Machine Learning

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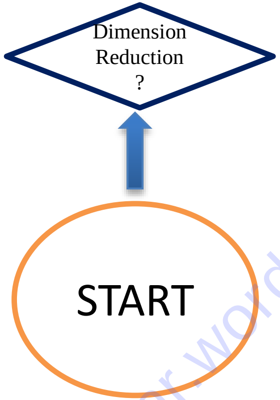
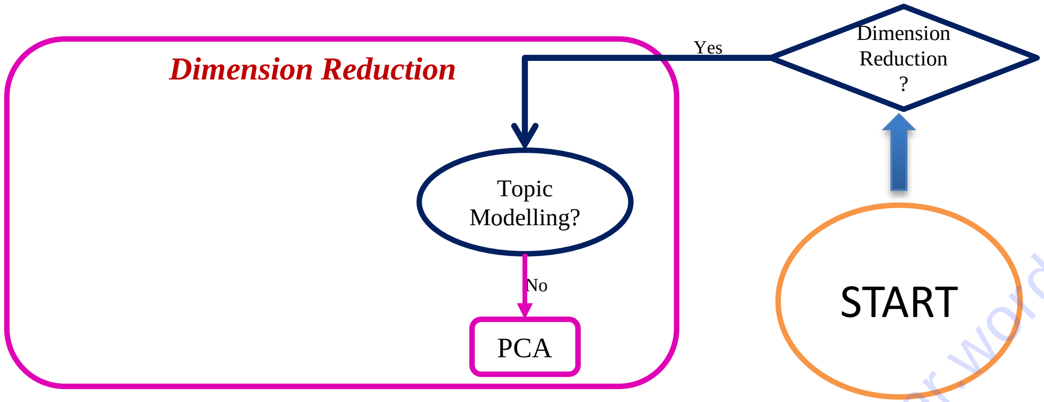

Dimension
Reduction
?
START

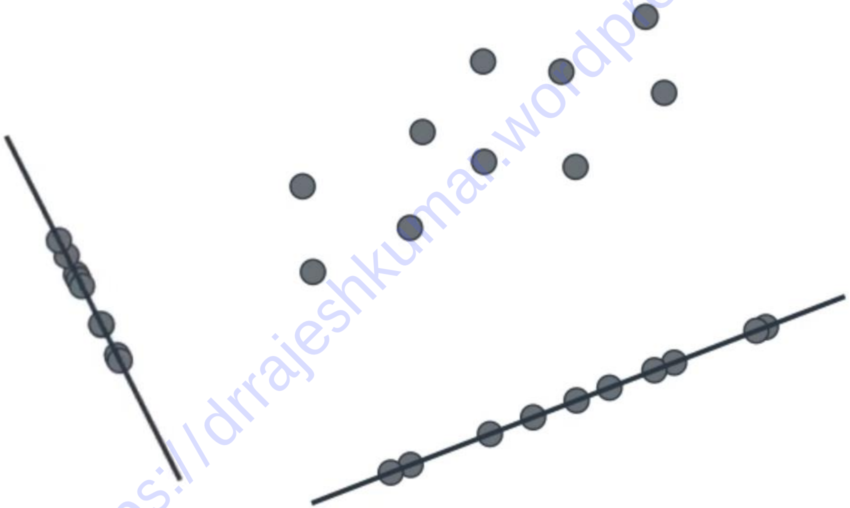

Dimension Reduction
Yes
Dimension Reduction ?
Topic Modelling?
No
PCA
START

Principal Component Analysis (PCA)

