An Introduction to Machine Learning with Python Programming
11 Sep 2023 - 20 Oct 2023

Principal Component Analysis

iHUB Divya Sampark, IIT Roorkee
Ritvij Bharat Private Limited (RBPL)

Presented by:
Shreyas Shukla

fig ref: pierian data

Unsupervised learning, so far, focused on clustering techniques, which seek to “discover” labels on feature data that has no historical labels.

Let’s now talk about unsupervised algorithms that focus on **dimension reduction.**

Motivation of Dimension Reduction:

- Imagine a dataset with 30+ features
- How would you understand the key features?
- Visualization and Data Analysis have limitations when the number of feature dimensions increases.

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Dimensionality Reduction Outcomes:

- Understand which features describe the most variance in the data set.
- Aid human understanding of large feature sets, especially through visualization.

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Dimensionality Reduction algorithms such as PCA **do not** simply choose a subset of the existing features.

They create **new** dimensional components that are combinations of proportions of the existing features.

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Theory and Intuition - Part One

Presented by:
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Principal Component Analysis Outcomes:

- Reduce number of dimensions in data.
- Show which features explain the most variance in the data.

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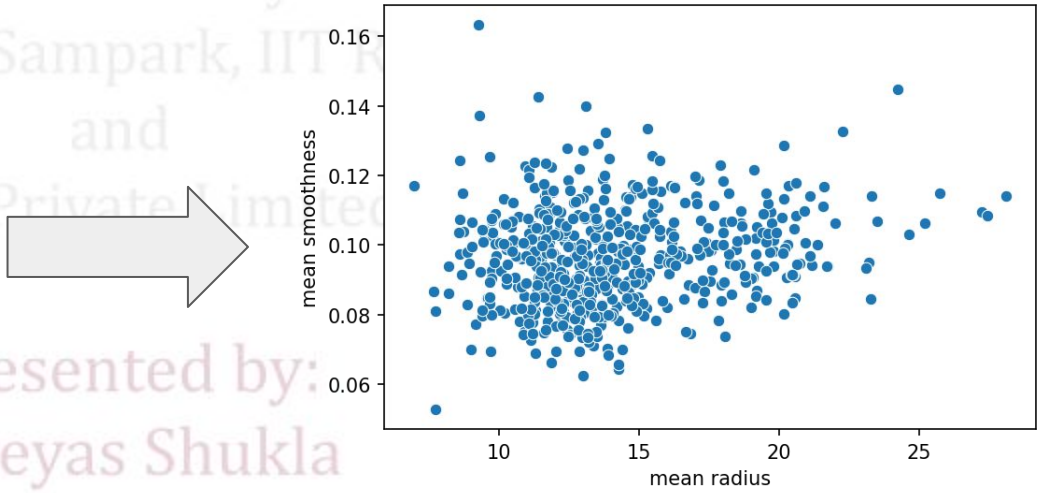
Let's talk about Dimension Reduction

	mean radius	mean smoothness
0	17.99	0.11840
1	20.57	0.08474
2	19.69	0.10960
3	11.42	0.14250
4	20.29	0.10030
...	...	...
564	21.56	0.11100
565	20.13	0.09780
566	16.60	0.08455
567	20.60	0.11780
568	7.76	0.05263



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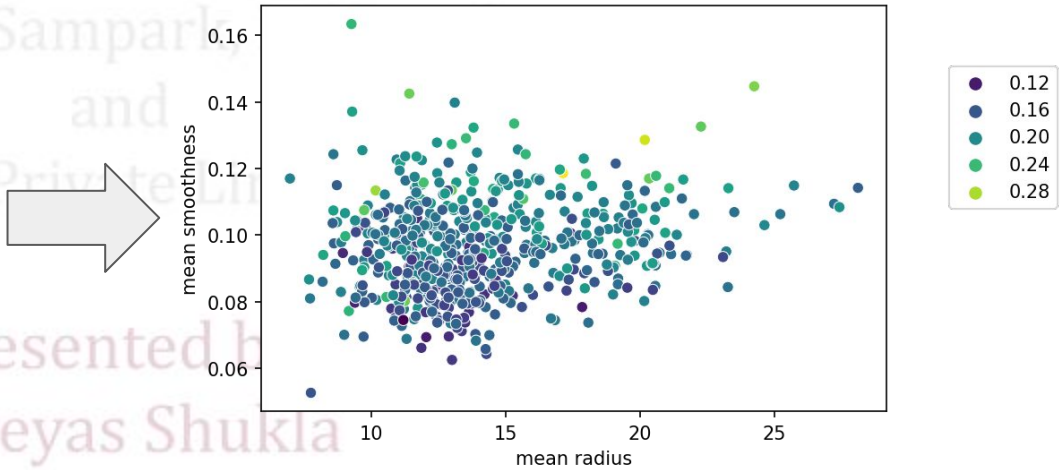
	mean radius	mean smoothness	mean symmetry
0	17.99	0.11840	0.2419
1	20.57	0.08474	0.1812
2	19.69	0.10960	0.2069
3	11.42	0.14250	0.2597
4	20.29	0.10030	0.1809
...	...	...	...
564	21.56	0.11100	0.1726
565	20.13	0.09780	0.1752
566	16.60	0.08455	0.1590
567	20.60	0.11780	0.2397
568	7.76	0.05263	0.1587



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	mean radius	mean texture	mean perimeter	mean area	mean smoothness	mean compactness	mean concavity	mean concave points	mean symmetry	mean fractal dimension	...
0	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.30010	0.14710	0.2419	0.07871	...
1	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.08690	0.07017	0.1812	0.05667	...
2	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.19740	0.12790	0.2069	0.05999	...
3	11.42	20.38	77.58	386.1	0.14250	0.28390	0.24140	0.10520	0.2597	0.09744	...
4	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.19800	0.10430	0.1809	0.05883	...
...	...	...	...	...	...	...	...	...	...	...	...
564	21.56	22.39	142.00	1479.0	0.11100	0.11590	0.24390	0.13890	0.1726	0.05623	...
565	20.13	28.25	131.20	1261.0	0.09780	0.10340	0.14400	0.09791	0.1752	0.05533	...
566	16.60	28.08	108.30	858.1	0.08455	0.10230	0.09251	0.05302	0.1590	0.05648	...
567	20.60	29.33	140.10	1265.0	0.11780	0.27700	0.35140	0.15200	0.2397	0.07016	...
568	7.76	24.54	47.92	181.0	0.05263	0.04362	0.00000	0.00000	0.1587	0.05884	...

569 rows × 30 columns

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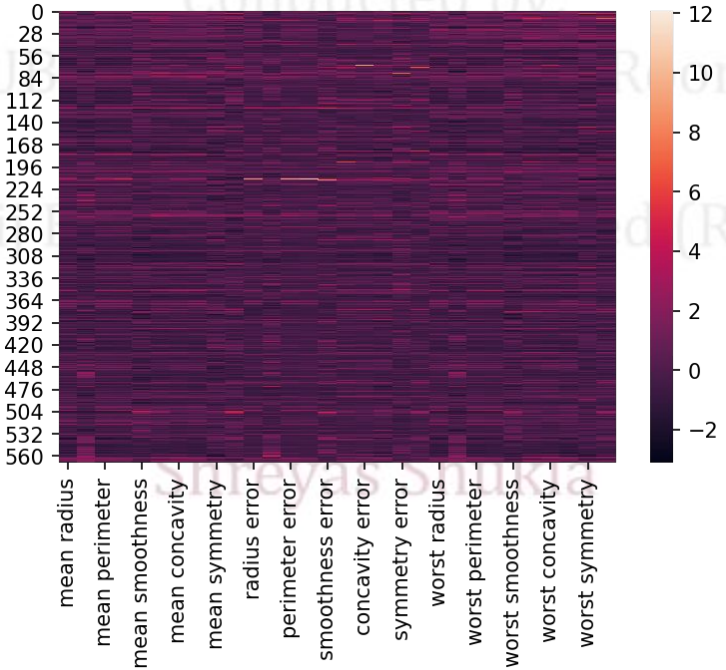

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Dimension Reduction

- Helps visualize and understand complex data sets.
- Can also act as a simpler data set for training data for machine learning algorithms.
  - Reduce dimensions then train ML Algorithm on smaller data set.

fig ref: pierian data

Dimension Reduction

- Helps reduce N features to a desired smaller set of components through a **transformation**.
- It does **not** simply select a subset of features.

fig ref: pierian data

Variance Explained

- Often, certain features are more important or have more explanatory power than other features.
- Eg: Size of a house is probably much more important than the color of a house when explaining the price of a house for sale.

fig ref: pierian data

- This idea of more important features is easy to understand when we can directly correlate features to a known label. But what about unlabeled data?
- What measurement can we use to determine feature “importance”?

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Measure the proportion to which each feature accounts for dispersion in the data set.

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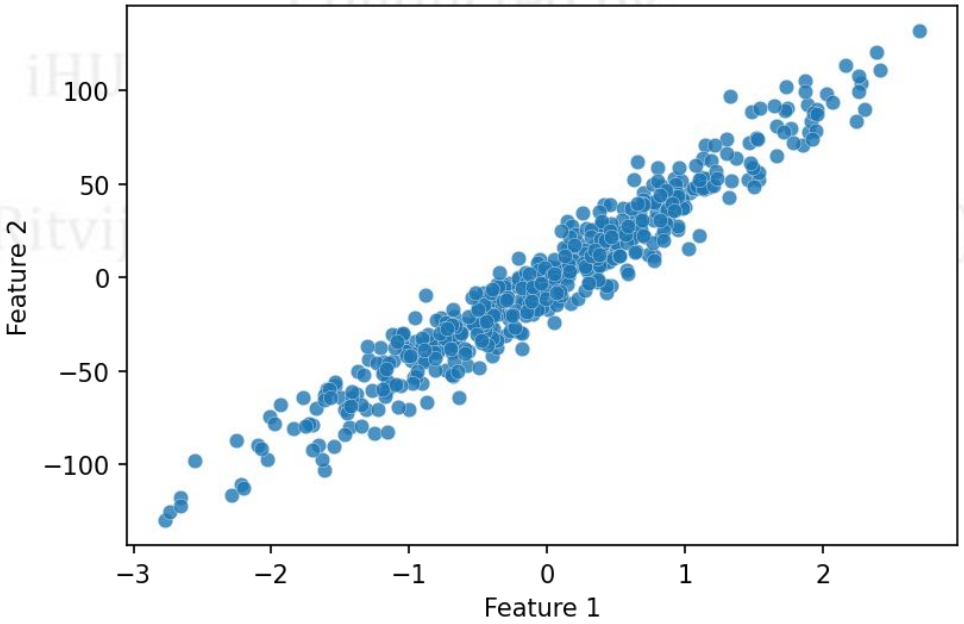

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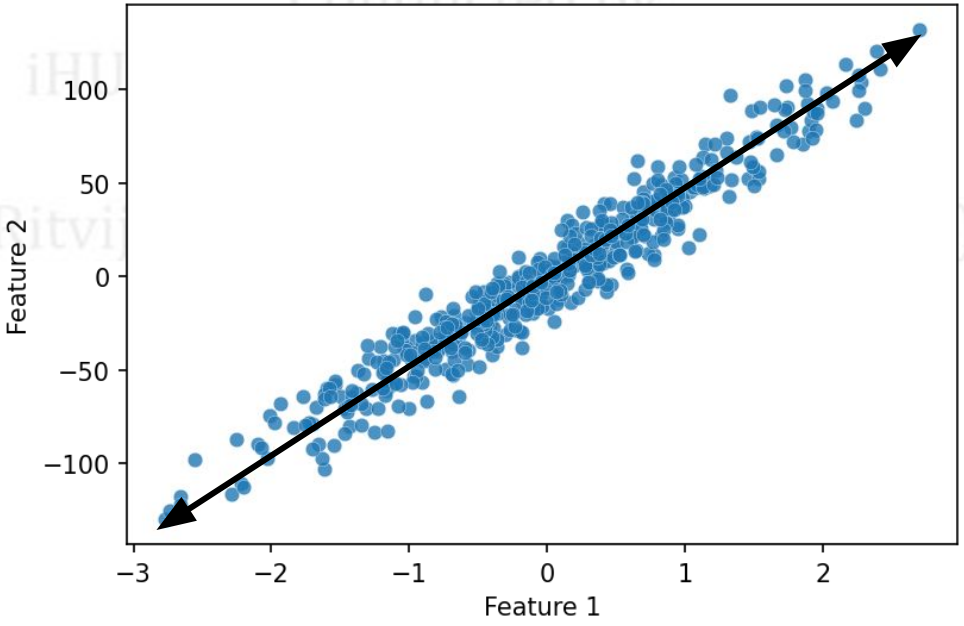

