

# Dimensionality reduction techniques

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# Overview

## 1 Motivation

## 2 Background mathematics

- Population vs sample
- Mean, standard deviation, variance
- Covariance, covariance matrix
- Eigenvectors, eigenvalues

## 3 Dimensionality reduction techniques

- PCA (Principal component analysis)
- SNE (Stochastic neighbor embedding)

## 4 Visualizations

- IRIS dataset
- MNIST dataset

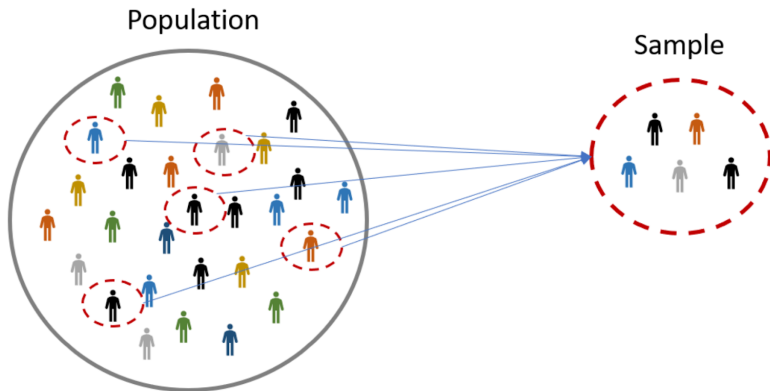
## 5 Summary

- Conclusion
- Practicum

# Motivation

- Relationships between data

# Population vs sample



# Population vs sample

## Population mean

$$\mu = \frac{\sum_{i=1}^N x_i}{N} \quad (1)$$

$N$  is number of items in the population

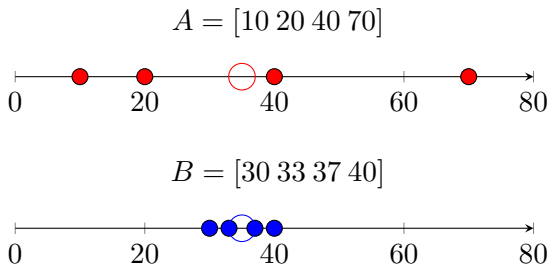
## Sample mean

$$\bar{X} = \frac{\sum_{i=1}^n x_i}{n} \quad (2)$$

$n$  is number of items in the sample

# Standard deviation

Let's take a look on two samples:



Here,  $\bar{A} = \bar{B} = 35$ . Unfortunately, mean doesn't tell us a lot except for a middle point.

# Standard deviation

For our two sets,  $A = [10\ 20\ 40\ 70]$  and  $B = [30\ 33\ 37\ 40]$ , we would be more interested in the *spread* of the data. So, how do we calculate it?

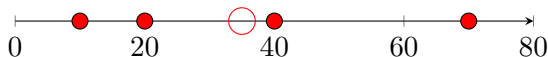
## Standard deviation

$$s = \sqrt{\frac{\sum_{i=1}^n (X_i - \bar{X})^2}{(n - 1)}} \quad (3)$$

In plain English, it is the "average distance from the mean of the data set to a point."

# Standard deviation

Set 1:  $A = [10\ 20\ 40\ 70]$ , and  $\bar{A} = 35$



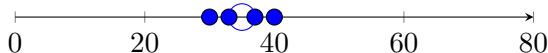
Let's calculate standard deviation:

$A$	$(A - \bar{A})$	$(A - \bar{A})^2$
10	-25	625
20	-15	225
40	5	25
70	35	1,225
Total		2,100
Divided by (n-1)		700
Square root		<b>26.4575</b>



# Standard deviation

Set 2:  $B = [30\ 33\ 37\ 40]$ , and  $\bar{B} = 35$



Let's calculate standard deviation:

$B$	$(B - \bar{B})$	$(B - \bar{B})^2$
30	-5	25
33	-2	4
37	2	4
40	5	25
Total		58
Divided by (n-1)		19.333
Square root		<b>4.397</b>

# Variance

Similar to standard deviation So, how do we calculate it?

## Variance

$$s^2 = \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{(n - 1)} \quad (4)$$

Almost identical to the standard deviation (there is no square root in the formula).

# Covariance

Previous measures are 1-dimensional. How do we check relationship between the dimensions?

## Covariance

### Variance

$$\text{var}(X) = \frac{\sum_{i=1}^n (X_i - \bar{X})(X_i - \bar{X})}{(n - 1)} \quad (5)$$

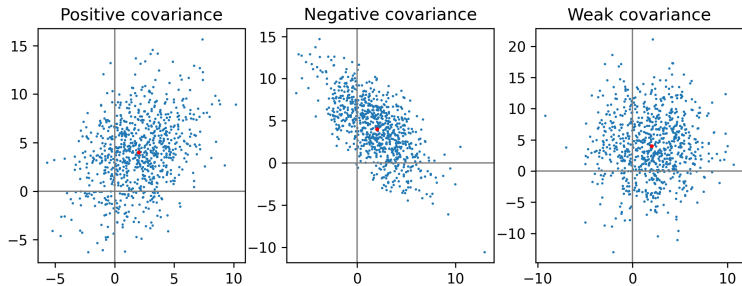
### Covariance

$$\text{covar}(X, Y) = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{(n - 1)} \quad (6)$$

How much dimensions vary from the mean *with respect to each other*.

- Covariance between one dimension and itself gives variance.

