2\text{🍌} & 0\text{🍌} \\ 1\text{🍒} & 10\text{🍒} \end{pmatrix}$$

- a two-dimensional array of real numbers
- usually denoted by capital letters
- dimension n x m (rows x columns) ⚠️
- a table with data for many practical matters
- addition, subtraction and scalar multiplication are very similar to vectors

Matrices in Numpy

⚠️ `.shape` is the most important operation for debugging vectors and matrices!

Matrices in Numpy

⚠️ `.shape` is the most important operation for debugging vectors and matrices!

In [ ]:
```
import numpy as np

D = np.array([
    [3, 6],
    [2, 0],
    [1, 10],
])
D.shape  # -> 3, 2 (rows, columns)
```

Transpose operation

$$D^T = \begin{pmatrix} d_{11} & d_{21} & d_{31} \\ d_{12} & d_{22} & d_{32} \end{pmatrix} = \begin{pmatrix} 3\text{🍎} & 2\text{🍌} & 1\text{🍒} \\ 6\text{🍎} & 0\text{🍌} & 10\text{🍒} \end{pmatrix}$$

- Swaps the axes of a matrix
- converts **column vectors** to **row vectors** and vice versa
- to transpose vectors in numpy, use `.reshape()`

Matrix-vector product (1)

Calculate the total cost for each shopper:

$$D^T \vec{prices} = \begin{pmatrix} 3\,\text{🍎} & 2\,\text{🍌} & 1\,\text{🍒} \\ 6\,\text{🍎} & 0\,\text{🍌} & 10\,\text{🍒} \end{pmatrix} \begin{pmatrix} 2€ \\ 1€ \\ 3€ \end{pmatrix}$$

$$= \begin{pmatrix} 3\,\text{🍎} \cdot 2€ + 2\,\text{🍌} \cdot 1€ + 1\,\text{🍒} \cdot 3€ \\ 6\,\text{🍎} \cdot 2€ + 0\,\text{🍌} \cdot 1€ + 10\,\text{🍒} \cdot 3€ \end{pmatrix} = \begin{pmatrix} 11€ \\ 42€ \end{pmatrix}$$

- like the dot product, but with each row or column
- multiplies a **(2, 3)** matrix with a **(3, 1)** column vector
- result is a vector of size **2**
- non-commutative!

Matrix-vector product (2)

Calculate the total cost for each shopper, reversed:

$$\vec{prices}^T D = \begin{pmatrix} 2€ & 1€ & 3€ \end{pmatrix} \begin{pmatrix} 3\text{🍎} & 6\text{🍎} \\ 2\text{🍌} & 0\text{🍌} \\ 1\text{🍒} & 10\text{🍒} \end{pmatrix}$$

$$= \begin{pmatrix} 3\text{🍎} \cdot 2€ + 2\text{🍌} \cdot 1€ + 1\text{🍒} \cdot 3€ \\ 6\text{🍎} \cdot 2€ + 0\text{🍌} \cdot 1€ + 10\text{🍒} \cdot 3€ \end{pmatrix} = \begin{pmatrix} 11€ & 42€ \end{pmatrix}$$

- multiplies a **(1, 3)** row vector with a **(3, 2)** matrix
- result is a **(1, 2)** row vector
- one dimension has to be the same, watch the indices!

Matrix Multiplication

Generally, in matrix multiplication the corresponding values in the **inner** dimension are subject to a dot product:

$$C = AB$$

$$C_{ij} = \sum_{k} = 1^n A_{ik} \cdot B_{kj}$$

Properties

- non-commutative: $AB \neq BA$
- associative:
  $(AB)C$
  $= A(BC)$
- distributive:
  $A(B + C)$
  $= AB + AC$

Matrix Multiplication

$$\begin{array}{ccc} & B & \\ & \begin{pmatrix}\boxed{1} & 3\\ \boxed{2} & 4\end{pmatrix} & \\ A\ \begin{pmatrix}\boxed{1} & \boxed{7}\\ 3 & 8\\ 5 & 0\end{pmatrix} & \begin{array}{|c|c|}\hline 15 & 31\\ \hline 19 & \\ \hline & \\ \hline\end{array} & AB \end{array}$$

Square Matrices

Square matrices have two identical dimensions *(n, n)*.