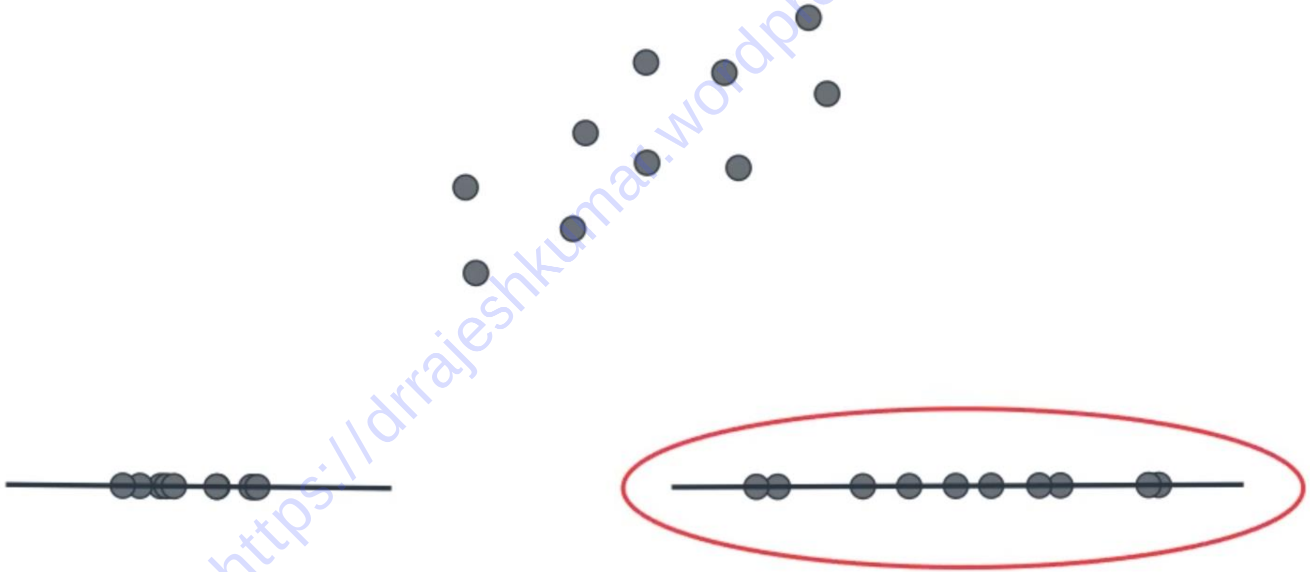
What is PCA?

- Unsupervised exploratory statistical technique used to:
  - **Simplify** and **reduce dimensionality** of the given dataset
  - **Visualize data** with high dimensionality
- Considers **maximized variance**
  - Maximum variance of a component ➔ a more significant factor
- Dimensions – different features that describe the data
  - Example: For 20 students, the number of hours studied and the marks obtained are provided.
    - Here number of hours and marks obtained are the dimensions

Dimensionality Reduction



Dimensionality Reduction



- Linear Transformation to determine a new coordinate system for the dataset
  - Greatest variance for any projection of the data set lies on the first axis → First Principal Component
  - 2nd greatest variance gives the Second Principal Component
- Dimensionality may be reduced by eliminating the principal components with least variance

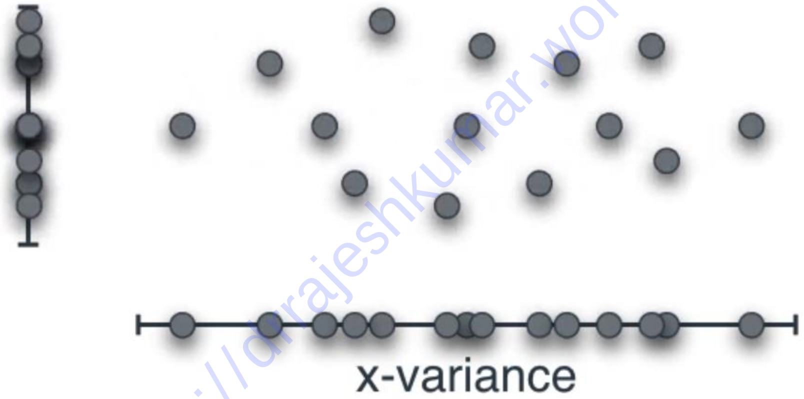
Variance and Covariance

- Measure how the data is distributed around the mean of that data.

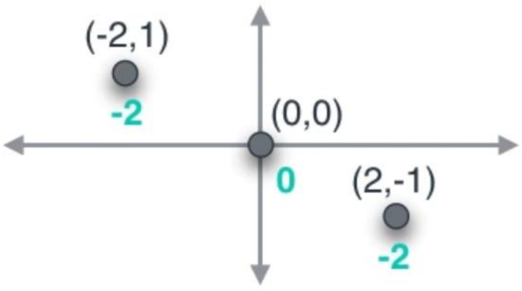
- **Variance** – Gives the deviation from the mean for data points in a single dimension.

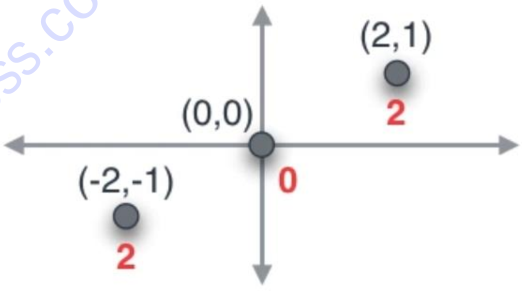
- **Covariance** – Measures the variation from the mean of each dimension with respect to the other.
    - Measures the existence of a relationship between 2 dimensions.
    - Square of the standard deviation

Variance?