# Covariance



# Covariance

Exercise: Find covariance between 2-dimensional dataset

Item number:	1	2	3	4	5
x	10	39	19	23	28
y	43	13	32	21	20

**Ans:** -120.55

## Covariance matrix

When we have more than two dimensions, covariances between individual dimensions could be described in covariance matrix

### Covariance matrix

$$C^{n \times n} = (c_{i,j} : c_{i,j} = \text{cov}(\text{Dim}_i, \text{Dim}_j)) \quad (7)$$

where  $C^{m \times n}$  is a matrix with  $n$  rows and  $m$  columns. Example for three dimensions:

$$c = \begin{pmatrix} \text{cov}(x, x) & \text{cov}(x, y) & \text{cov}(x, z) \\ \text{cov}(y, x) & \text{cov}(y, y) & \text{cov}(y, z) \\ \text{cov}(z, x) & \text{cov}(z, y) & \text{cov}(z, z) \end{pmatrix} \quad (8)$$

Since  $\text{cov}(a, b) = \text{cov}(b, a)$ , the matrix is symmetrical about the main diagonal.

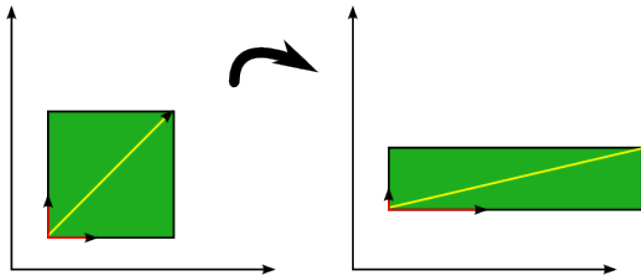
# Covariance matrix

Exercise: Find covariance matrix for the 3-dimensional dataset

Item number:	1	2	3
x	1	-1	4
y	2	1	3
z	1	3	-1

**Ans:** 
$$\begin{pmatrix} 4.222 & 1.667 & -3.333 \\ 1.667 & 0.667 & -1.333 \\ -3.333 & -1.333 & 2.667 \end{pmatrix}$$

# Eigenvectors



- Eigenvectors (red) do not change direction when a linear transformation (e.g. scaling) is applied to them. Other vectors (yellow) do.



# Eigenvectors

An example of non-eigenvector:

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \boxed{\begin{pmatrix} 1 \\ 3 \end{pmatrix}} = \begin{pmatrix} 11 \\ 5 \end{pmatrix} \quad (9)$$

An example of eigenvector:

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \boxed{\begin{pmatrix} 3 \\ 2 \end{pmatrix}} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} \quad (10)$$

# Eigenvalues

The amount by which the original vector was scaled after multiplication by the square matrix

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4 \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} \quad (11)$$

# PCA

# Iris flower dataset

# Iris flower dataset

**iris setosa**



petal

sepal

**iris versicolor**



petal

sepal

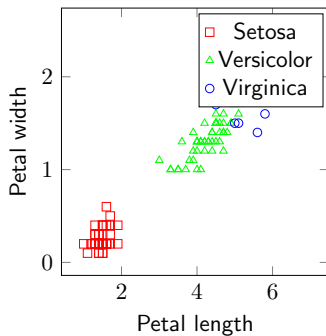
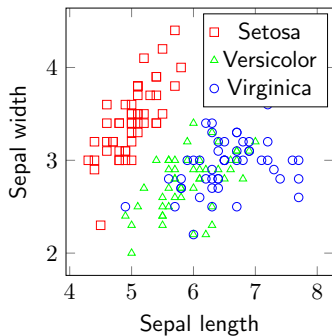
**iris virginica**



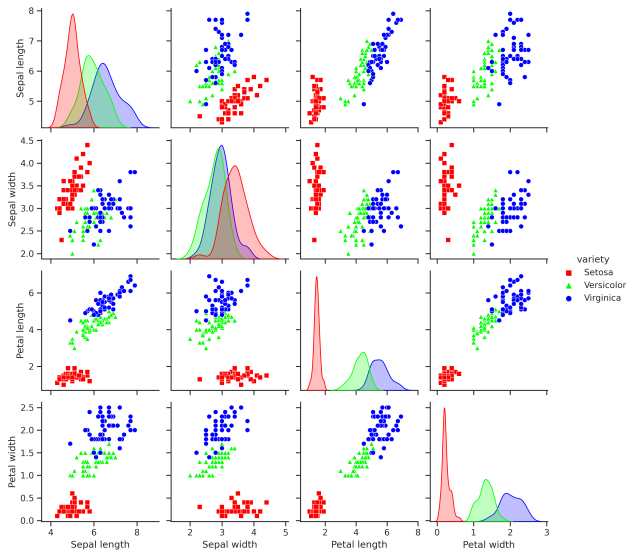
petal

sepal

# Iris flower dataset



# Iris flower dataset











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# Experiment

# Experiment

# Experiment

# Conclusion

## Thank you for your attention!

- Workshop contents:

<https://github.com/CodeSeoul/machine-learning/tree/master/221210-pca>

- Follow-up QA?

<http://discord.com/users/tuttelikz>



# References



Ning Qian. “On the momentum term in gradient descent learning algorithms”. In: *Neural networks* 12.1 (1999), pp. 145–151.



John Duchi, Elad Hazan, and Yoram Singer. “Adaptive subgradient methods for online learning and stochastic optimization.”. In: *Journal of machine learning research* 12.7 (2011).



Sebastian Ruder. “An overview of gradient descent optimization algorithms”. In: *arXiv preprint arXiv:1609.04747* (2016).



Mykola Novik. *torch-optimizer – collection of optimization algorithms for PyTorch*. Version 1.0.1. Jan. 2020.