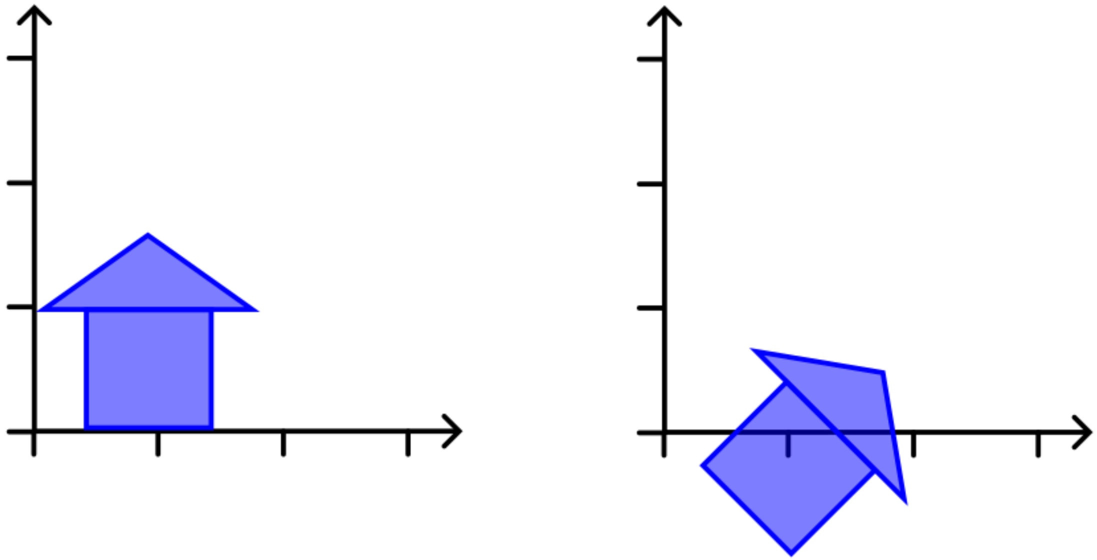
$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

⚠️ **You will mess up the dimensions without causing an error!**

Takeaways

- Linear algebra is a set of shortcuts for common math operation on large datasets.
- Vectors are arrays of numbers that represent geometrical entities or just data.
- there are four ways to multiply vectors.
- **matrices are tables of numbers with *n x m* (rows x columns).**
- **vectors and matrices are multiplied similar to a dot product.**

3. Linear Transformations



- Matrices represent linear transformations of coordinate systems
- multplication with a matric transforms a vector
- if it is not a square matrix, the number of dimensions changes
- applications: 3D vector graphics, CAD, Unreal engine, 3D molecules

Rotation by 90°

$$R_{90} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Example:

$$R_{90}\vec{a} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 3 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \cdot 3 + 1 \cdot 1 \\ -1 \cdot 3 + 0 \cdot 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -3 \end{pmatrix}$$