Covariance





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

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

Covariance

- Covariance between two variables *x, y*

$$\boldsymbol{cov}(\boldsymbol{x},\boldsymbol{y}) = \frac{\sum_{i=1}^{n}(\overline{\boldsymbol{x}}_i - \boldsymbol{x})(\overline{\boldsymbol{y}}_i - \boldsymbol{y})}{\boldsymbol{n}-\boldsymbol{1}}$$

- *Covariance matrix*: represents the covariance between dimensions
  - Forms a symmetric *N X N* matrix for N dimensional data
  - Diagonal gives the variances of the dimensions

Covariance

- Covariance between two variables *x, y*

$$\boldsymbol{cov(x,y) = \frac{\sum_{i=1}^{n}(\bar{x}_i - x)(\bar{y}_i - y)}{n-1}}$$

- *Covariance matrix*: represents the covariance between dimensions
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$$\boldsymbol{C = \begin{bmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{bmatrix}}$$

Covariance matrix for 3 dimensions

Covariance

- Covariance between two variables *x, y*

$$cov(x, y) = \frac{\sum_{i=1}^{n}(\overline{x}_i - x)(\overline{y}_i - y)}{n-1}$$

$$C = \begin{bmatrix} cov(x,x) & cov(x,y) & cov(x,z) \\ cov(y,x) & cov(y,y) & cov(y,z) \\ cov(z,x) & cov(z,y) & cov(z,z) \end{bmatrix}$$

Covariance matrix for 3 dimensions

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Covariance Evaluation

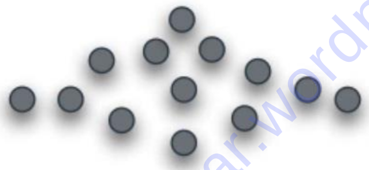
Covariance(x,y)	**Nature of Relationship**
= 0	*x*, *y* are **independent**
> 0	*x*, *y* move in **same direction**
< 0	*x*, *y* move in **opposing directions**

Covariance

$$\text{covariance} = \frac{-2 + 0 + 2 + 0 + 0 + 0 + 2 + 0 + -2}{9} = 0$$

Covariance

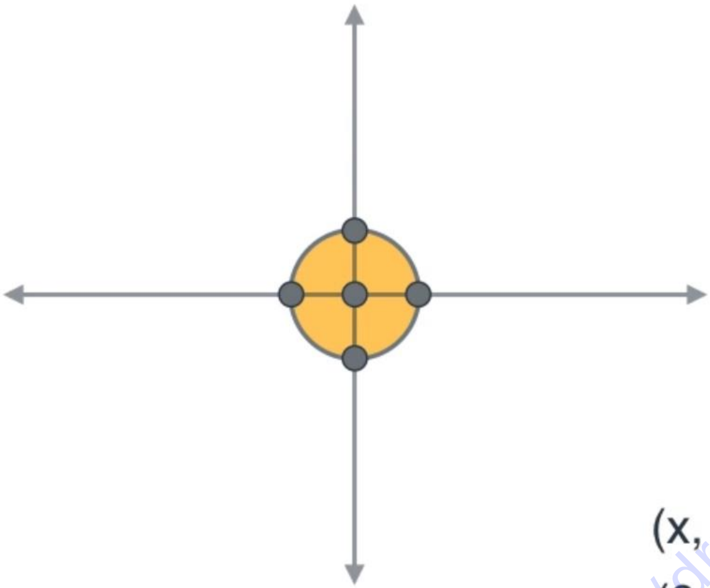
negative
covariance



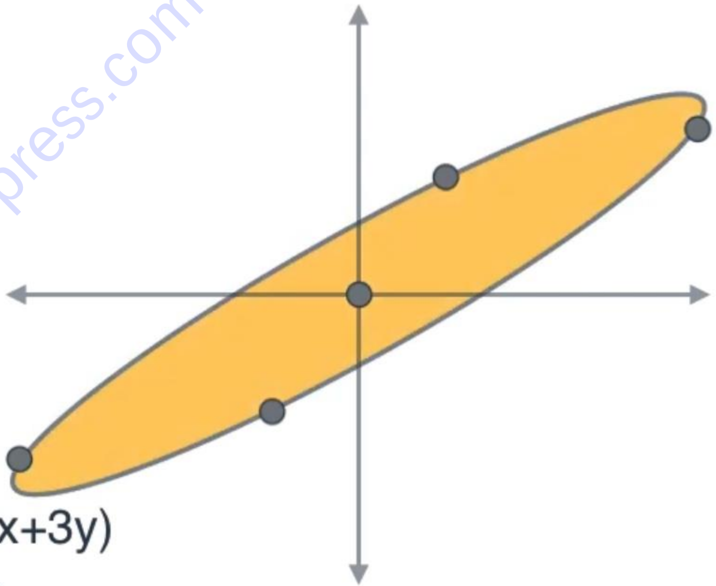
covariance zero
(or very small)

