Dimensionality reduction techniques: Part 1

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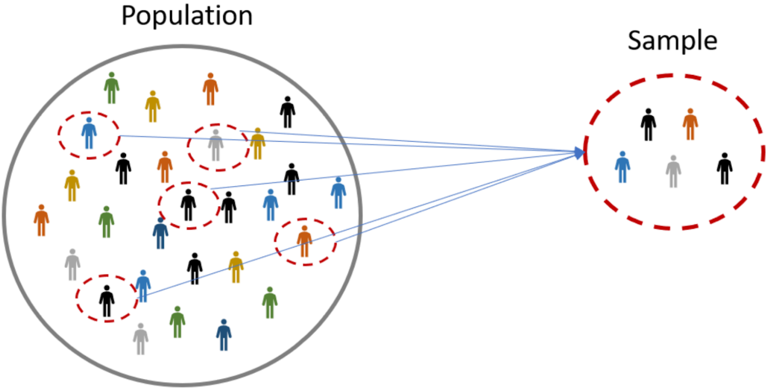
Motivation

Why dimensionality reduction?

Important "toolkit" in machine learning:

- Preprocessing step for other algorithms (reduce size)
- Visualization
- Compression
- Interpolation

Population vs sample



Population vs sample

Population mean

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

N is number of items in the population

Sample mean

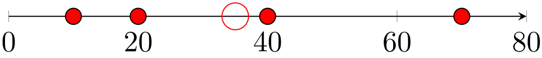
$$\bar{X} = \frac{\sum_{i=1}^{n} x_i}{n} \qquad (2)$$

n is number of items in the sample

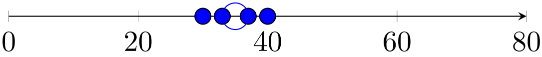
Standard deviation

Let's take a look on two samples:

$$A = [10\ 20\ 40\ 70]$$



$$B = [30\ 33\ 37\ 40]$$



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?

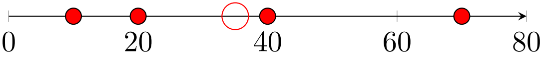
Standard deviation

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

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 $\bar{A} = 35$

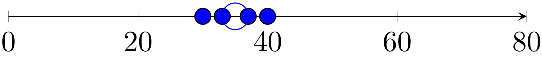


Let's calculate standard deviation:

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		**26.4575**

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		**4.397**

Variance

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

Variance

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

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

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

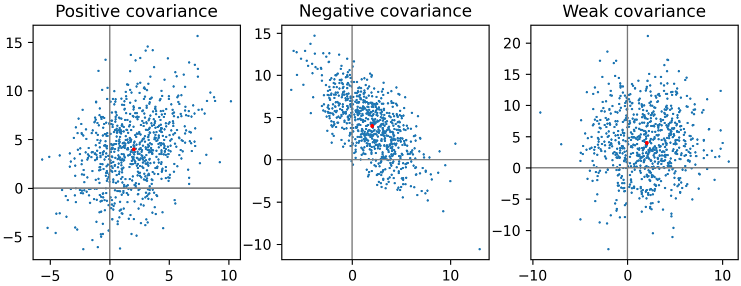
Covariance

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

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

- Covariance between one dimension and itself gives variance.

Covariance



Positive covariance
Negative covariance
Weak 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

$$C^{n \times n} = (c_{i,j} : c_{i,j} = cov(Dim_i, Dim_j)) \tag{7}$$

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

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

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

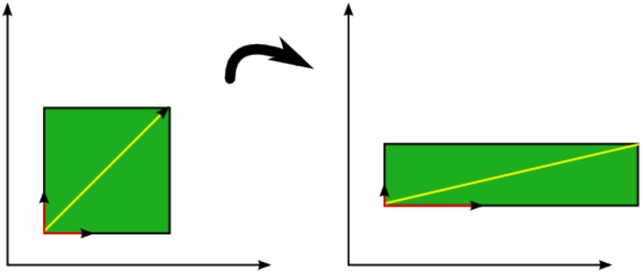
Covariance matrix

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:

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

An example of eigenvector:

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

Eigenvalues

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

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = \boxed{4} \times \begin{pmatrix} 3 \\ 2 \end{pmatrix} \tag{11}$$

PCA

What is Principal Component Analysis?

