Applied
Machine Learning

Lecture 14
Dimensionality Reduction:
Principal Components Analysis

Ekarat Rattagan, Ph.D.

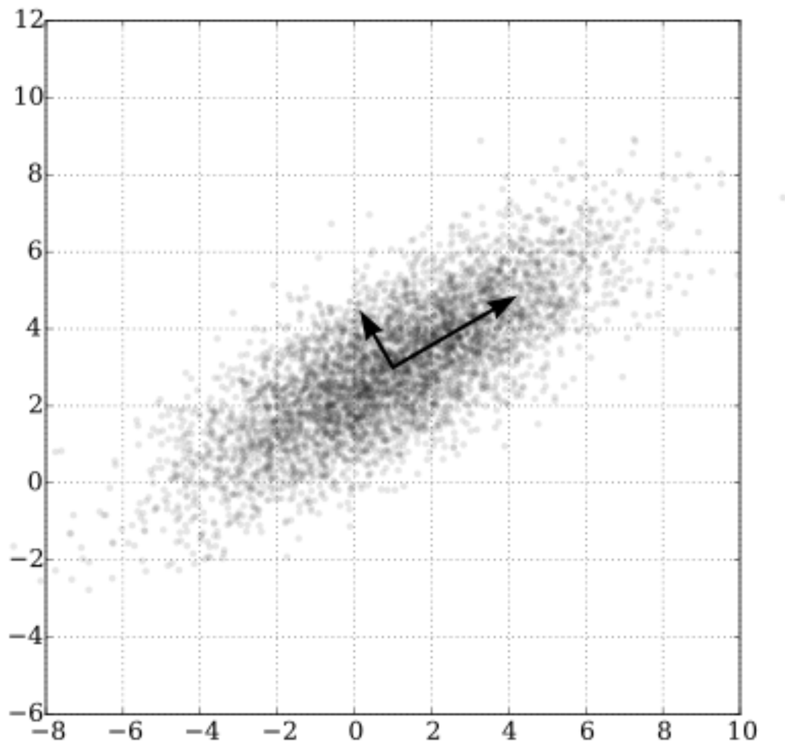
Principal Components Analysis (PCA)

- PCA: most popular instance of second main class of unsupervised learning methods, projection methods, aka dimensionality-reduction methods

- We have some data $X \in \mathbb{R}^{N \times D}$
- D may be huge, etc.
- We would like to find a new representation $Z \in \mathbb{R}^{N \times K}$ where K << D.

Principal Components Analysis (PCA)

- Aim: find a small number of "directions" in input space that explain variation in input data; re-represent data by projecting along those directions
- Important assumption: variation contains information



Principal Components Analysis (PCA)

- Can be used to:
  - Reduce number of dimensions in data
  - Find patterns in high-dimensional data
  - Visualise data of high dimensionality
- Example applications:
  - Face recognition
  - Image compression

Steps of PCA

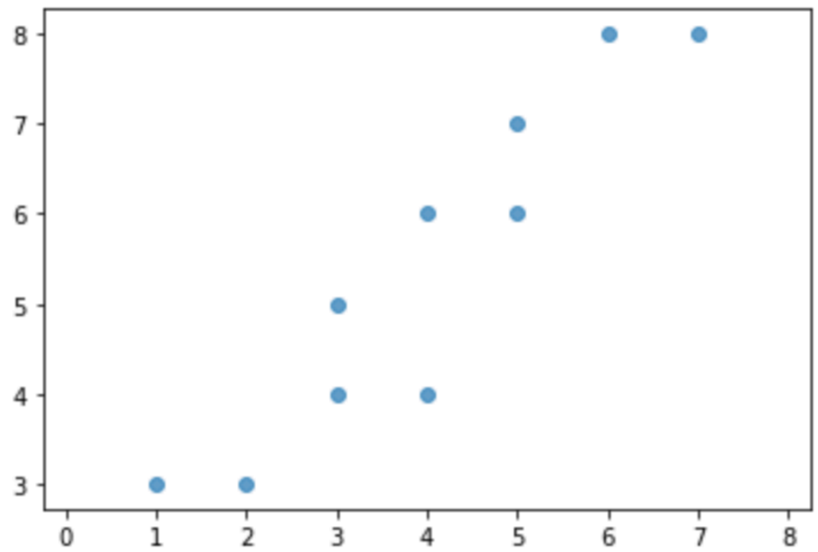
For each column:

1. Let $\overline{X}$ be the mean vector (taking the mean of all rows)
2. Adjust the original data by the mean $X' = X - \overline{X}$
3. Compute the covariance matrix A of X'
4. Find the eigenvectors and eigenvalues of A.

Example

Step 1 & 2

	X1	X2	X1'	X2'
	1	3	-3	-2.4
	2	3	-2	-2.4
	3	4	-1	-1.4
	3	5	-1	-0.4
	4	4	0	-1.4
	4	6	0	0.6
	5	6	1	0.6
	5	7	1	1.6
	6	8	2	2.6
	7	8	3	2.6
Mean	4	5.4		



$\bar{X}_1$ Mean1=4

$\bar{X}_2$ Mean2=5.4

Covariance Matrix

Covariance: measures the correlation between X and Y

- Cov(X,Y)=0: independent
- Cov(X,Y)>0: move same direction
- Cov(X,Y)<0: move oppo dirrection

mean of X_i column

$$\text{cov}(X,Y) = \frac{\sum_{i=1}^{n}(X_i - \overline{X})(Y_i - \overline{Y})}{(n-1)}$$

$$\begin{bmatrix} \text{cov}(X_1,X_1) & \text{cov}(X_1,X_2) & \cdots & \text{cov}(X_1,X_n) \\ \text{cov}(X_2,X_1) & \text{cov}(X_2,X_2) & \cdots & \text{cov}(X_2,X_n) \\ \vdots & \vdots & \vdots & \vdots \\ \text{cov}(X_n,X_1) & \text{cov}(X_n,X_2) & \cdots & \text{cov}(X_n,X_n) \end{bmatrix}$$

https://dmitry.ai/t/topic/242

$$A = \begin{bmatrix} cov(X_1', X_1') & cov(X_1', X_2') \\ cov(X_2', X_1') & cov(X_2', X_2') \end{bmatrix}$$

Step 3

- $A = \begin{bmatrix} 3.33 & 3.22 \\ 3.22 & 3.60 \end{bmatrix}$

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

	X1	X2	X1'	X2'
	1	3	-3	-2.4
	2	3	-2	-2.4
	3	4	-1	-1.4
	3	5	-1	-0.4
	4	4	0	-1.4
	4	6	0	0.6
	5	6	1	0.6
	5	7	1	1.6
	6	8	2	2.6
	7	8	3	2.6
Mean	$\bar{X}_1$ 4	$\bar{X}_2$ 5.4		

Ex. $cov(X_1', X_1') = \frac{\sum_{i=1}^{10}(X_1' - \bar{X}_1')(X_1' - \bar{X}_1')}{9}$

$(-3-0)(-3-0)+$ 9 +
$(-2-0)(-2\ 0)+$ 4 +
$(-1-0)(-1-0)+$ 1 +
$(-1-0)(-1\cdot 0)+$ 1 +
$(0-0)(0-0)+$ 0 +
$(0-0)(0-0)+$ 0 +
$(1-0)(1-0)+$ 1 +
$(1-0)(1-0)+$ 1 +
$(2-0)(2-0)+$ 4 +
$(3-0)(3-0)$ 9

$\frac{30}{9}$

4

3.33

$$\begin{bmatrix} 3.33 & 3.20 \\ 3.20 & 3.60 \end{bmatrix} X = \lambda X$$

Eigenvalues & eigenvectors

- Vectors x having same direction as Ax are called eigenvectors of A. (A is a cov matrix)
- In the equation Ax=λx, λ is called an eigenvalue of A.

$$\begin{pmatrix} 2 & 3 \\ 2 & 1 \end{pmatrix} x \begin{pmatrix} 3 \\ 2 \end{pmatrix} = \begin{pmatrix} 12 \\ 8 \end{pmatrix} = 4x \begin{pmatrix} 3 \\ 2 \end{pmatrix}$$

multiply multiply

Eigenvectors make understanding linear transformations easy. They are the "axes" (directions) along which a linear transformation acts simply by "stretching/compressing" and/or "flipping"; **eigenvalues** give you the factors by which this compression occurs.

