# Principal Component Analysis

# Principal Component Analysis

- Our discussions of **unsupervised learning** have focused on clustering techniques, which seek to “discover” labels on feature data that has no historical labels.
- We will now shift towards unsupervised algorithms that focus on **dimension reduction**.

# Principal Component Analysis

- 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.

# Principal Component Analysis

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

# Principal Component Analysis

- Important Note:
  - Dimensionality Reduction algorithms such as PCA <u>**do not**</u> simply choose a subset of the existing features.
  - They create <u>**new**</u> dimensional components that are combinations of proportions of the existing features.

# Principal Component Analysis

- Section Overview
    - Theory and Intuition of PCA.
    - Manually create PCA Algorithm.
    - Utilize Scikit-Learn to perform PCA.
    - PCA Exercise Project Overview
    - PCA Exercise Solution

# Principal Component Analysis

## Theory and Intuition - Part One

# Principal Component Analysis

- Hotelling’s paper perfectly describes the purpose of PCA:
  - Analyzing a complex set of variables into its principal components.
- Let’s review the motivation and basic idea behind Principal Component Analysis.

# Principal Component Analysis

- Principal Component Analysis Outcomes:
  - Reduce number of dimensions in data.
  - Show which features explain the most variance in the data.

# Principal Component Analysis

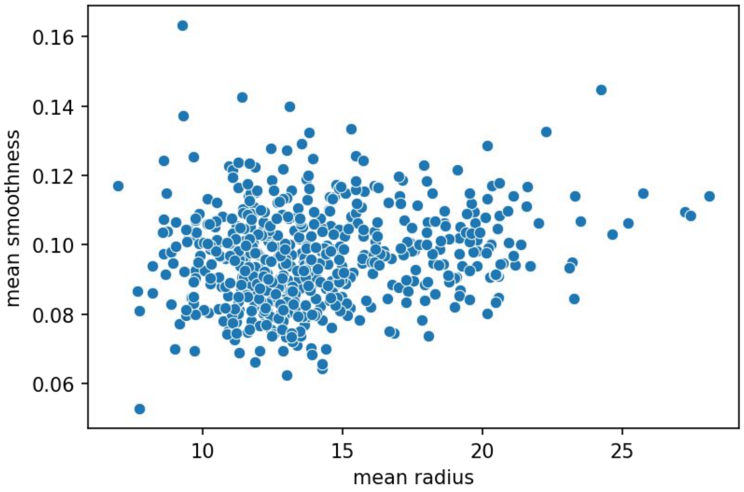
- Dimension Reduction

| | 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 |

# Principal Component Analysis

- 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 |



# Principal Component Analysis

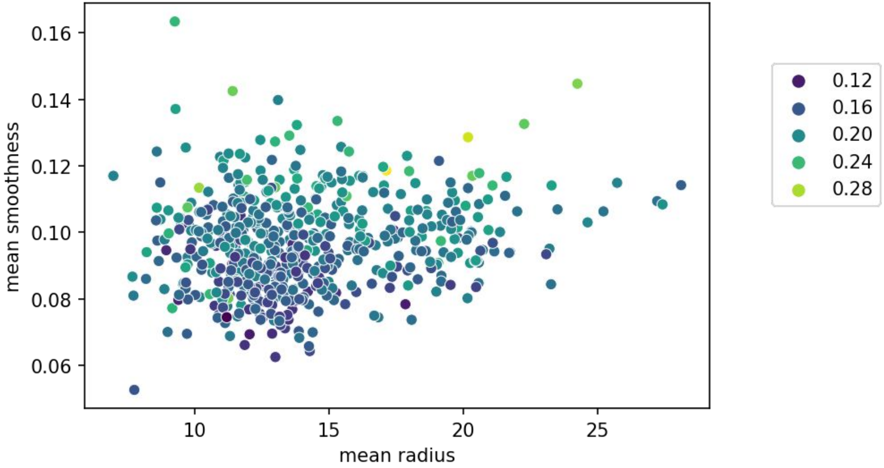
- Dimension Reduction

| | 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 |

# Principal Component Analysis

- Dimension Reduction

| | 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 |



# Principal Component Analysis

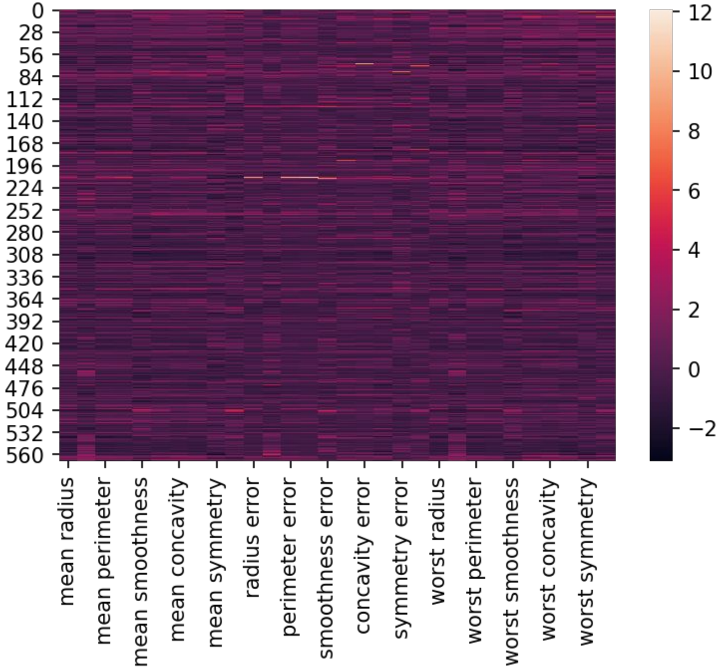
- Dimension Reduction

| | 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

# Principal Component Analysis

- Dimension Reduction



# Principal Component Analysis

- 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.

# Principal Component Analysis

- 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.

# Principal Component Analysis

- Variance Explained
  - We’ve often seen that certain features are more important or have more explanatory power than other features.
  - For example, size of a house is probably much more important than the color of a house when explaining the price of a house for sale.

# Principal Component Analysis

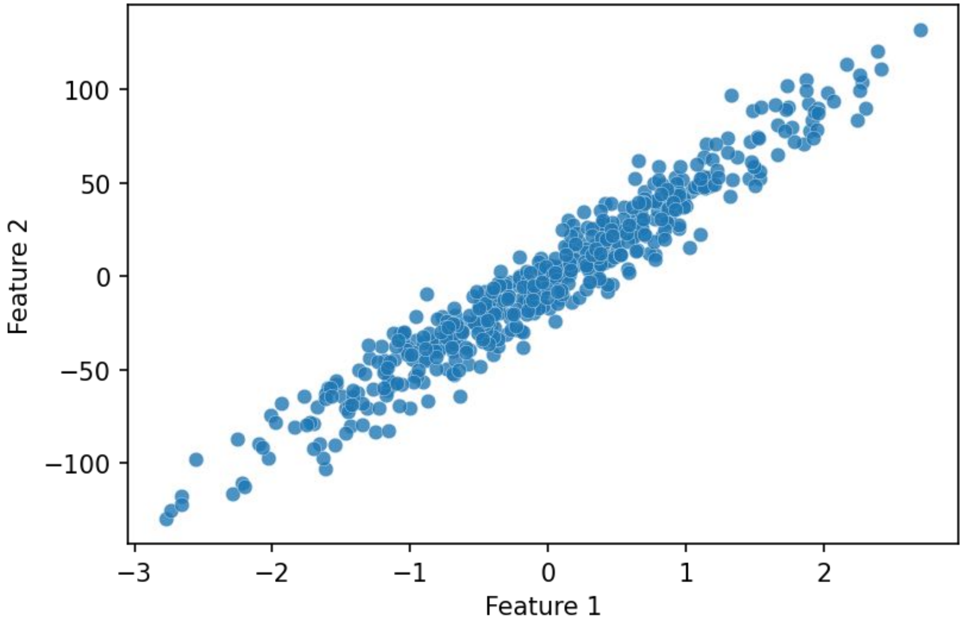
- Variance Explained
  - This idea of more important features is easy to understand when we can directly correlate features to a known label. But what about unlabeled data?
  - What measurement can we use to determine feature “importance”?

