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# Principal Component Analysis

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**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**.

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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.

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

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# Theory and Intuition - Part One

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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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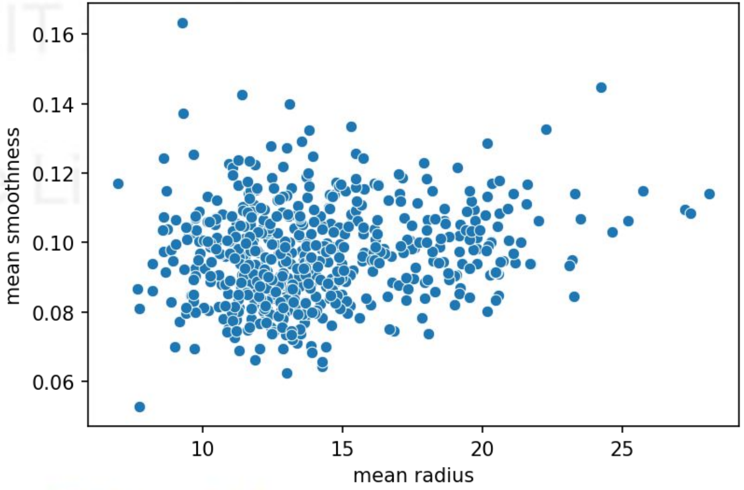
# Let’s talk about Dimension Reduction

| | 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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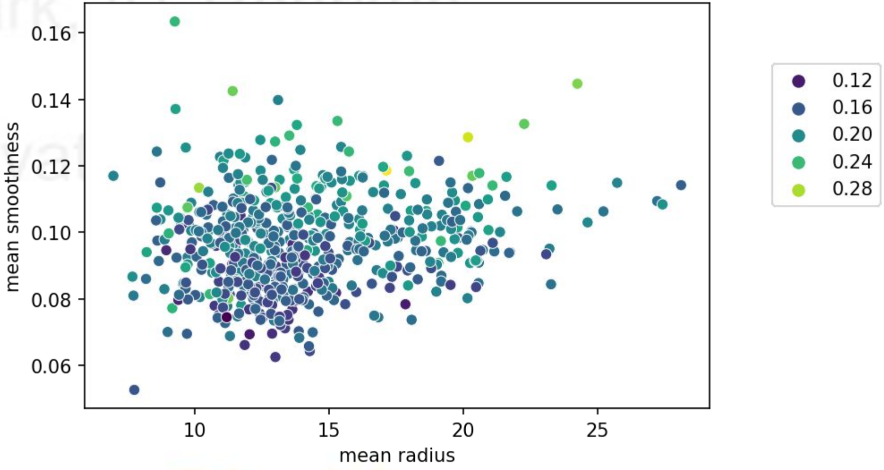
| | mean radius | mean smoothness | mean symmetry |
|---|---|---|---|
| **0** | 17.99 | 0.11840 | 0.2419 |
| **1** | 20.57 | 0.08474 | 0.1812 |
| **2** | 19.69 | 0.10960 | 0.2069 |
| **3** | 11.42 | 0.14250 | 0.2597 |
| **4** | 20.29 | 0.10030 | 0.1809 |
| **...** | ... | ... | ... |
| **564** | 21.56 | 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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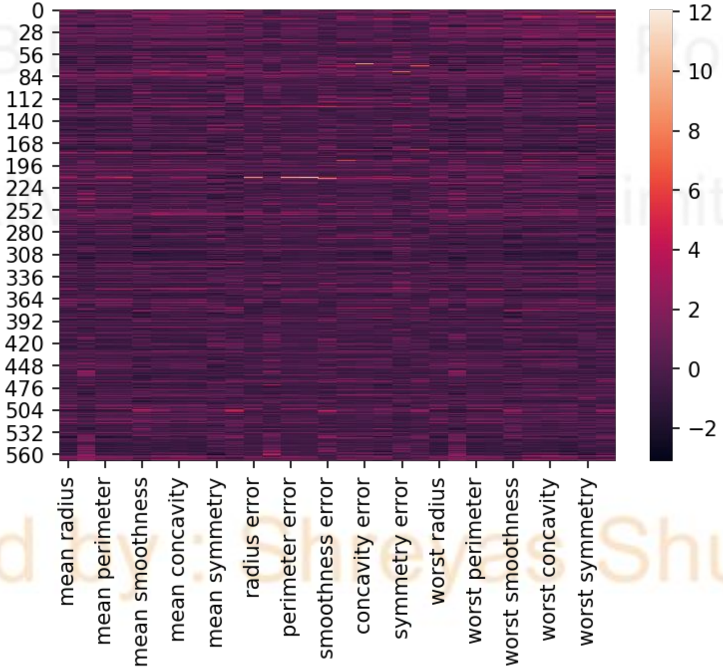

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Dimension Reduction

- 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.

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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.

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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.

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- 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”?

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

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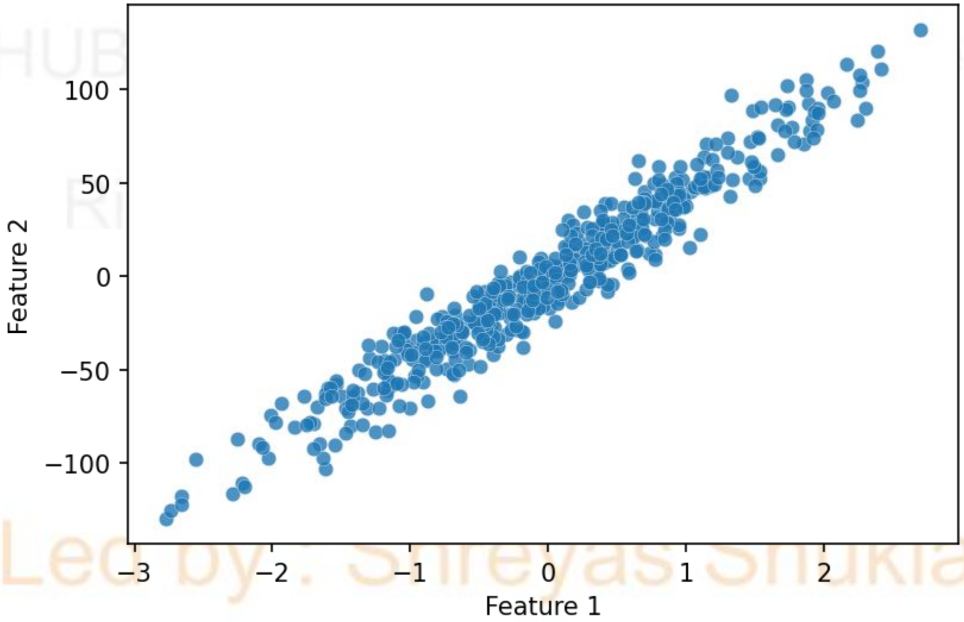


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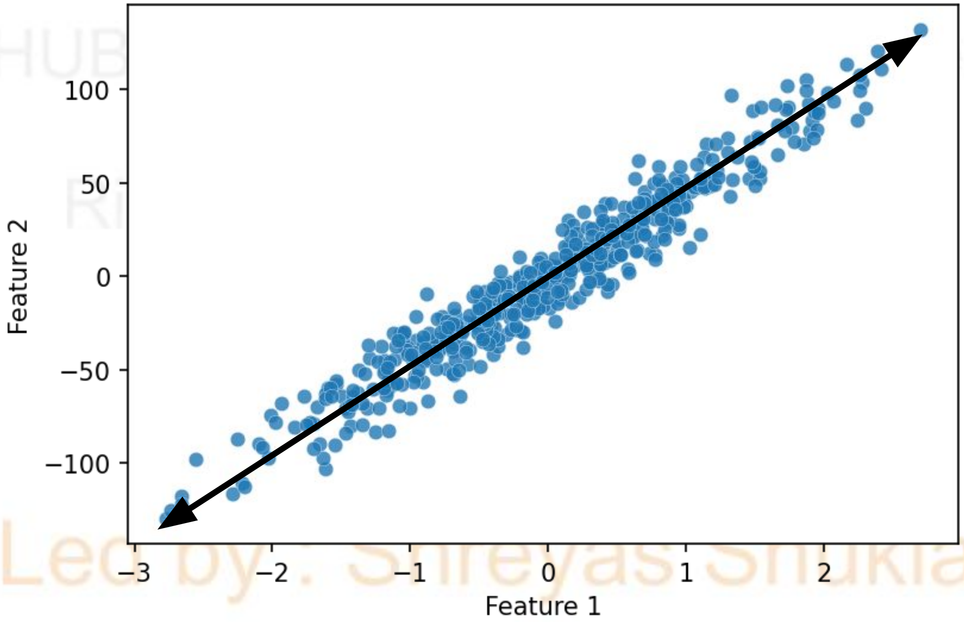


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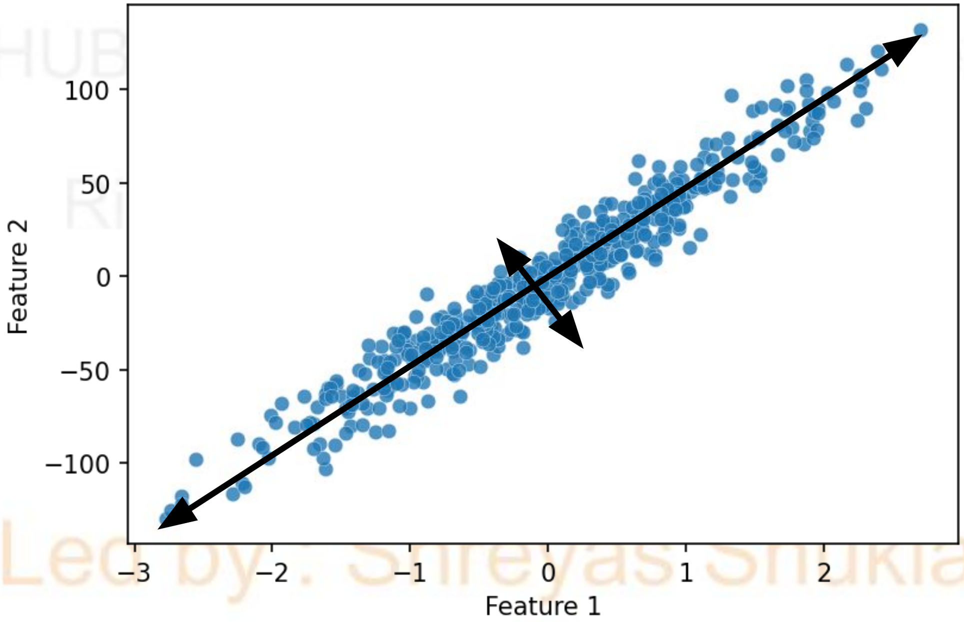


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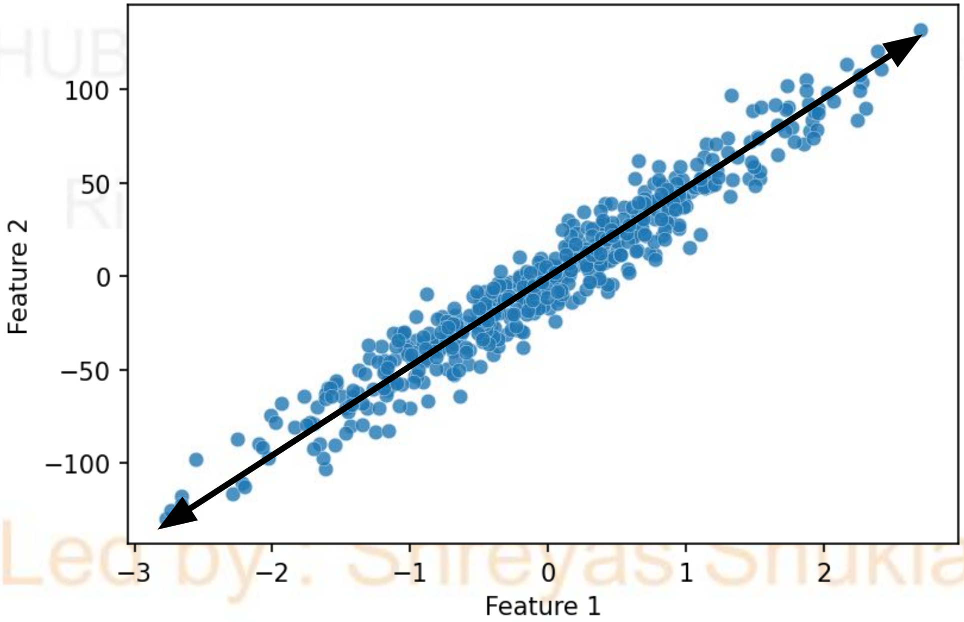