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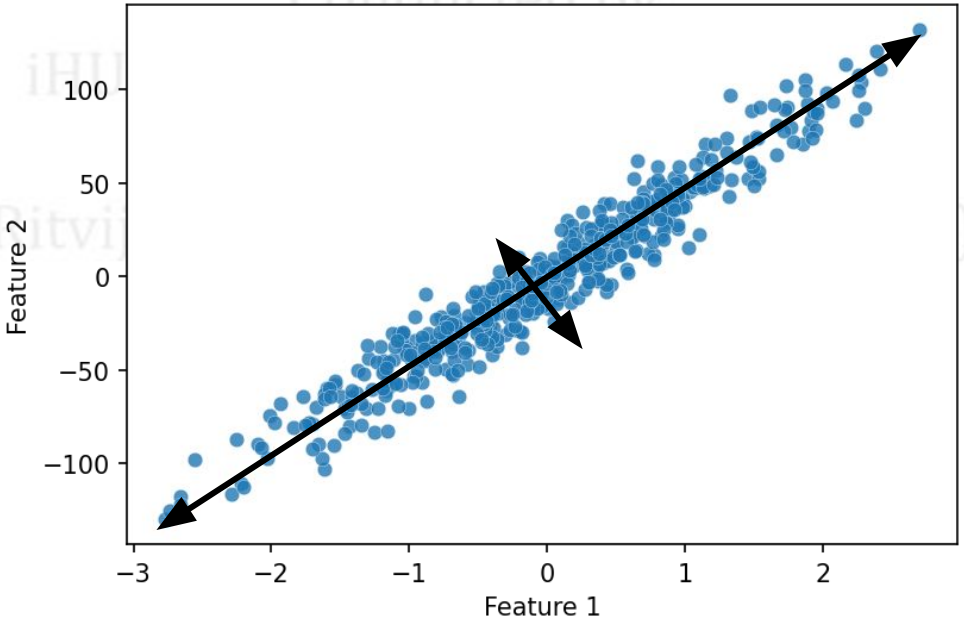

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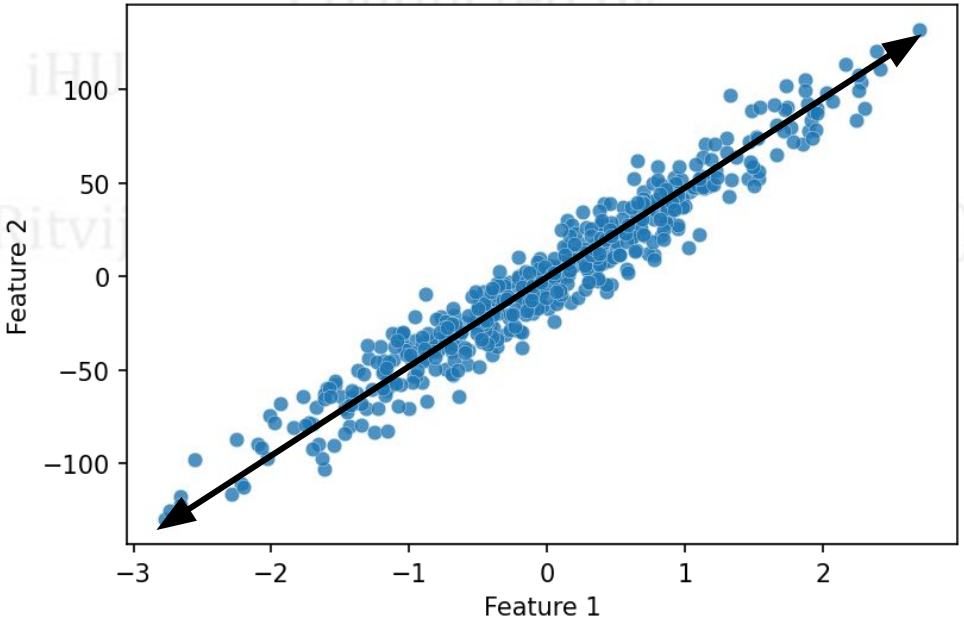

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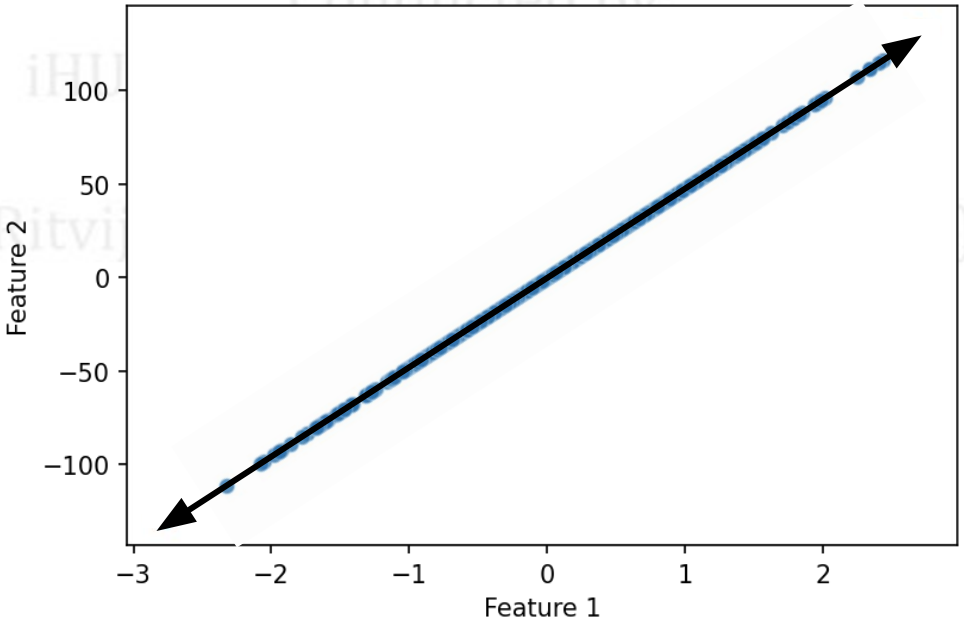

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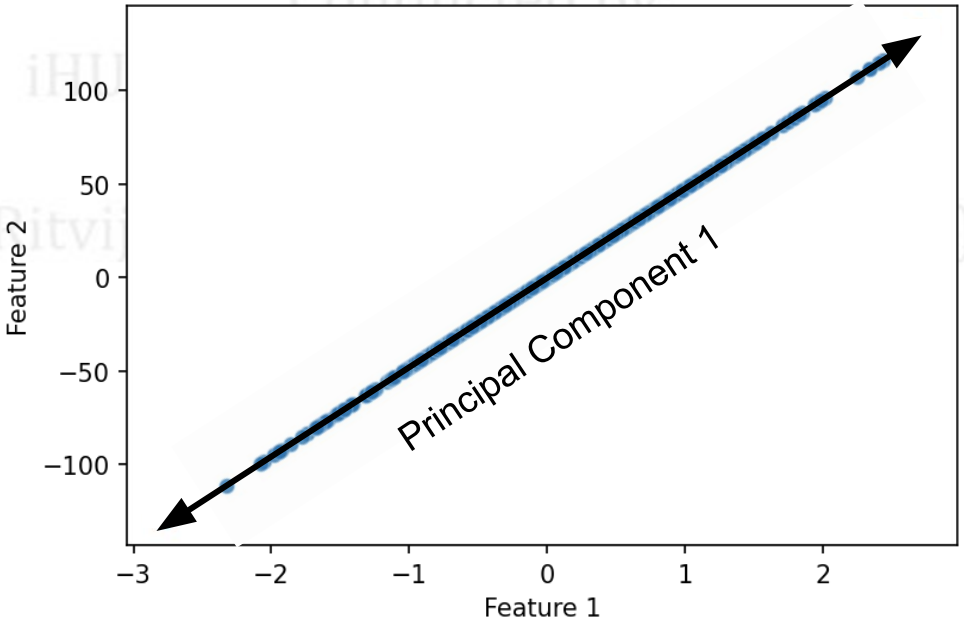

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Principal Component 1

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Variance Explained

- Principal Component is basically a linear combination of original features.
- The more variance the original feature accounts for, the more influence it has over the principal components.

Here we went from 2 features down to 1 principal component.

This single principal component can “explain” some percentage of the original data, for example 90% of variance explained by principal component.

fig ref: pierian data

100% of the variance in the data is explained by all the original features.

We trade off some of the explained variance for less dimensions.

This can be significant savings for data sets with many dimensions, but only a few strong features.

fig ref: pierian data

Let’s see how PCA actually works mathematically.

fig ref: pierian data

PCA operates by creating a new set of dimensions, that is the principal components, that are normalized linear combinations of the original features.

$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2 + \ldots + \phi_{p1} X_p$$

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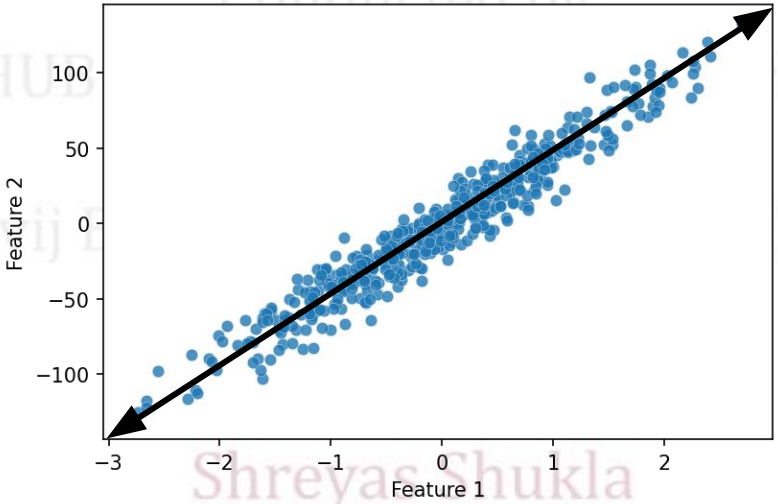

$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2$$

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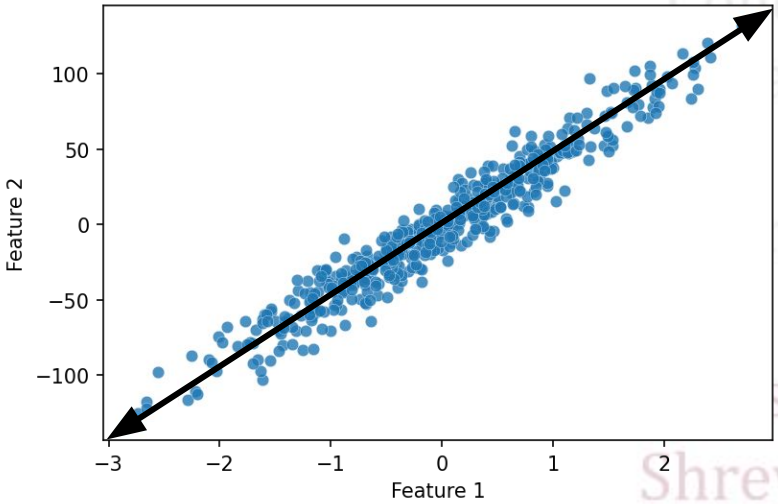

