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)

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

Why dimensionality reduction?

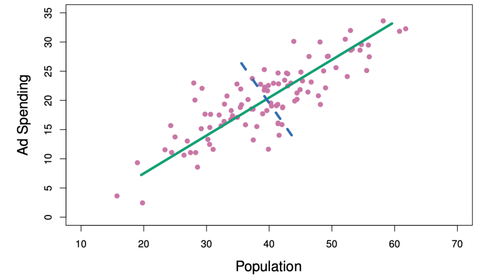
- Data visualization (2-d or 3-d)
- Preprocess data before machine learning
  - ✓ algorithms can focus on important features/patterns
  - ✓ training can be more efficient
- Removing noise and redundant information
- Data compression

Principal component analysis

eigendecomposition of the covariance matrix

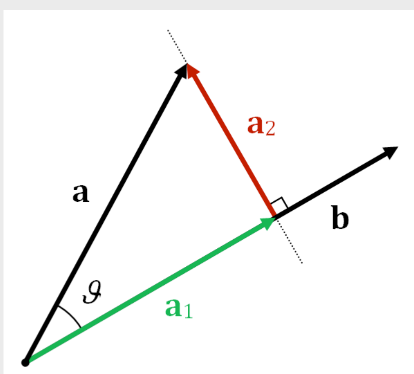
Principal component analysis

- 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**:

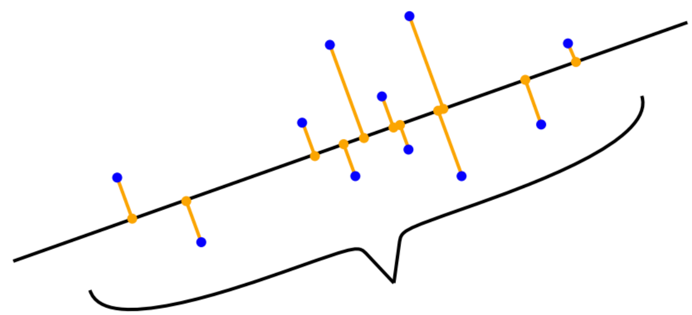
$$\mathbf{a_1} = a_1 \hat{\mathbf{b}}$$

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:

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

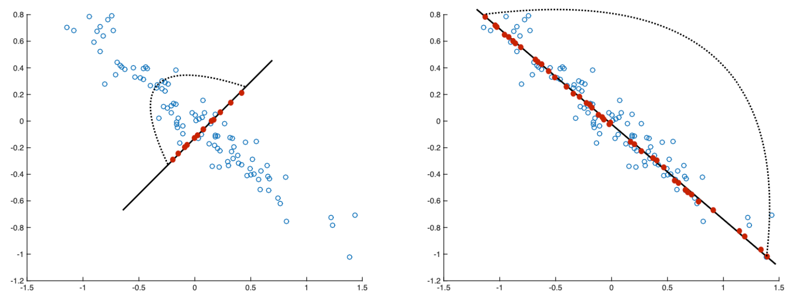
https://en.wikipedia.org/wiki/Vector_projection

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

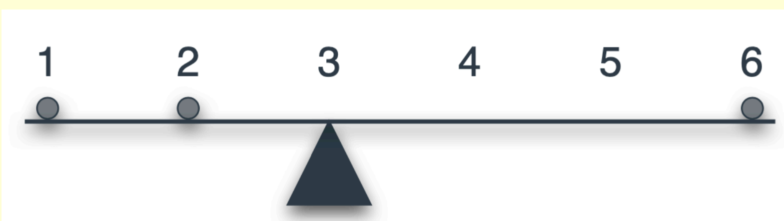


Idea: minimize sum of square distances to the line (or maximize the sum of squares of the scalar projections)

Disclaimer

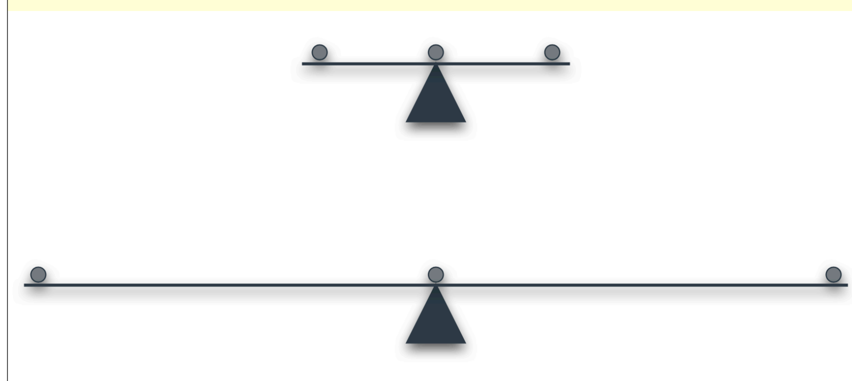
- The following slides contain figures adapted from:
  - ✓ Unsupervised Learning SERRANO.ACADEMY the art of understanding
    - ✓ https://serrano.academy/unsupervised-learning/
- Video:
  - ✓ https://www.youtube.com/watch?v=g-Hb26agBFg