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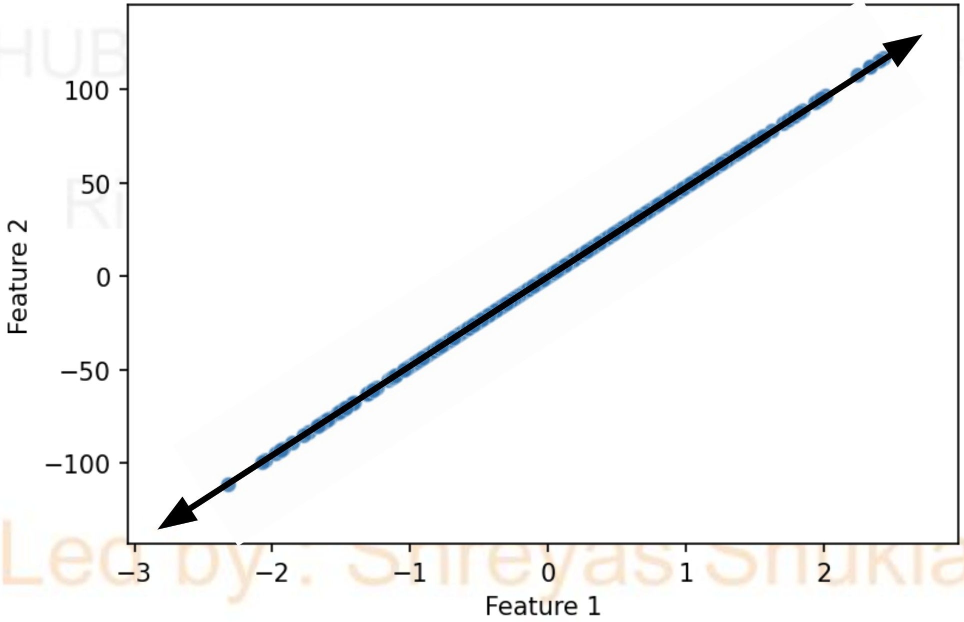

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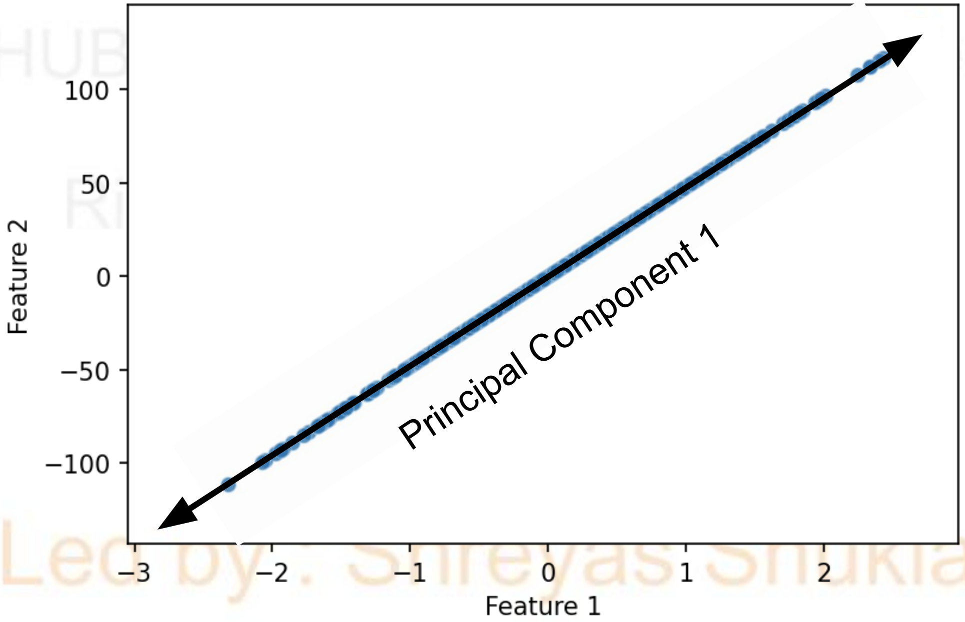

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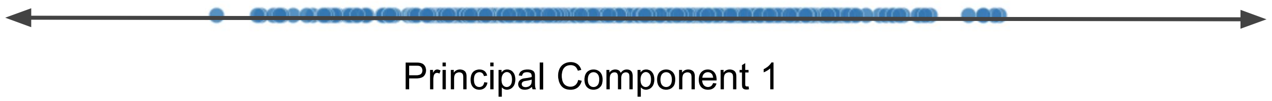

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Variance Explained

- 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.

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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.

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.

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Let’s see how PCA actually works mathematically.

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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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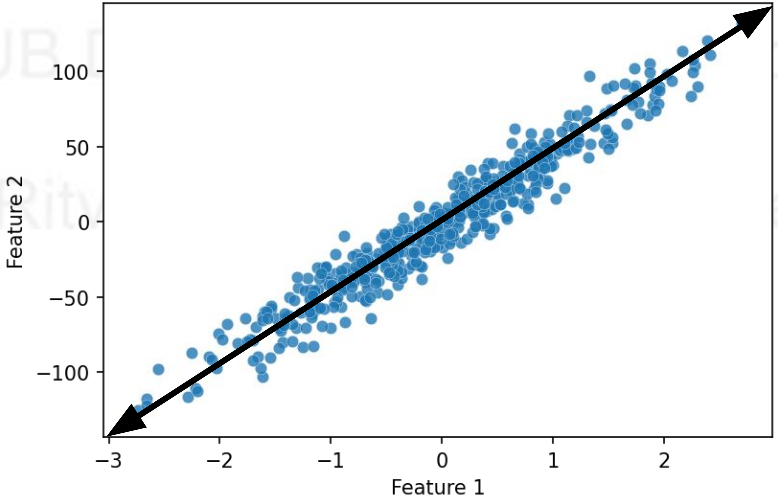


$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2$$

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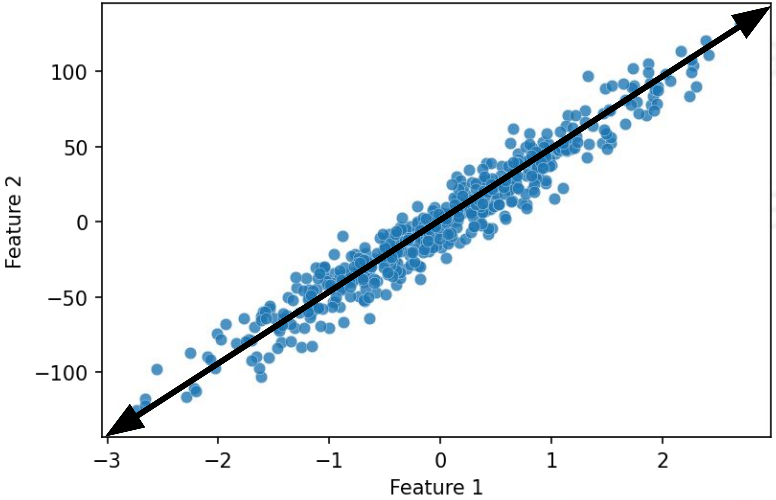


$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2$$

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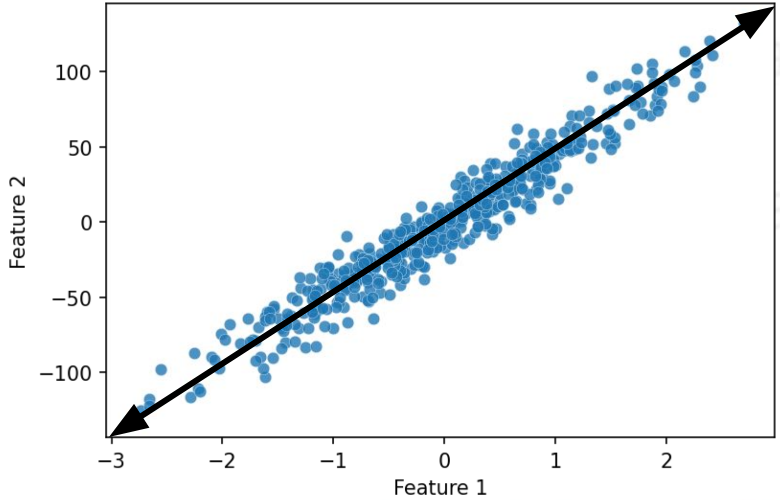
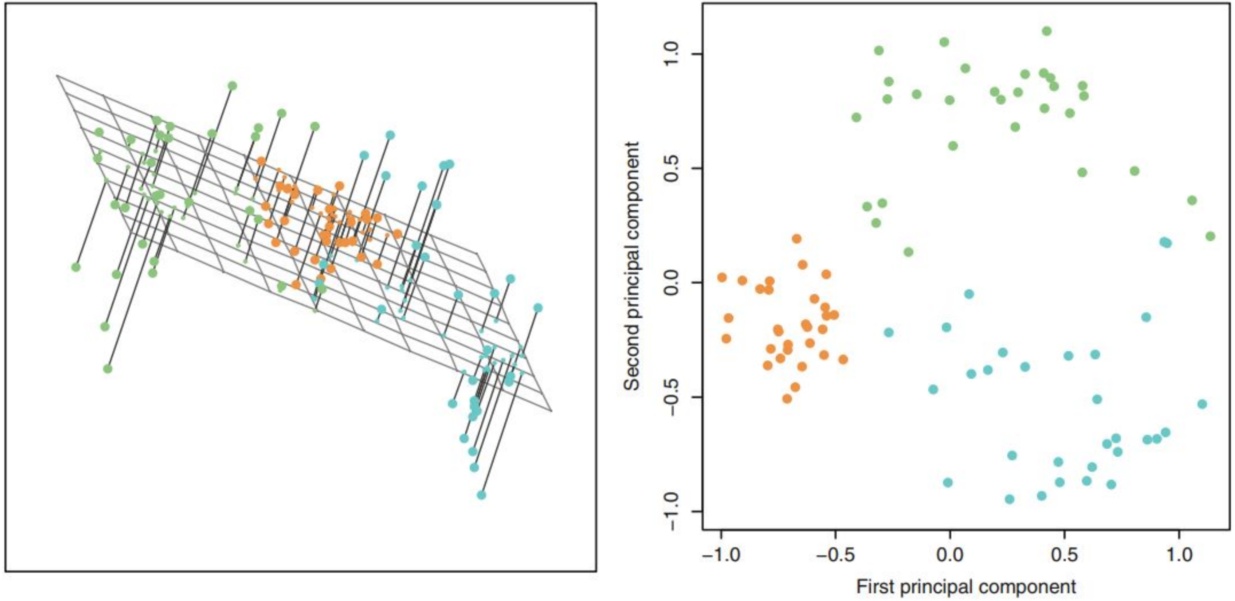



$$Z_1 = \phi_{11} X_1 + \phi_{21} X_2$$


Second principal component
First principal component
1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

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How do we calculate these components?

Let’s walk through the steps visually.