$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2$$

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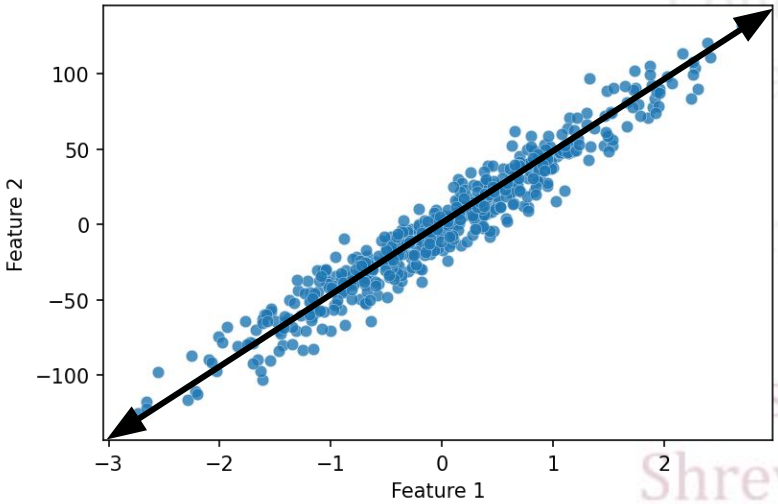

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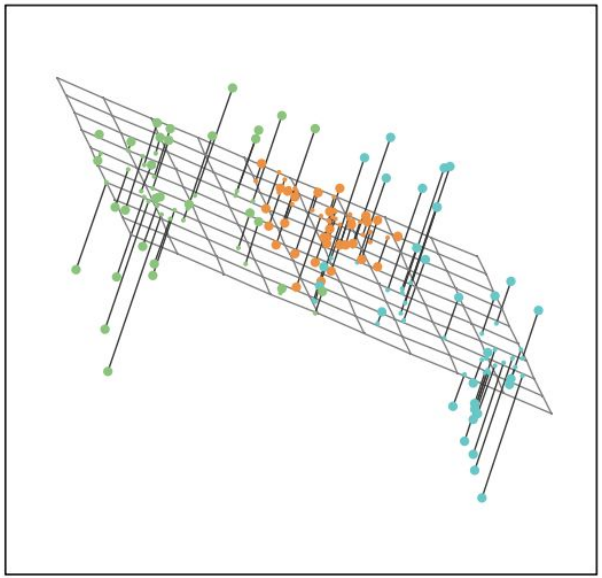

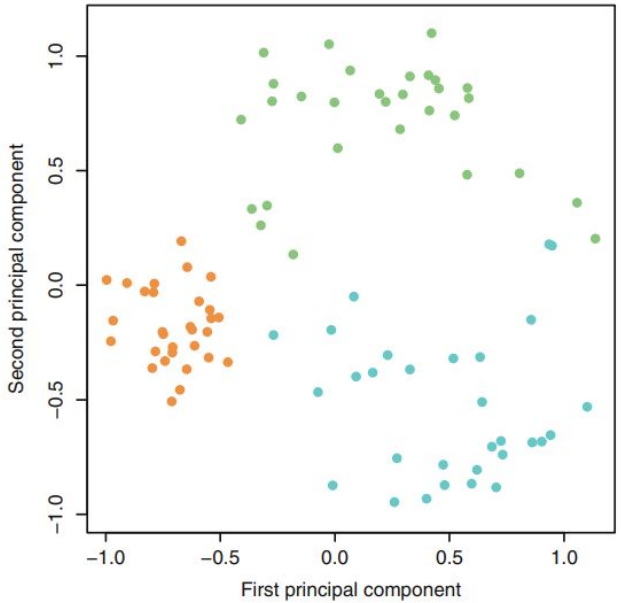

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How do we calculate these components?

Let’s walk through the steps visually.

fig ref: pierian data

X1	X2
1	2
2	1
3	2
4	4
5	3
6	5

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X1	X2
1	2
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4	4
5	3
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Standardize the data:

X1	X2
1	2
2	1
3	2
4	4
5	3
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X1	X2
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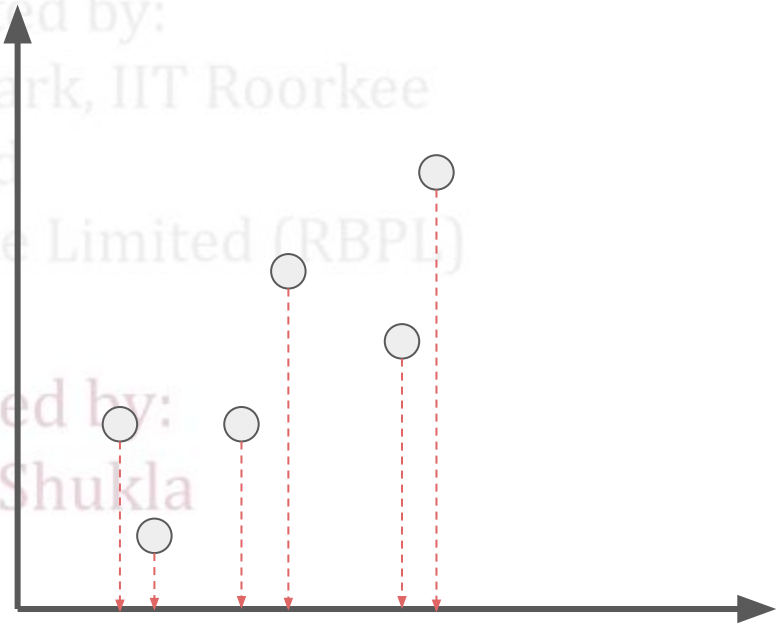

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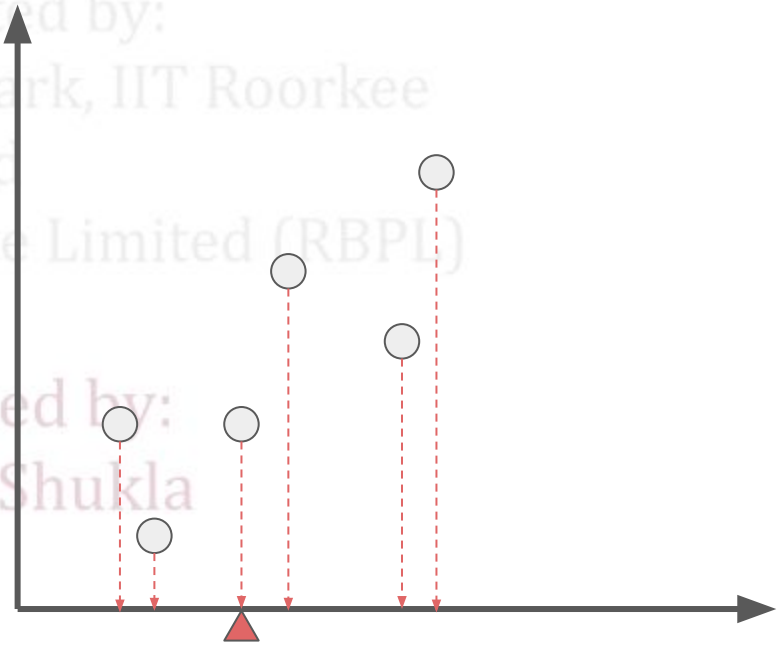

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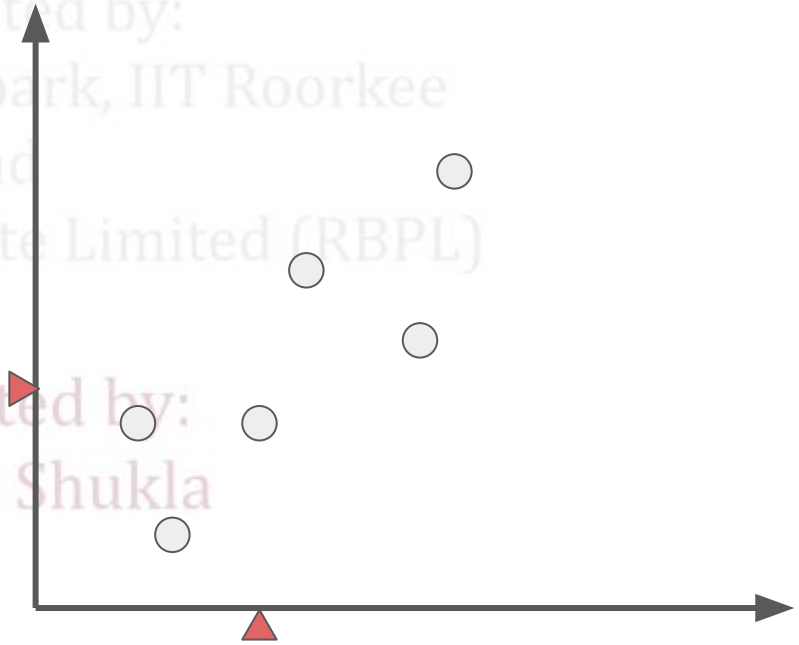

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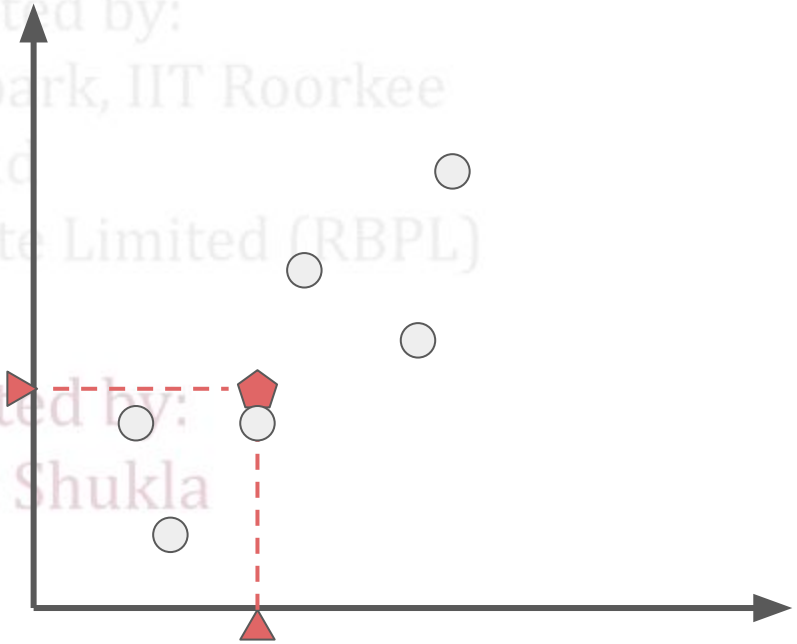