# Principal Component Analysis

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

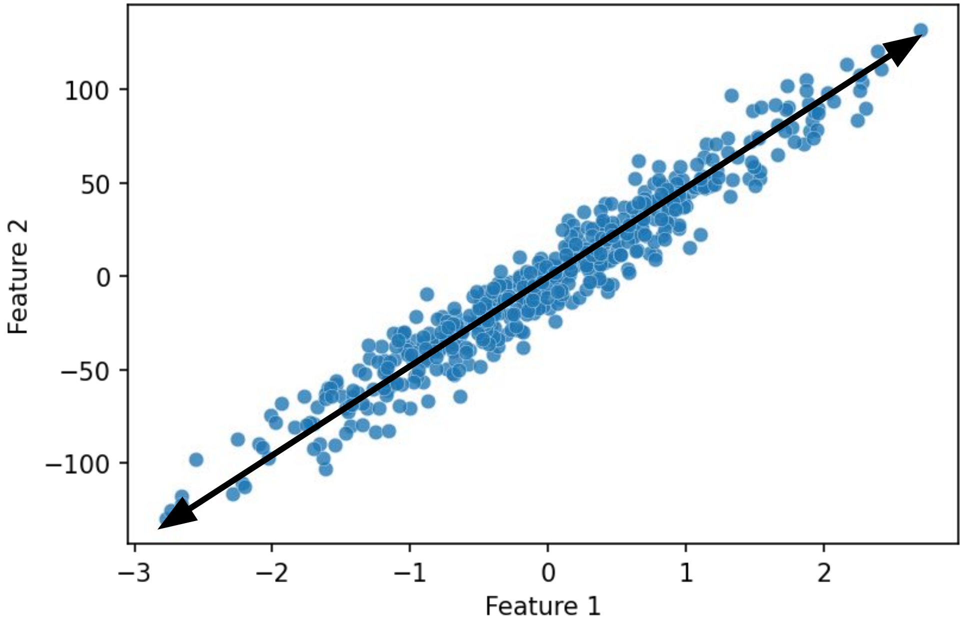
# Principal Component Analysis

- Variance Explained



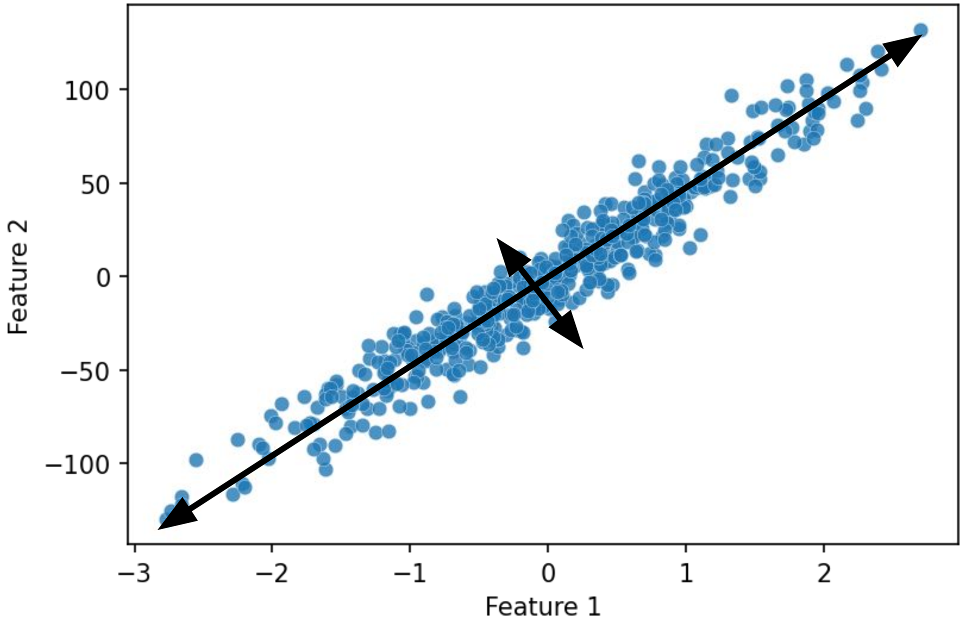
# Principal Component Analysis

- Variance Explained



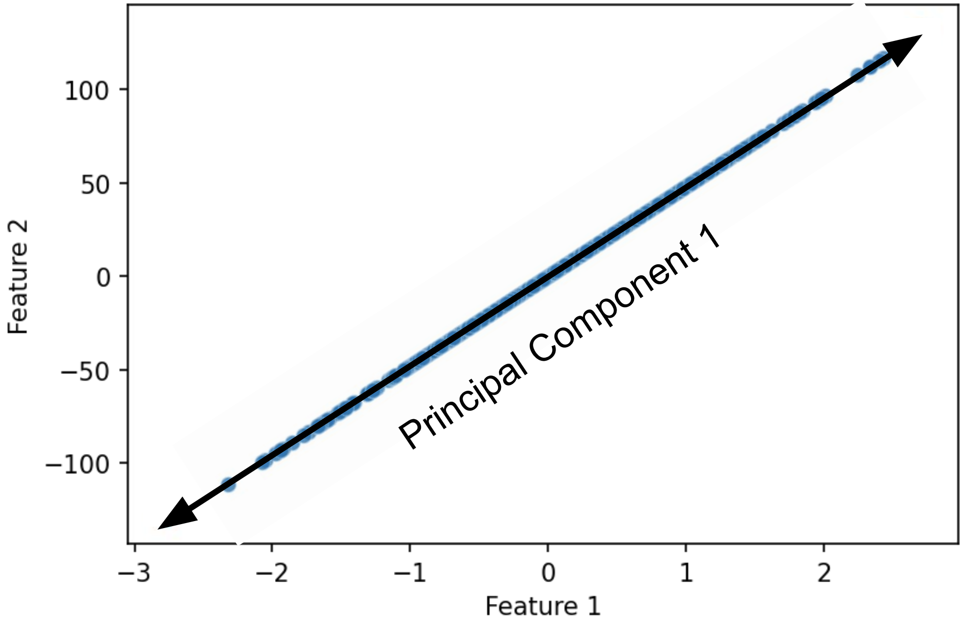
# Principal Component Analysis

- Variance Explained



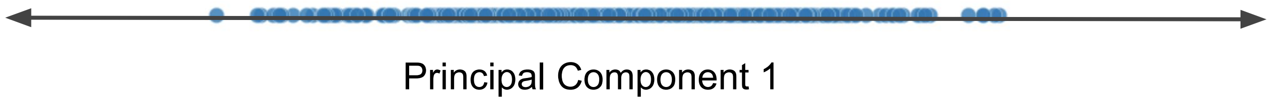
# Principal Component Analysis

- Variance Explained



# Principal Component Analysis

- Variance Explained



# Principal Component Analysis

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

# Principal Component Analysis

- Variance Explained
  - 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.

# Principal Component Analysis

- Variance Explained
  - 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.

# Principal Component Analysis

Theory and Intuition - Part Two

# Principal Component Analysis

- Suggested Reading:
  - Section 10.1 of ISLR covers the topic of Principal Component Analysis.

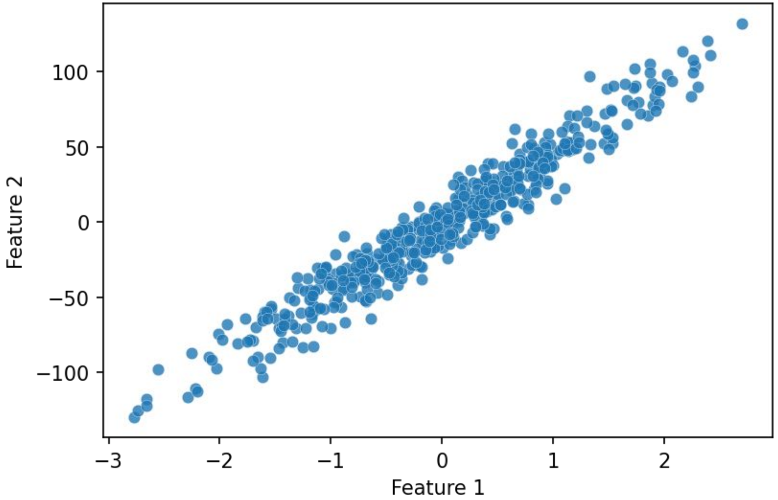
# Principal Component Analysis

- Principal Component Analysis operates by creating a new set of dimensions (the principal components) that are normalized linear combinations of the original features.

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

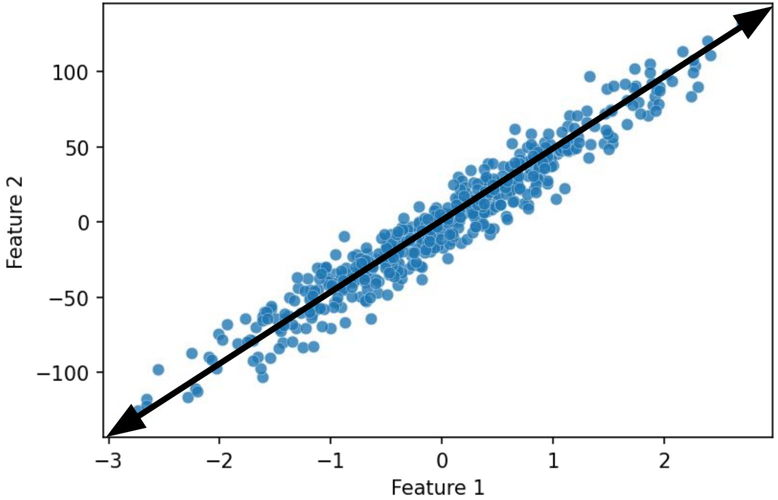
# Principal Component Analysis

- Principal Component Analysis:



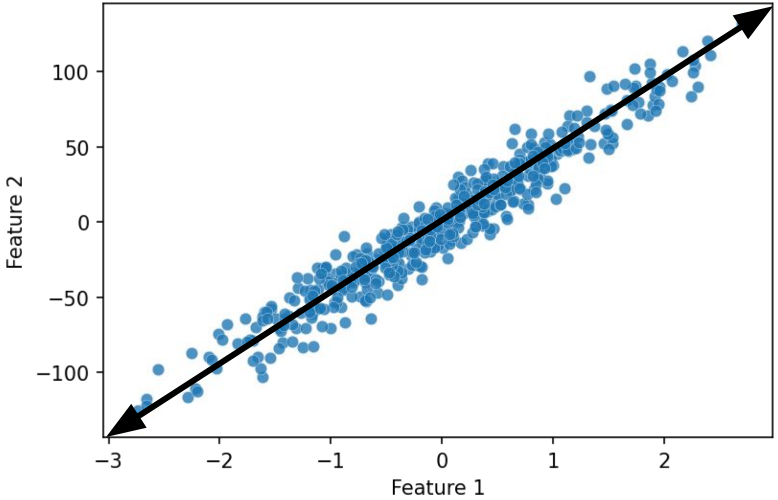
# Principal Component Analysis

- Principal Component Analysis:



# Principal Component Analysis

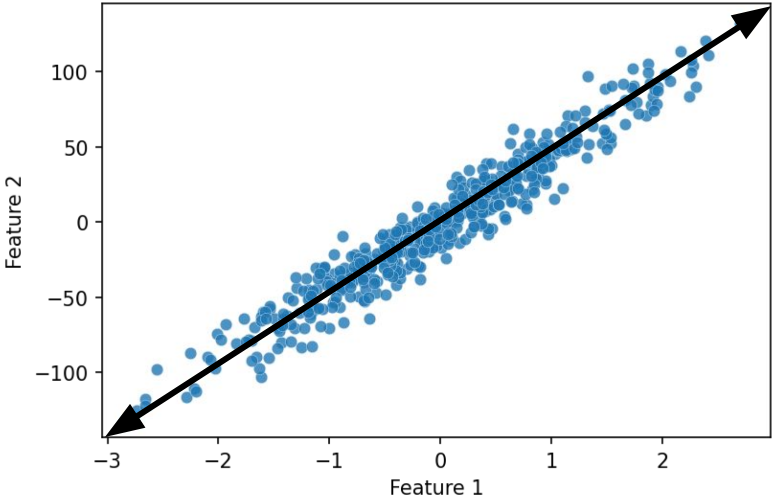
- Principal Component Analysis:




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

# Principal Component Analysis

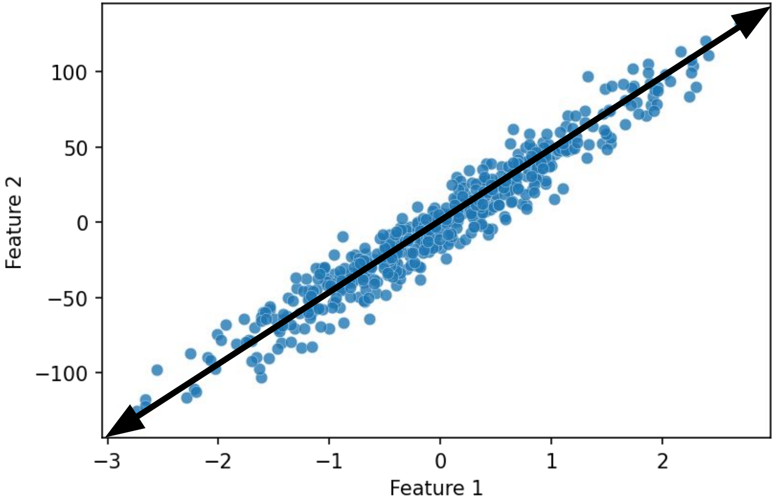
- Principal Component Analysis:




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

# Principal Component Analysis

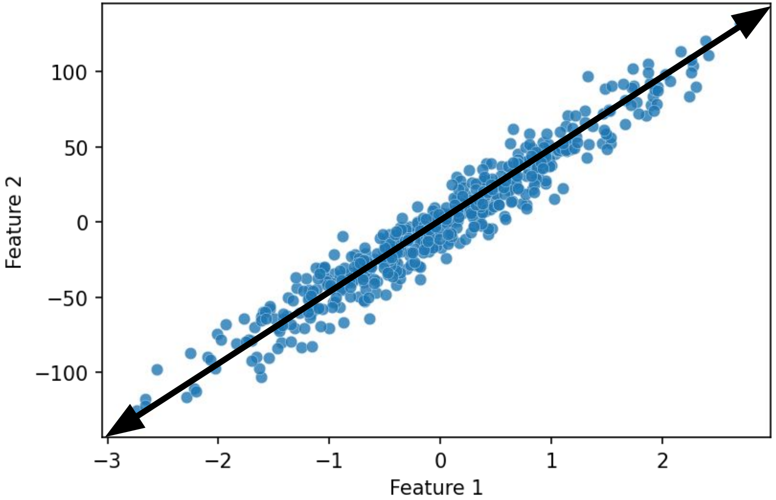
- Principal Component Analysis:




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

# Principal Component Analysis

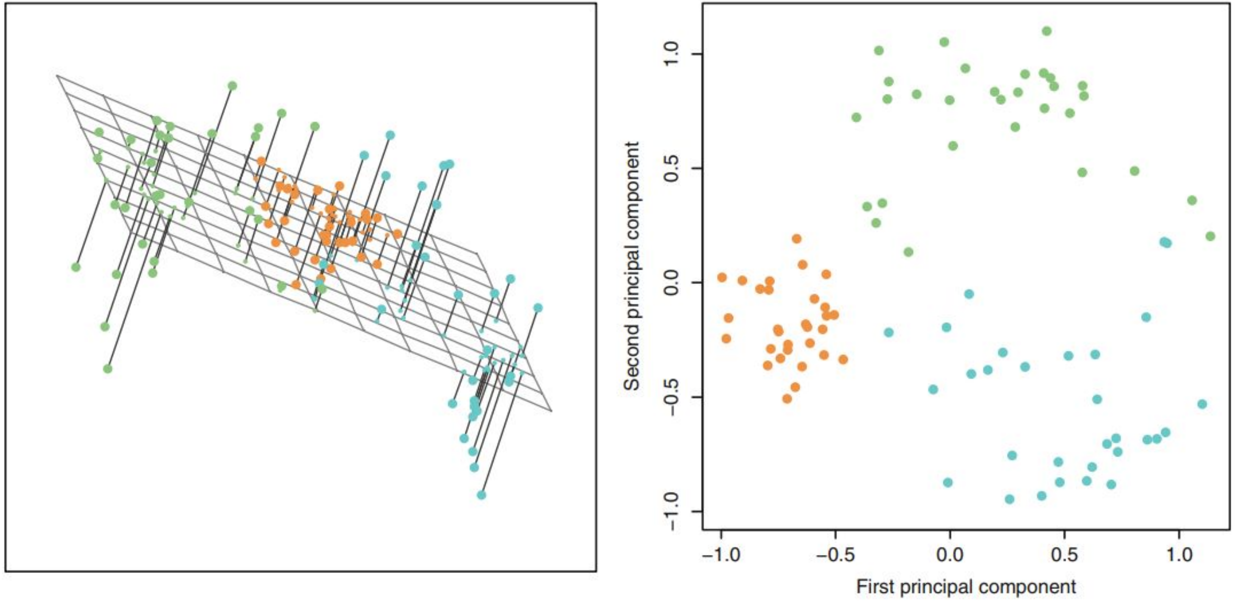
- Principal Component Analysis:




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

# Principal Component Analysis

- Principal Component Analysis:



# Principal Component Analysis

- How do we actually calculate these components?
- Let’s walk through the steps visually.

# Principal Component Analysis

- Begin with a two dimensional data set:

# Principal Component Analysis

- Begin with a two dimensional data set:

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

# Principal Component Analysis

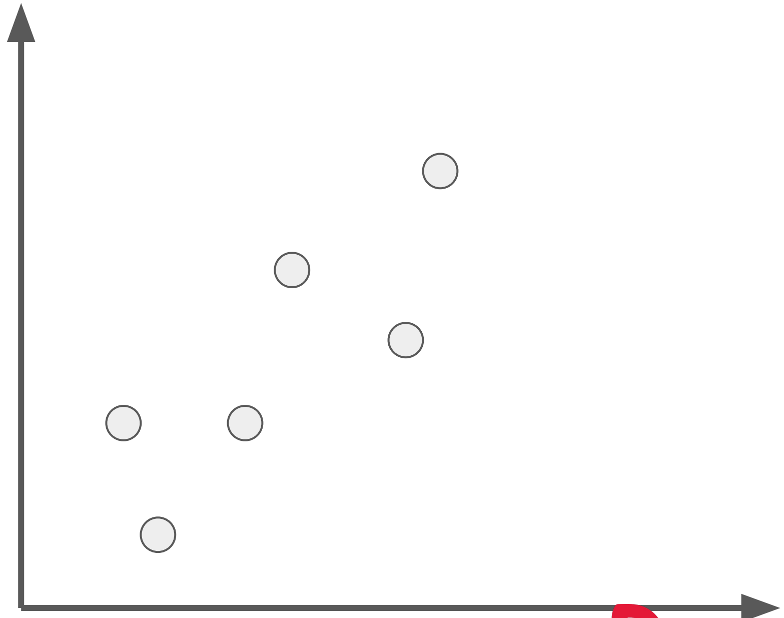
- Begin with a two dimensional data set:

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

# Principal Component Analysis

- Begin with a two dimensional data set:

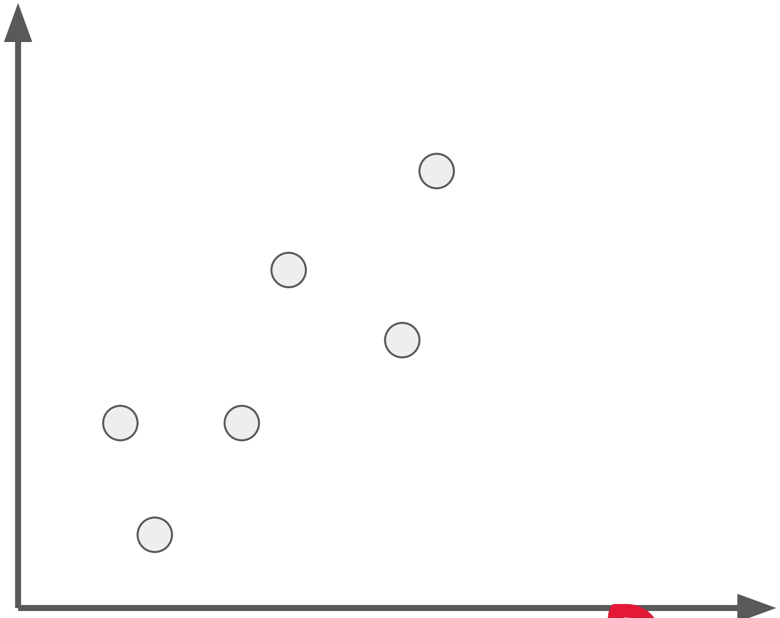
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

- Standardize the data:

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



# Principal Component Analysis

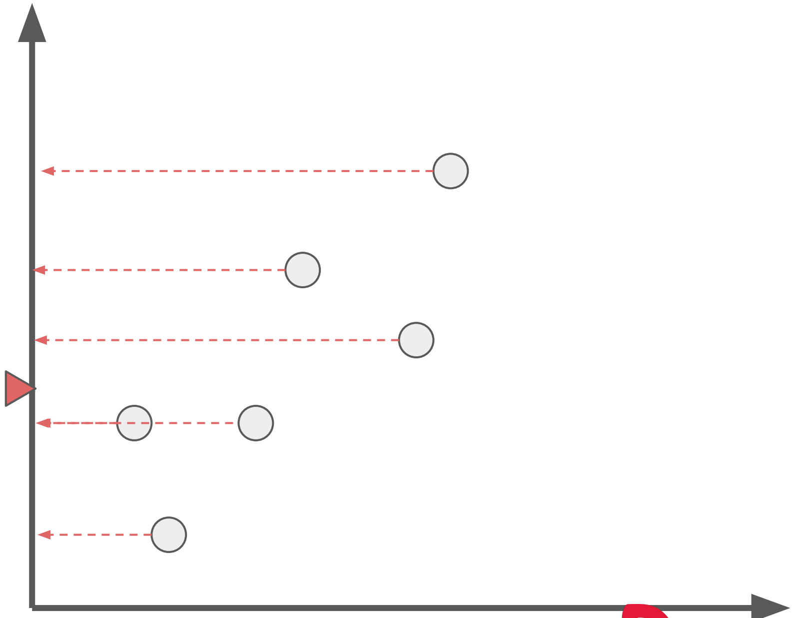
- Standardize the data:

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

# Principal Component Analysis

- Standardize the data:

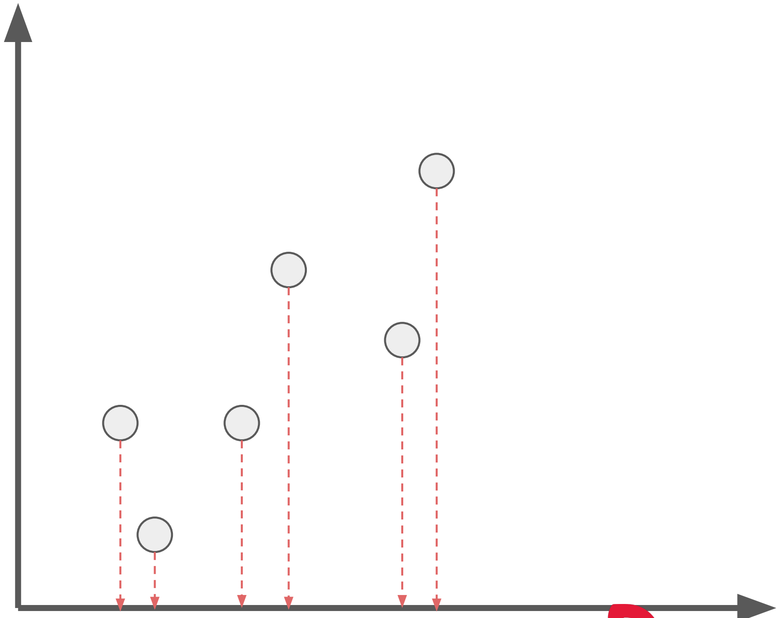
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

- Standardize the data:

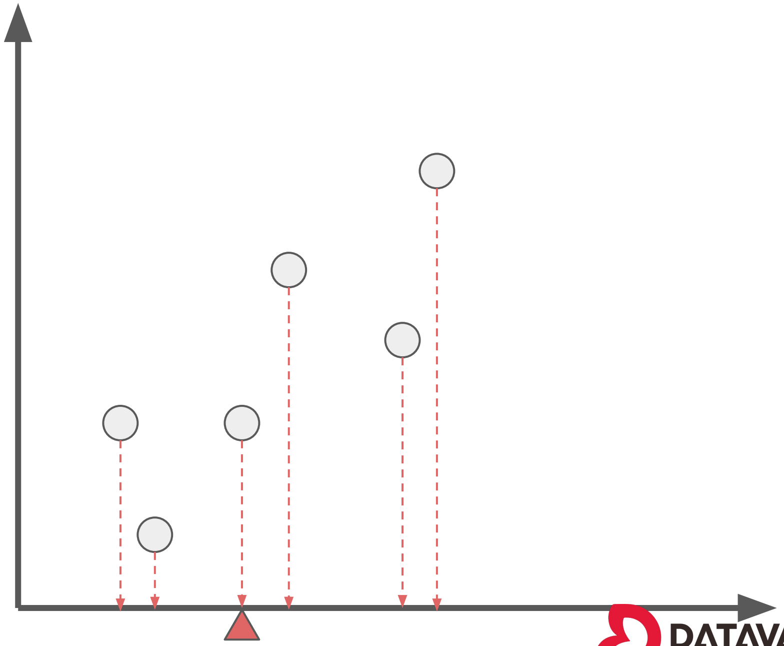
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

- Standardize the data:

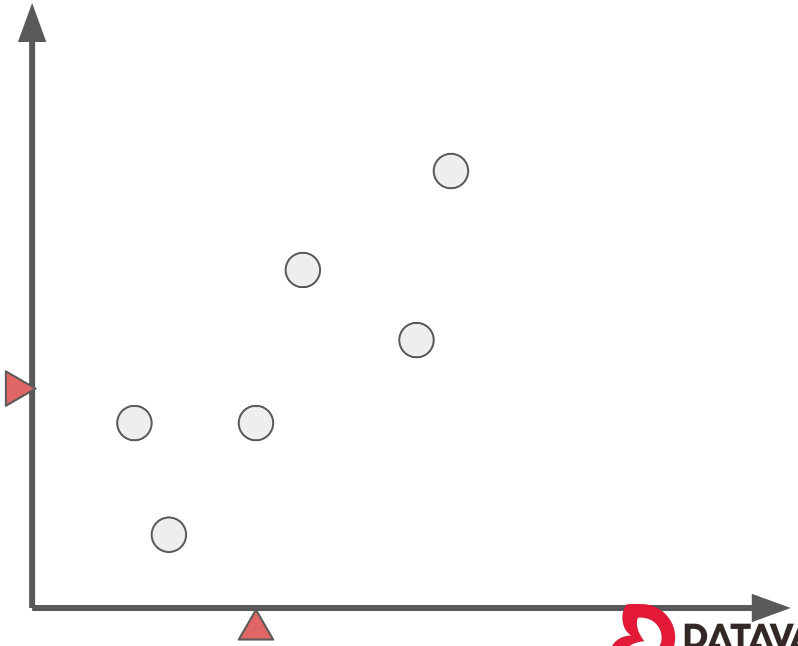
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

- Standardize the data:

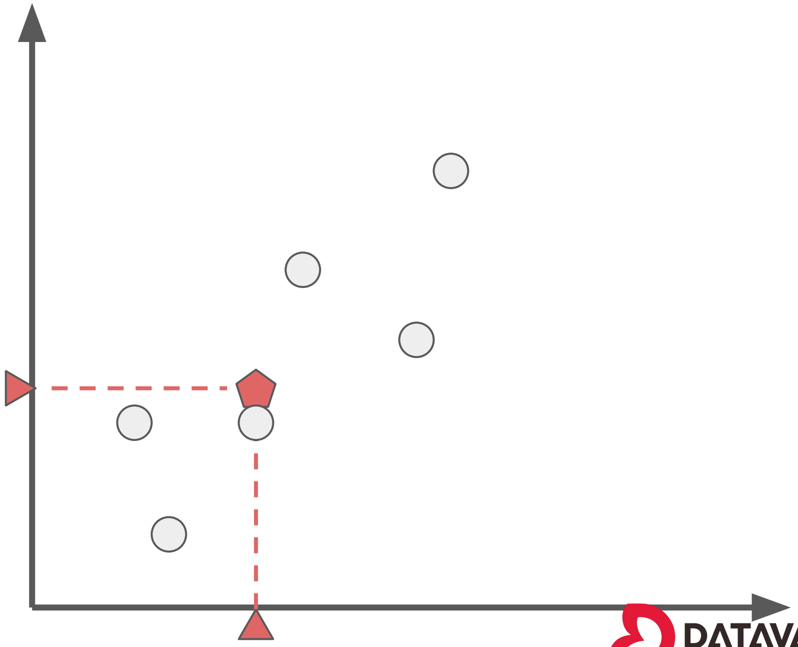
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

- Standardize the data:

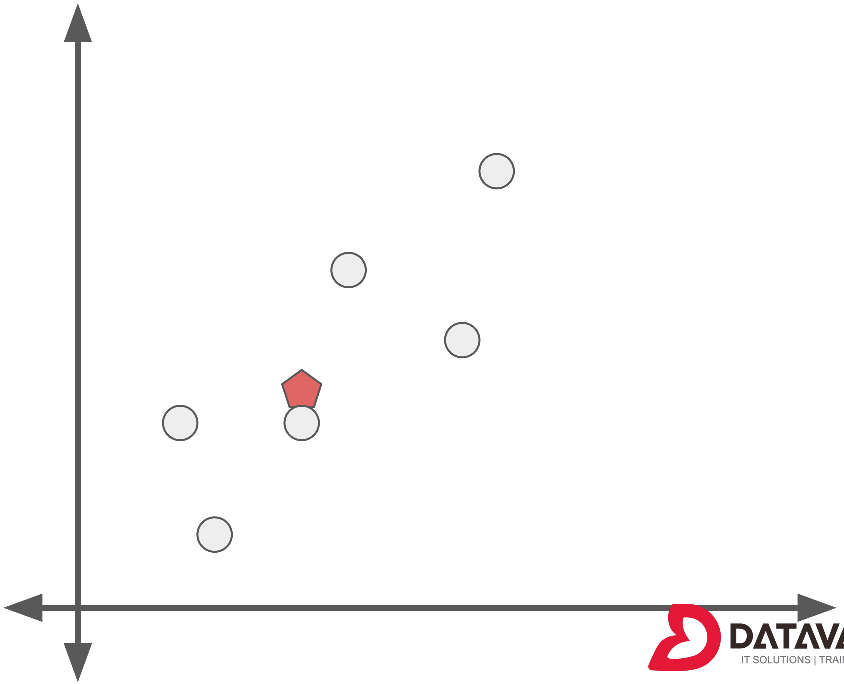
| X1 | X2 |
|---|---|
| 1 | 2 |
| 2 | 1 |
| 3 | 2 |
| 4 | 4 |
| 5 | 3 |
| 6 | 5 |



# Principal Component Analysis

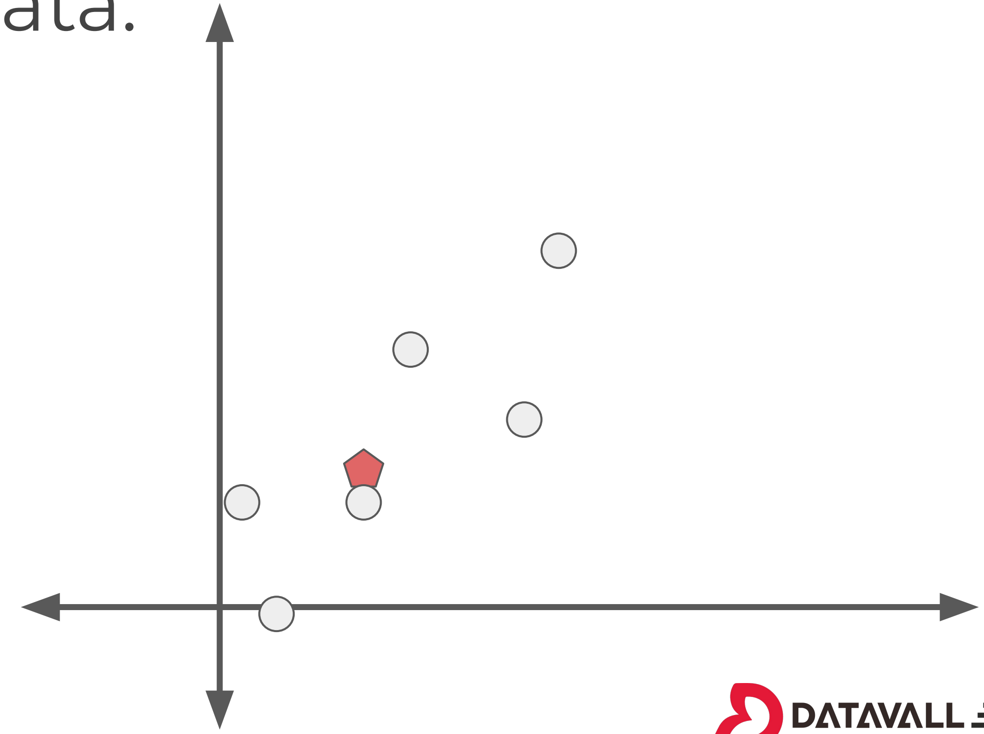
- Standardize the data:

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



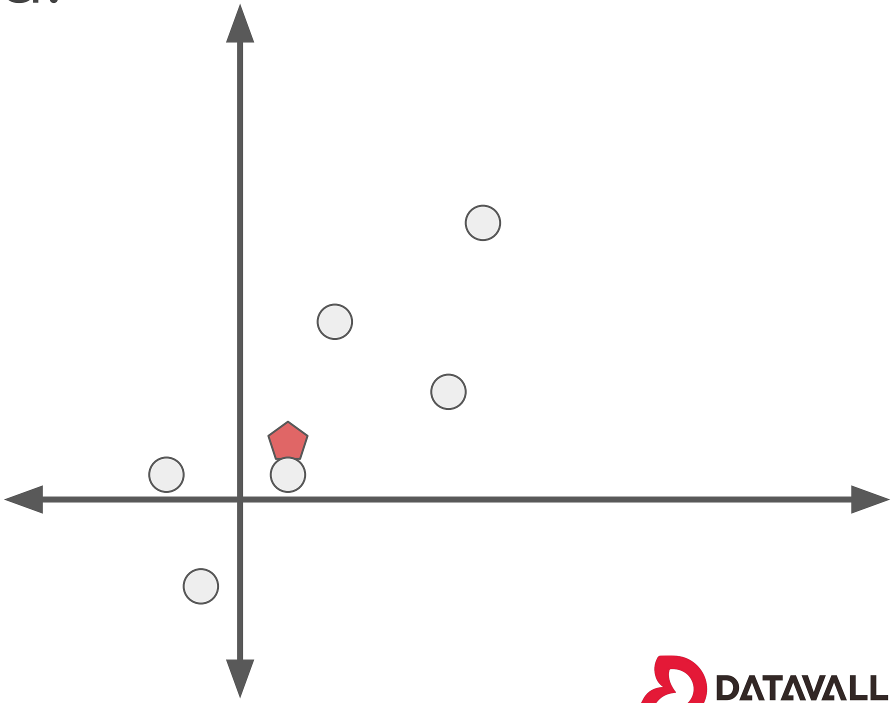
# Principal Component Analysis

- Standardize the data:



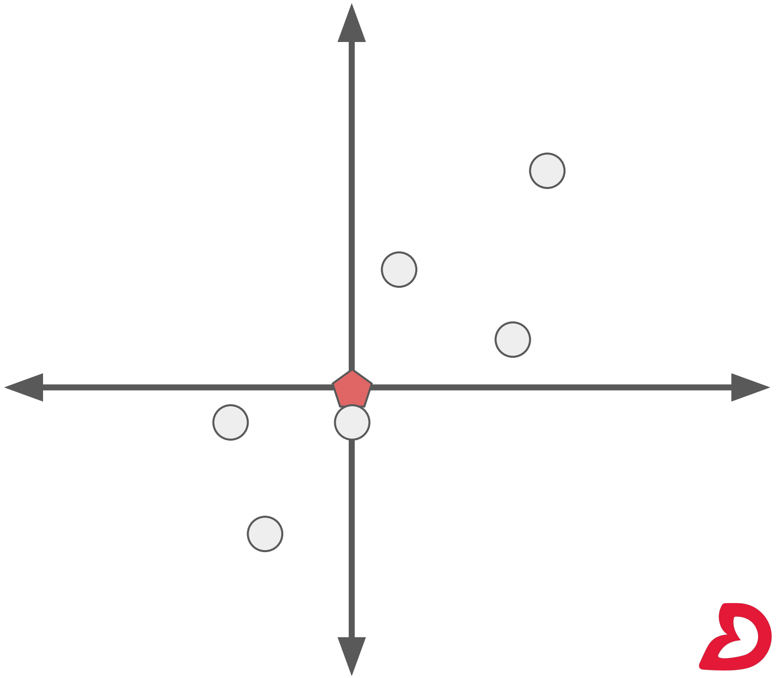
# Principal Component Analysis

- Standardize the data:



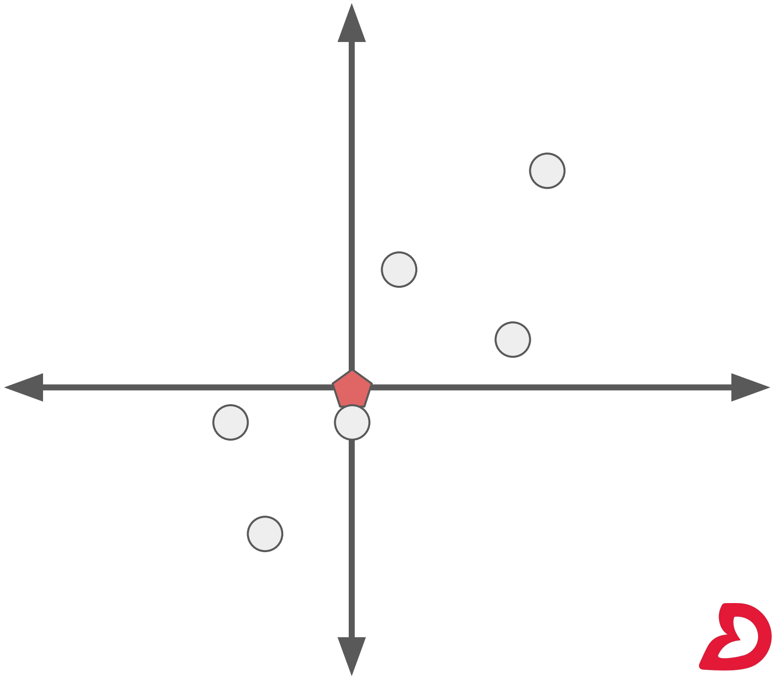
# Principal Component Analysis

- Standardize the data:



# Principal Component Analysis

- Calculate covariance matrix for data:

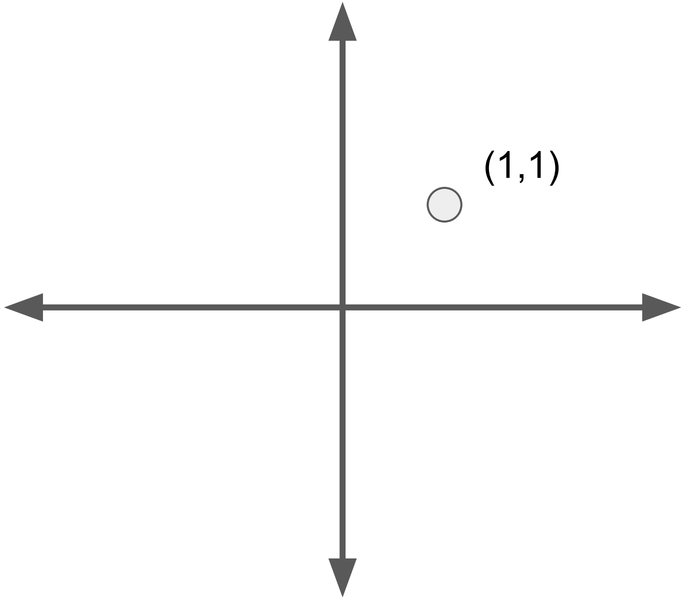


# Principal Component Analysis

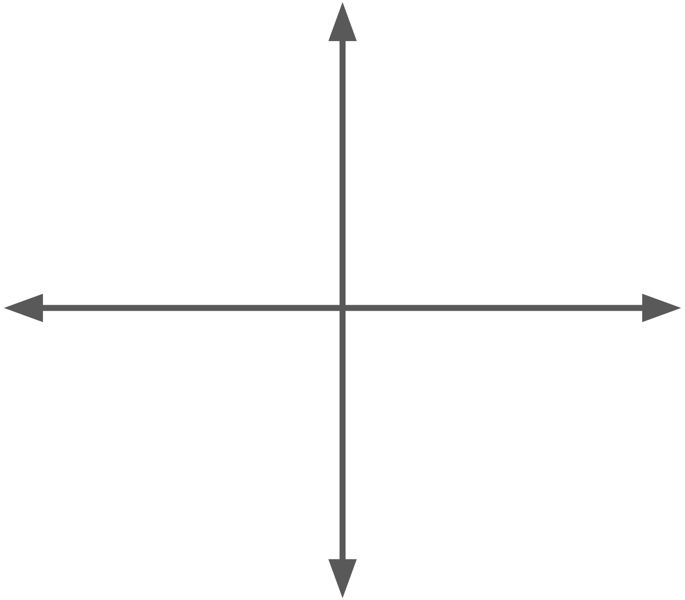
- Linear transformation of data:

# Principal Component Analysis

- Linear transformation of data:

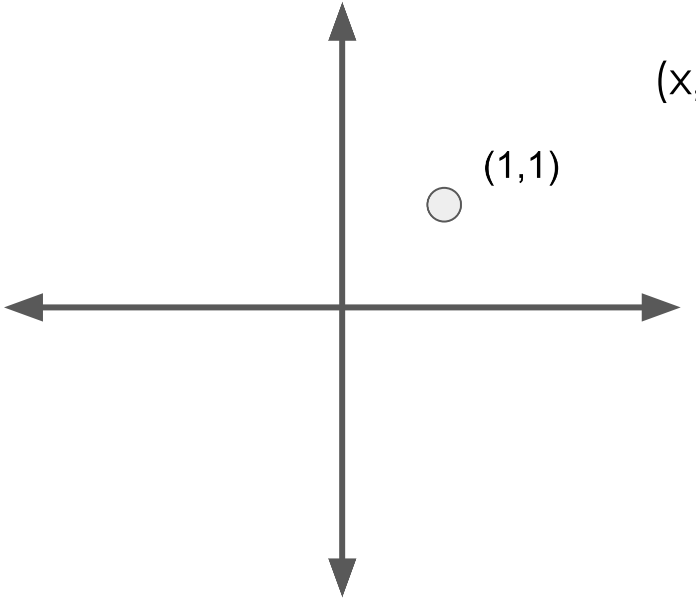



$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$



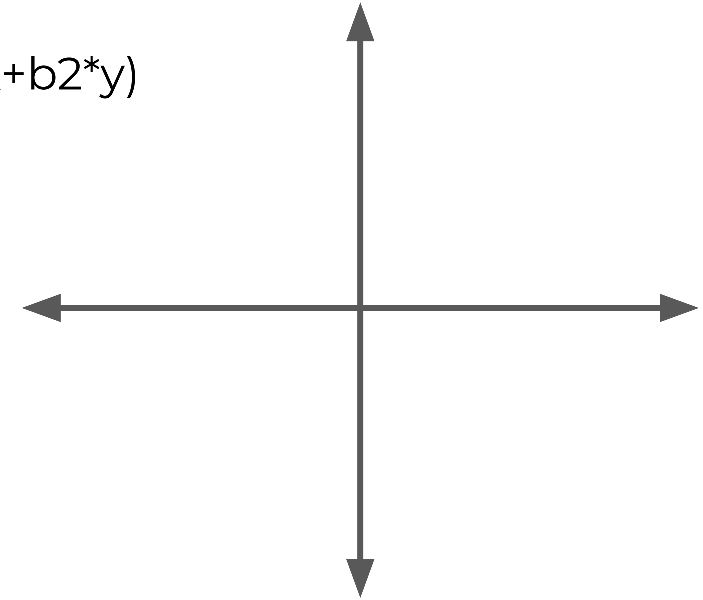
# Principal Component Analysis

- Linear transformation of data:



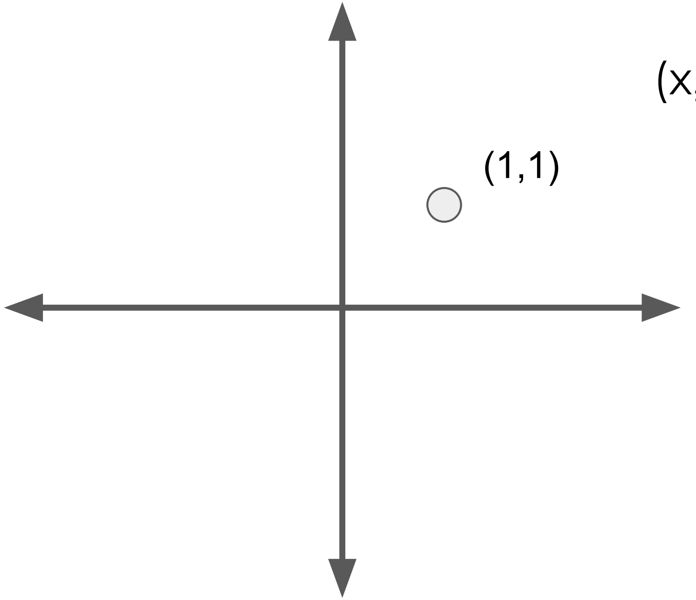

$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$

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



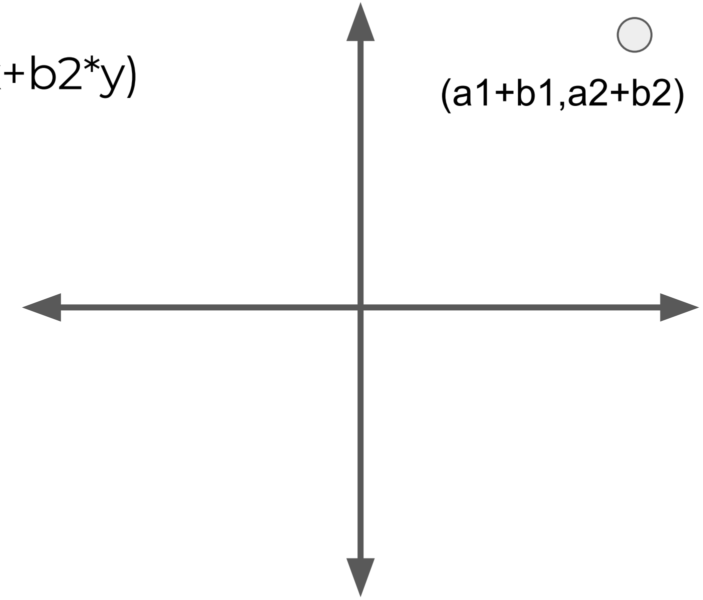
# Principal Component Analysis

- Linear transformation of data:



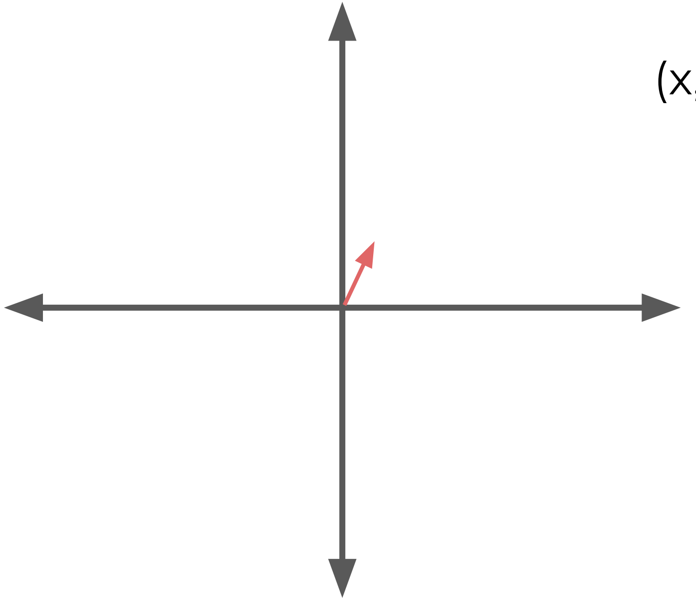

$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$

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



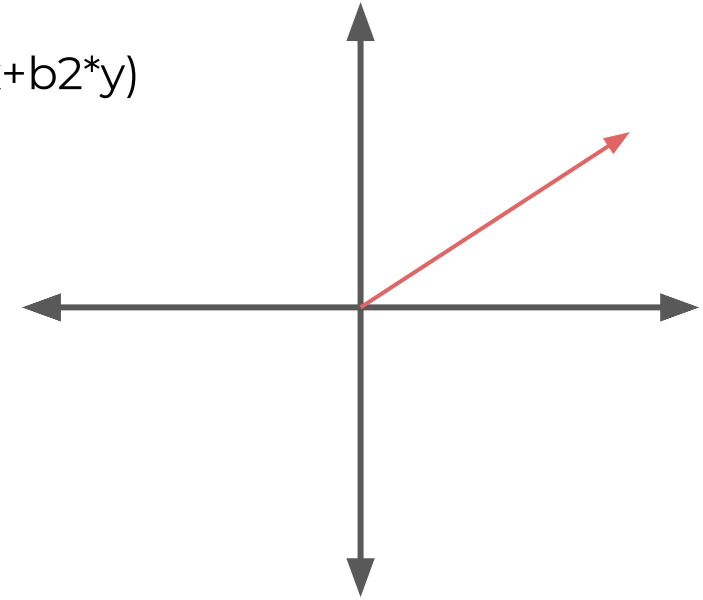
# Principal Component Analysis

- Linear transformation of data:



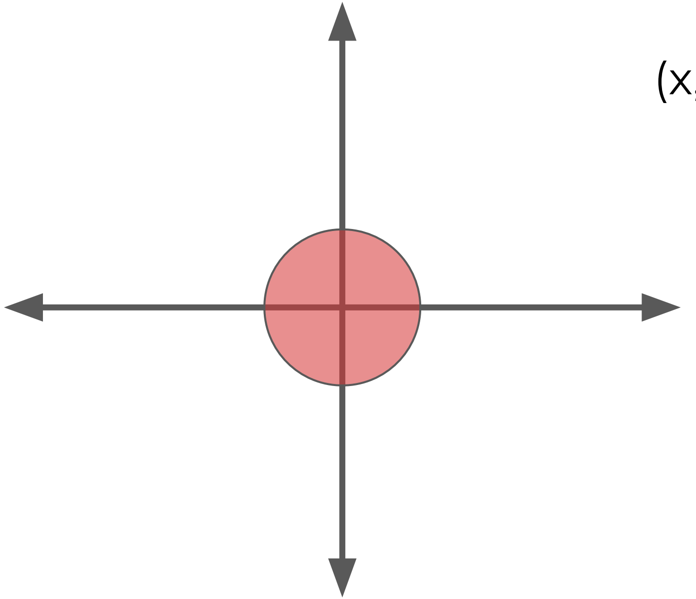
$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$

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



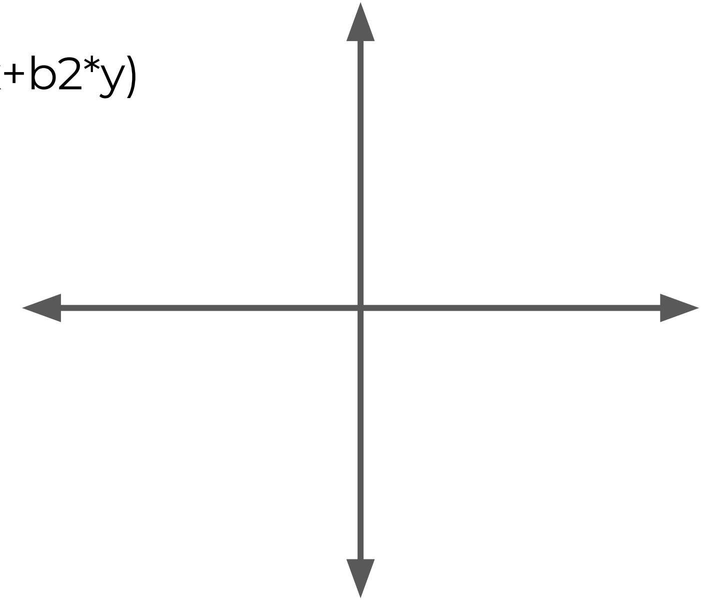
# Principal Component Analysis

- Linear transformation of data:



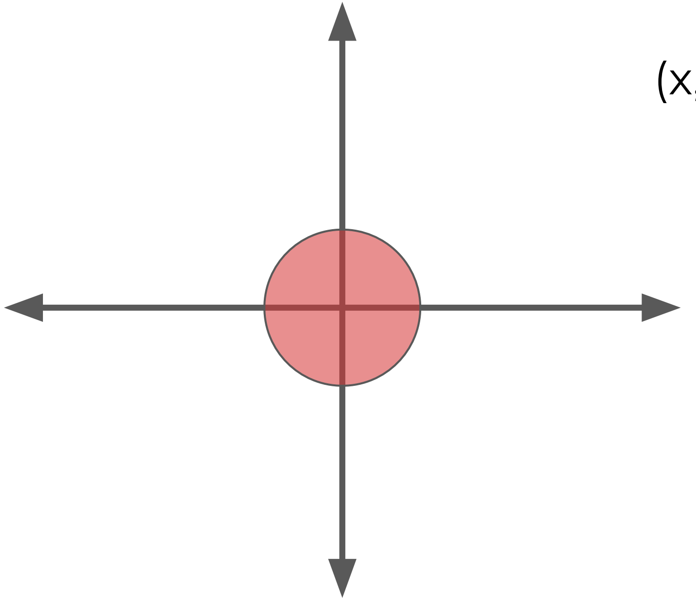
$$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$$

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



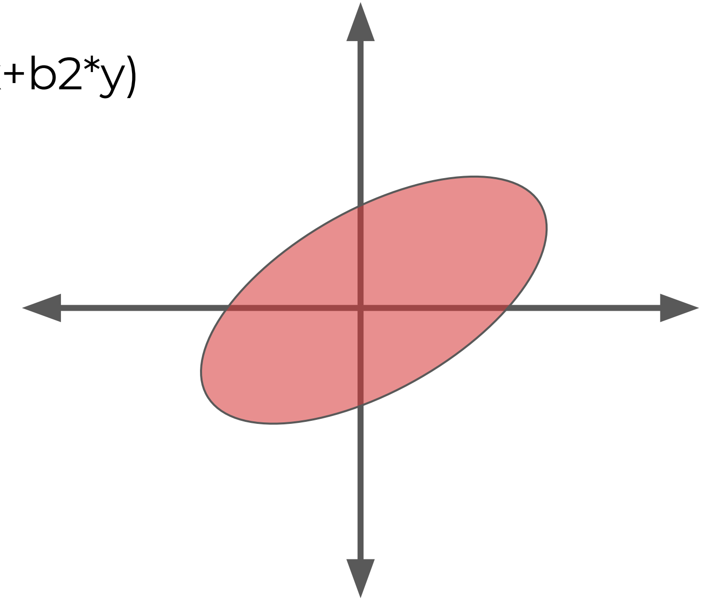
# Principal Component Analysis

- Linear transformation of data:



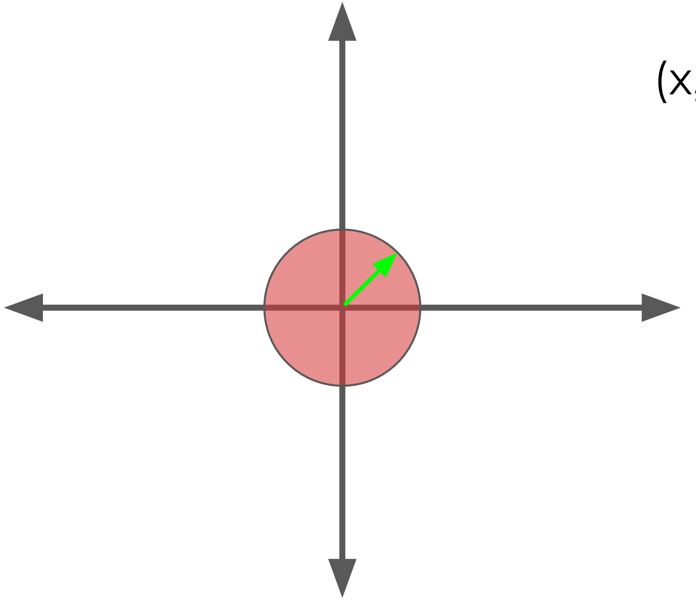
$$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$$

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



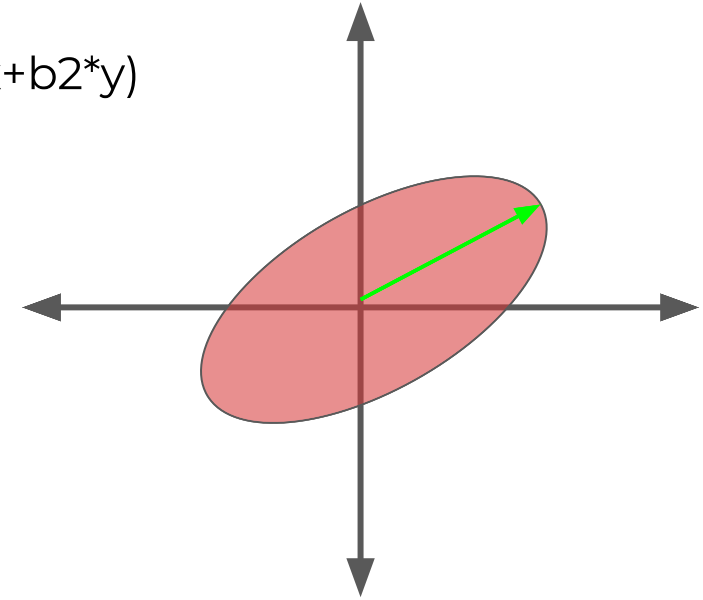
# Principal Component Analysis

- Linear transformation of data:



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

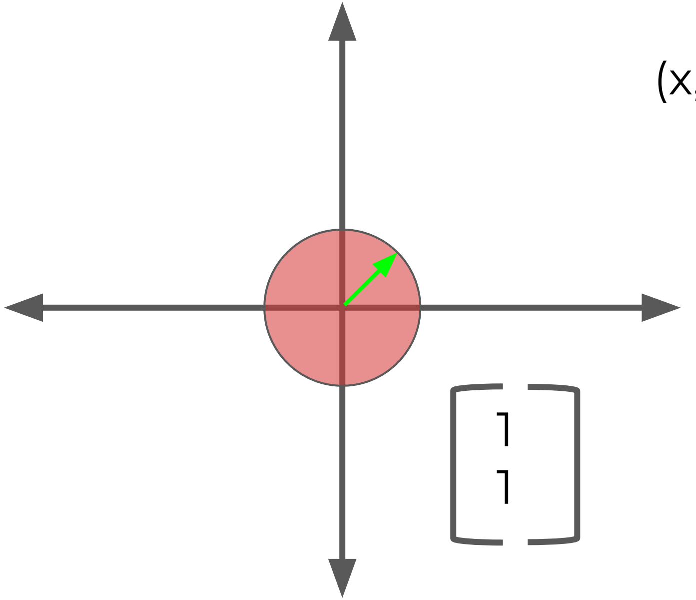
$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