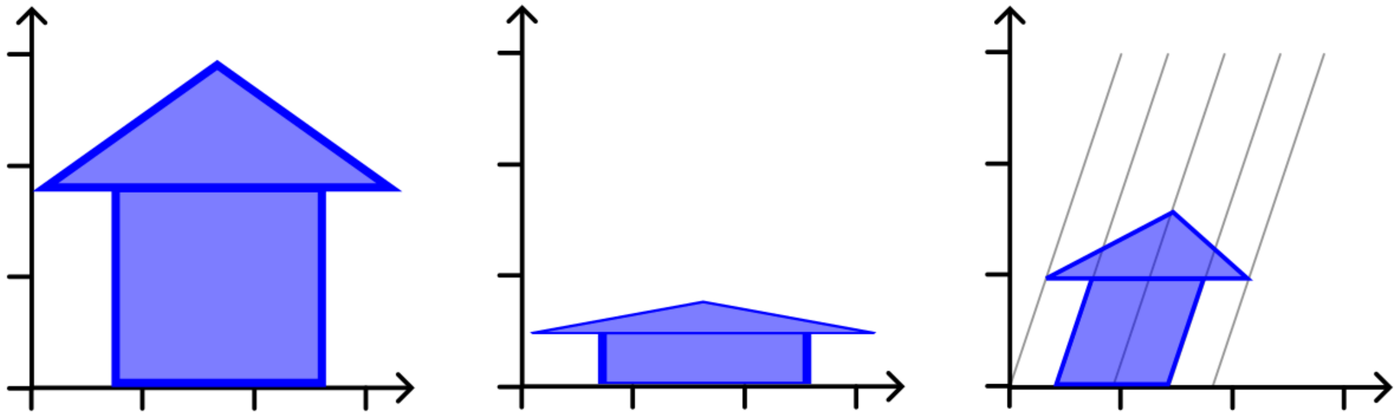
Rotation by other angles

$$R(\theta) = \begin{pmatrix} cos\theta & sin\theta \\ -sin\theta & cos\theta \end{pmatrix}$$

In a 3D coordinate system:

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & cos\theta & -sin\theta \\ 0 & sin\theta & cos\theta \end{pmatrix}$$

Other linear transformations



- scale, flip, shear
- proportions on each axis stay the same
- angle between axes may change

Special Transformation Matrices

Identity Matrix

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

Multiplication of a vector with an identita matrix results in the same vector.