positive
covariance

Linear Transformations



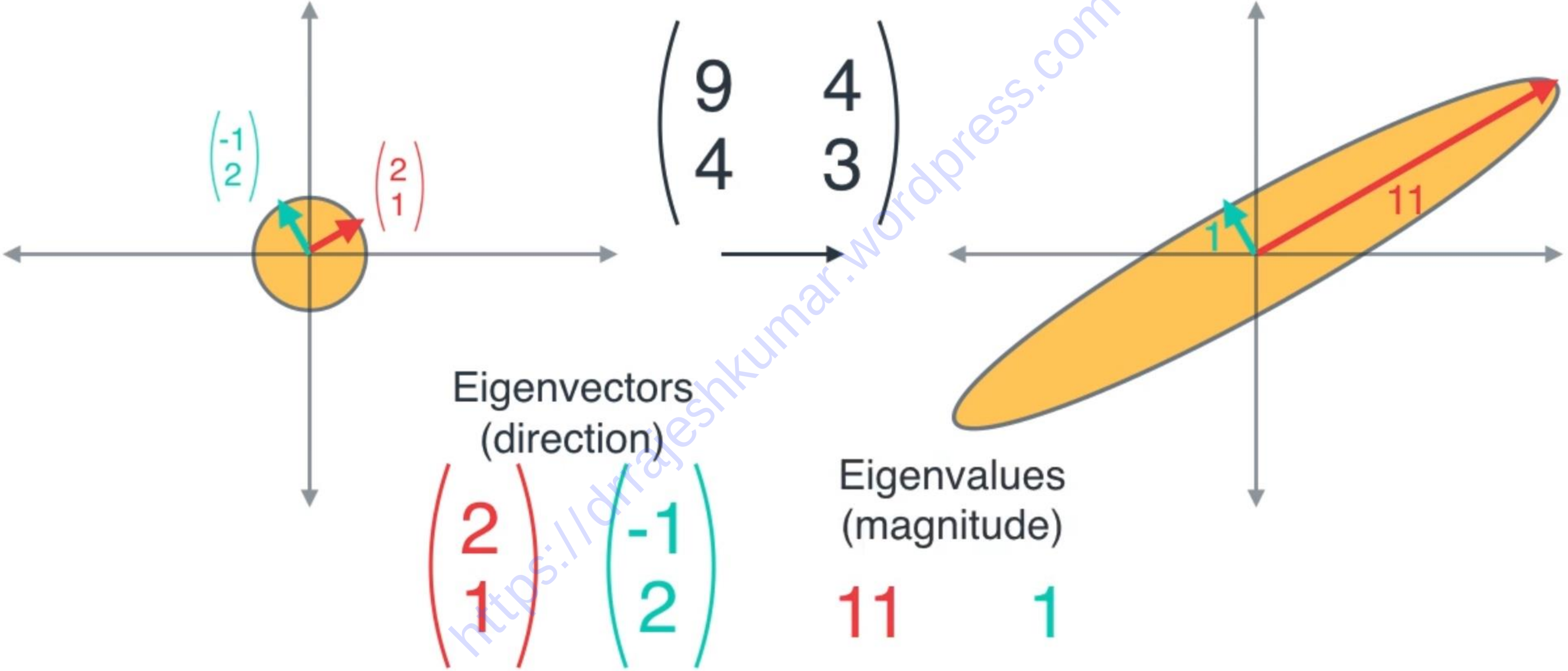
$$\begin{pmatrix} 9 & 4 \\ 4 & 3 \end{pmatrix} \longrightarrow$$



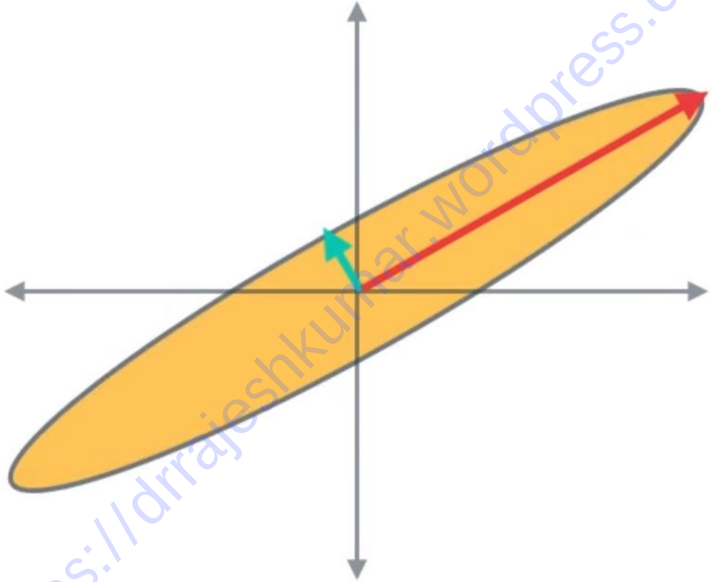
(x, y) ⟶ (9x+4y, 4x+3y)