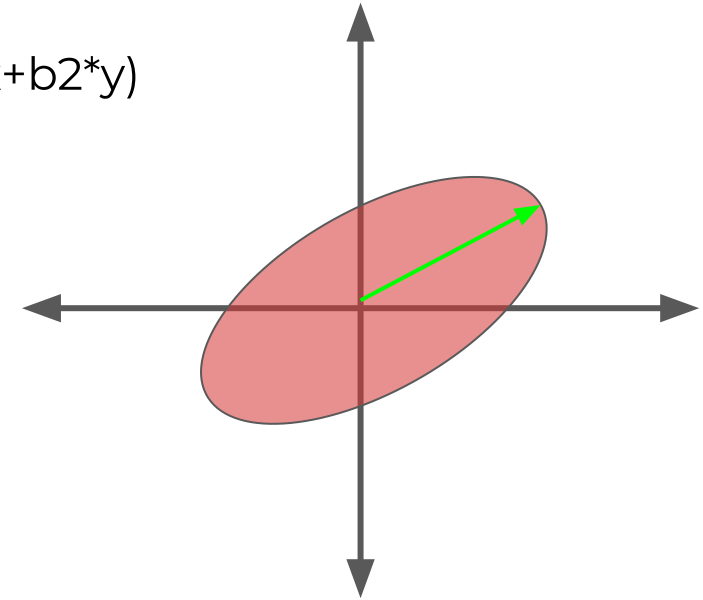


# Principal Component Analysis

- EigenVector: Directional Information

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

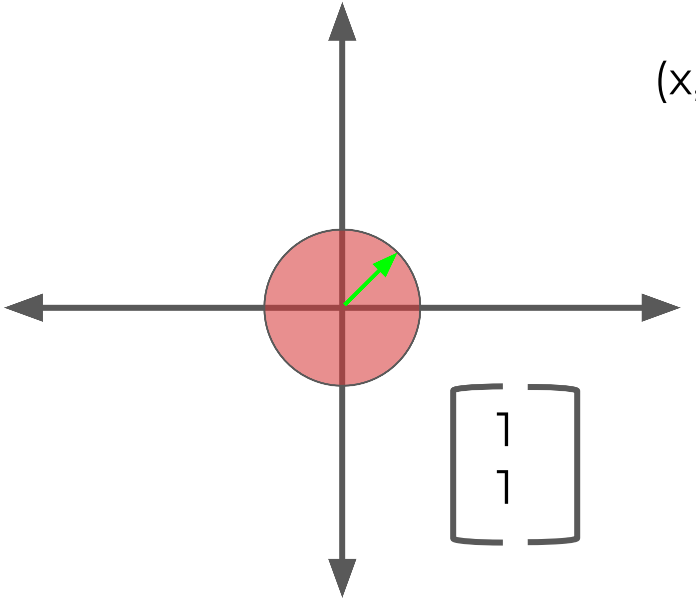


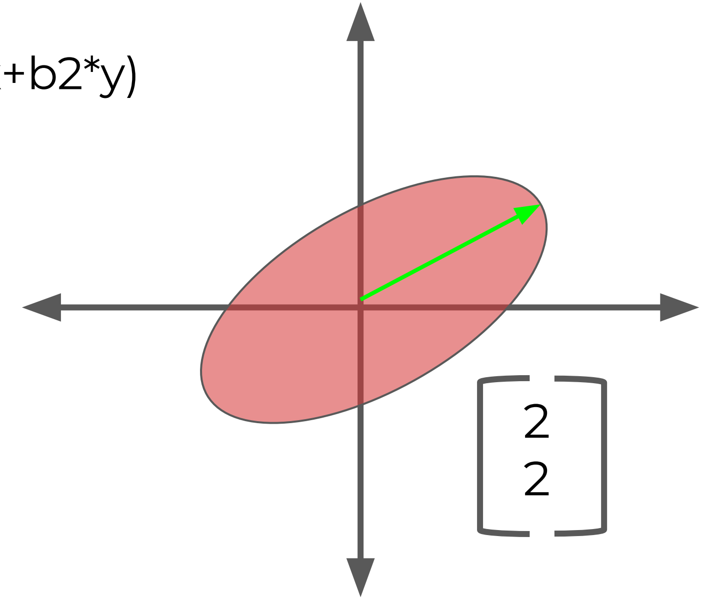



# Principal Component Analysis

- EigenVector: Directional Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)

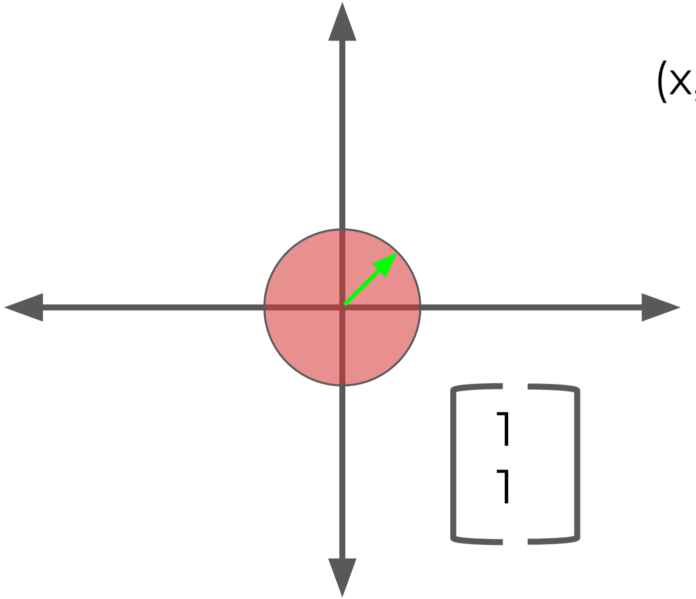


# Principal Component Analysis

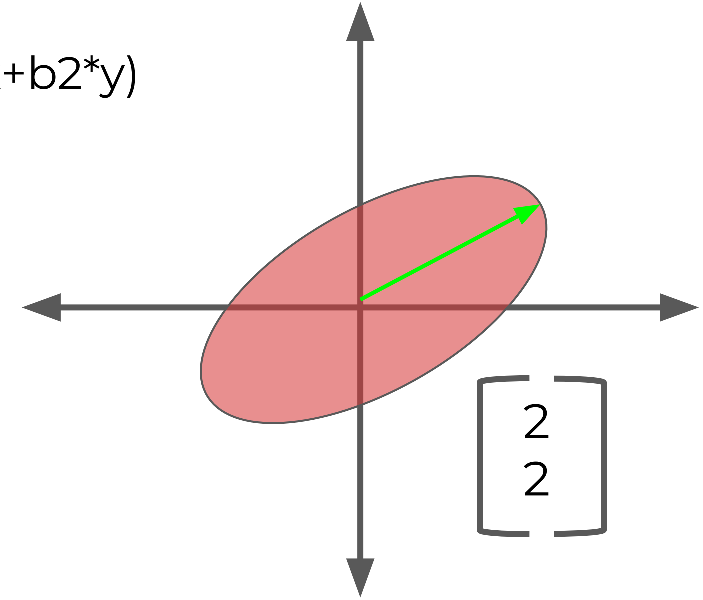
- EigenValue: Magnitude Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)



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

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

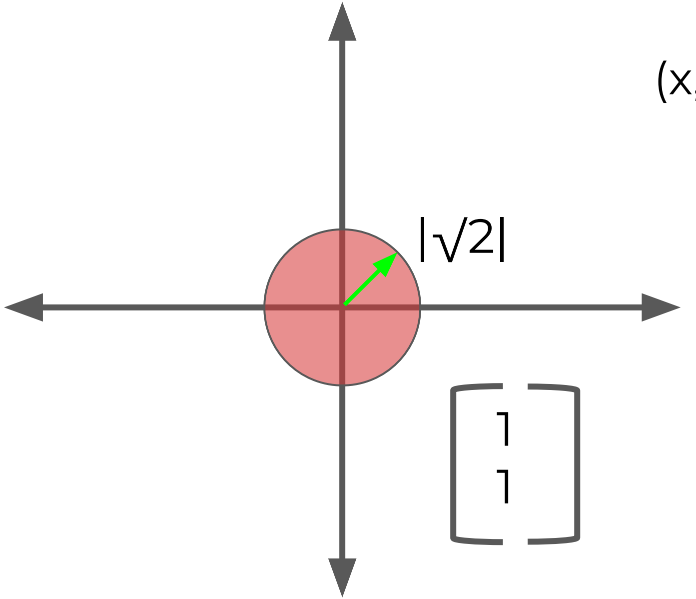


$$\begin{bmatrix} 2 \\ 2 \end{bmatrix}$$

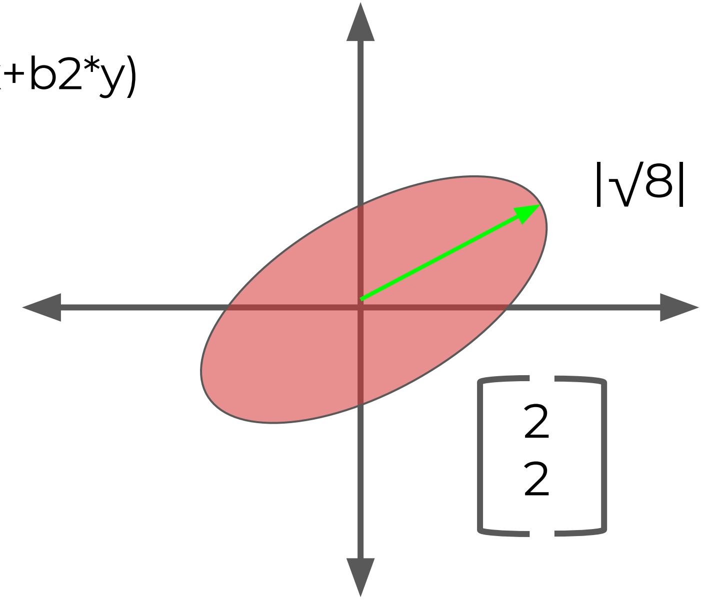
# Principal Component Analysis

- EigenValue: Magnitude Information

(x,y) → (a1*x+b1*y,a2*x+b2*y)