The more directions you have along which you understand the behavior of a linear transformation, the easier it is to understand the linear transformation

Arturo Magidin (https://math.stackexchange.com/users/742/arturo-magidin), What is the importance of eigenvalues/eigenvectors?, URL (version: 2018-01-15): https://math.stackexchange.com/q/23325

Eigenvalues & eigenvectors

A singular matrix has no inverse

- We want to find x and λ.
- Ax=λx ⇔ (A-λI)x = 0, let say x != 0, then

not equal

vector

(A- λI) must be zero or det(A-λI) = 0

* matrix is zero when determinant is zero.

- How to calculate x and λ:
  - Calculate det(A-λI), yields a polynomial (degree n)
  - Determine roots to det(A-λI)=0, roots are eigenvalues λ
  - Solve (A- λI) x=0 for each λ to obtain eigenvectors x

– **Why det(A-λI) ?**

1 An **eigenvector** $\boldsymbol{x}$ lies along the same line as $A\boldsymbol{x}$: $\boxed{A\boldsymbol{x} = \lambda\boldsymbol{x}.}$ The **eigenvalue** is λ.

2 If $A\boldsymbol{x} = \lambda\boldsymbol{x}$ then $A^2\boldsymbol{x} = \lambda^2\boldsymbol{x}$ and $A^{-1}\boldsymbol{x} = \lambda^{-1}\boldsymbol{x}$ and $(A + cI)\boldsymbol{x} = (\lambda + c)\boldsymbol{x}$: the same $\boldsymbol{x}$.

3 If $A\boldsymbol{x} = \lambda\boldsymbol{x}$ then $(A–\lambda I)\boldsymbol{x} = \boldsymbol{0}$ and $A–\lambda I$ is singular and $\boxed{\mathbf{det}(\boldsymbol{A}-\boldsymbol{\lambda I}) = \mathbf{0}.}$ n eigenvalues.

$$\det\left(\begin{bmatrix} 3.33 & 3.22 \\ 3.22 & 3.60 \end{bmatrix} - \lambda \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right) = 0 \rightarrow \det\left(\begin{bmatrix} 3.33-\lambda & 3.22 \\ 3.22 & 3.60-\lambda \end{bmatrix}\right) = 0$$

Step 4

$$\rightarrow (3.33-\lambda)(3.60-\lambda) - (3.22)(3.22)$$

$$\rightarrow 11.98 - 6.93\lambda + \lambda^2 - 10.36$$

$$\rightarrow 1.62 - 6.93\lambda + \lambda^2$$

$$\rightarrow \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}, \quad \lambda_1 = 0.24, \quad \lambda_2 = 6.69$$

- Python
  - Eigenvectors:
  - x1 = (-0.722, 0.692), λ1 = 0.24
  - x2 = (0.6923, 0.722), λ2 = 6.69
  - ~~Thus the second eigenvector is more important!~~

$$\begin{bmatrix} 3.33 & 3.22 \\ 3.22 & 3.60 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = 6.69 \begin{bmatrix} x \\ y \end{bmatrix}$$