A way of identifying patterns in data: by highlighting their similarities and differences

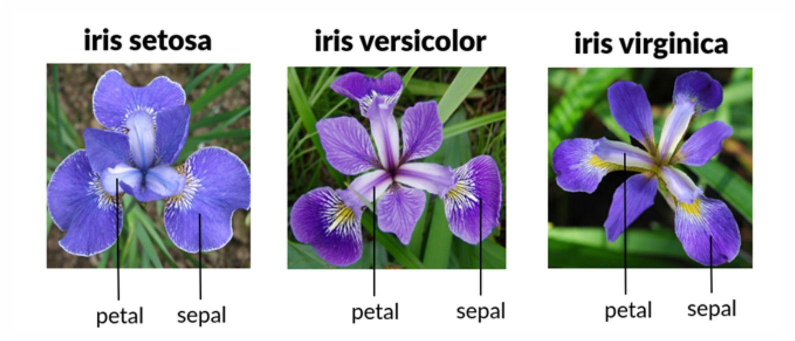
Pros

- Once patterns in the data, and you compress the data, ie. by reducing the number of dimensions, without much loss of information.

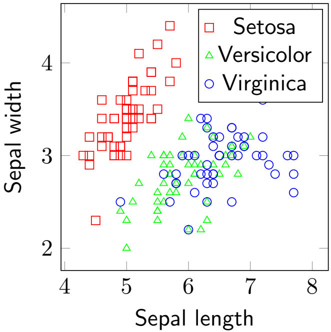
Cons

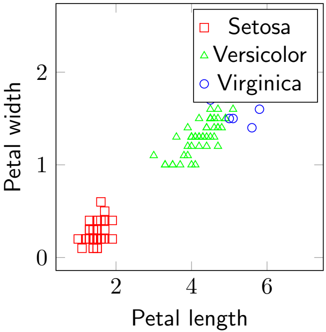
- Linear $\therefore$ difficult to unfold single ambiguous object really belongs in several disparate locations in the low-dimensional space.