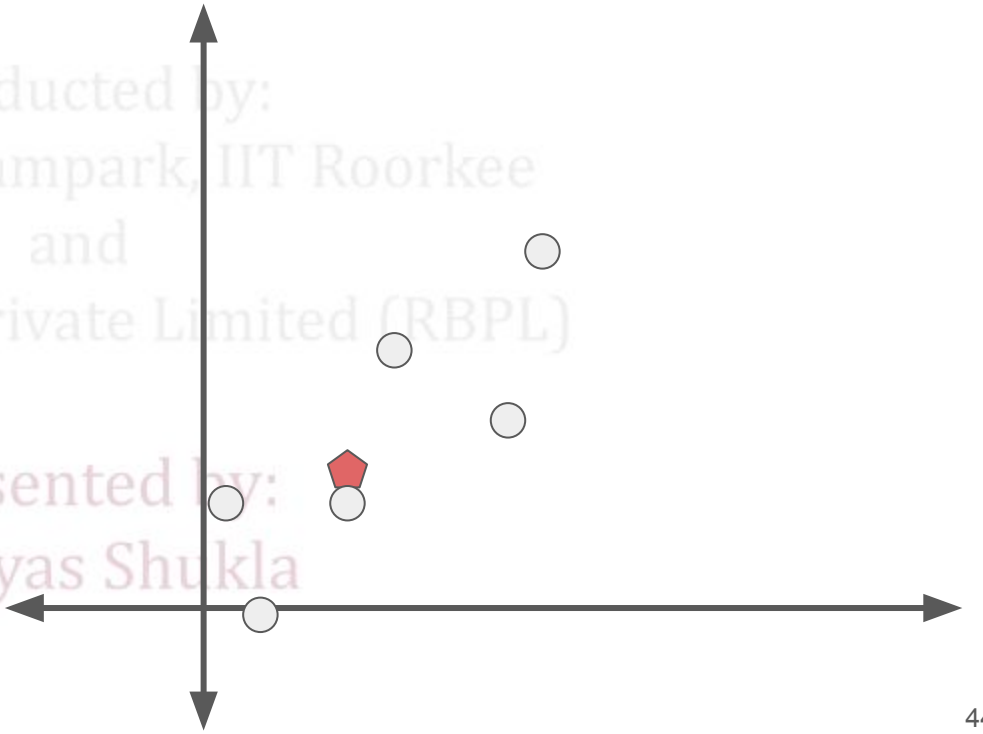
fig ref: pierian data

Standardize the data:

X1	X2
1	2
2	1
3	2
4	4
5	3
6	5

fig ref: pierian data

Standardize the data:



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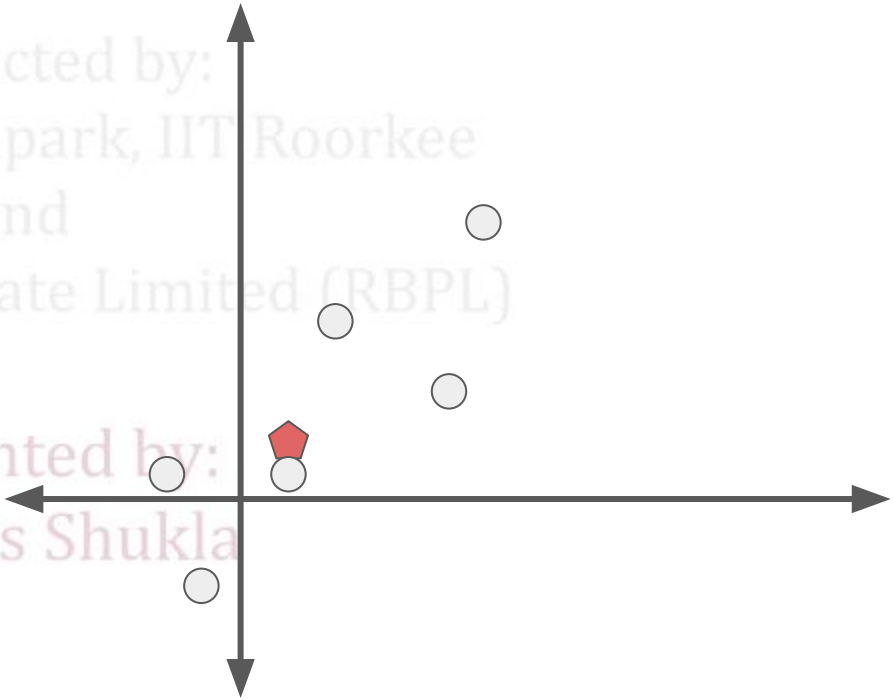

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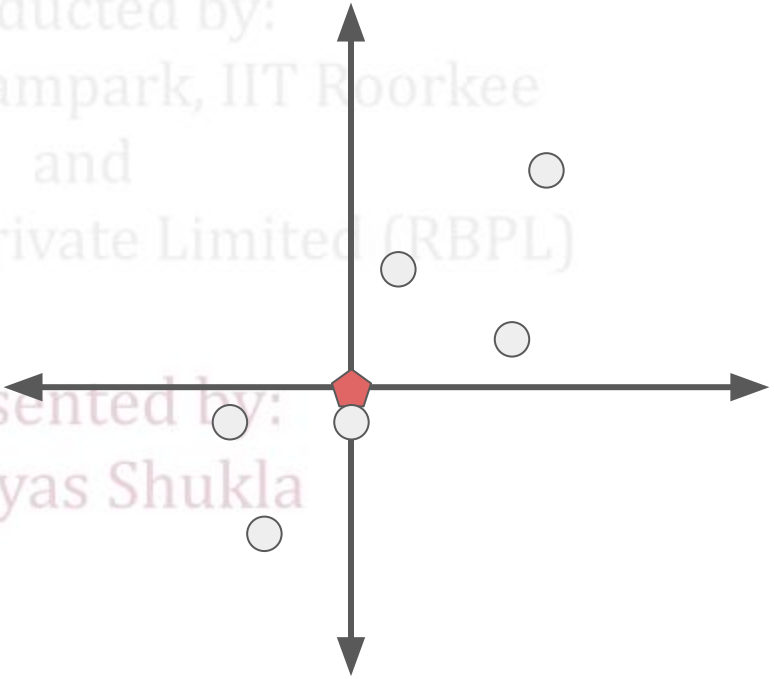
Standardize the data:



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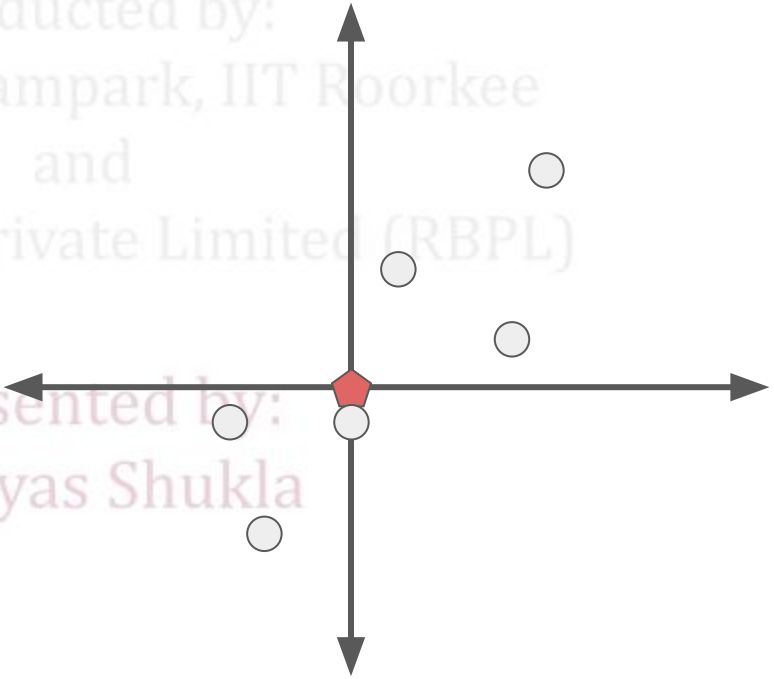
Calculate covariance matrix for data:



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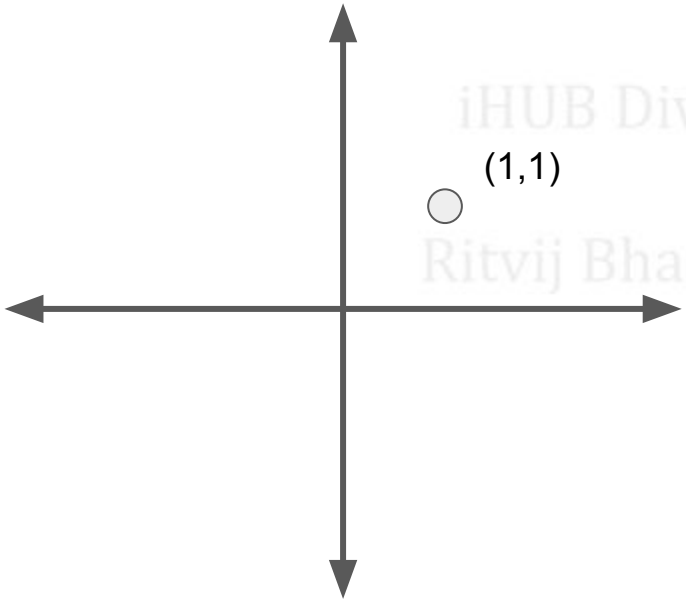
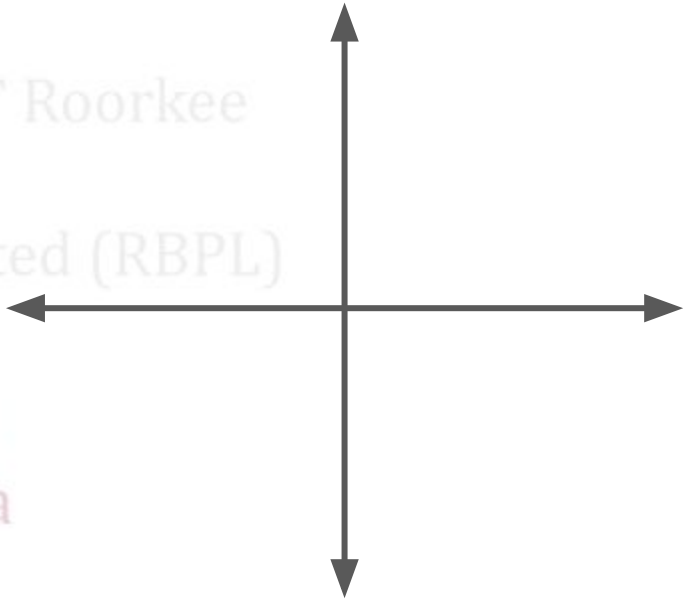
Linear transformation of data:





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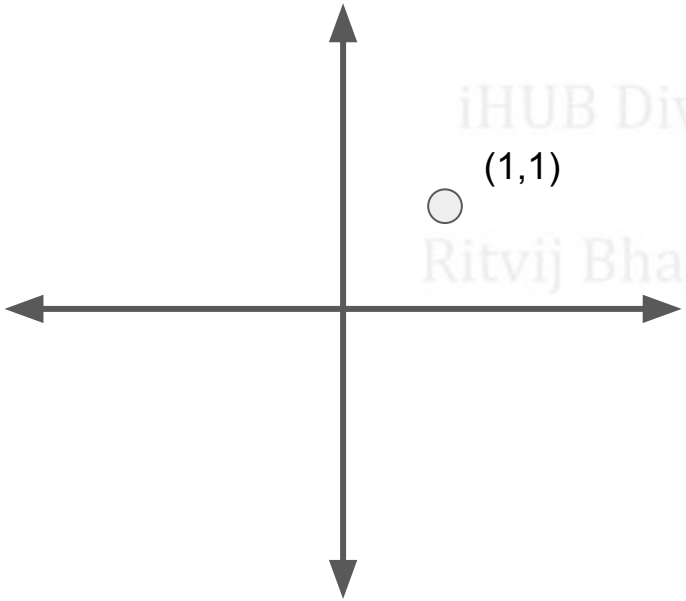
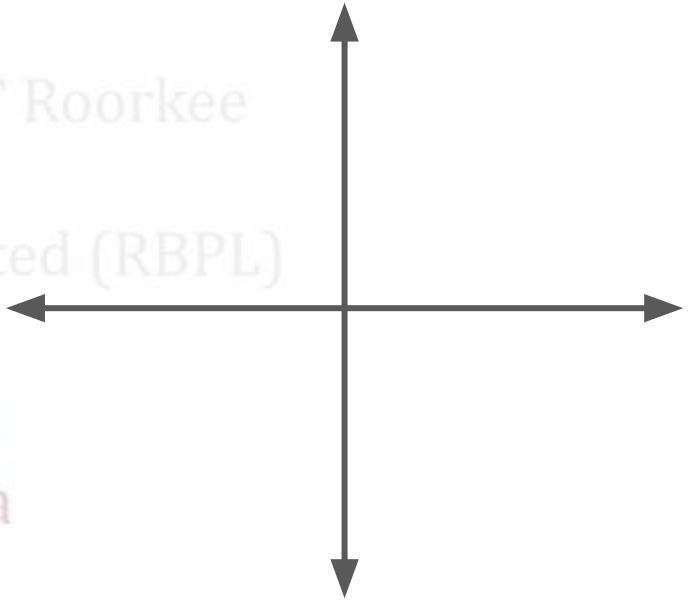