$$3.33x + 3.22y = 6.69x$$

$$3.22x + 3.60y = 6.69y$$

$$-3.36x + 3.22y = 0$$

$$\frac{3.22x - 3.09y = 0}{x = 0.958y}$$

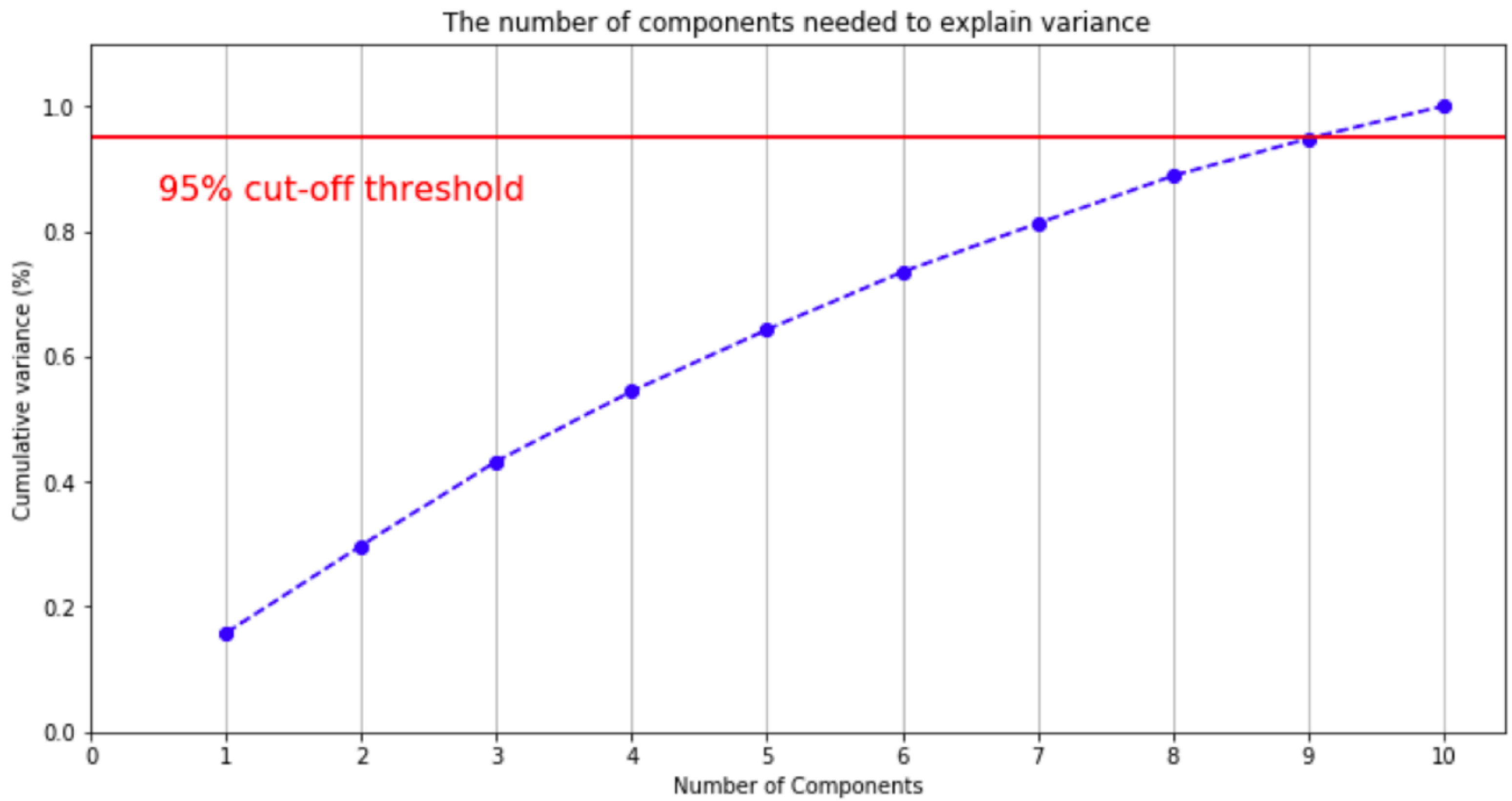
vector $\approx \begin{bmatrix} 0.958 \\ 1 \end{bmatrix}$

Interesting !!!

normalize $= \begin{bmatrix} 0.692 \\ 0.722 \end{bmatrix}$

- https://lpsa.swarthmore.edu/MtrxVibe/EigMat/MatrixEigen.html
- Test
  - https://octave-online.net/

PCA — how to choose the number of components?