(0,0)	(0,0)
(1,0)	(9,4)
(0,1)	(4,3)
(-1,0)	(-9,-4)
(0,-1)	(-4,-3)

Linear Transformations



Linear Transformations



Eigenvectors (direction)

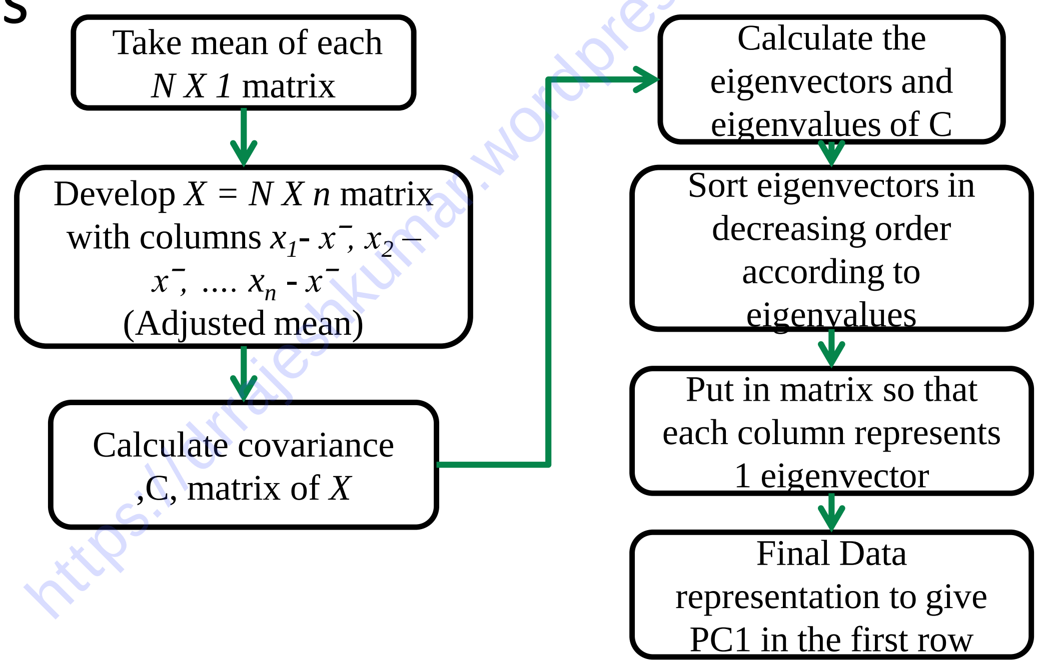
$$\begin{pmatrix}2\\1\end{pmatrix} \quad \begin{pmatrix}-1\\2\end{pmatrix}$$

Eigenvalues (magnitude)