$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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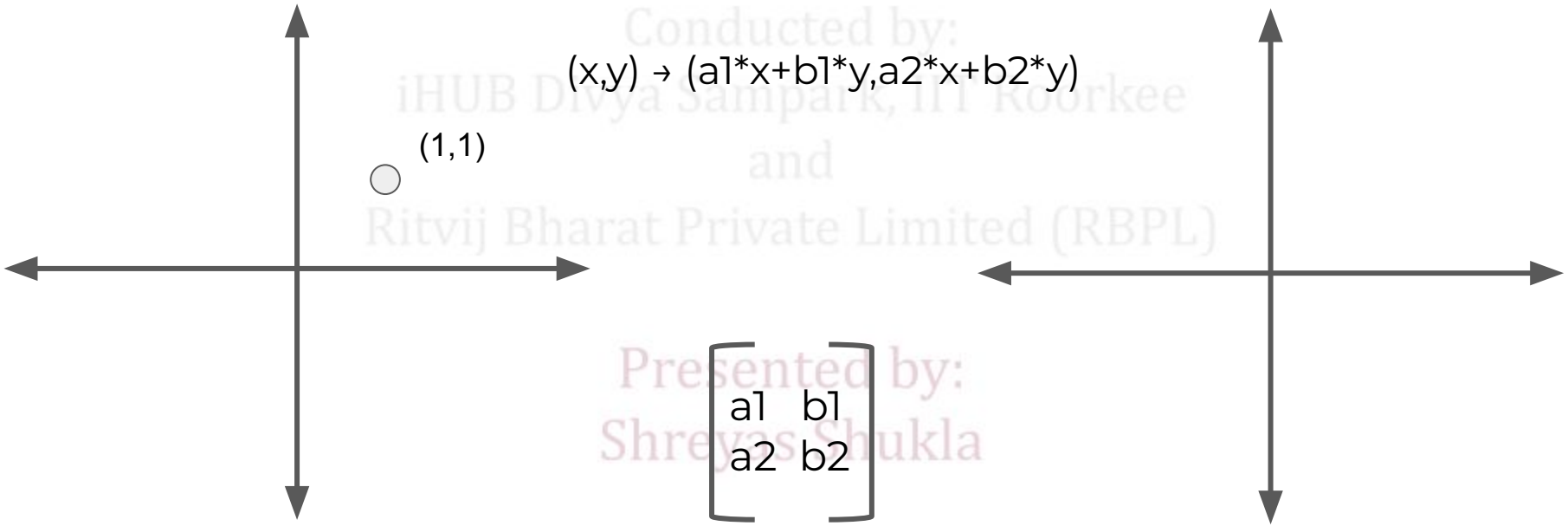

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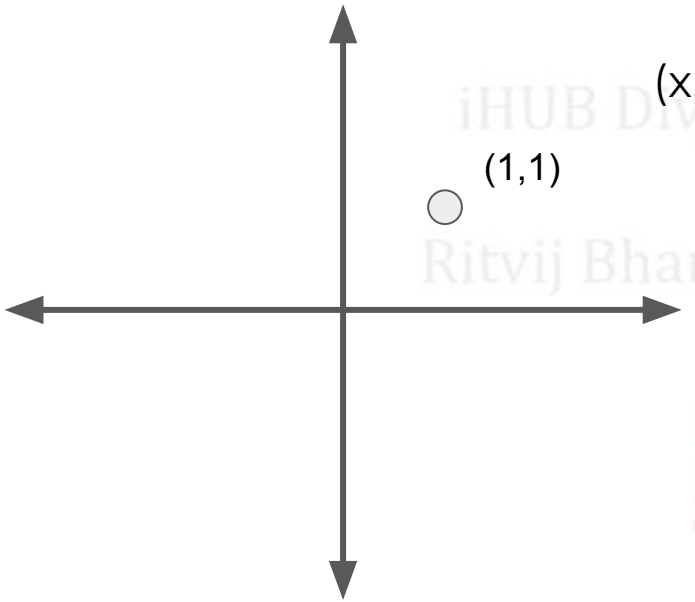
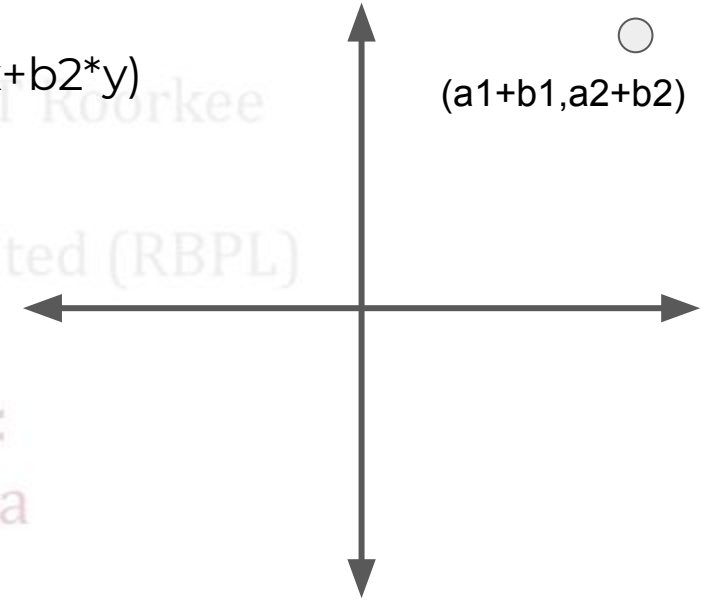


(x,y) → (a1*x+b1*y,a2*x+b2*y)

$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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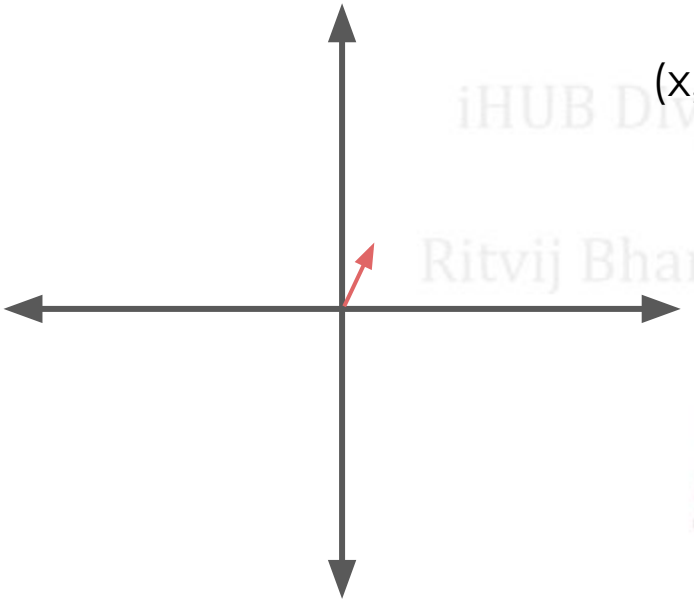

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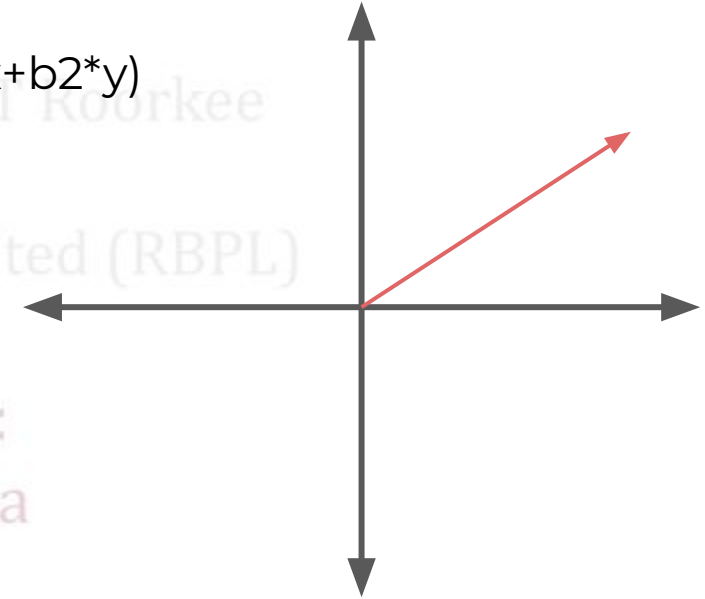

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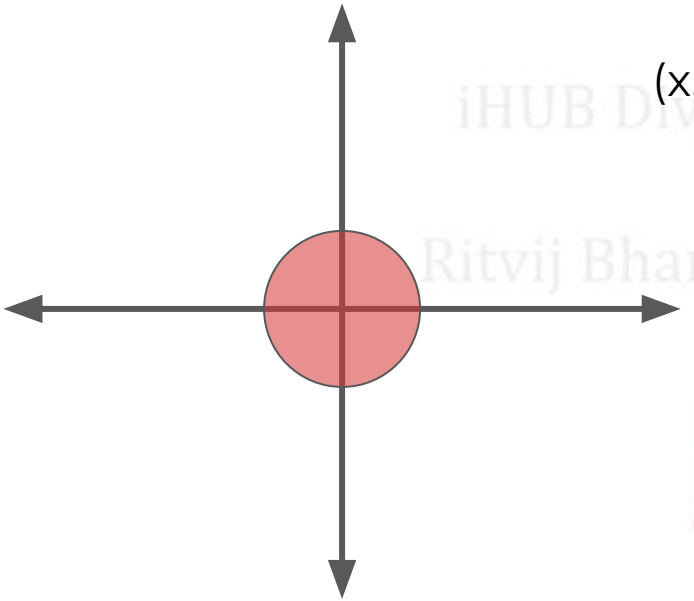