In this case, to get 95% of variance explained I need 9 principal components.

https://www.mikulskibartosz.name/pca-how-to-choose-the-number-of-components/

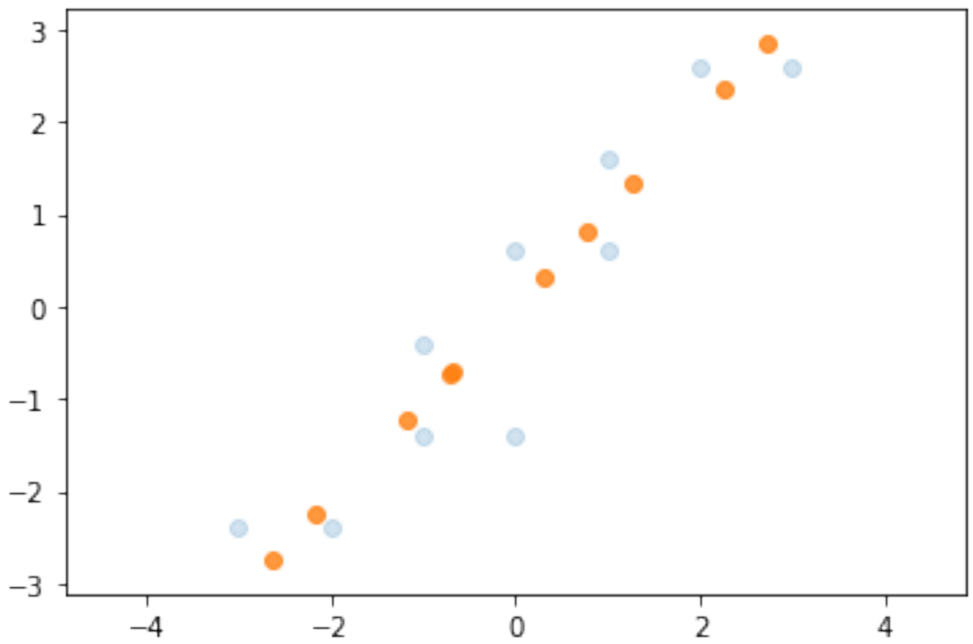
Assume we keep only one dimension

- We keep the dimension of
  $x2 = (0.6923, 0.722)$, $\lambda 2 = 6.69$
- Finally, we can obtain the data as

$[0.69, 0.72]$
1×2

$\begin{bmatrix} -3 & -2.4 \\ & \end{bmatrix}$
2×10

$x2 * X'$



Variance of sample = 6.693

```
[[-3.81]
 [-3.12]
 [-1.70]
 [-0.98]
 [-1.01]
 [0.43]
 [1.13]
 [1.85]
 [3.26]
 [3.95]]
```

1×10

PCA –> Original Data

- Retrieving old data (x_1, x_2)

$$\left[\underbrace{\begin{bmatrix}[-3.81]\\ [-3.12]\\ [-1.70]\\ [-0.98]\\ [-1.01]\\ [0.43]\\ [1.13]\\ [1.85]\\ [3.26]\\ [3.95]\end{bmatrix}}_{10\times 1} * \underbrace{(\,0.6923,\ 0.722)}_{1\times 2}\right]_{10\times 2} + \bar{X}$$

PCA –> Original Data

- Retrieving old data (x_1, x_2)