11   1

Steps for PCA - Flowchart

- Given $x_1, x_2, \ldots, x_n$ is a set of *n (N X 1)* vectors



Steps for PCA - Flowchart

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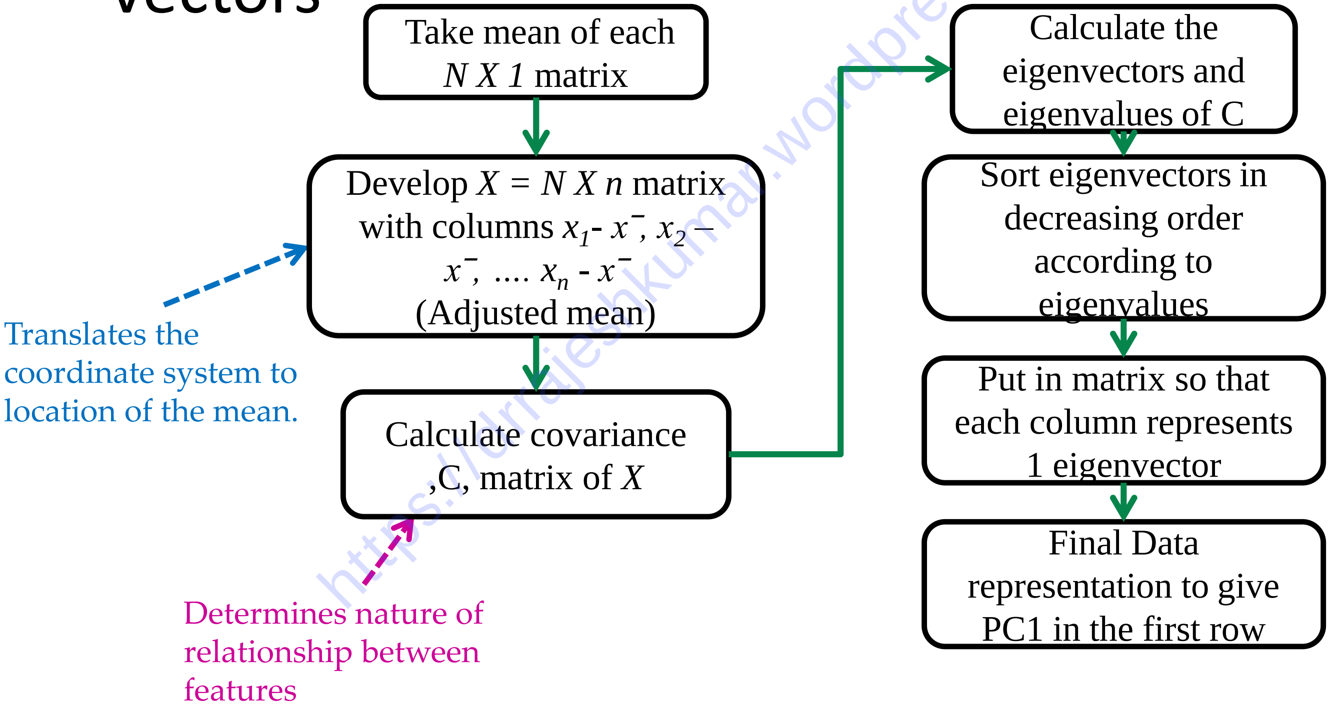

Steps for PCA - Flowchart

- Given x_1, x_2, ….,x_n is a set of *n (N X 1)* vectors

1. Take mean of each *N X 1* matrix
2. Develop $X = N \times n$ matrix with columns $x_1 - \bar{x}$, $x_2 - \bar{x}$, …. $x_n - \bar{x}$ (Adjusted mean)
3. Calculate covariance ,C, matrix of *X*
4. Calculate the eigenvectors and eigenvalues of C
5. Sort eigenvectors in decreasing order according to eigenvalues
6. Put in matrix so that each column represents 1 eigenvector
7. Final Data representation to give PC1 in the first row

Eigenvector with the highest eigenvalue gives the Principal Component .

Steps of PCA

- Given $x_1, x_2, ..., x_n$ is a set of *n (N X 1)* vectors

$$x_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{iN} \end{bmatrix}$$

- Calculate the average of each

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n}\begin{bmatrix} x_{i1} \\ \vdots \\ x_{iN} \end{bmatrix}$$

- X is the *N X n* matrix with columns

$$X = [x_1 - \bar{x} \quad x_2 - \bar{x} \quad \dots \quad xn - \bar{x}]$$

This is the mean adjusted data

Steps for PCA

- Develop the covariance matrix by calculating the covariance matrix C from X

- Each term may be written as

$$x_j = \bar{x} + \sum_{i=1}^{i=n} g_{ji} eg_i$$

Steps for PCA

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Eigenvector

- Calculate eigenvectors → $eg_1, eg_2, \ldots .eg_n$ will be *NX1* orthonormal vectors

Steps for PCA

- Develop the covariance matrix by calculating the covariance matrix C from X

- Each term may be written as

$$x_j = \bar{x} + \sum_{i=1}^{i=n} g_{ji} eg_i$$

Coordinates

- Calculate eigenvectors → $eg_1, eg_2, \ldots eg_n$ will be *NX1* orthonormal vectors
- Here, g_{ji} are the coordinates of x_j in the space

$$g_{ji} = (xj - \bar{x}).eg_i$$

Steps for PCA – Reduced Dimension Data Derivation

- Sort eigenvectors according to eigenvalue.
  - Matrix *E* gives the sorted eigenvalues with each column representing an eigenvector.
  - $E = [eg_1\ eg_2 \ldots\ eg_n]$

- Final Data Representation (Feature Vectors):
  - Determine **Row Feature Vector (RFV)** – matrix E transposed so that eigenvectors are <u>in rows</u>
    - Most significant eigenvector is at the top