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

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

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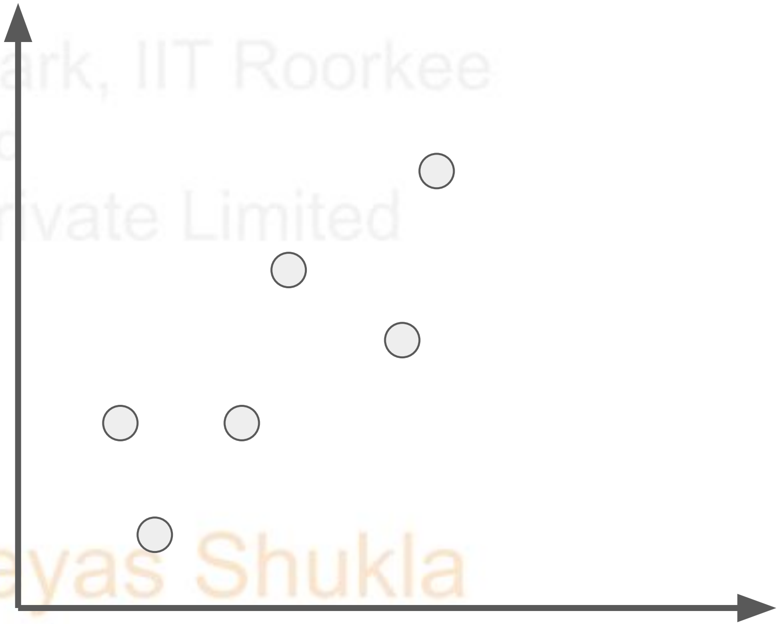

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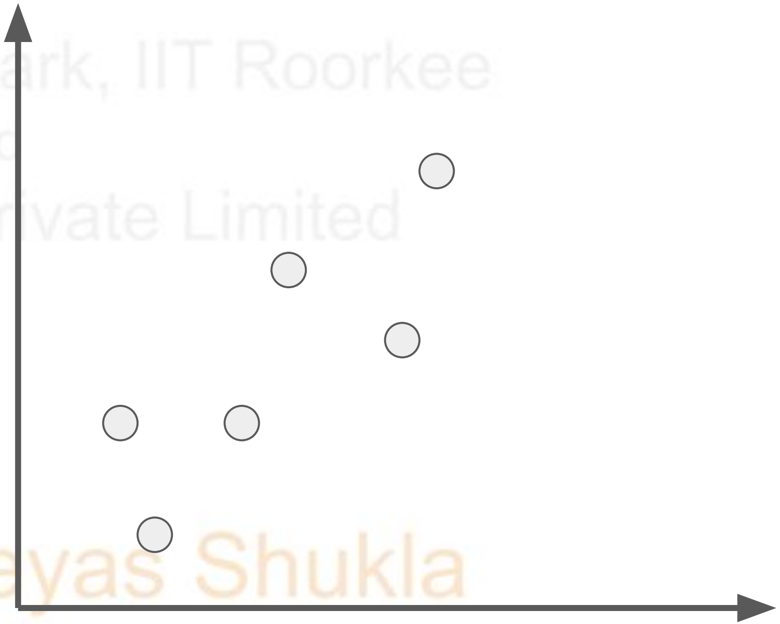
# Standardize the data:

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



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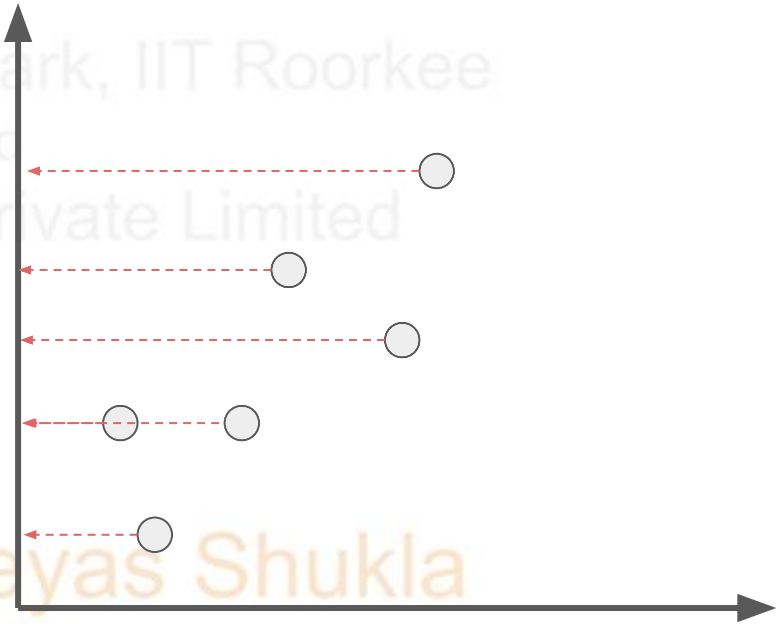
| 6 | 5 |



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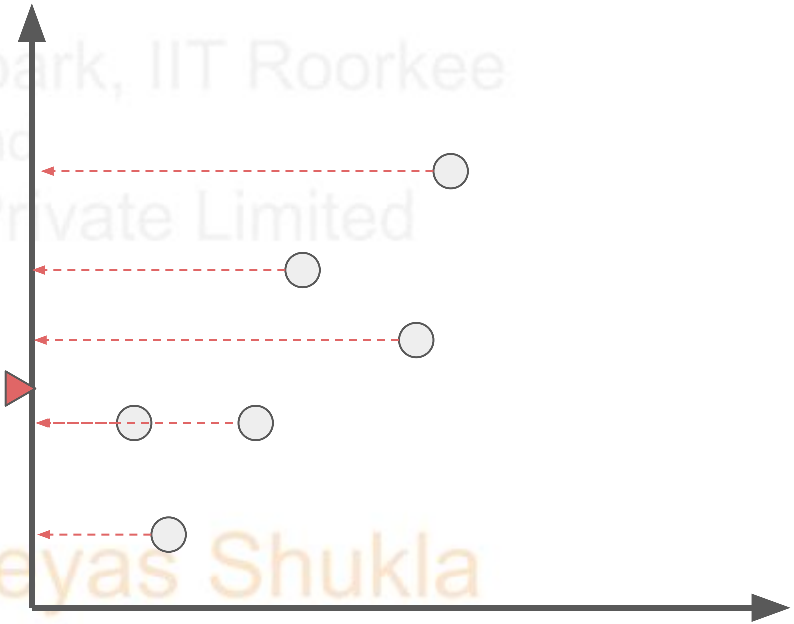
| 6 | 5 |



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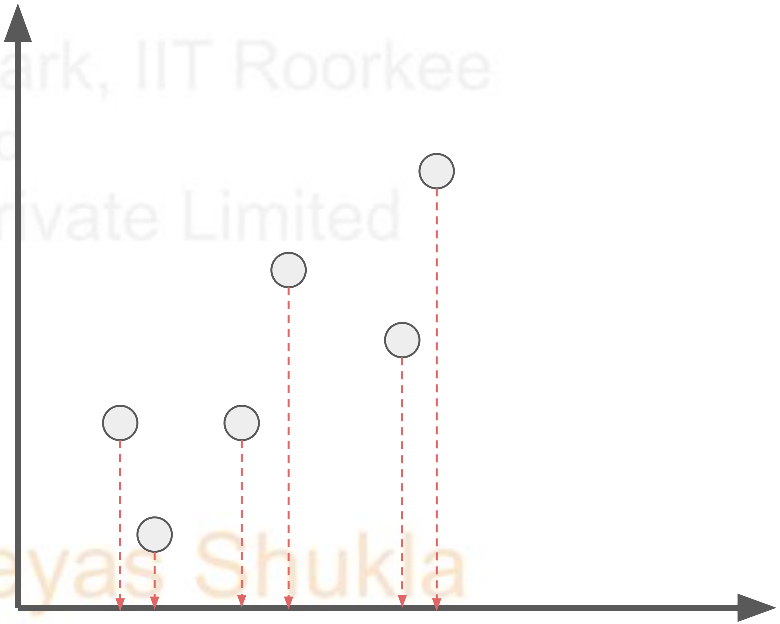
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



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| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |

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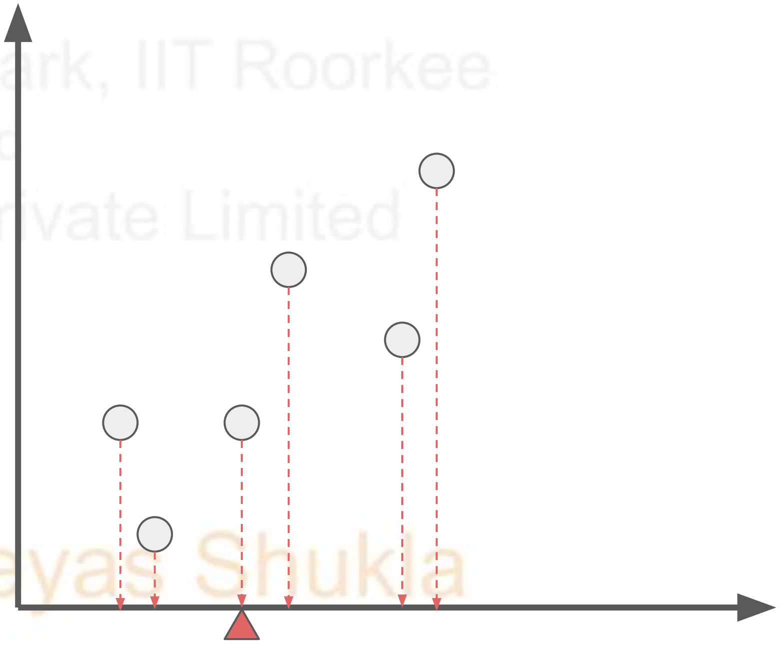

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| X1 | X2 |
|---|---|
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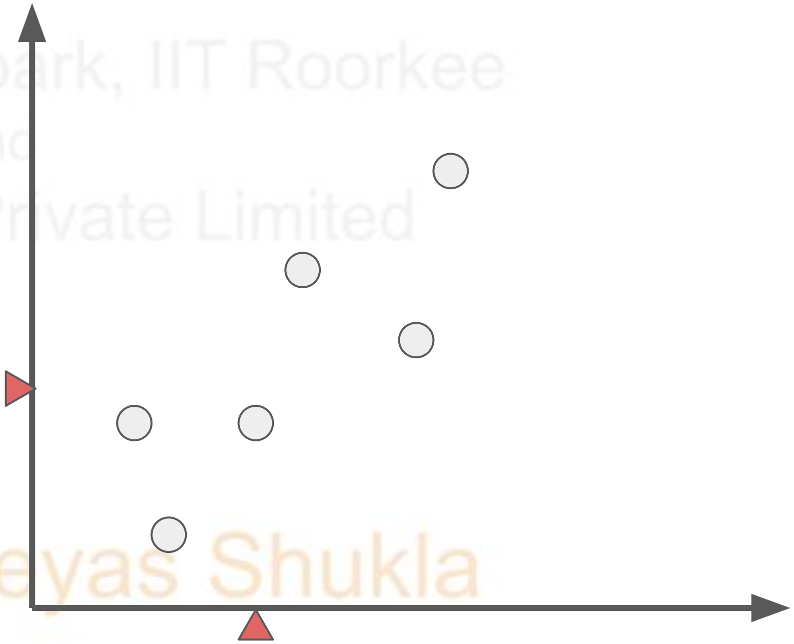
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



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# Standardize the data:

| X1 | X2 |
| --- | --- |
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| 2 | 1 |
| 3 | 2 |
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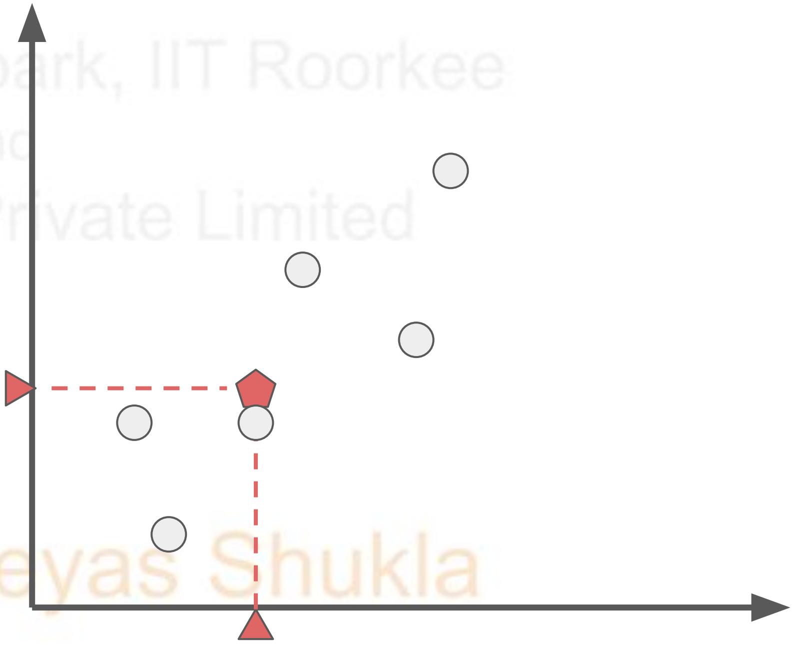