$$I\vec{v} = \vec{v}$$

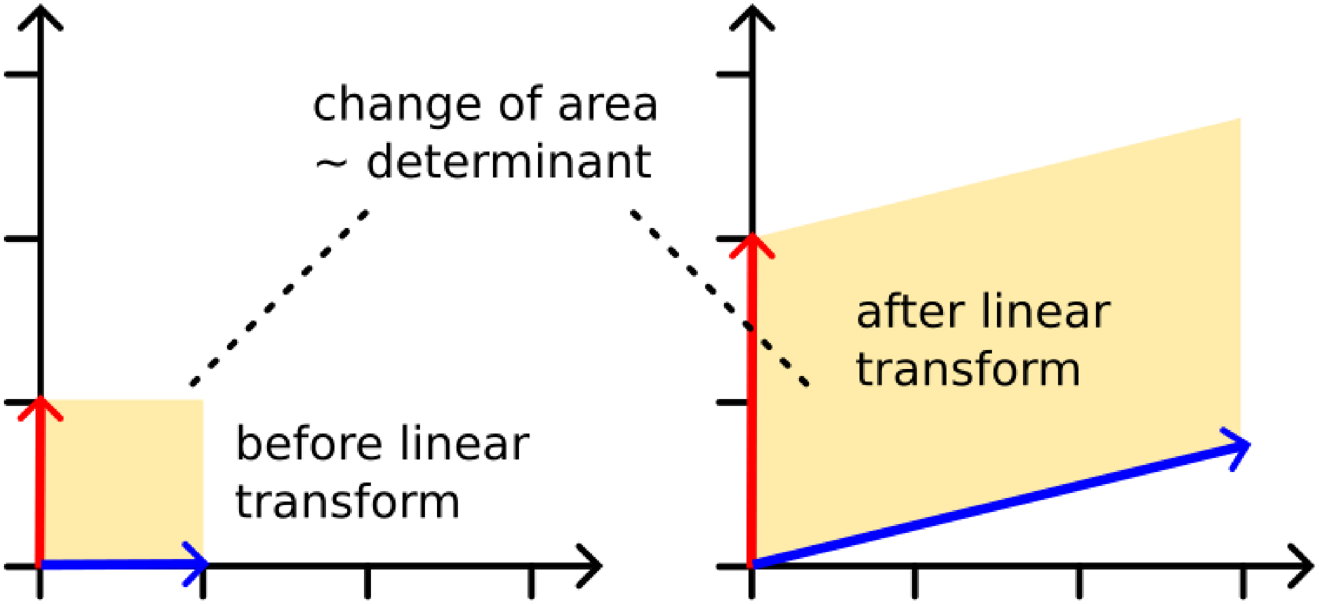
Null Matrix

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Multiplication of a vector with a null matrix results in a null vector.

Determinants

a key characteristic to describe linear transformation matrices



The determinant of a matrix $det A$ specifies by what factor the area spanned by unit vectors changes during a linear transformation