  - Determine **Zero Mean Data (ZMD)** - Mean adjusted data matrix (X) transposed so that separate dimensions are in each row

$$\boldsymbol{Final\ Data = RFV \times ZMD}$$

Example

http://kybele.psych.cornell.edu/~edelman/Psych-465-Spring-2003/PCA-tutorial.pdf

Original Data

x	y
2.5	2.4
0.5	0.7
2.2	2.9
1.9	2.2
3.1	3
2.3	2.7
2	1.6
1	1.1
1.5	1.6
1.1	0.9

Adjusted Mean Data

x	y
0.69	0.49
-1.31	-1.21
0.39	0.99
0.09	0.29
1.29	1.09
0.49	0.79
0.19	-0.31
-0.81	-0.81
-0.31	-0.31
-0.71	-1.01

Example

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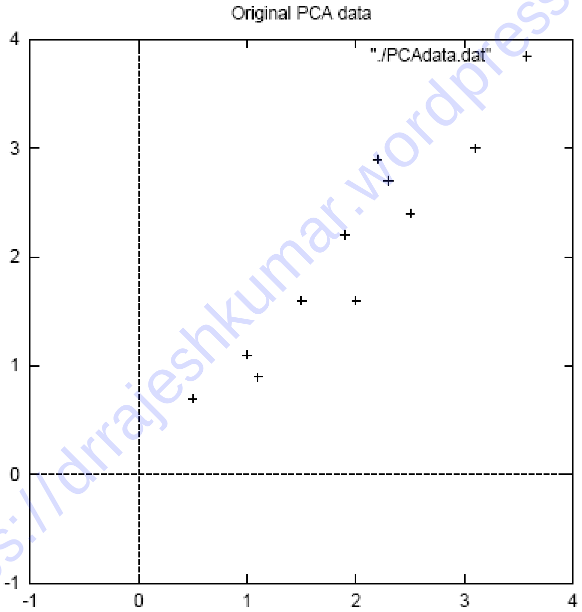

Plot of the Data

Example

- Covariance matrix

$$C = \begin{bmatrix} .616555556 & .615444444 \\ .615444444 & .716555556 \end{bmatrix}$$

- Non-diagonal elements > 0
  - Variables increase/ decrease together.

- Eigenvectors and eigenvalues of C

$$eigenvectors = \begin{bmatrix} .0490833989 \\ 1.28402771 \end{bmatrix}$$

$$eigenvectors = \begin{bmatrix} -.735178656 & -.677873399 \\ .677873399 & -.735178656 \end{bmatrix}$$

Example

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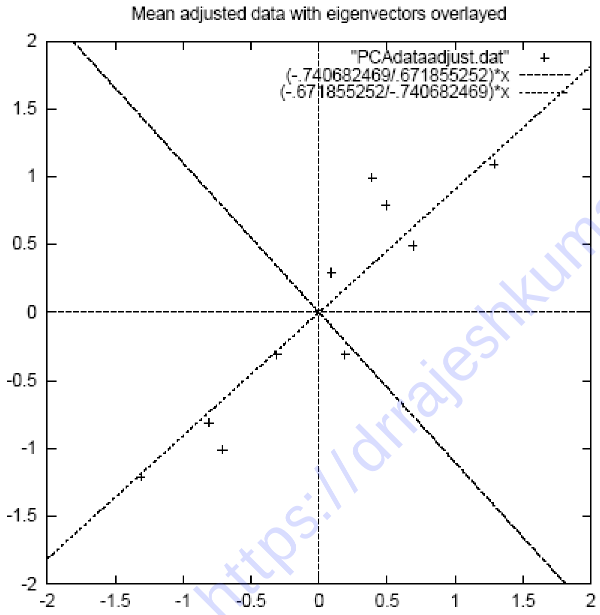


- One of the eigenvectors goes through the middle of the points, like drawing a line of best fit.
- The second eigenvector gives us the other, less important, pattern in the data.

Example

- **Principal Component → Eigenvector with the highest eigenvalue.**
- Order the eigenvectors by eigenvalue in decreasing order
  - This gives the significance of each eigenvector.
- The less significant vectors may be ignored.
  - May result in loss of information
  - Smaller the eigenvalues, lesser is the loss of information
- Final data set contains reduced dimensions!

