# Principal Component Analysis

CSC 461: Machine Learning

Fall 2022

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# Dimensionality reduction

- Basically …
  - ✓ mapping **high-dimensional** data into **low dimensional** data
  - ✓ can be as simple as dropping some features or using a combination of all features
- Given $\mathscr{D} = \{\mathbf{x_1}, \ldots, \mathbf{x_n}\}$ with $\mathbf{x_i} \in \mathbb{R}^d$, find a representation $\mathscr{Z} = \{\mathbf{z_1}, \ldots, \mathbf{z_n}\}$ with $\mathbf{z_i} \in \mathbb{R}^{d'}$ and $d' \ll d$
  - ✓ properties should be preserved (e.g., variance, distances, neighborhood)

$$\begin{bmatrix} \text{---} & \mathbf{x_1}^T & \text{---} \\ & \vdots & \\ \text{---} & \mathbf{x_n}^T & \text{---} \end{bmatrix}_{n \times d} \Rightarrow \begin{bmatrix} \mathbf{z_1}^T \\ \vdots \\ \mathbf{z_n}^T \end{bmatrix}_{n \times d'}$$

# Why dimensionality reduction?

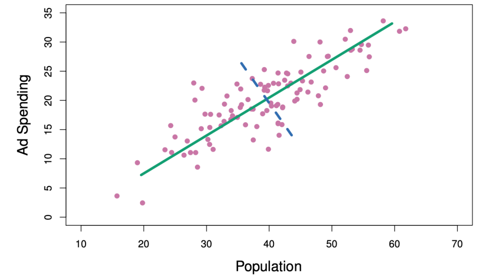
- Data visualization (2-d or 3-d)
- Preprocess data before machine learning
  - ✓ algorithms can focus on important features/patterns
  - ✓ training can be more efficient
- Removing noise and redundant information
- Data compression

# Principal component analysis

eigendecomposition of the covariance matrix

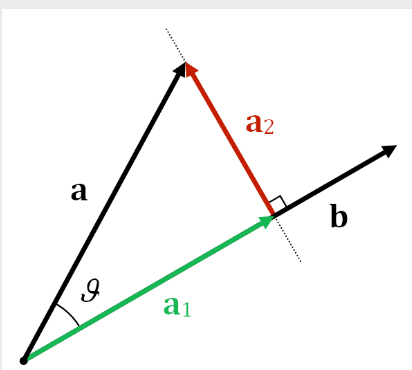
# Principal component analysis

- Find projections of the data onto directions that maximize variance
  - ✓ directions are **orthogonal** to each other




https://www.dataschool.io/15-hours-of-expert-machine-learning-videos/

# Preliminaries




The **vector projection** of vector **a** onto a nonzero vector **b** is the orthogonal projection of **a** onto a straight line parallel to **b**:

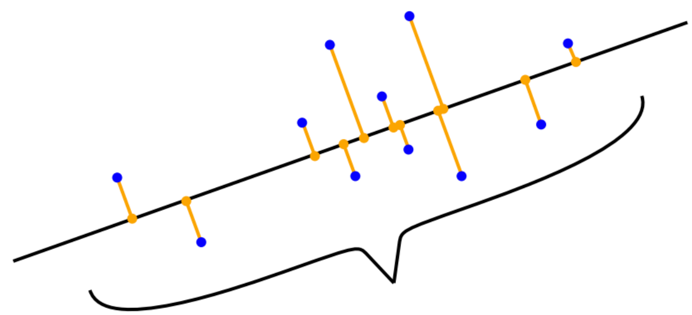
$$\mathbf{a_1} = a_1 \hat{\mathbf{b}}$$

where $a_1$ is a scalar, called the **scalar projection** of **a** onto **b**, and $\hat{\mathbf{b}}$ is the unit vector in the direction of **b**. The scalar projection is defined as:

$$a_1 = \mathbf{a} \cdot \hat{\mathbf{b}}$$

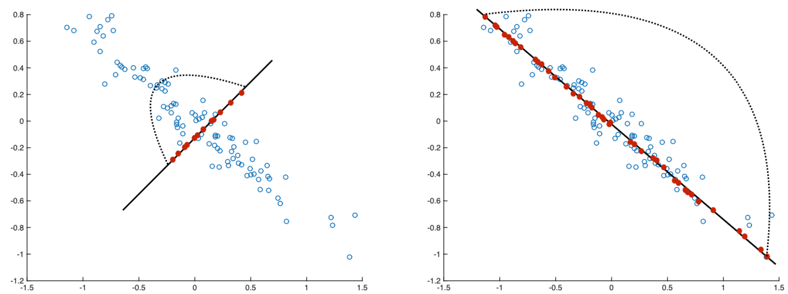
https://en.wikipedia.org/wiki/Vector_projection

# Data projection on a line



PCA idea is finding a line that maintains as much variance (spread) as possible when the data is projected.