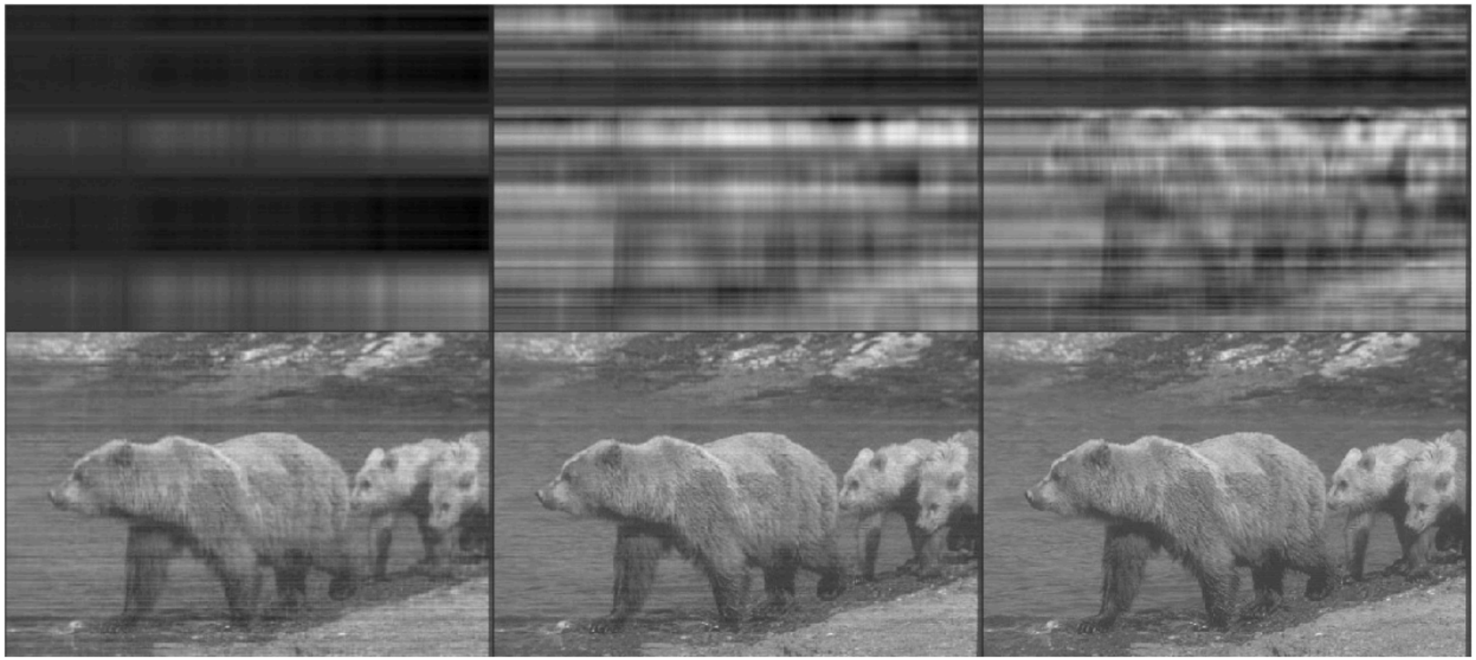
$$\begin{bmatrix} -2.64 & -2.75 \\ -2.16 & -2.25 \\ -1.18 & -1.23 \\ -0.68 & -0.71 \\ -0.70 & -0.73 \\ 0.30 & 0.31 \\ 0.78 & 0.81 \\ 1.28 & 1.33 \\ 2.26 & 2.35 \\ 2.74 & 2.85 \end{bmatrix}_{10\times 2} + \bar{X} = \begin{bmatrix} 1.36 & 2.65 \\ 1.84 & 3.15 \\ 2.82 & 4.17 \\ 3.32 & 4.69 \\ 3.30 & 4.67 \\ 4.30 & 5.71 \\ 4.78 & 6.21 \\ 5.28 & 6.73 \\ 6.26 & 7.75 \\ 6.74 & 8.25 \end{bmatrix} \sim \begin{bmatrix} 1.0 & 3.0 \\ 2.0 & 3.0 \\ 3.0 & 4.0 \\ 3.0 & 5.0 \\ 4.0 & 4.0 \\ 4.0 & 6.0 \\ 5.0 & 6.0 \\ 5.0 & 7.0 \\ 6.0 & 8.0 \\ 7.0 & 8.0 \end{bmatrix}$$

$$\bar{X} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 \\ & \\ & \end{bmatrix}_{10\times 2}$$

Mean1=4
Mean2=5.4

Applications

PCA for Compression



321x481 image, D is the number of basis vectors used