Calculating Determinants

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

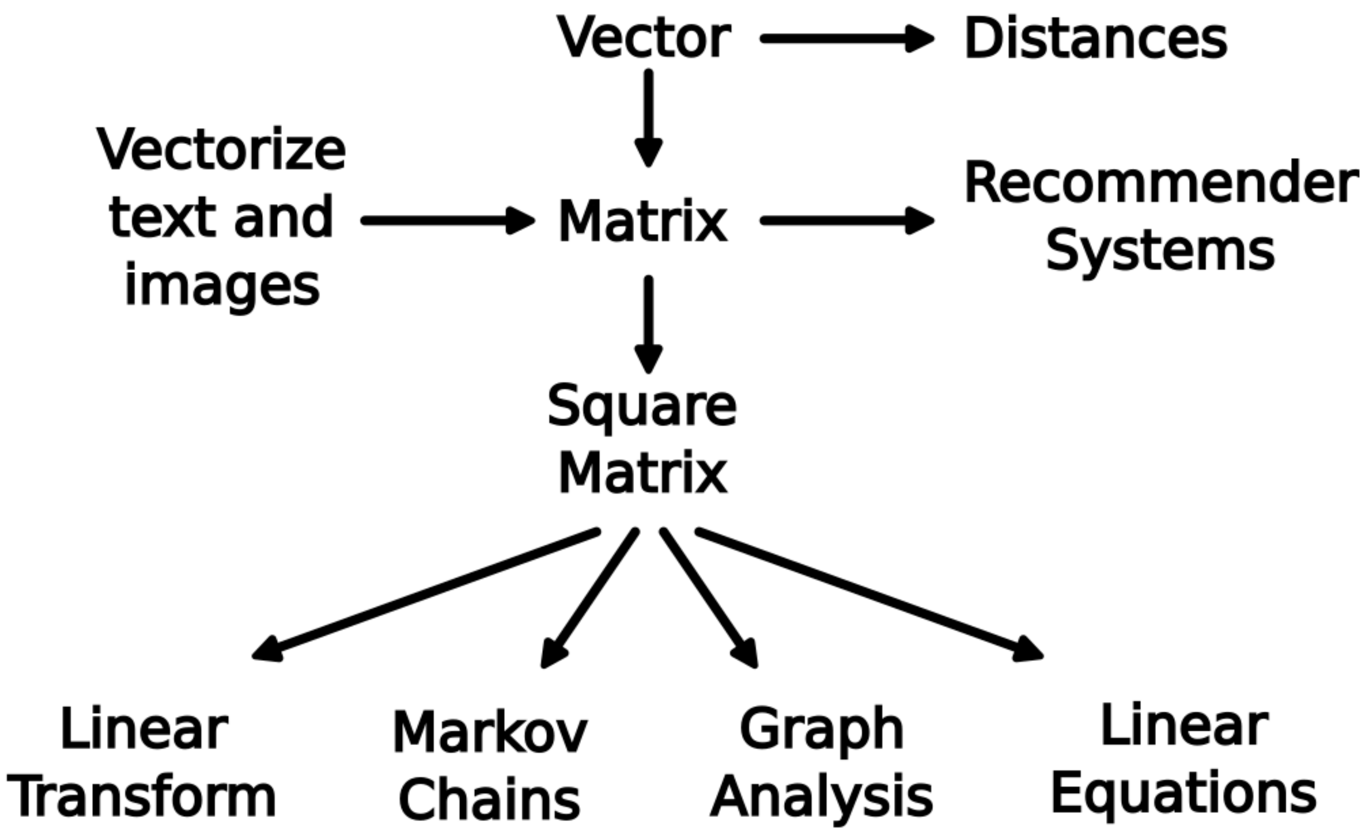
$$det A = ad - bc$$

- if $det A$ is 1, the scale of the image does not change (e.g. rotation)
- if $det A$ is negative, the orientation of the coordinate system reverses
- if $det A$ is 0, some axes fall together during the transformation

Takeaways

- Linear algebra is a set of shortcuts for common math operation on large datasets.
- Vectors are arrays of numbers that represent geometrical entities or just data.
- there are four ways to multiply vectors.
- matrices are tables of numbers with $n \times m$ (rows x columns).
- vectors and matrices are multiplied similar to a dot product.
- **matrix multiplication rotates, scales, flips, shears vectors to a new coordinate system.**
- **the determinant tells how a transformation matrix changes the area spanned by unit vectors.**

Overview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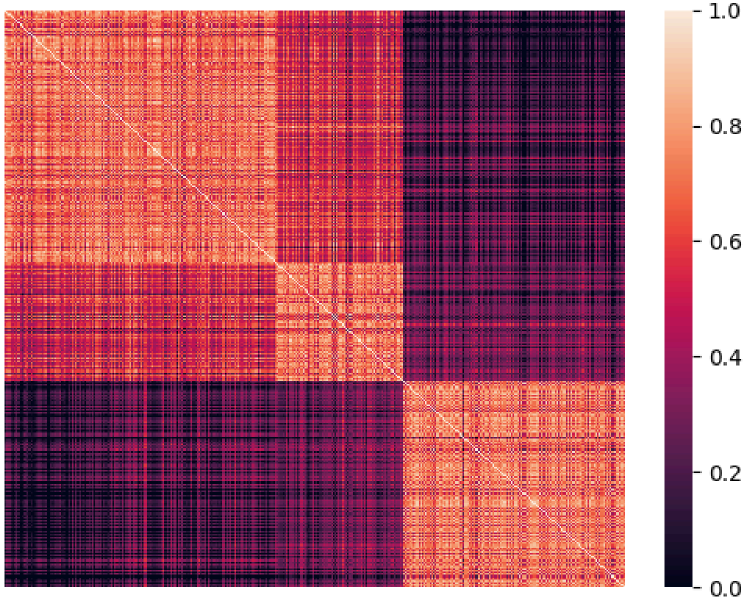
4. Distances and Norms

A distance matrix of 333 penguins:



We have seen how we can combine vectors and matrices in different ways. Now, we will compare two vectors.

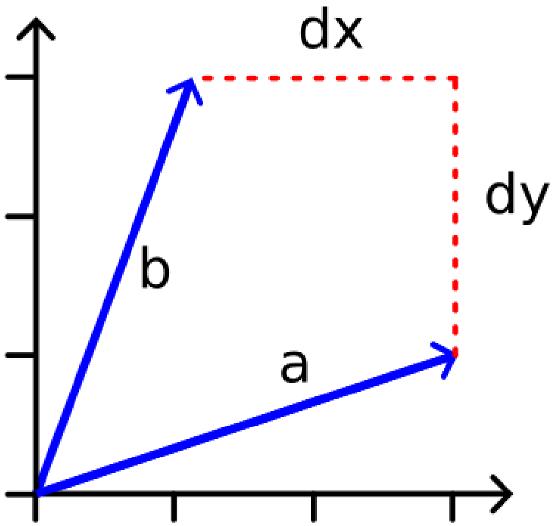
Comparing vectors

How can we measure the distance between 2 data points?