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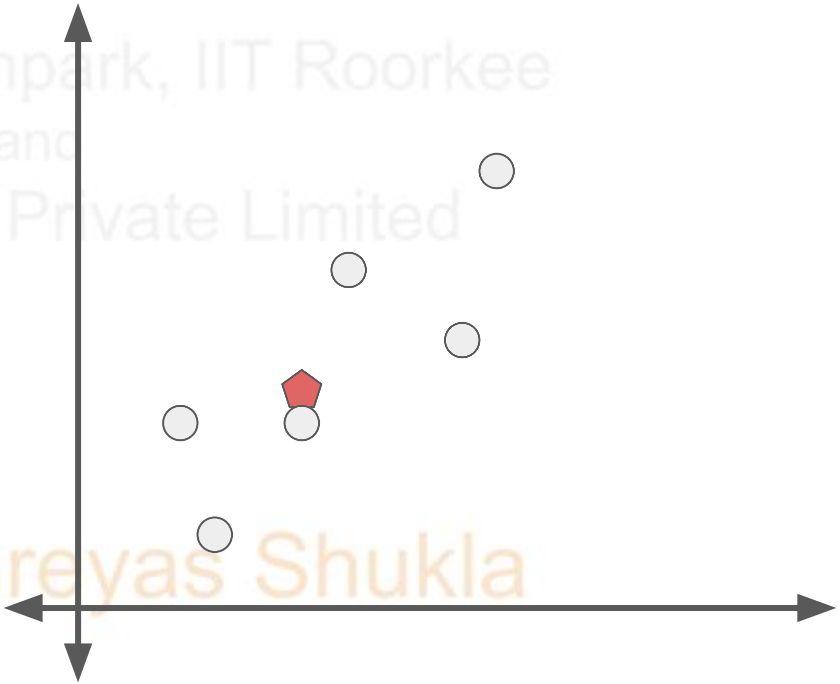

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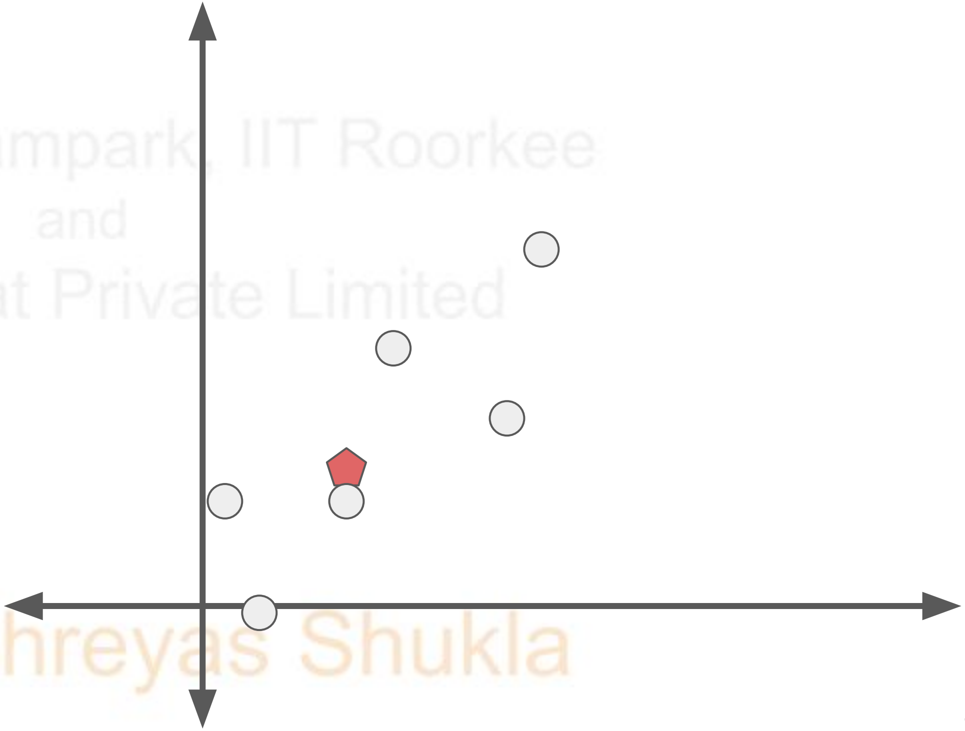

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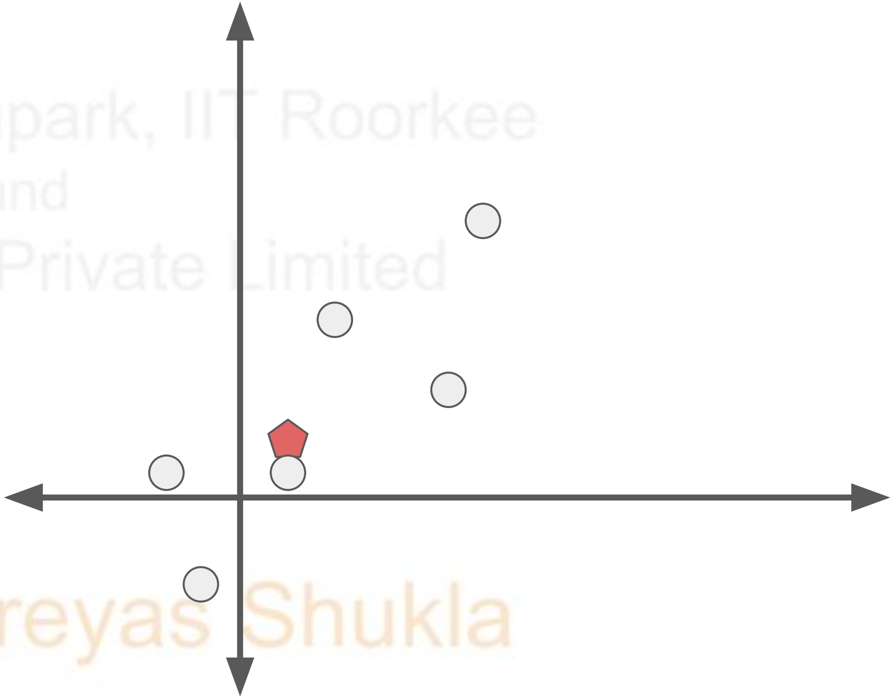

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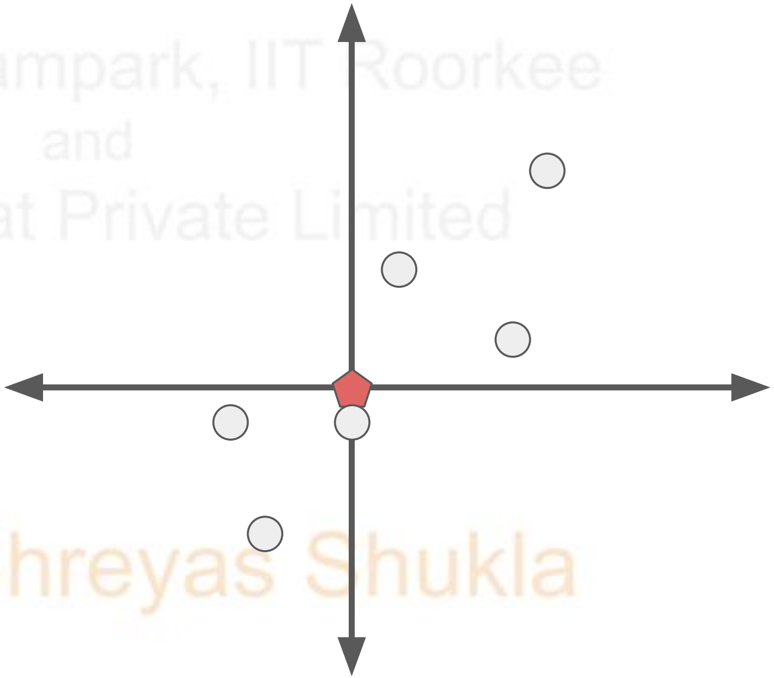

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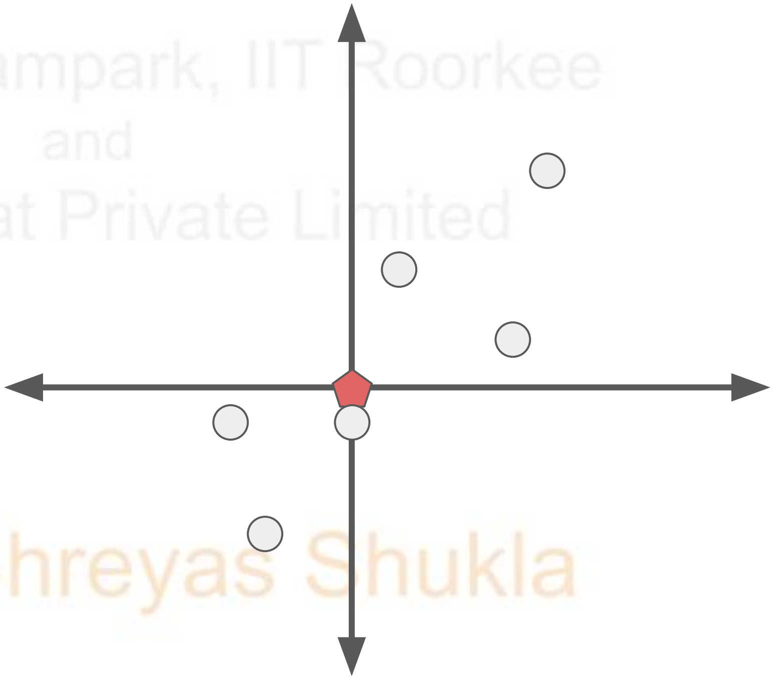
# Calculate covariance matrix for data:



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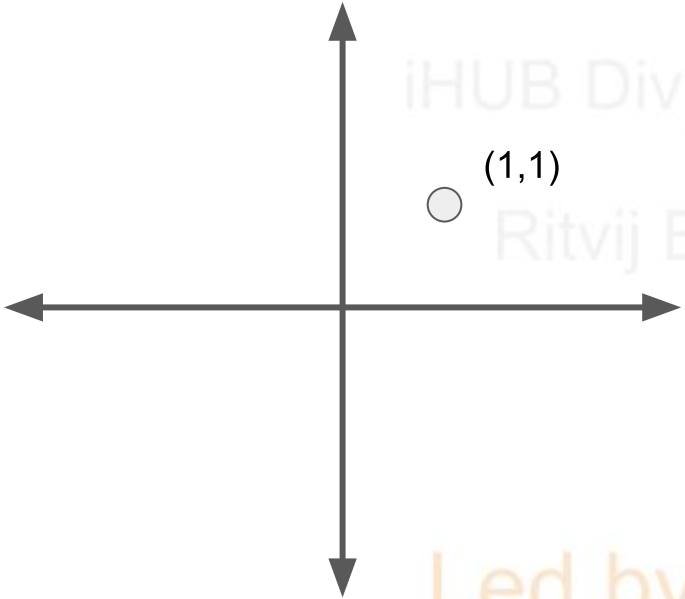
# Linear transformation of data:

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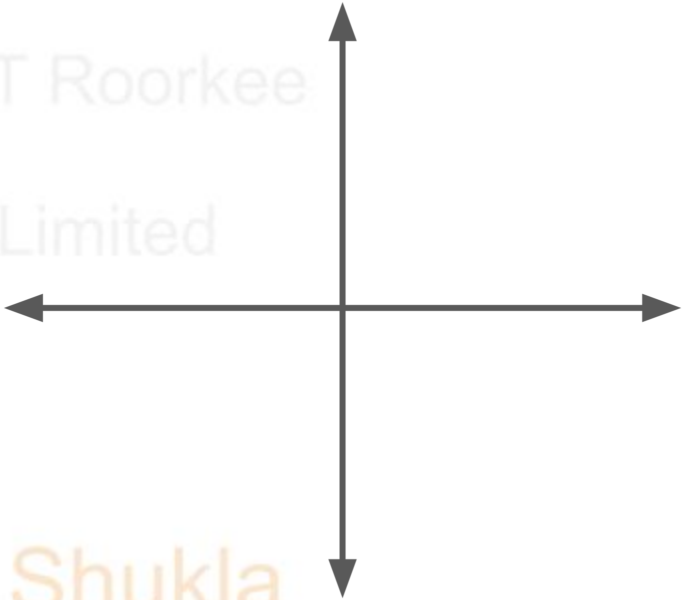