## What is the best line? — maximize variance



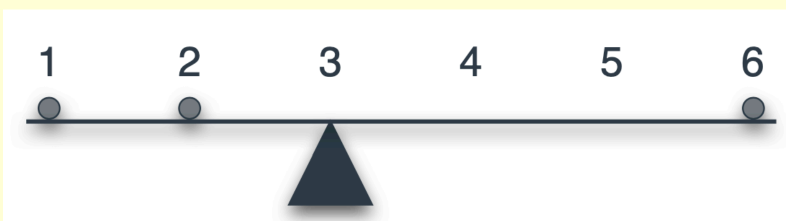
Idea: minimize sum of square distances to the line (or maximize the sum of squares of the scalar projections)



## Disclaimer

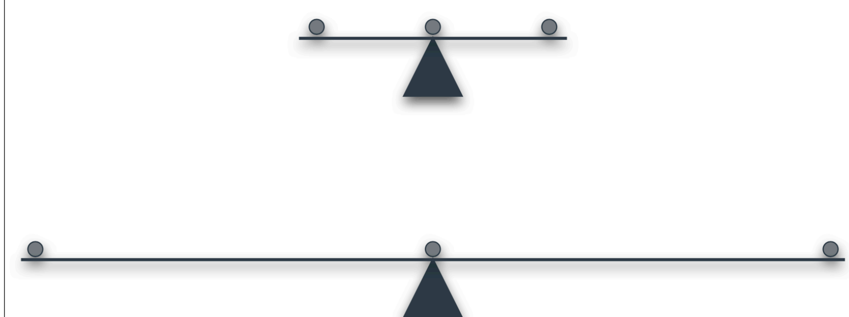
- The following slides contain figures adapted from:
  - ✓ Unsupervised Learning SERRANO.ACADEMY the art of understanding
    - ✓ https://serrano.academy/unsupervised-learning/
- Video:
  - ✓ https://www.youtube.com/watch?v=g-Hb26agBFg

## The mean




$$\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$$

## Doesn’t always help



# The variance

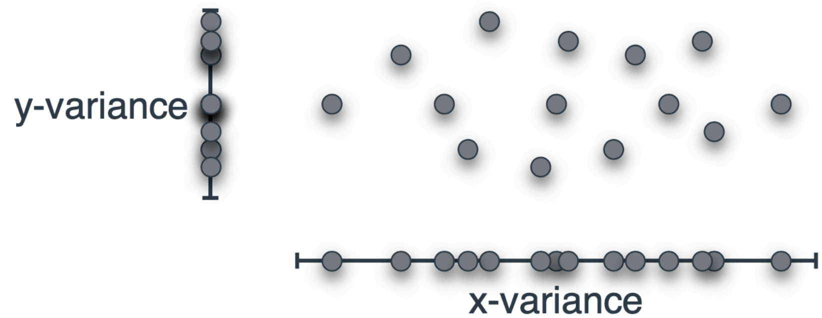

Variance = $\frac{1^2+0^2+1^2}{3}$ = 2/3


Variance = $\frac{5^2+0^2+5^2}{3}$ = 10/3

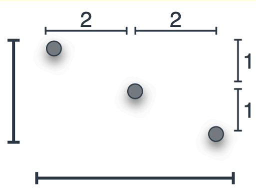
“biased” estimator
default in numpy

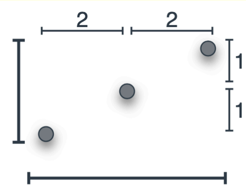
$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