Example – Feature Vector and Data

- Feature Vector with both eigenvectors ($[eg_2\ eg_1]$)

$$E = \begin{bmatrix} -.677873399 & -.735178656 \\ -.735178656 & .677873399 \end{bmatrix}$$

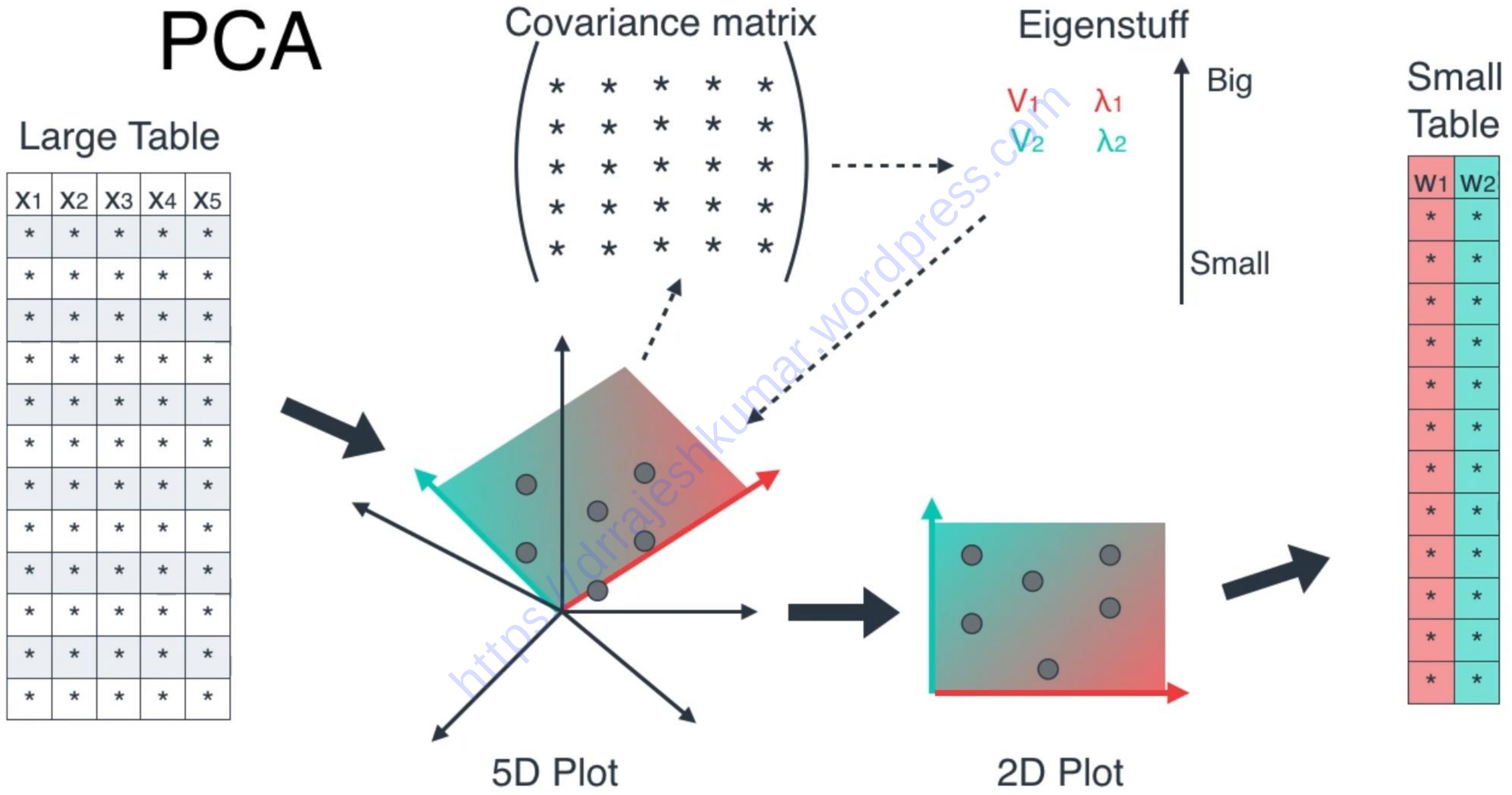
Can remove the less significant feature from matrix for reduced version.

- Data reconstruction with reduced features based on E and X!

$$\boldsymbol{Final\ Data = RFV\ \times ZMD}$$

Example – Final Data

x	y
-0.827970186	-0.175115307
1.77758033	0.142857227
-0.992197494	0.384374989
-0.274210416	0.130417207
-1.67580142	-0.209498461
-0.912949103	0.175282444
0.099109438	-0.349824698
1.14457216	0.046417258
0.438046137	0.01776463
1.22382056	-0.162675287


PCA
Large Table
x1 x2 x3 x4 x5
Covariance matrix
Eigenstuff
V1 λ1
V2 λ2
Big
Small
Small Table
w1 w2
5D Plot
2D Plot
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