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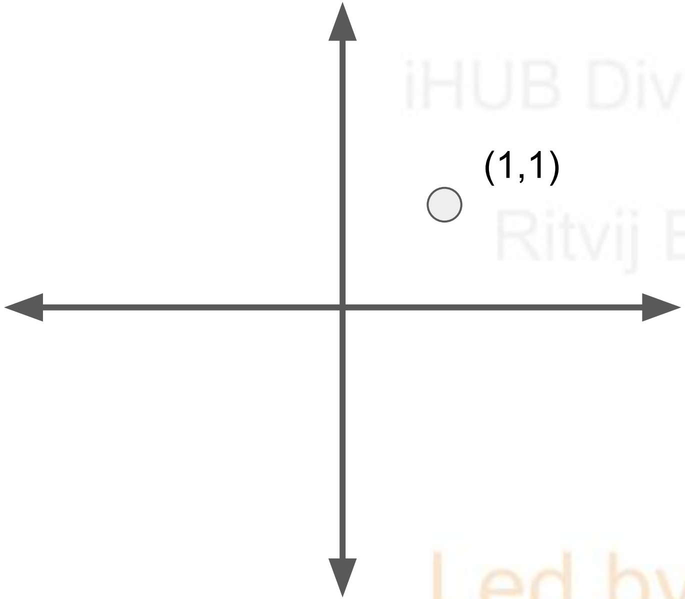
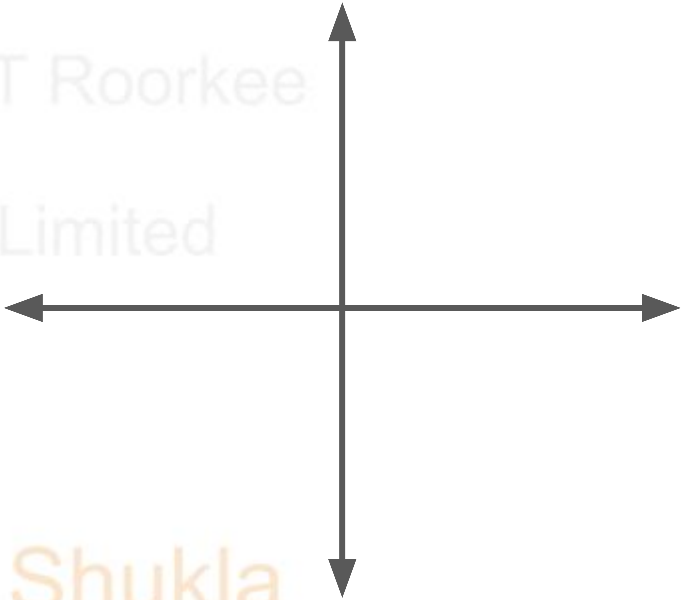



$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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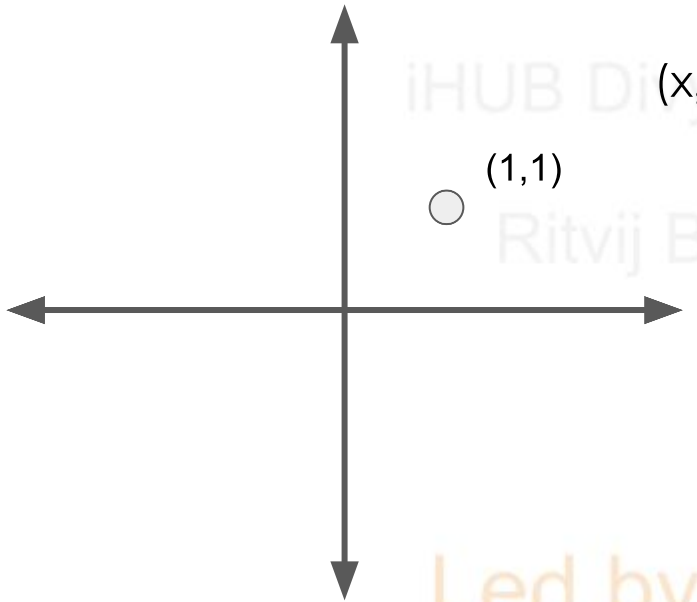
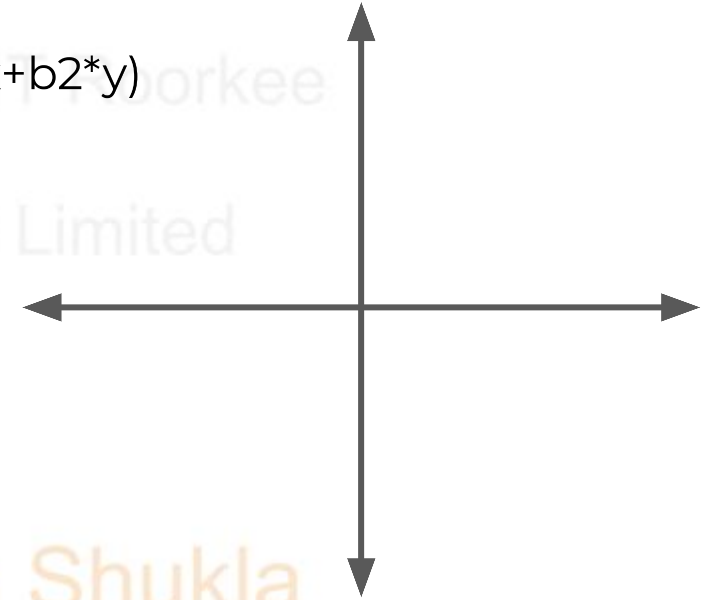
$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$




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



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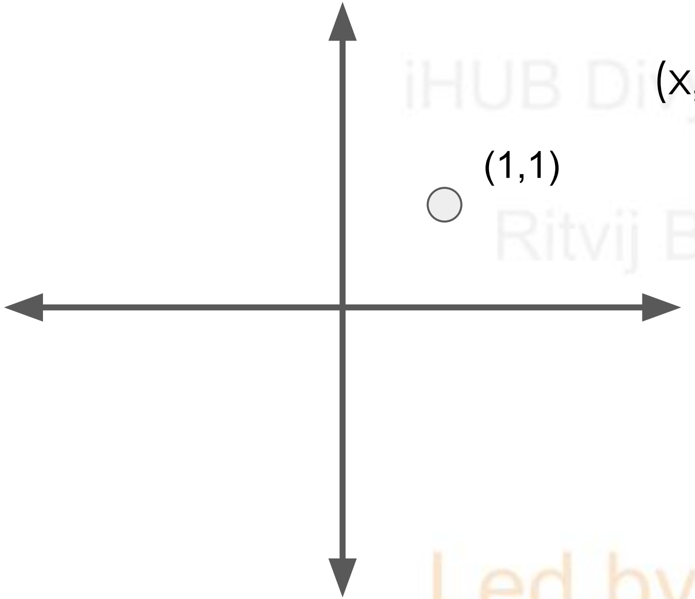


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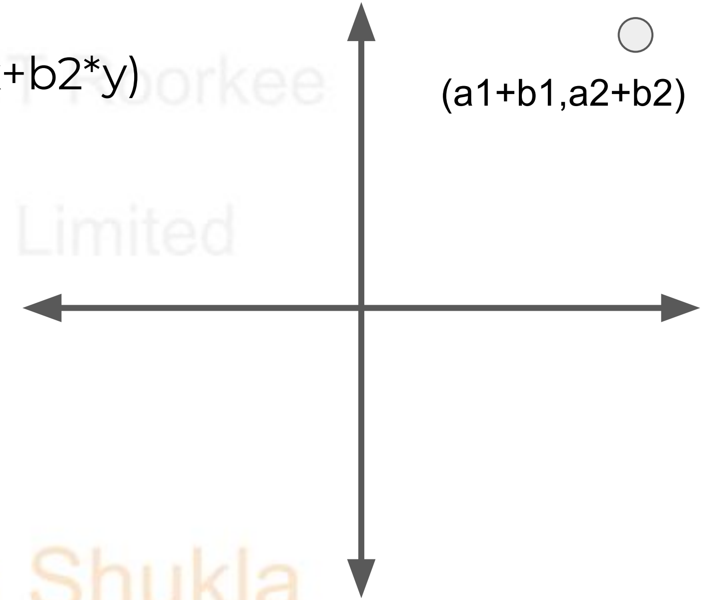


$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

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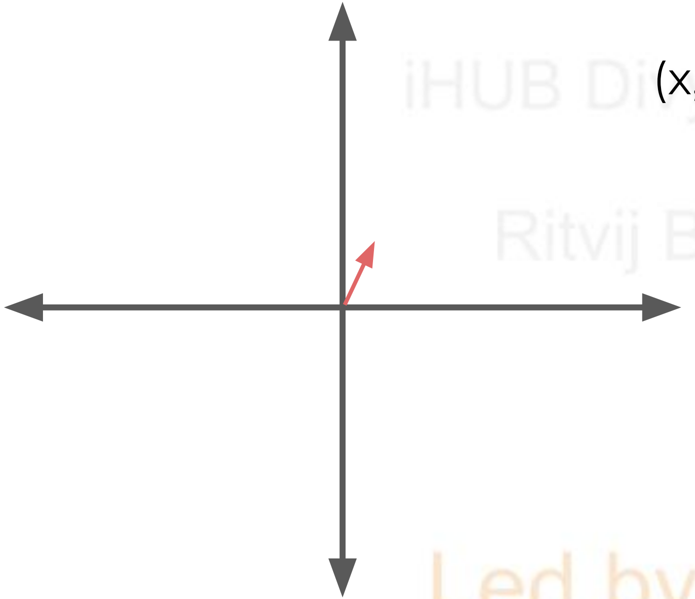

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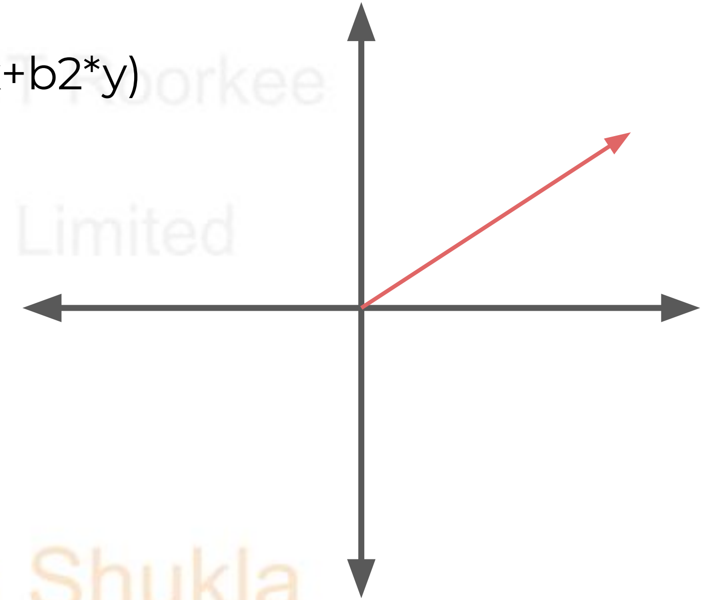
$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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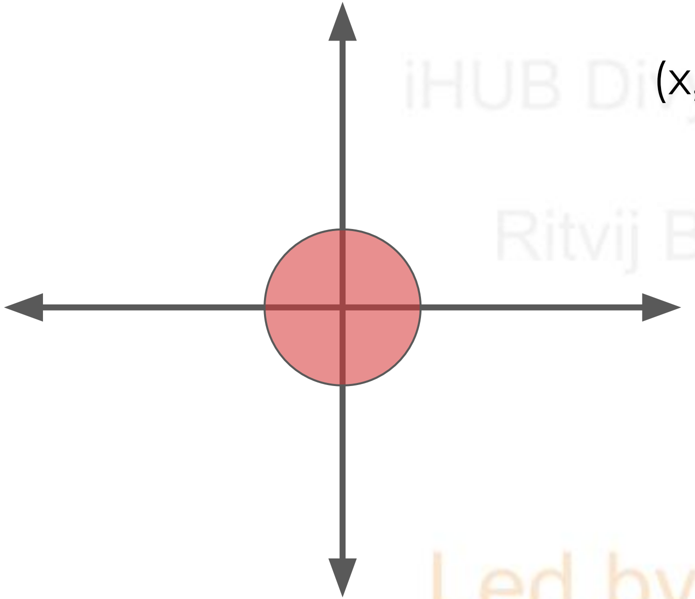
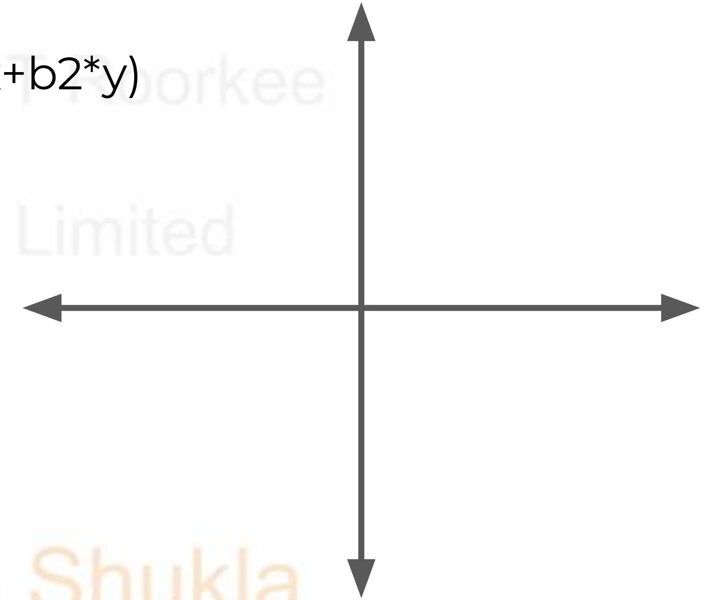