The mean



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

Doesn’t always help



The variance

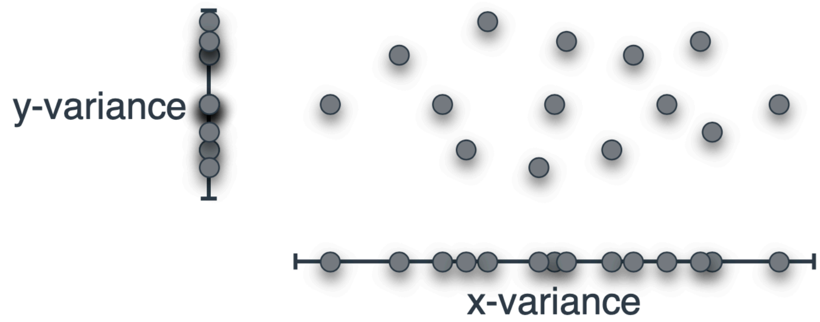
Variance = $\dfrac{1^2+0^2+1^2}{3}$ = 2/3

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

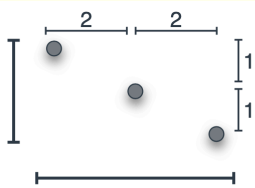
“biased” estimator
default in numpy

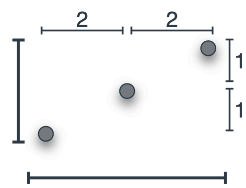
$$\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu)^2$$

Variance and data



Doesn’t always help

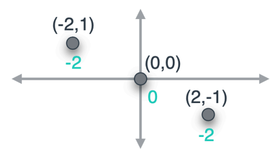




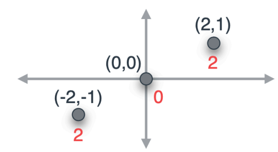
x-variance = $\dfrac{2^2+0^2+2^2}{3}$ = 8/3

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

Covariance



zero mean



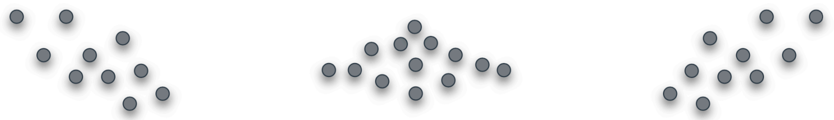
zero mean

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

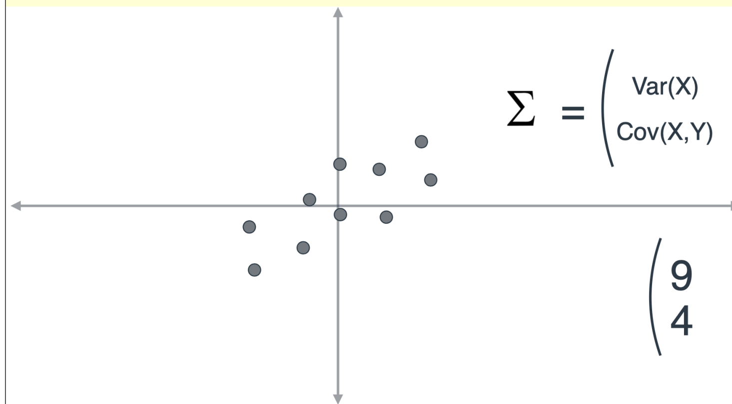
covariance = $\dfrac{2 + 0 + 2}{3}$ = 4/3

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

Covariance



Covariance matrix

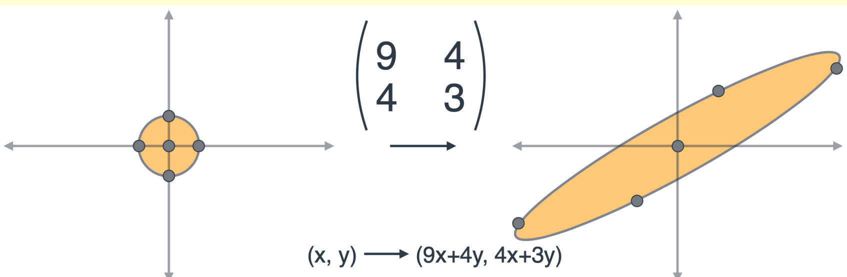


$$\Sigma = \begin{pmatrix} \mathrm{Var}(X) & \mathrm{Cov}(X,Y) \\ \mathrm{Cov}(X,Y) & \mathrm{Var}(Y) \end{pmatrix}$$