$$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$$

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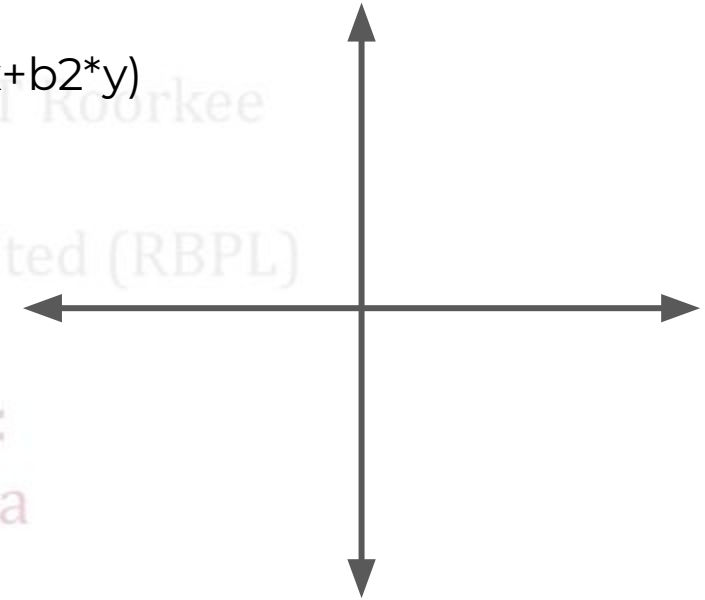
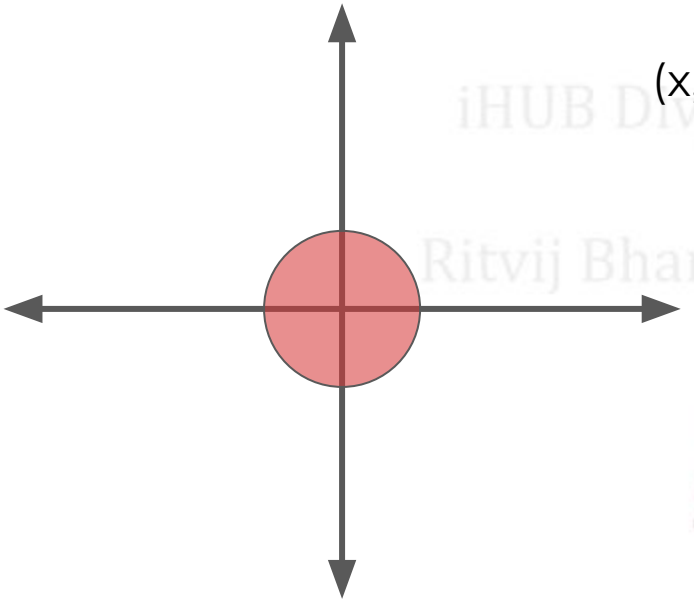
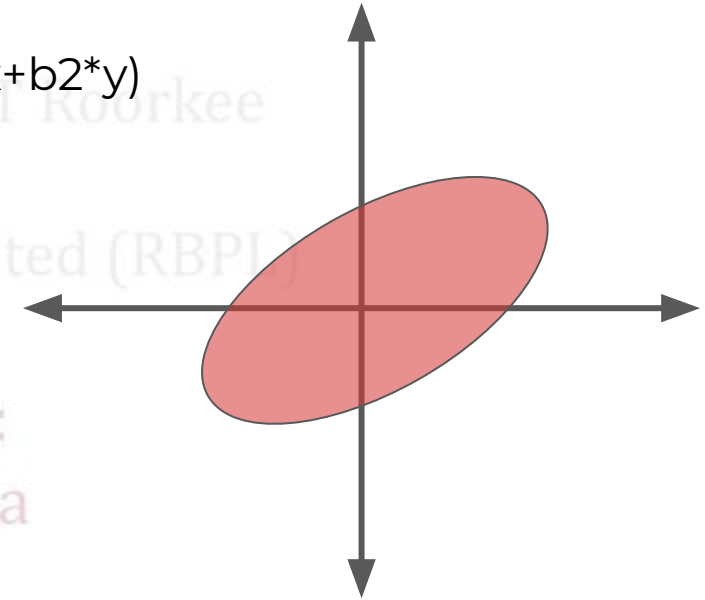


fig ref: pierian data



(x,y) → (a1*x+b1*y,a2*x+b2*y)

$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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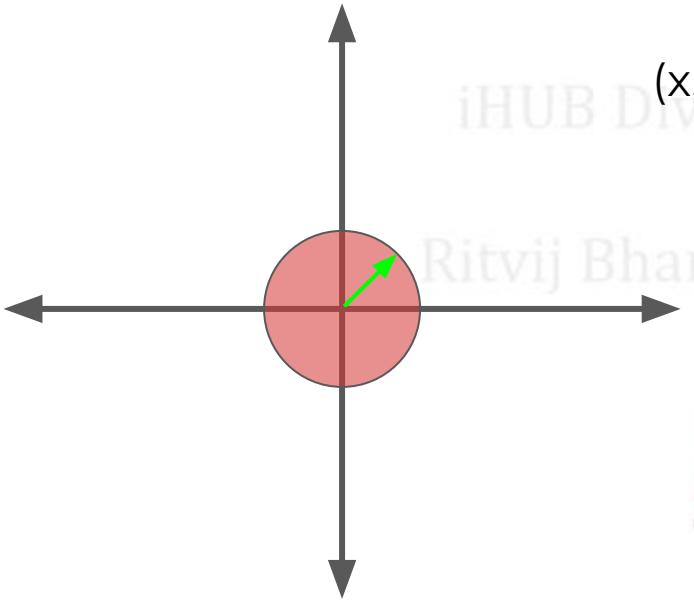


(x,y) → (a1*x+b1*y,a2*x+b2*y)

$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

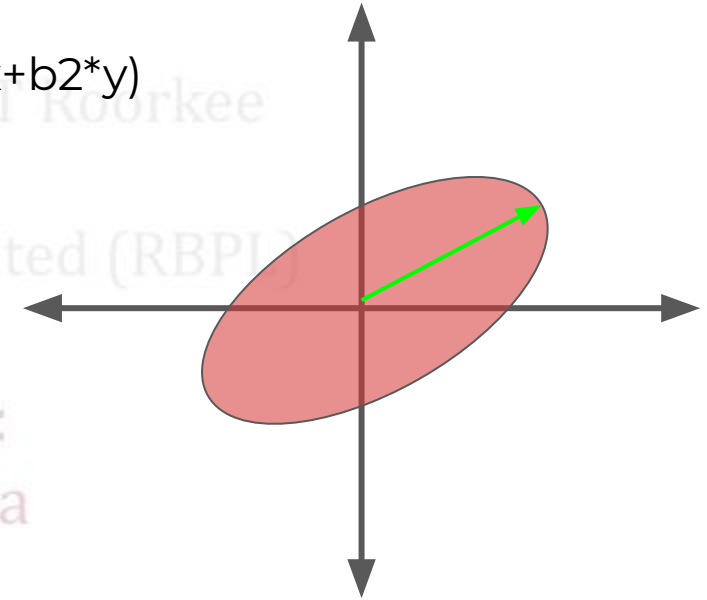
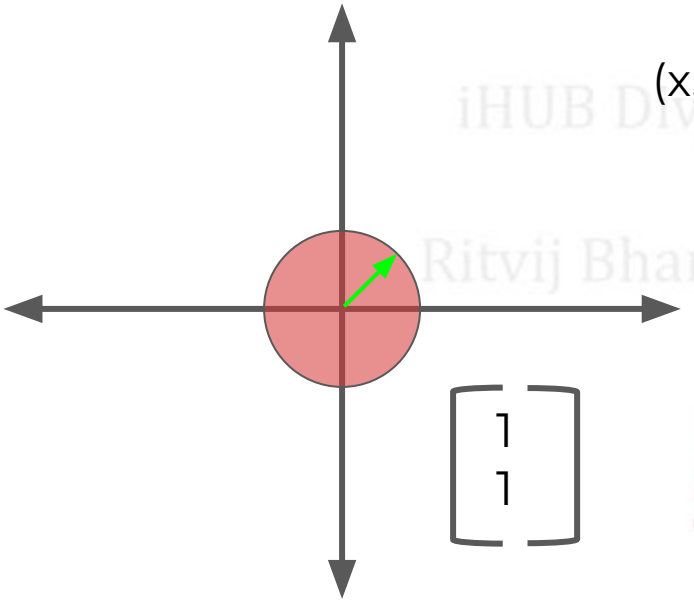


fig ref: pierian data

EigenVector: Directional Information



(x,y) → (a1*x+b1*y,a2*x+b2*y)

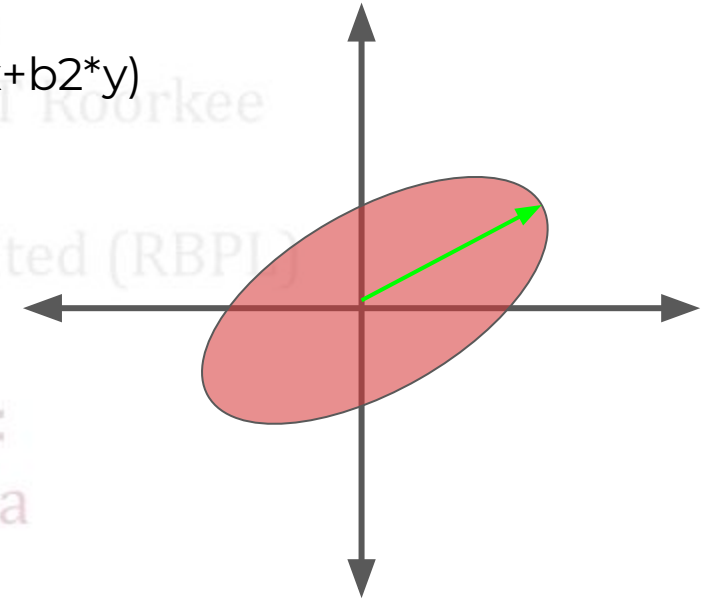
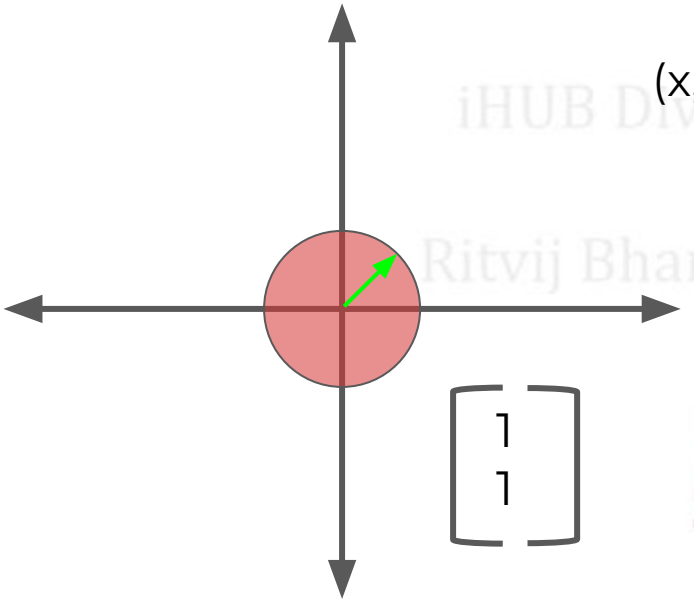


fig ref: pierian data

EigenVector: Directional Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)



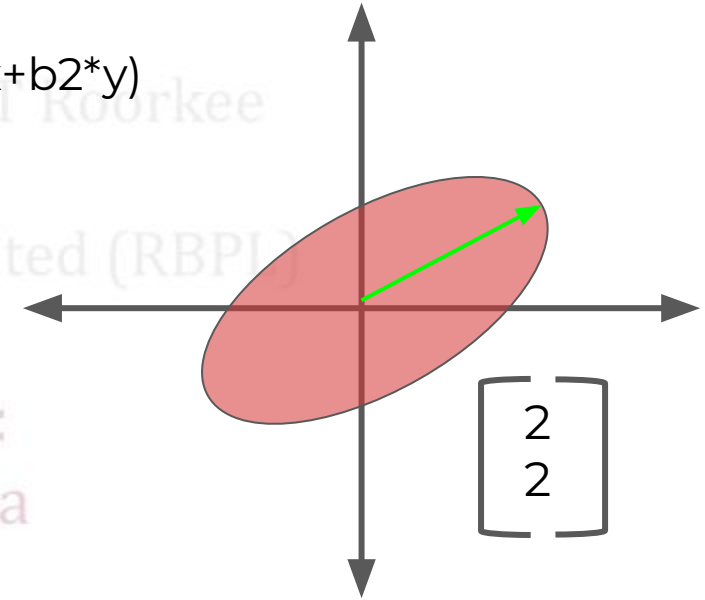
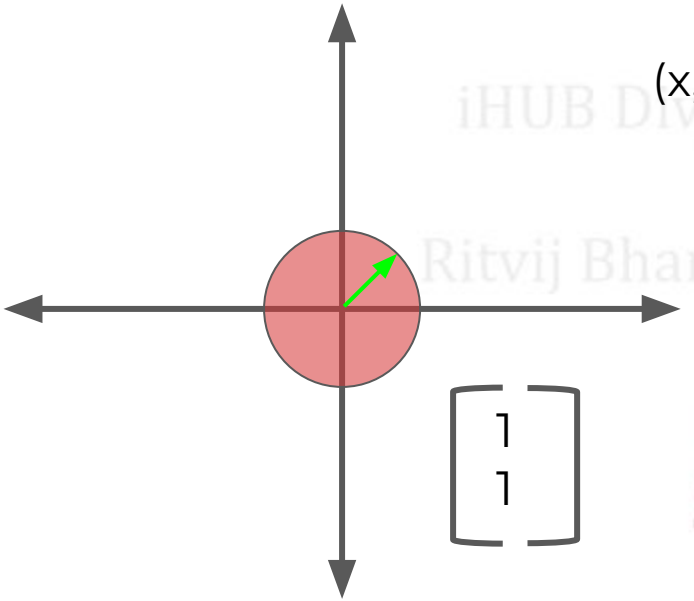


fig ref: pierian data

EigenValue: Magnitude Information



(x,y) → (a1*x+b1*y,a2*x+b2*y)