# Variance and data




# Doesn’t always help

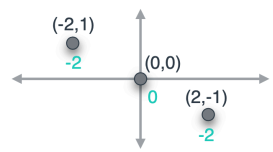


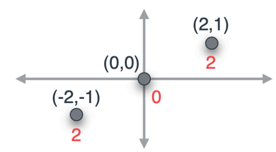

x-variance = $\frac{2^2+0^2+2^2}{3}$ = 8/3

y-variance = $\frac{1^2+0^2+1^2}{3}$ = 2/3

# Covariance




zero mean




zero mean

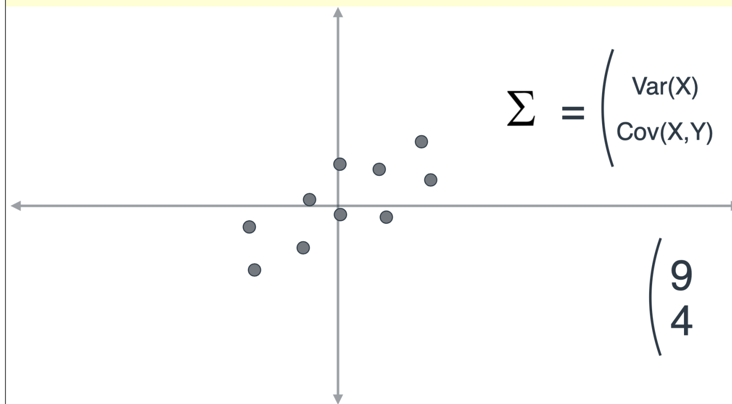
covariance = $\frac{(-2) + 0 + (-2)}{3}$ = -4/3

covariance = $\frac{2 + 0 + 2}{3}$ = 4/3

$$\operatorname{cov}(\mathbf{x}, \mathbf{y}) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

# Covariance


# Covariance matrix

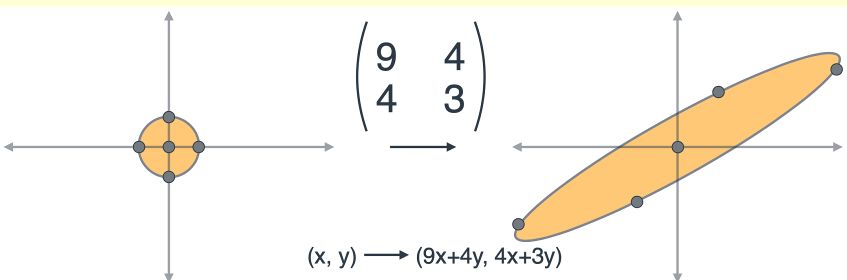


$$\Sigma = \begin{pmatrix} \text{Var(X)} & \text{Cov(X,Y)} \\ \text{Cov(X,Y)} & \text{Var(Y)} \end{pmatrix}$$

$$\begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix}$$

Every element $\Sigma_{ij}$ of the covariance matrix is the covariance between variable *i* and variable *j*

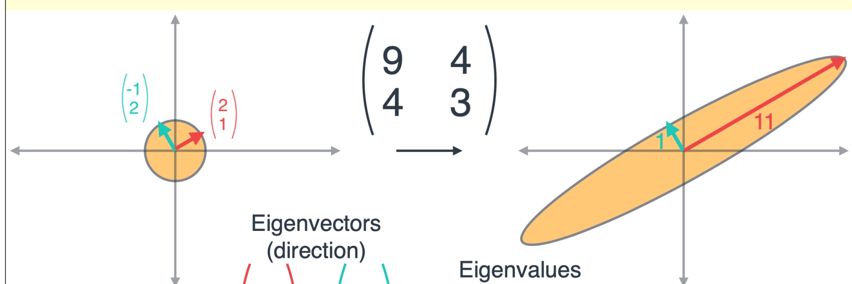
# Linear transformations



$$\begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix} \longrightarrow$$

| (x, y) ⟶ | (9x+4y, 4x+3y) |
|---|---|
| (0,0) | (0,0) |
| (1,0) | (9,4) |
| (0,1) | (4,3) |
| (-1,0) | (-9,-4) |
| (0,-1) | (-4,-3) |

# Eigenvectors and eigenvalues




$$\begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix} \longrightarrow$$

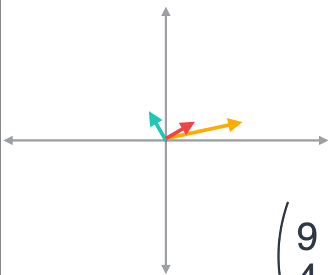
Eigenvectors
(direction)