$$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$$

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



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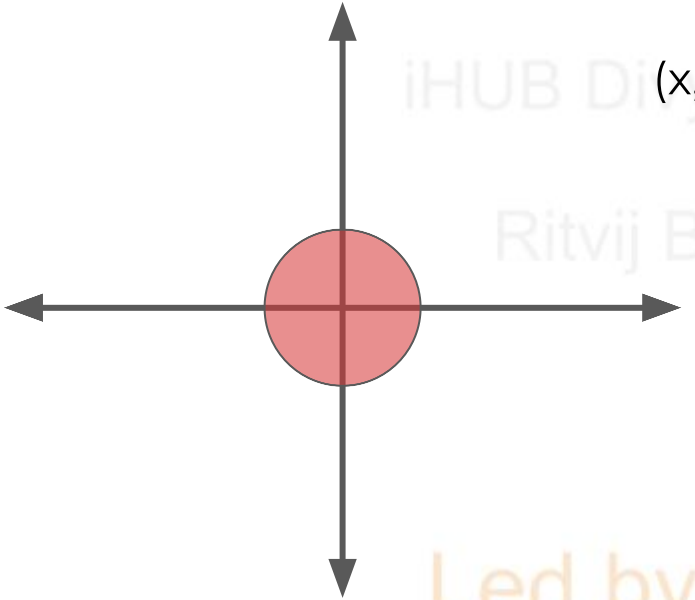
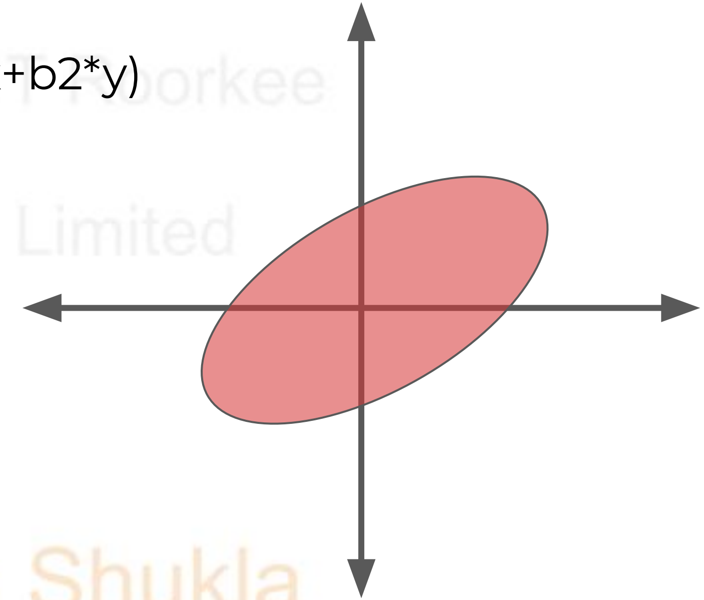


$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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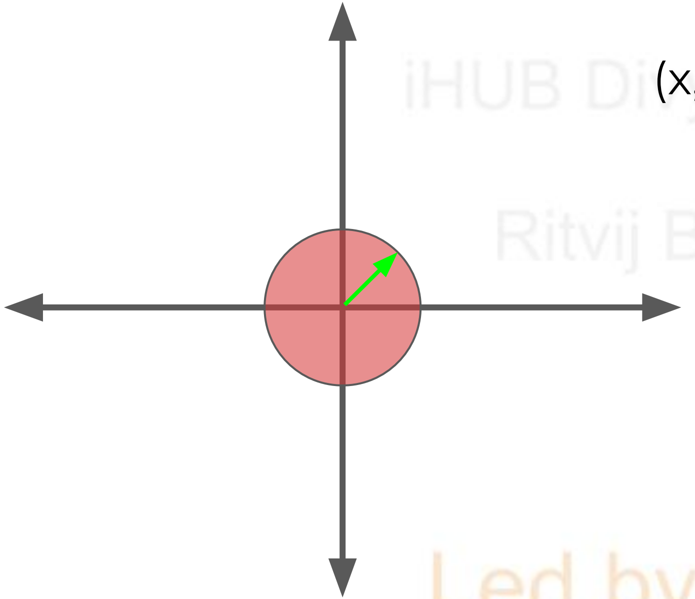

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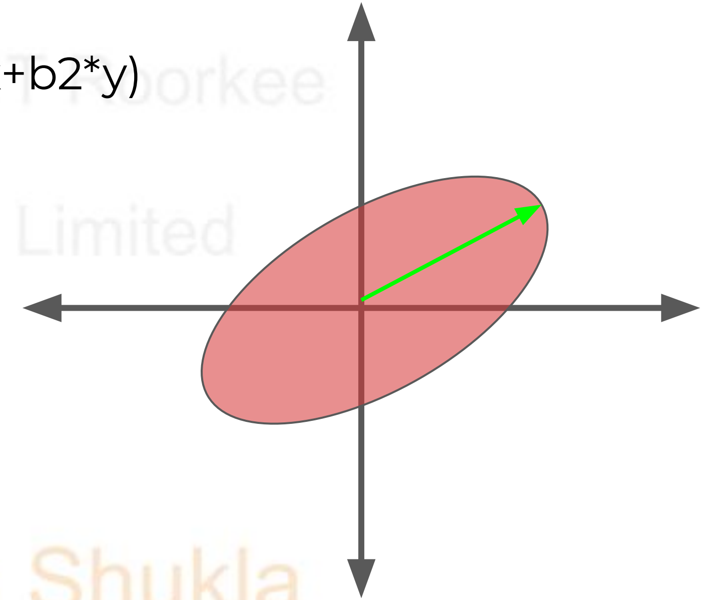
$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



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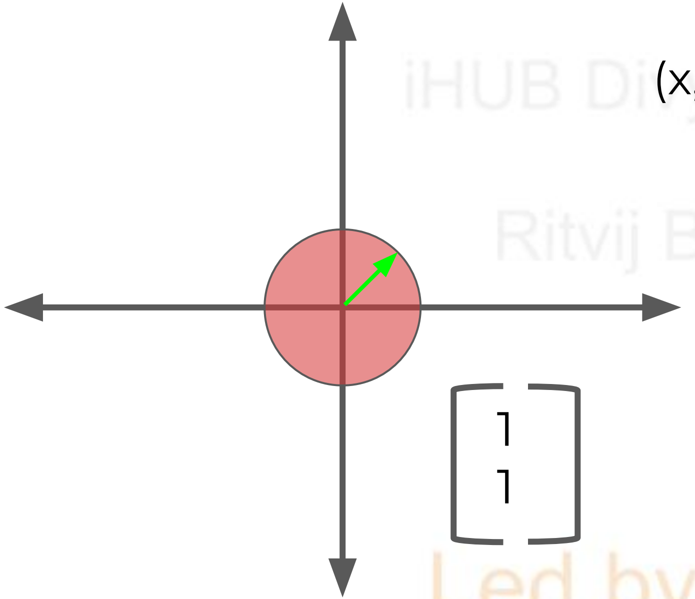
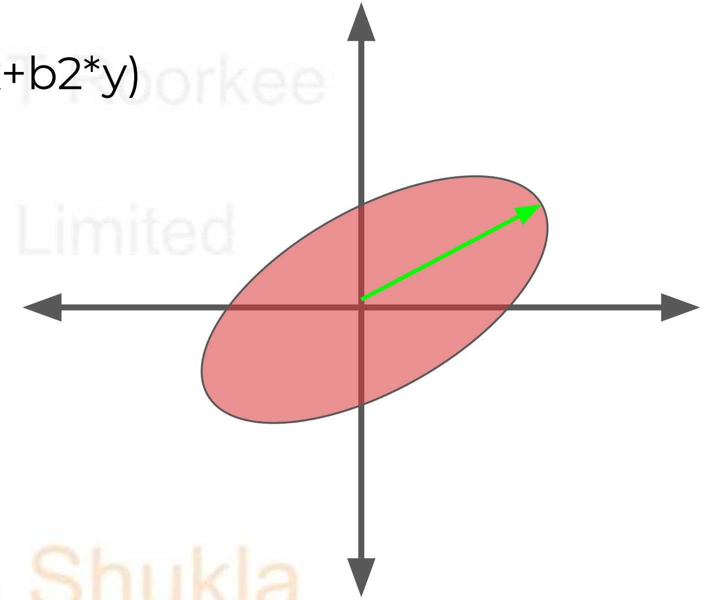
# EigenVector: Directional Information



$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

(x,y) → (a1*x+b1*y,a2*x+b2*y)



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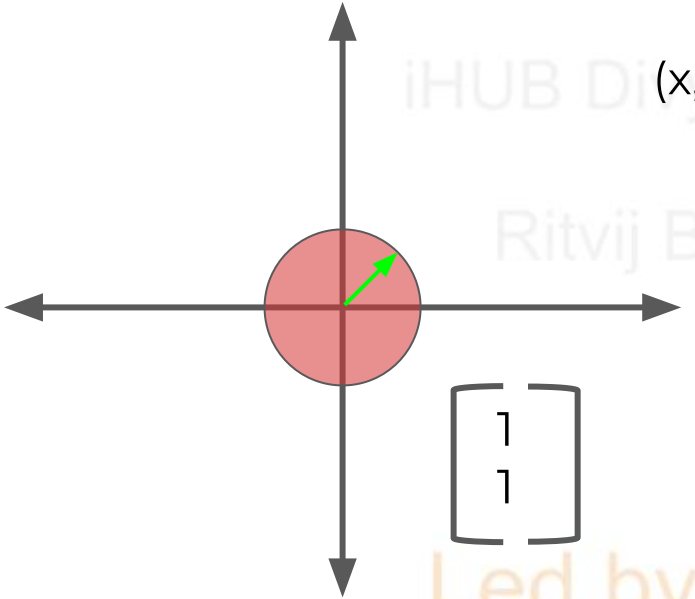
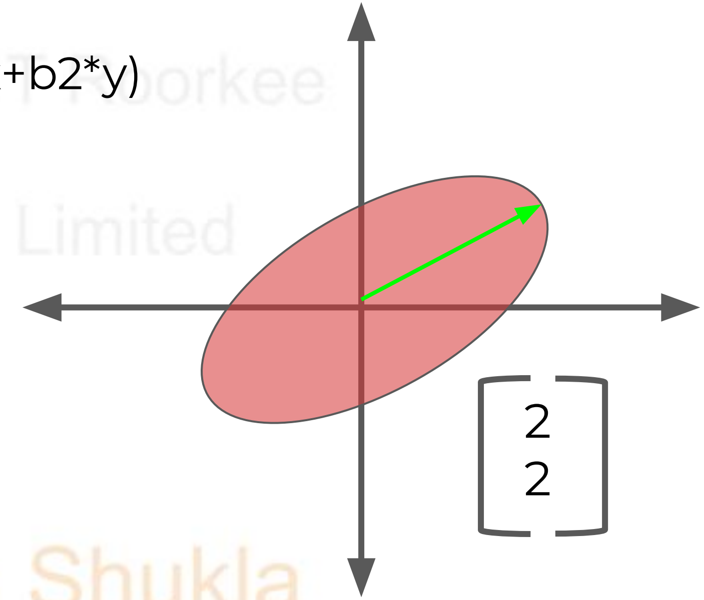
# EigenVector: Directional Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)