$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

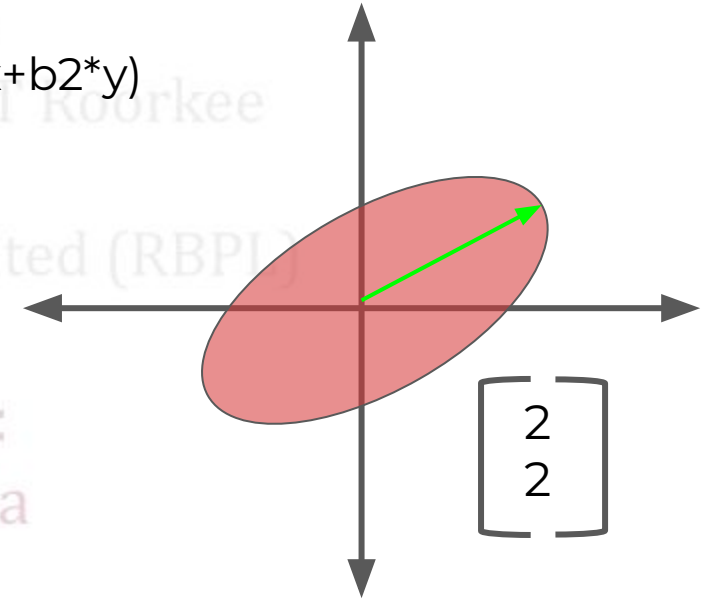
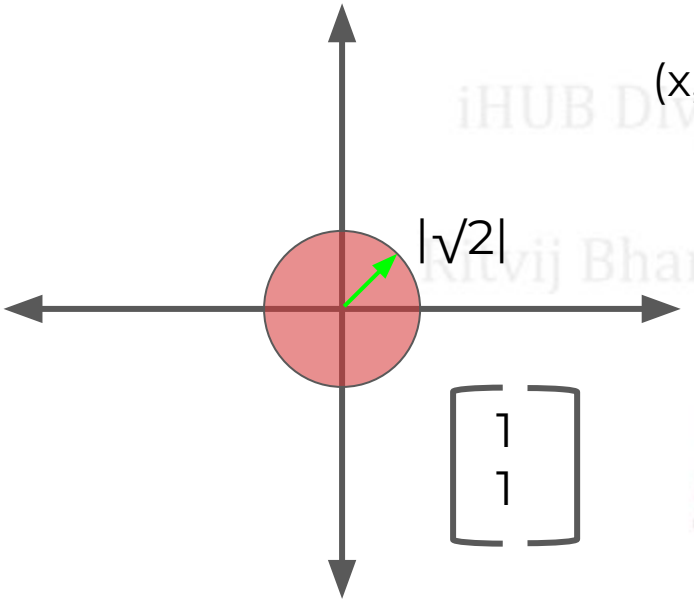


fig ref: pierian data

EigenValue: Magnitude Information



(x,y) → (a1*x+b1*y,a2*x+b2*y)

$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

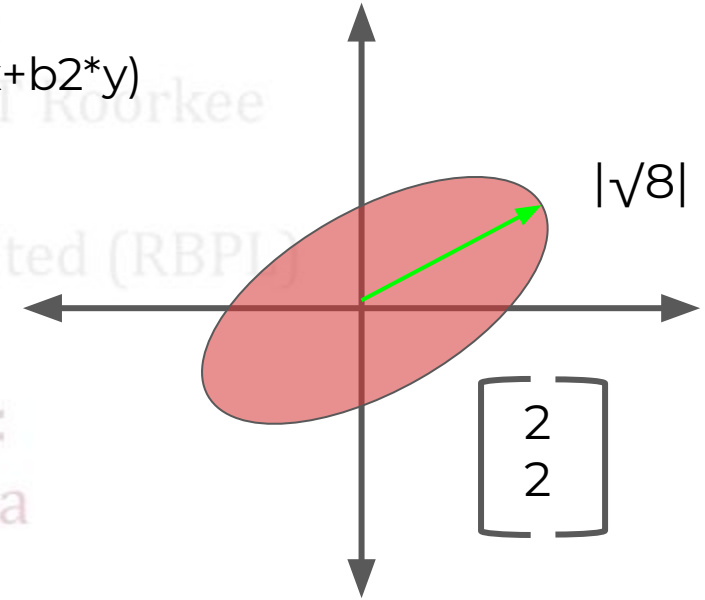
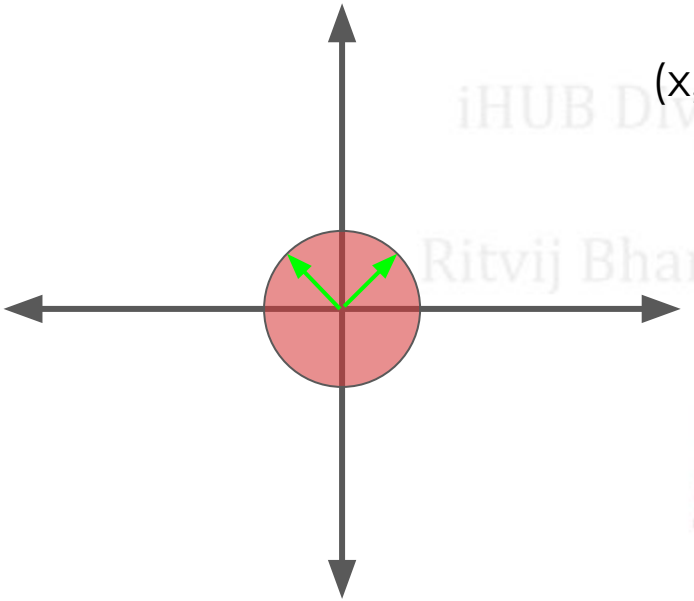


fig ref: pierian data

Orthogonal EigenVector



(x,y) → (a1*x+b1*y,a2*x+b2*y)

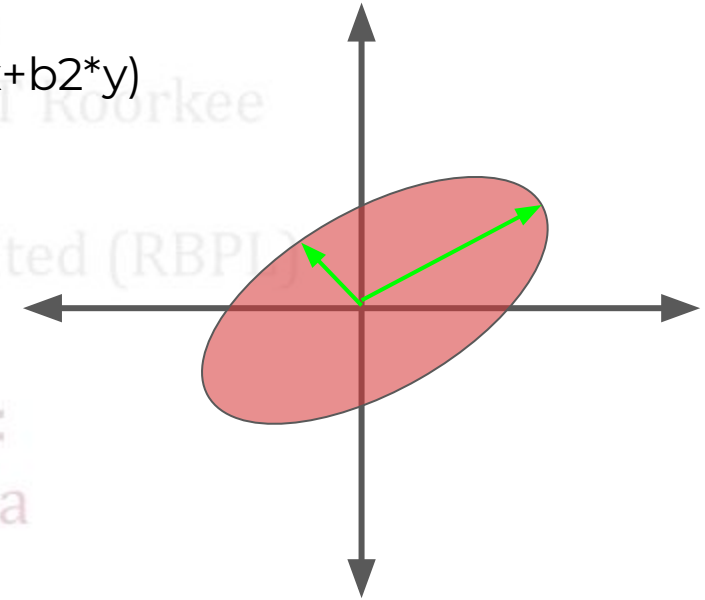
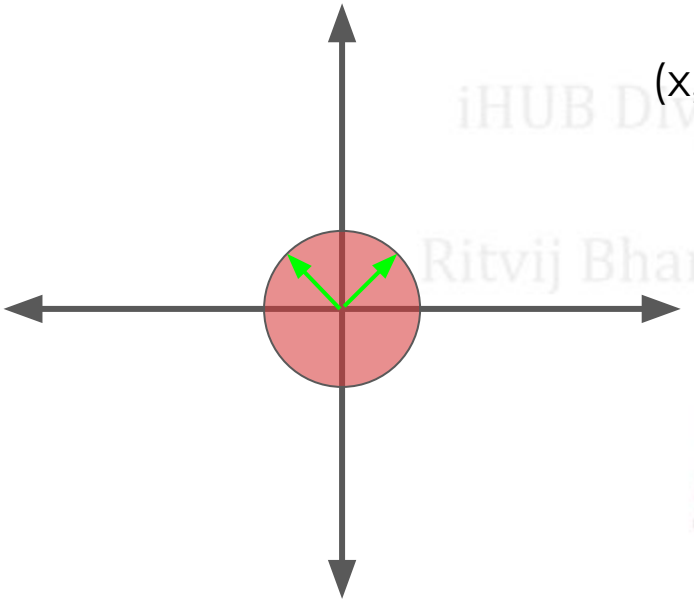


fig ref: pierian data

EigenVector is just a linear transformation

(x,y) → (a1*x+b1*y,a2*x+b2*y)



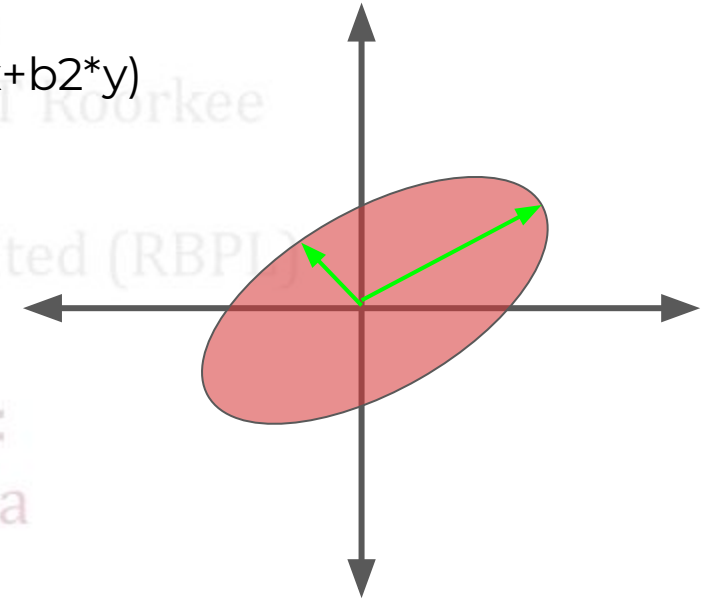


fig ref: pierian data

Apply Linear Transformation:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$