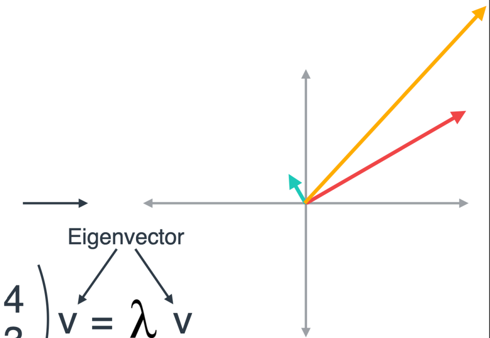
$$\begin{pmatrix} 2 \\ 1 \end{pmatrix} \quad \begin{pmatrix} -1 \\ 2 \end{pmatrix}$$

Eigenvalues
(magnitude)

11 1

# Eigenvectors and eigenvalues





Eigenvector

$$\begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix} v = \lambda\, v$$

Eigenvalue

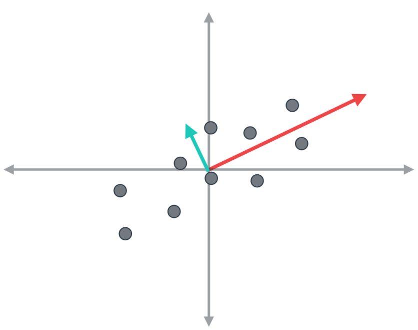
# Eigenvectors and eigenvalues

- The decomposition of a **square matrix A** into eigenvalues and eigenvectors is known as **eigen decomposition**
  - ✓ for **real symmetric matrices** eigenvectors can be chosen real and orthonormal

$$A = V \Lambda V^T \qquad A\mathbf{v} = \lambda \mathbf{v}$$

columns of V are the eigenvectors of A and $\Lambda$ is a diagonal matrix whose entries are the eigenvalues of A

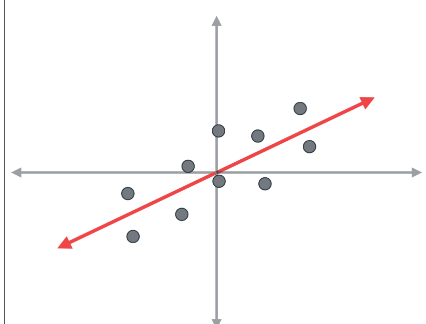
# Principal component analysis (PCA)



$$\Sigma = \begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix}$$

| | | |
|---|---|---|
| $\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ | $\begin{pmatrix} -1 \\ 2 \end{pmatrix}$ | Eigenvectors (direction) |
| 11 | 1 | Eigenvalues (magnitude) |

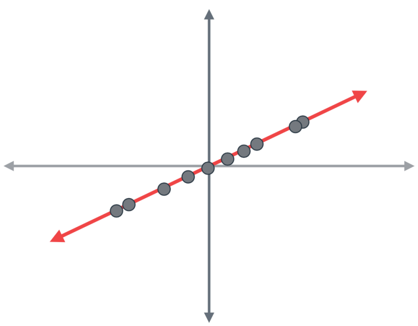
# Principal component analysis (PCA)



$$\Sigma = \begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix}$$

| | |
|---|---|
| $\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ | Eigenvectors (direction) |
| 11 | Eigenvalues (magnitude) |

# Principal component analysis (PCA)

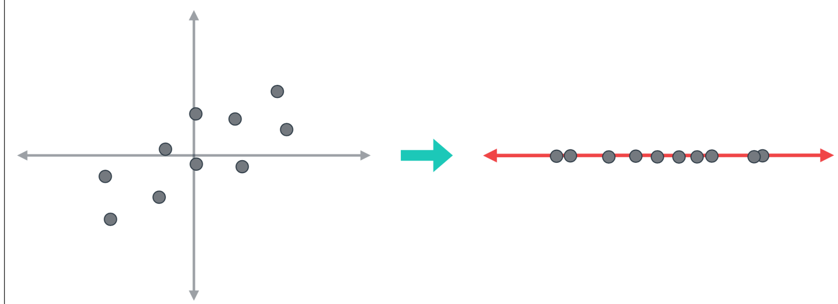


$$\Sigma = \begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix}$$

$\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ Eigenvectors (direction)