$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$



$$\begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

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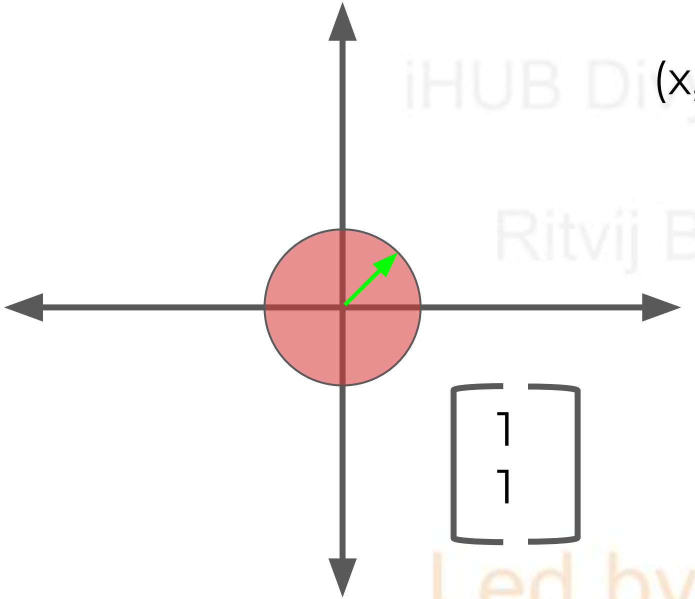
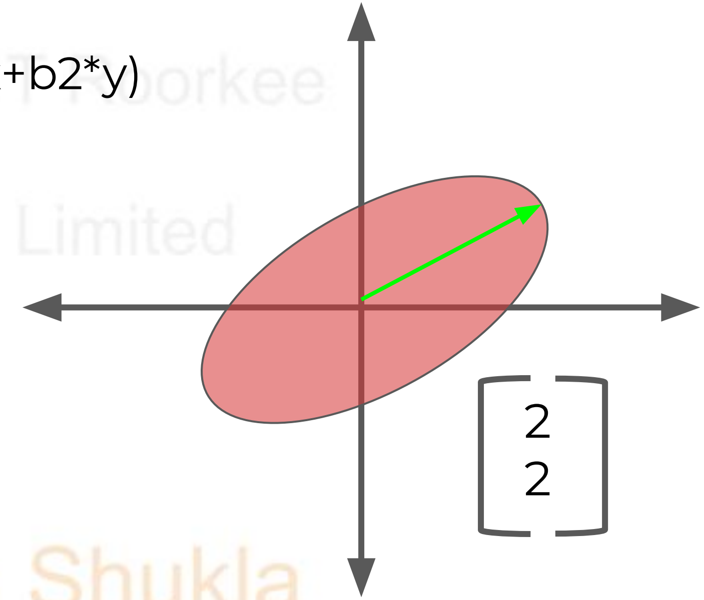
# EigenValue: Magnitude Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)



$$\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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



$$\begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

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# EigenValue: Magnitude Information

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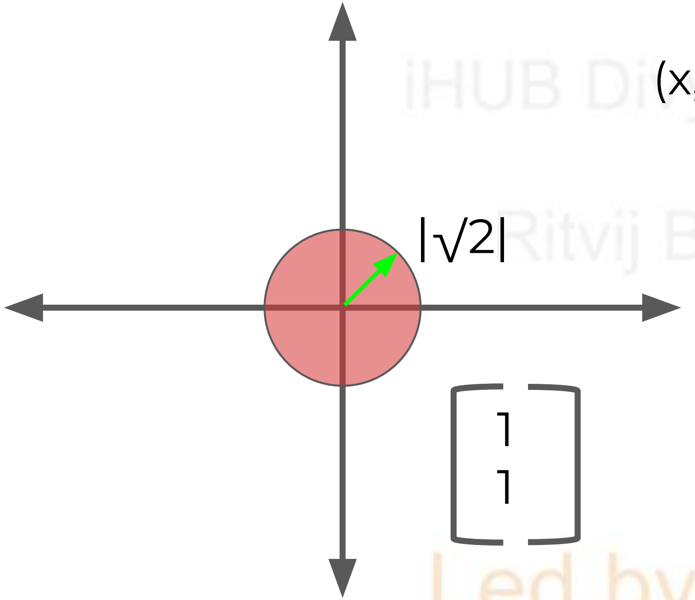
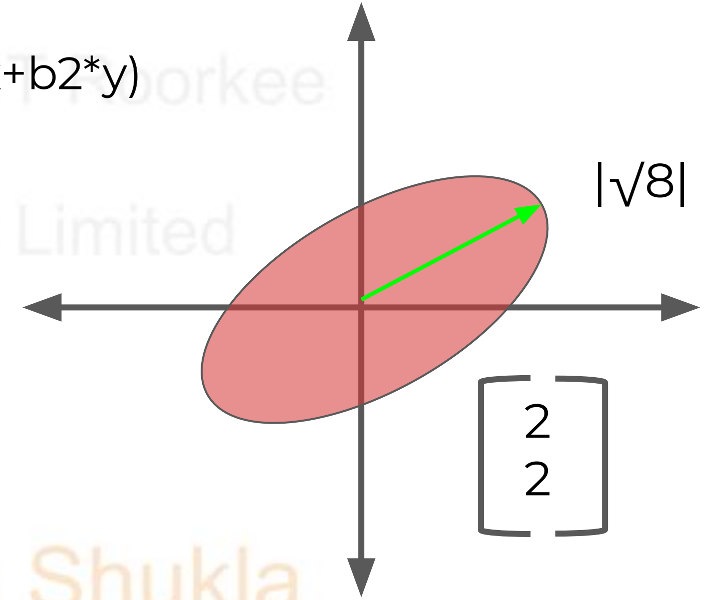
$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$




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

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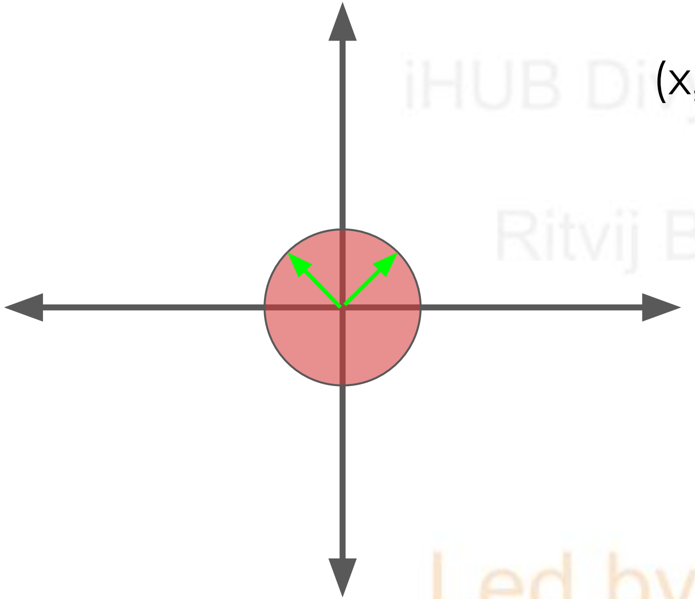
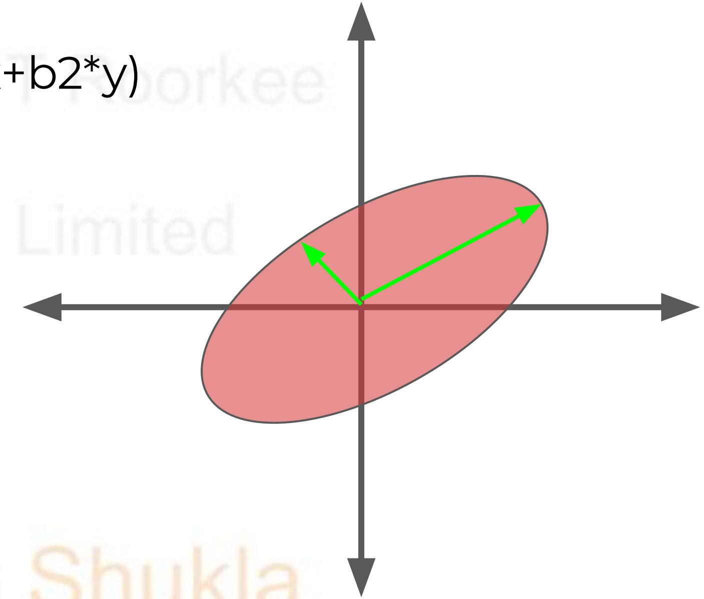
# Orthogonal EigenVector



(x,y) → (a1*x+b1*y,a2*x+b2*y)



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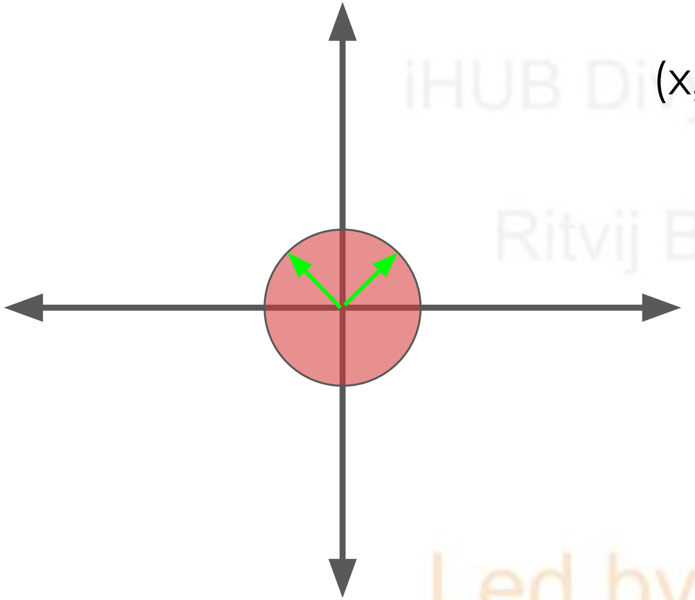
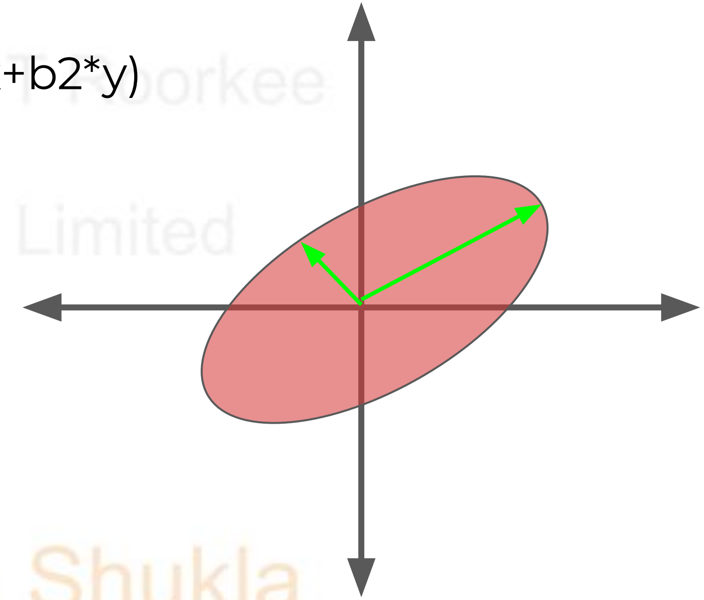
# EigenVector is just a linear transformation