Iris flower dataset

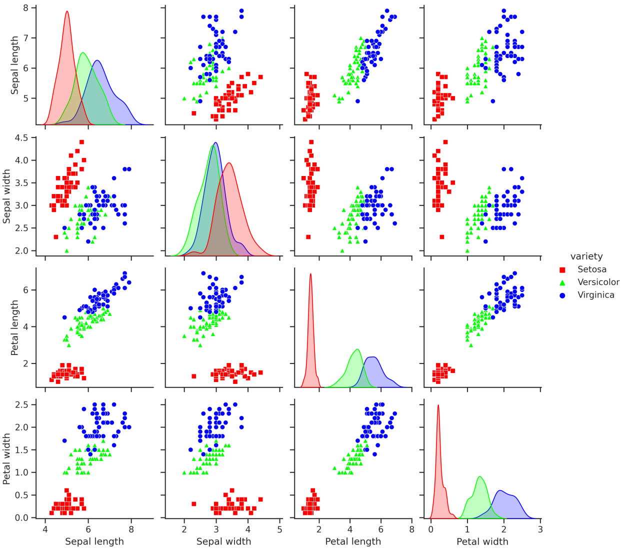


Iris flower dataset





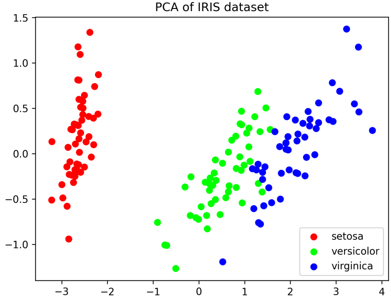
Iris flower dataset



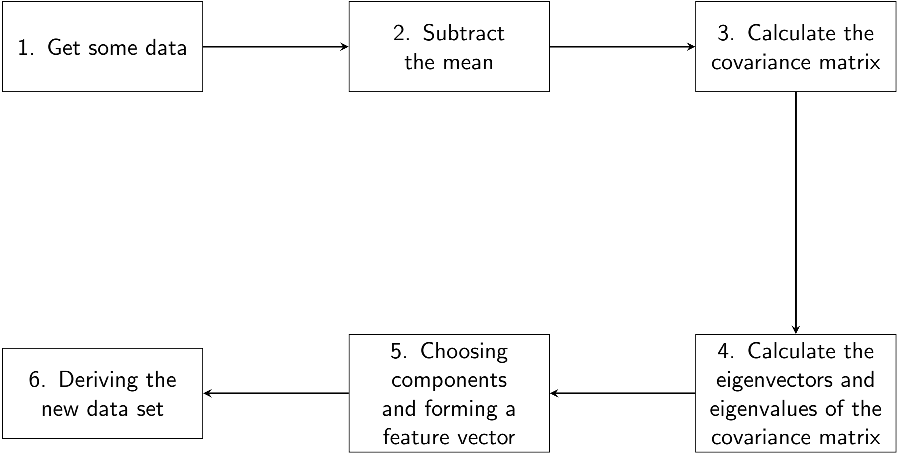
Applying PCA to Iris flower dataset

PCA automatically finds principal components (eg. *axes*) in feature space. Here, we defined two, so we can visualize in 2D easily.

```
from sklearn import datasets
from sklearn.decomposition import PCA

iris = datasets.load_iris()

X = iris.data
y = iris.target
target_names = iris.target_names

pca = PCA(n_components=2)
X_r = pca.fit(X).transform(X)
```



PCA under the hood



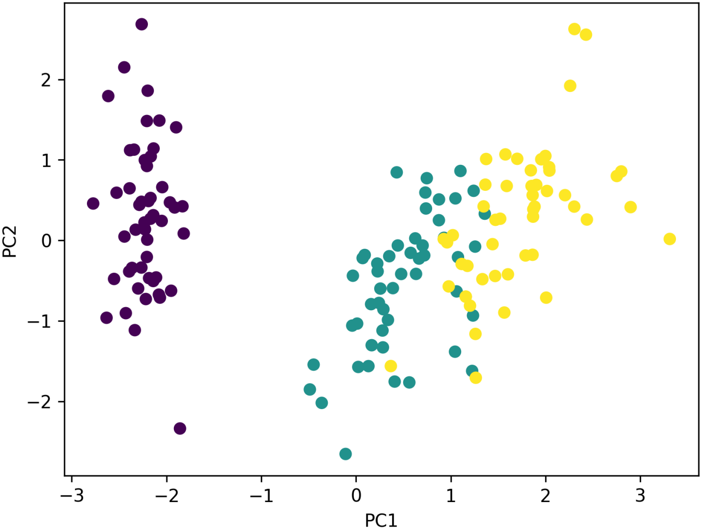
PCA under the hood

```
import numpy as np
from numpy.linalg import eig

def PCA_numpy(X,y):
    def mean(x): # np.mean(X, axis = 0)
        return sum(x)/len(x)

    def std(x): # np.std(X, axis = 0)
        return (sum((i - mean(x))**2 for i in x)/len(x))**0.5

    def Standardize_data(X):
        return (X - mean(X))/std(X)

    def covariance(x):
        return (x.T @ x)/(x.shape[0]-1)

    # Step 1: Standardize the data
    X_std = Standardize_data(X)
    # Step 2: Find the covariance matrix
    cov_mat = covariance(X_std) # np.cov(X_std.T)

    # Step 3: Find the eigenvectors and eigenvalues of the covariance matrix
    eig_vals, eig_vecs = eig(cov_mat)
```

PCA under the hood

```
max_abs_idx = np.argmax(np.abs(eig_vecs), axis=0)
signs = np.sign(eig_vecs[max_abs_idx, range(eig_vecs.shape[0])])
eig_vecs = eig_vecs*signs[np.newaxis,:]
eig_vecs = eig_vecs.T

# Step 4: Rearrange the eigenvectors and eigenvalues
eig_pairs = [(np.abs(eig_vals[i]), eig_vecs[i,:]) for i in range(len(eig_vals))]

# Then, we sort the tuples from the highest to the lowest based on eigenvalues magni
eig_pairs.sort(key=lambda x: x[0], reverse=True)
eig_vals_sorted = np.array([x[0] for x in eig_pairs])
eig_vecs_sorted = np.array([x[1] for x in eig_pairs])

# Step 5: Choose principal components
k = 2
W = eig_vecs_sorted[:k, :] # Projection matrix

# Step 6: Project the data
X_proj = X_std.dot(W.T)

return X_proj
```

PCA under the hood



t-SNE (Stochastic neighbor embedding)

To be continued

Conclusion

Practicum

Thank you for your attention!

References