11 Eigenvalues (magnitude)

# Principal component analysis (PCA)



# More formally

- Given $\mathscr{D} = \{\mathbf{x_1}, \ldots, \mathbf{x_n}\}$ with $\mathbf{x_i} \in \mathbb{R}^d$
  - ✓ find $\mathscr{Z} = \{\mathbf{z_1}, \ldots, \mathbf{z_n}\}$ with $\mathbf{z_i} \in \mathbb{R}^{d'}$ and $d' \ll d$
- Example from 3-d to 2-d

$$\mathbf{v_1} \in \mathbb{R}^3, \mathbf{v_2} \in \mathbb{R}^3$$

$$\mathbf{z_i} = [\mathbf{v_1}^T\mathbf{x_i}, \mathbf{v_2}^T\mathbf{x_i}]^T, \mathbf{z_i} \in \mathbb{R}^2$$

# PCA

- Input
  - ✓ data must be **centered**

$$X = \begin{bmatrix} | & & | \\ \mathbf{x_1} & \ldots & \mathbf{x_n} \\ | & & | \end{bmatrix}_{d \times n}$$

$$\frac{1}{n}\sum_{i=1}^{n} c_i = 0, \quad \text{for all rows } \mathbf{c} \text{ in } X$$

- Output
  - ✓ orthonormal eigenvectors $\mathbf{v_1}, \ldots \ \mathbf{v_k}$ (principal components)

## First principal component

$\|\mathbf{v_1}\|_2 = 1$

$$\arg\max_{\mathbf{v_1}} \sum_{i=1}^{n} (\mathbf{x_i}^T \mathbf{v_1})^2$$

$$\arg\max_{\mathbf{v_1}} \mathbf{v_1}^T \left[ \sum_{i=1}^{n} \mathbf{x_i} \mathbf{x_i}^T \right] \mathbf{v_1}$$

$$XX^T = \Sigma$$

construct lagrangian and set derivative to zero

solution $\mathbf{v_1}$ is the first eigenvector of $XX^T$

## Second principal component

$\|\mathbf{v_2}\|_2 = 1$

$\mathbf{v_2}^T \mathbf{v_1} = 0$

$$\arg\max_{\mathbf{v_2}} \sum_{i=1}^{n} (\mathbf{x_i}^T \mathbf{v_2})^2$$

$$\arg\max_{\mathbf{v_2}} \mathbf{v_2}^T \left(XX^T\right) \mathbf{v_2}$$

solution $\mathbf{v_2}$ is the second eigenvector of $XX^T$

**Other principal components will follow the same idea**

## PCA algorithm

- Assuming **X** and **K** as inputs
  - ✓ **Center** the data in X
  - ✓ Compute **eigendecomposition** $\left(V\Lambda V^T\right)$ of $XX^T$
  - ✓ Return the **top K eigenvectors** from $V$
- Eigenvectors can then be used for **projecting** the data into lower dimensions

## Remarks

- The **larger** the eigenvalue, the **more important** the corresponding eigenvector
  - ✓ that's why we **sort** eigenvalues (and corresponding eigenvectors) in **decreasing order**
- All eigenvalues of a positive semidefinite matrix are **non-negative**
  - ✓ **covariance matrix** is always symmetric and p.s.d.
- For dimensionality reduction, we can ignore eigenvectors that are "less important"
  - ✓ how many? … see explained variance next

# Explained variance

- The variance of each principal component is equal to their corresponding eigenvalues
  - ✓ variance is often presented as a percentage, i.e., eigenvalues divided by the total sum of eigenvalues
- The sum of percentages of the top-k principal components is usually referred as the “explained variance” (cumulative variance)
  - ✓ often used to select how many components to keep for a reduced dataset

# Explained variance

| PC | Eigenvalue | Variance (%) | Cumulative Variance |
|---|---|---|---|
| 1st | 23.31800 | 59.072% | 59.072% |
| 2nd | 7.01200 | 17.764% | 76.835% |
| 3rd | 4.61800 | 11.699% | 88.534% |
| 4th | 1.98100 | 5.018% | 93.553% |
| 5th | 1.00100 | 2.536% | 96.089% |
| 6th | 0.82100 | 2.080% | 98.168% |
| 7th | 0.64100 | 1.624% | 99.792% |
| 8th | 0.03100 | 0.079% | 99.871% |
| 9th | 0.02900 | 0.073% | 99.944% |
| 10th | 0.02200 | 0.056% | 100.000% |

# Google colab

https://colab.research.google.com/drive/1qOXOFEC3EdOZA1ONLvH-50Foqpel5wzw?usp=sharing