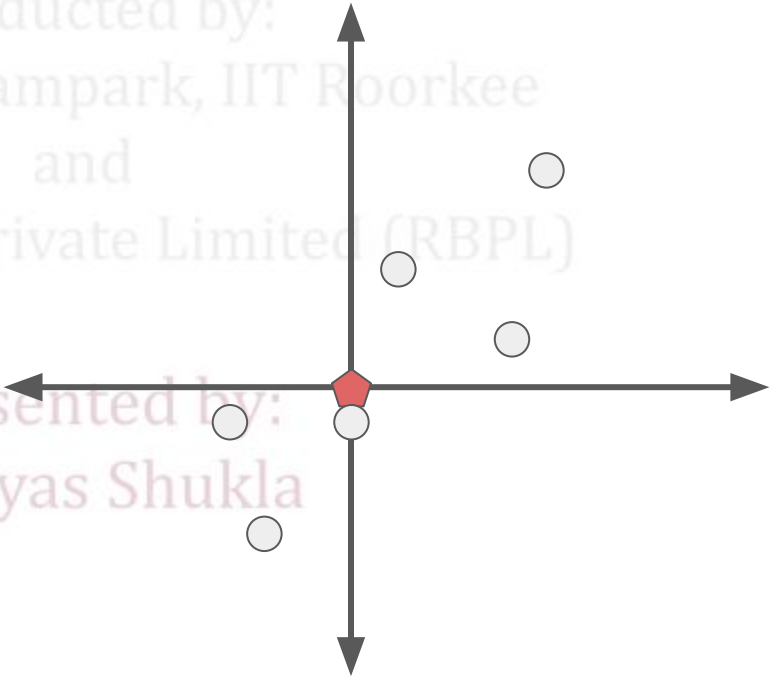


fig ref: pierian data

Apply Linear Transformation:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$

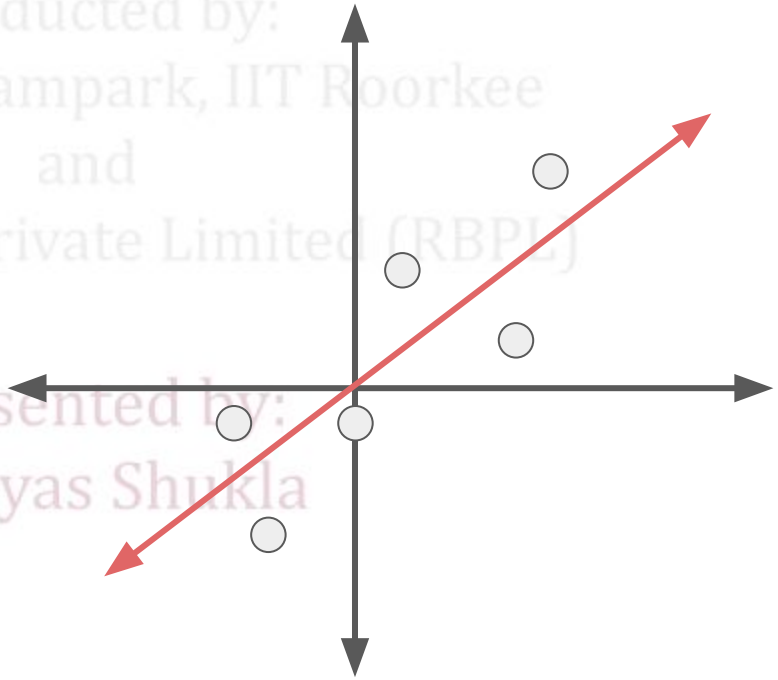


fig ref: pierian data

Apply Linear Transformation:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$

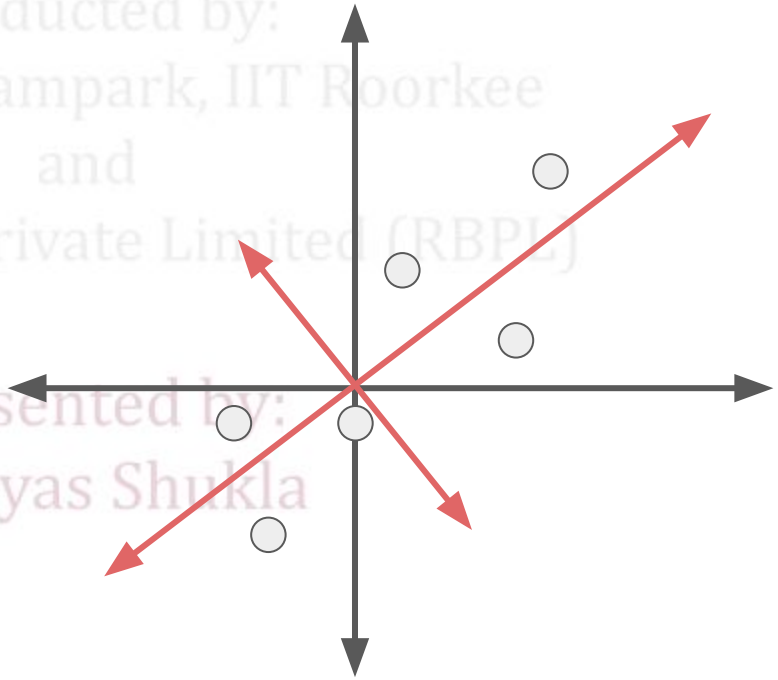
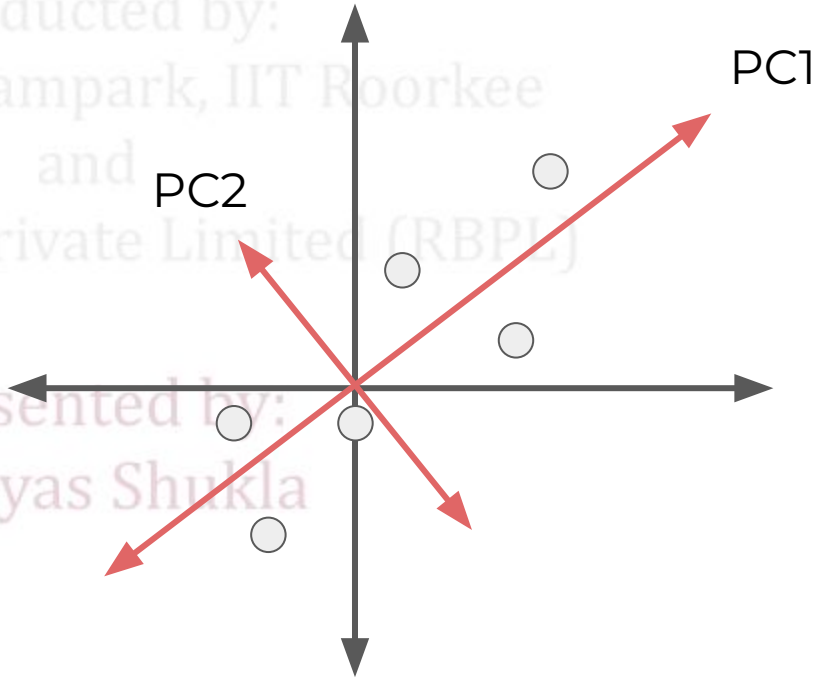


fig ref: pierian data

EigenValue measures variance explained:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$



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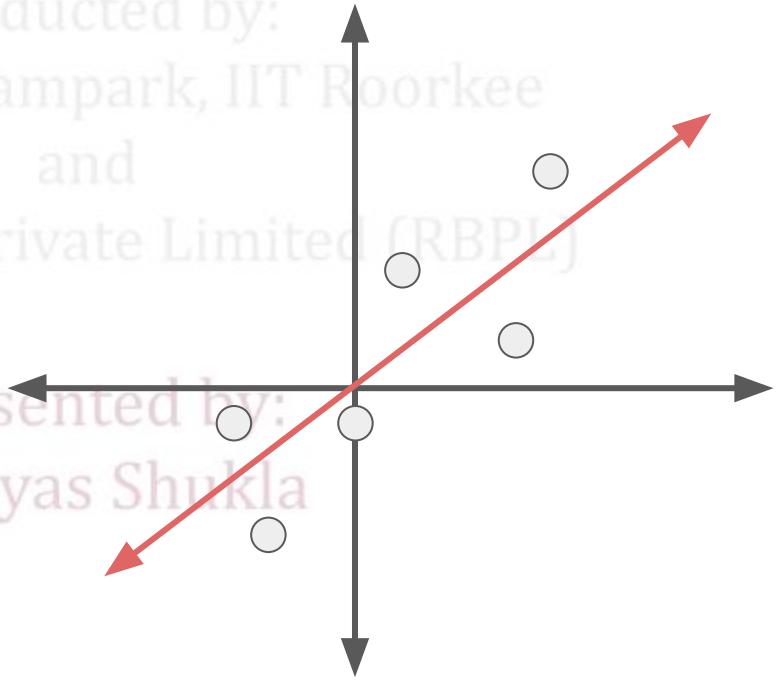
EigenValue measures variance explained:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$



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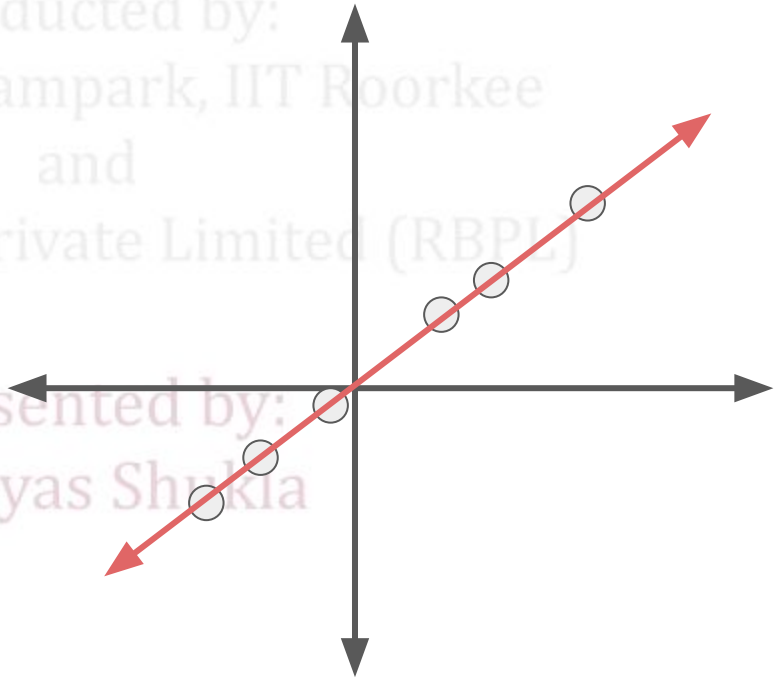

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$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$

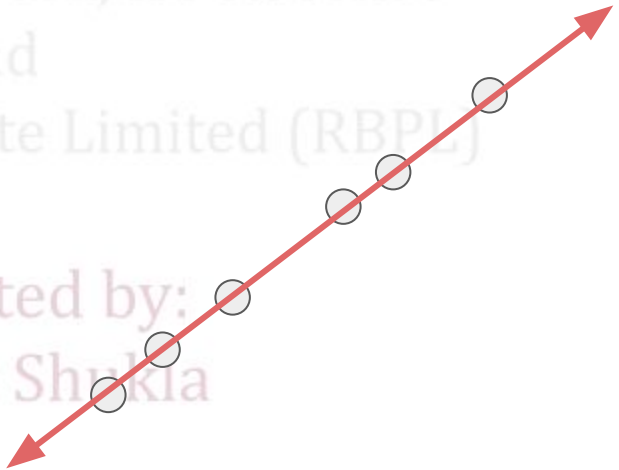

fig ref: pierian data

EigenValue measures variance explained:

$$\begin{bmatrix} \text{Var}(X) & \text{Cov}(X,Y) \\ \text{Cov}(X,Y) & \text{Var}(Y) \end{bmatrix}$$

Principal Component 1

fig ref: pierian data

PCA Steps

1. Get original data
2. Calculate Covariance Matrix
3. Calculate EigenVectors
4. Sort EigenVectors by EigenValues
5. Choose N largest EigenValues
6. Project original data onto EigenVectors

fig ref: pierian data