	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	sex
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0	Male
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0	Female
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0	Female
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0	Female
5	Adelie	Torgersen	39.3	20.6	190.0	3650.0	Male

- **norms** measure the length of the difference vector.
- **cosine similarity** measures the angle between two vectors.

L1 Norm: Manhattan distance

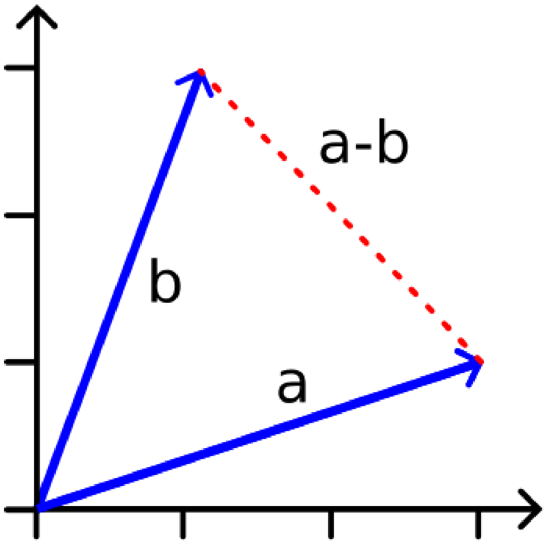


The Manhattan distance sums up the absolute of each component of a vector (or the difference of two)

$$||\vec{a}||_1 = \sum_i |a_i|$$

Application: regularization in Machine Learning.

L2 Norm: Euclidean distance

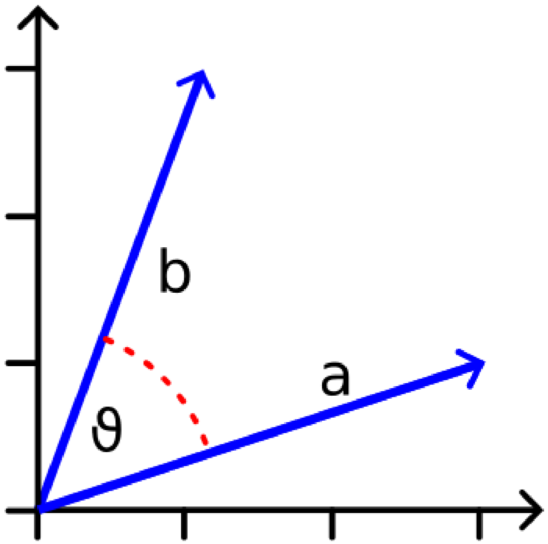


Euclidean distance does the same calculation as in the Pythagorean theorem: it sums up square differences and then takes the square root.

$$||\vec{a}||_2 = \sqrt{\sum_i a_i^2}$$

Application: regularization in Machine Learning

Cosine similarity



- Cosine similarity measures the angle between two vectors
- between 1 (perfect match) and 0 (orthogonal)
- cosine rule explains why dot product is zero if angle is 90°

$$cos(\theta) = \frac{\vec{a} \cdot \vec{b}}{||\vec{a}||_2 \cdot ||\vec{b}||_2}$$

Application: search in RAGs, clustering, anomaly detection and recommender systems

Takeaways

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- Vectors are arrays of numbers that represent geometrical entities or just data.
- there are four ways to multiply vectors.
- matrices are tables of numbers with *n x m* (rows x columns).
- vectors and matrices are multiplied similar to a dot product.
- matrix multiplication rotates, scales, flips, shears vectors to a new coordinate system.
- the determinant tells how a transformation matrix changes the area spanned by unit vectors.
- **The length of vectors can be measured by L1 and L2 norms.**
- **Cosine similarity measures the angle between vectors.**

Applications

Will be done in exercise notebooks

- Recommender Systems
- Graph Analysis
- Linear Equation Systems
- Vectorization

Further Material

See www.academis.eu/linear_algebra