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

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

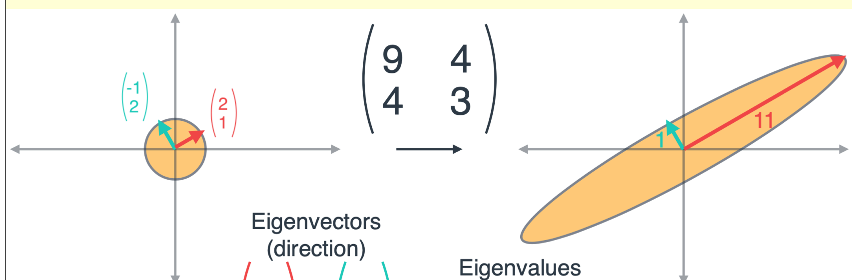
Linear transformations



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

(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



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

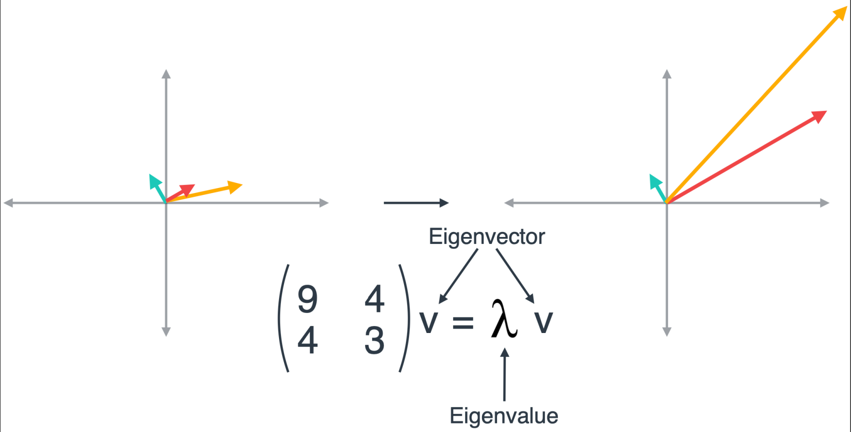
Eigenvectors (direction)

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

Eigenvalues (magnitude)

11 1

Eigenvectors and eigenvalues



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

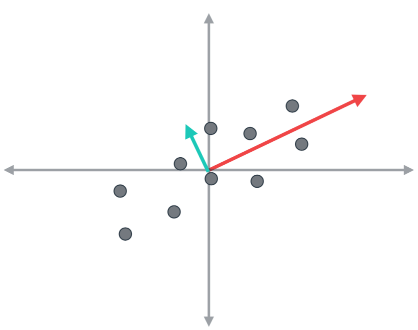
Eigenvectors and eigenvalues

- 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 Λ is a diagonal matrix whose entries are the eigenvalues of A

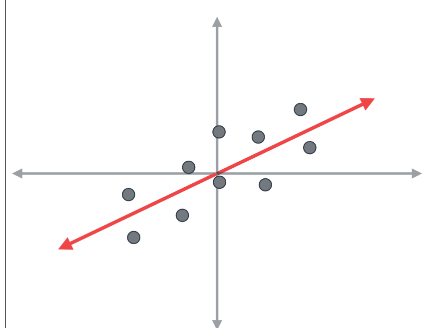
Principal component analysis (PCA)



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

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

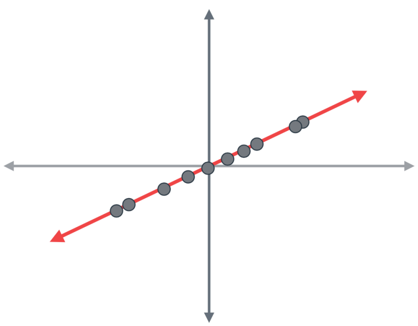
Principal component analysis (PCA)



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

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

Principal component analysis (PCA)

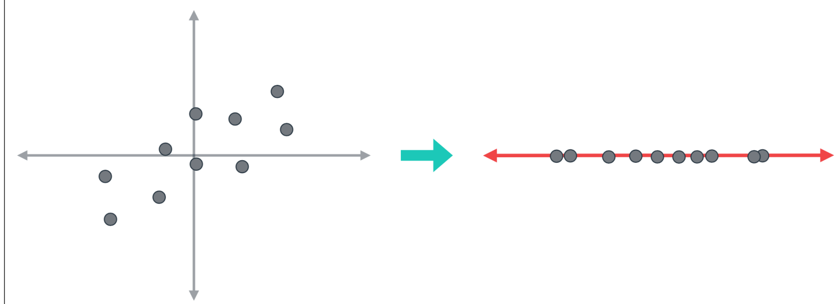


$$\Sigma = \begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix}$$

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

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

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

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

$$XX^T = \Sigma$$

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

Google colab