(x,y) → (a1*x+b1*y,a2*x+b2*y)



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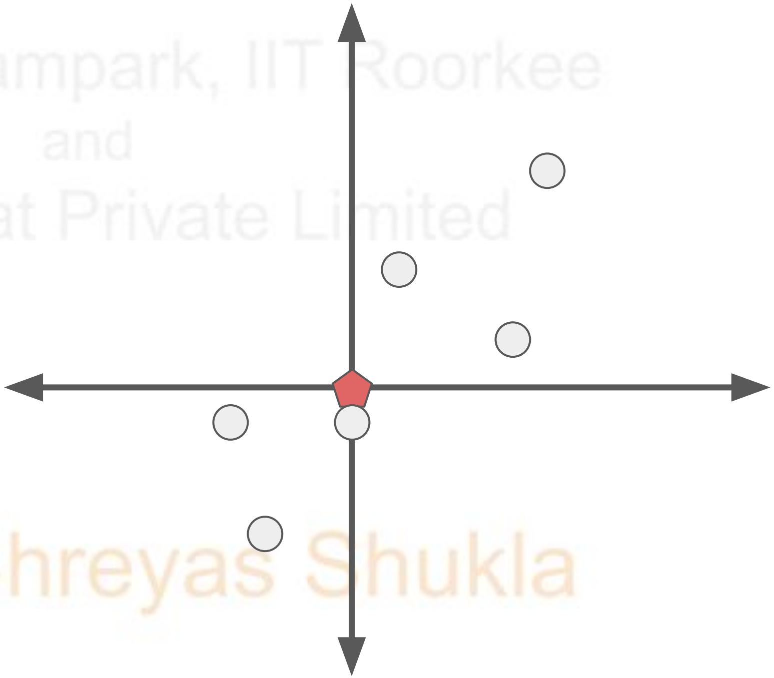
# Apply Linear Transformation:

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



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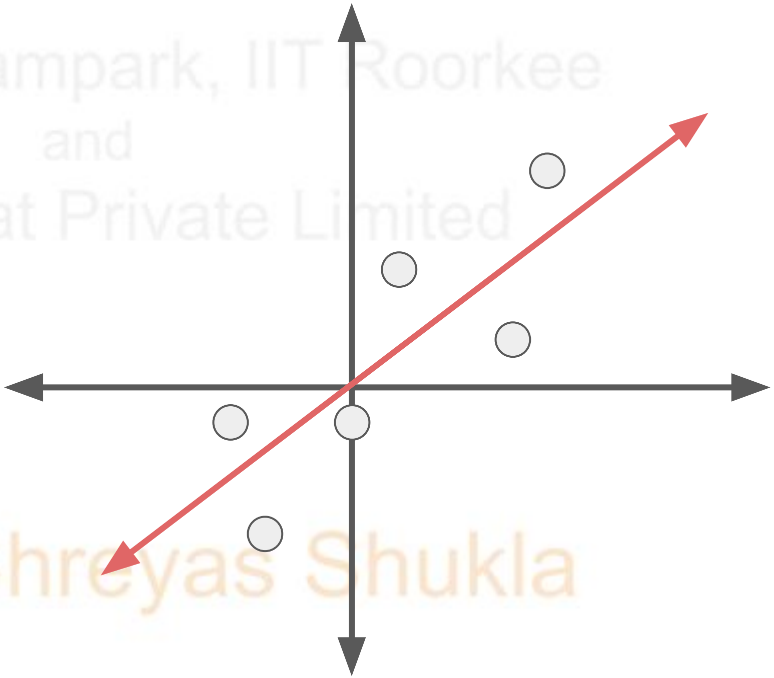
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



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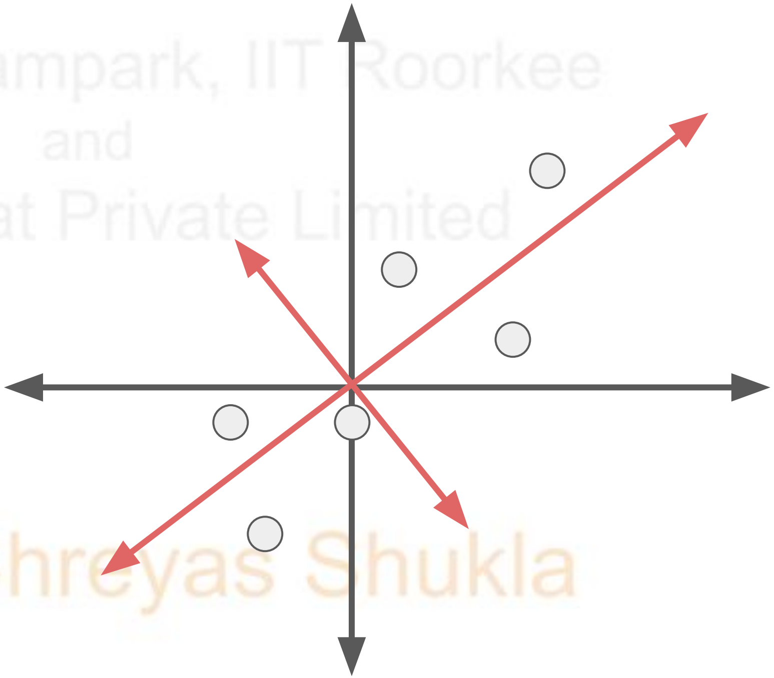
# Apply Linear Transformation:

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



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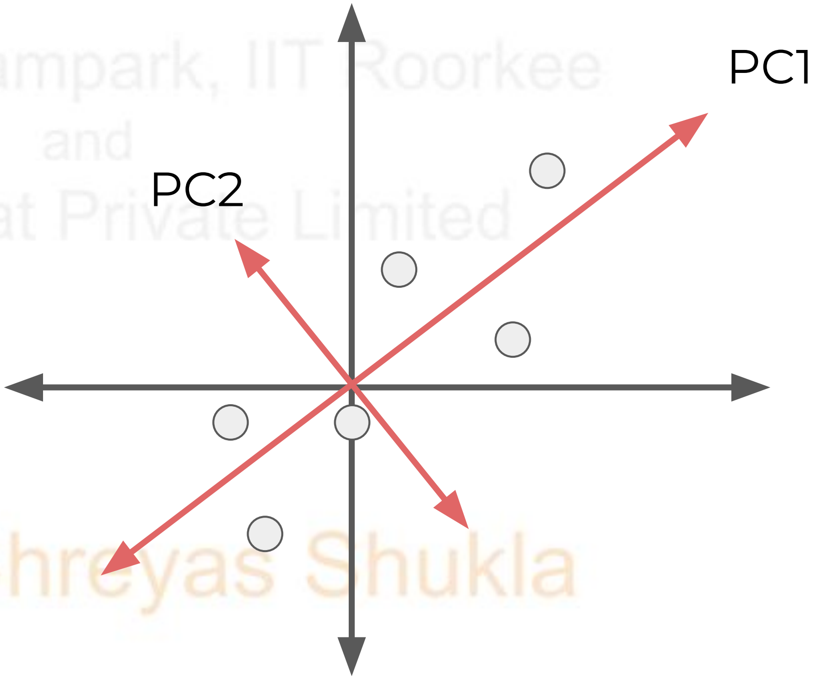
# EigenValue measures variance explained:

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



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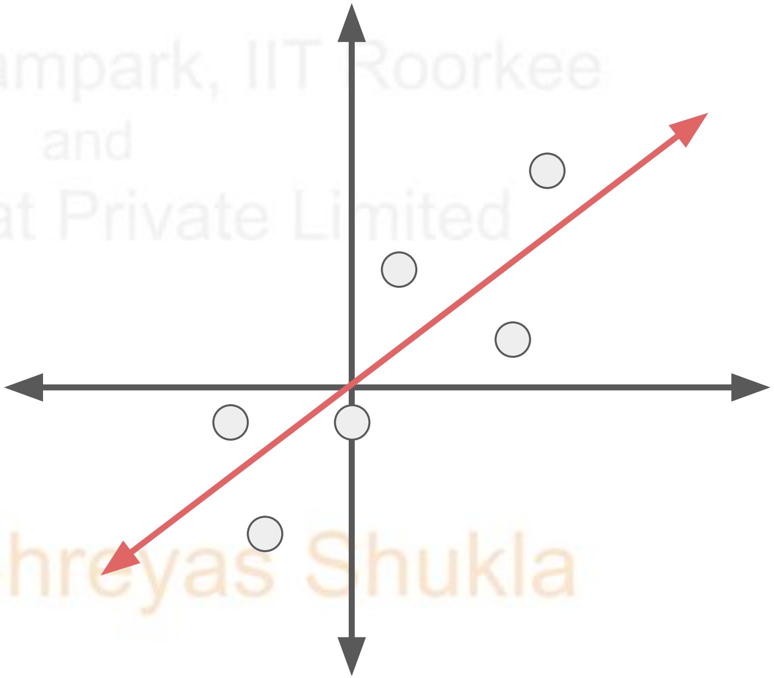
# EigenValue measures variance explained:

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



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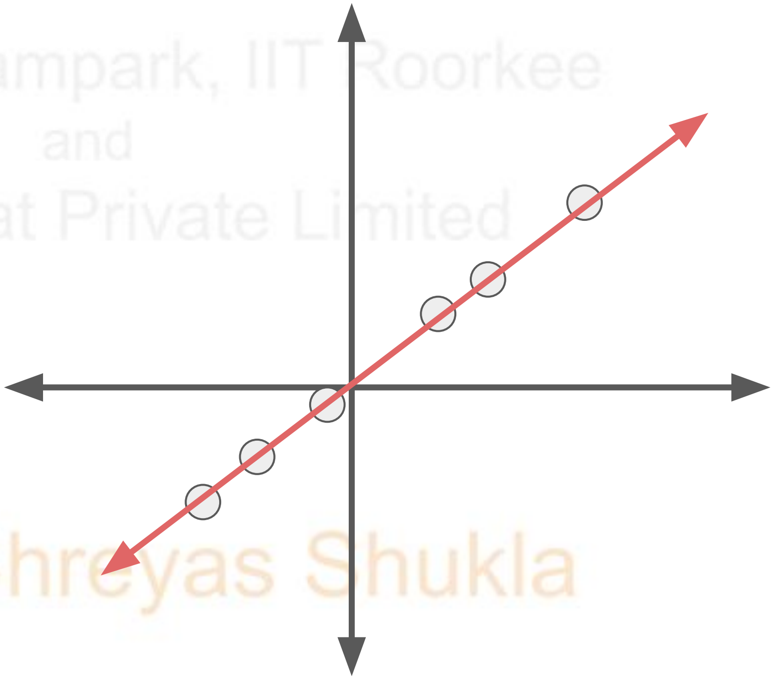
# EigenValue measures variance explained:

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



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# EigenValue measures variance explained:

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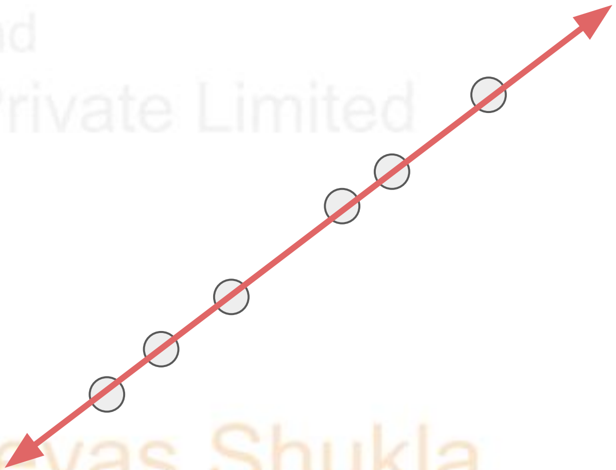
$$\begin{bmatrix} \mathrm{Var}(X) & \mathrm{Cov}(X,Y) \\ \mathrm{Cov}(X,Y) & \mathrm{Var}(Y) \end{bmatrix}$$



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# EigenValue measures variance explained:

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

Principal Component 1

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# PCA Steps

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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

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