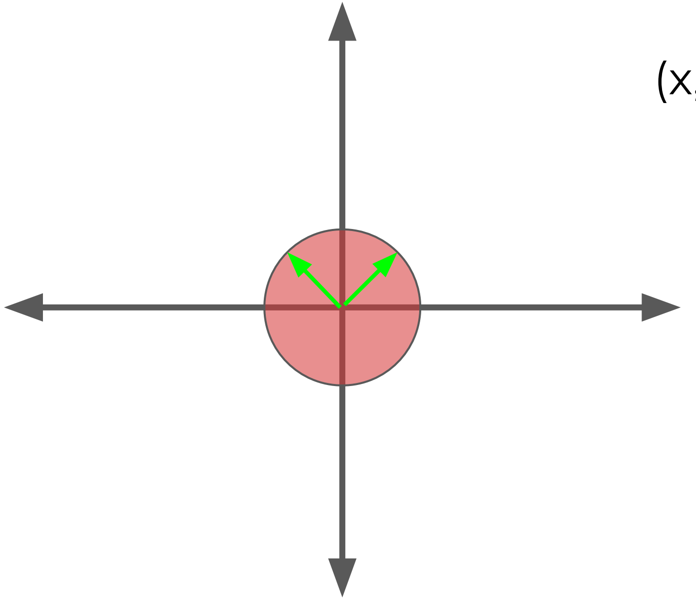



$$\begin{bmatrix} a1 & b1 \\ a2 & b2 \end{bmatrix}$$

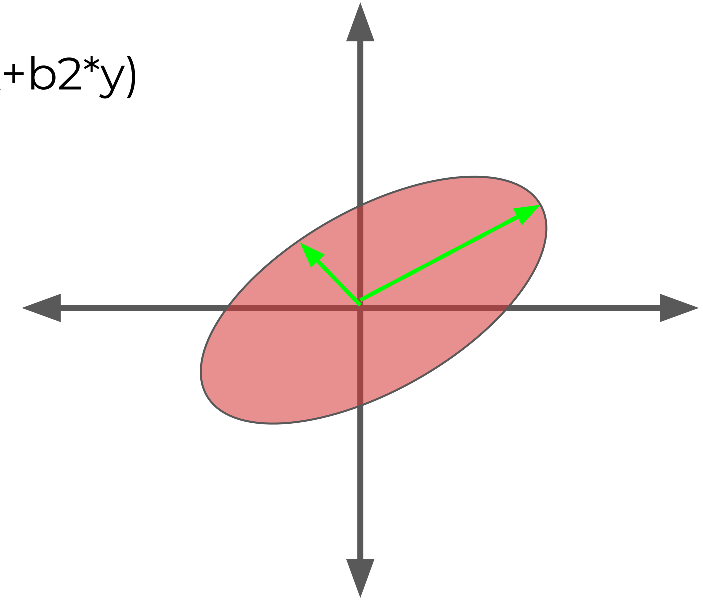


# Principal Component Analysis

- Orthogonal EigenVector

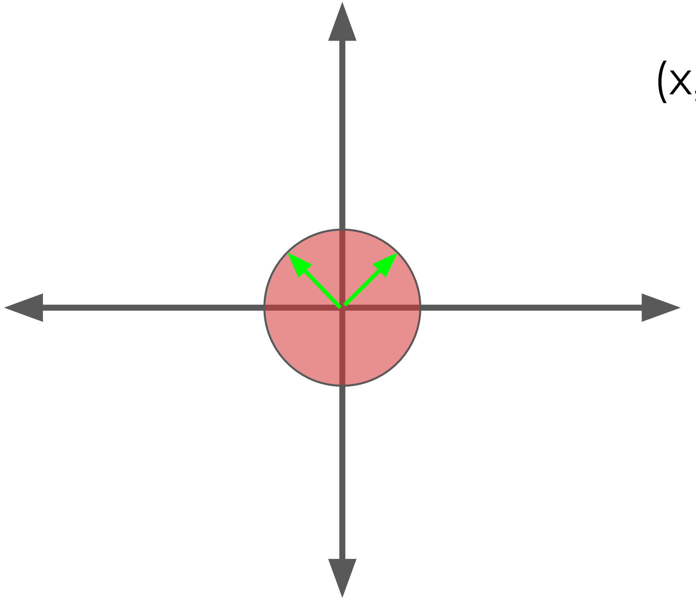


$(x,y) \rightarrow (a1*x+b1*y, a2*x+b2*y)$

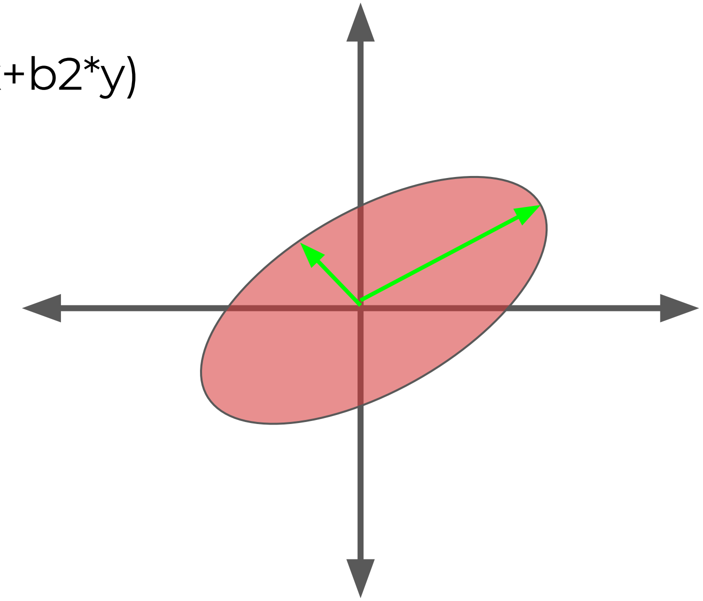


# Principal Component Analysis

- EigenVector is just a linear transformation



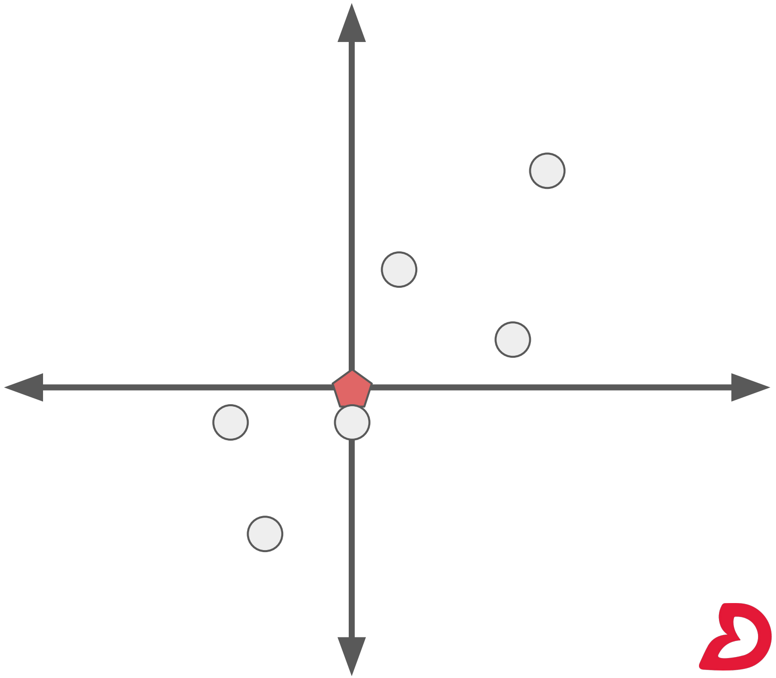
$$(x,y) \rightarrow (a1*x+b1*y,a2*x+b2*y)$$



# Principal Component Analysis

- Apply Linear Transformation:

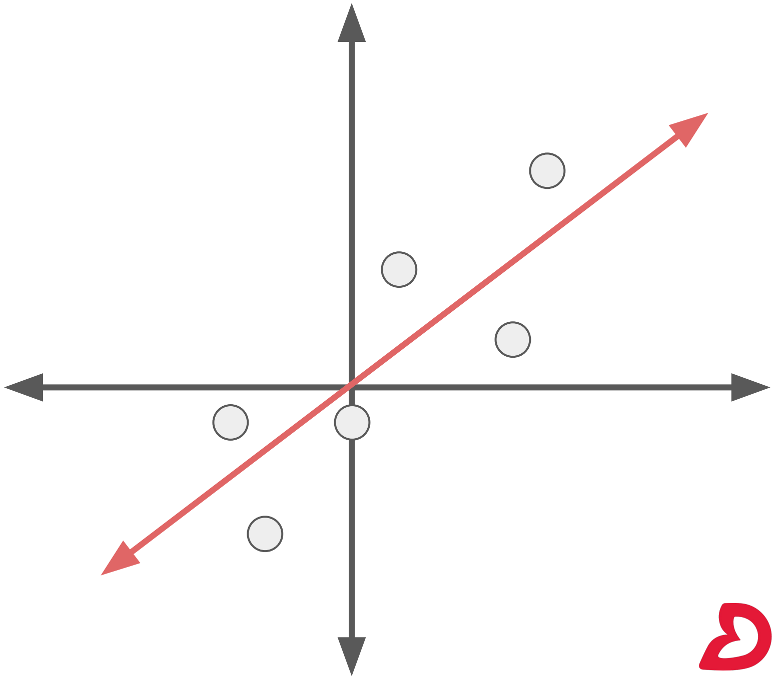
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



# Principal Component Analysis

- Apply Linear Transformation:

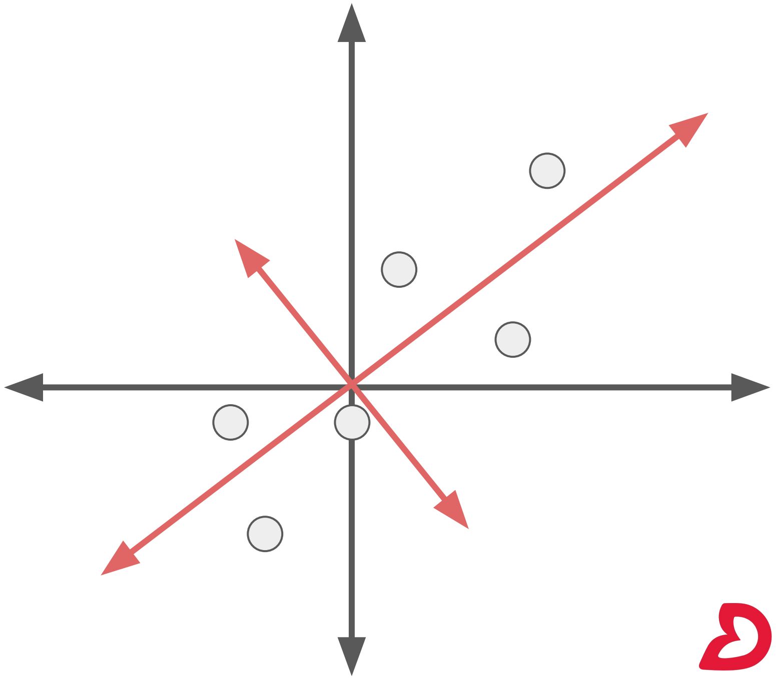
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



# Principal Component Analysis

- Apply Linear Transformation:

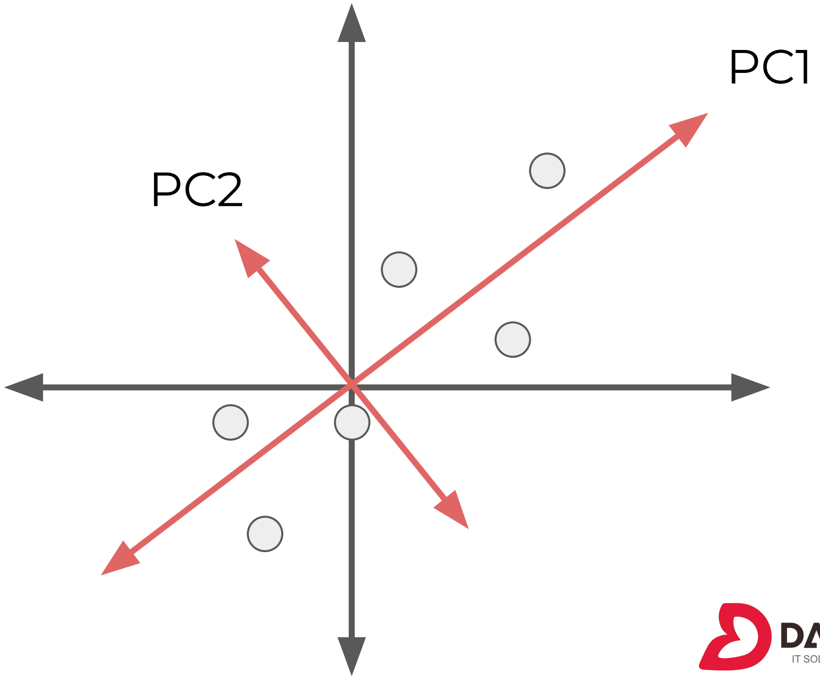
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



# Principal Component Analysis

- EigenValue measures variance explained:

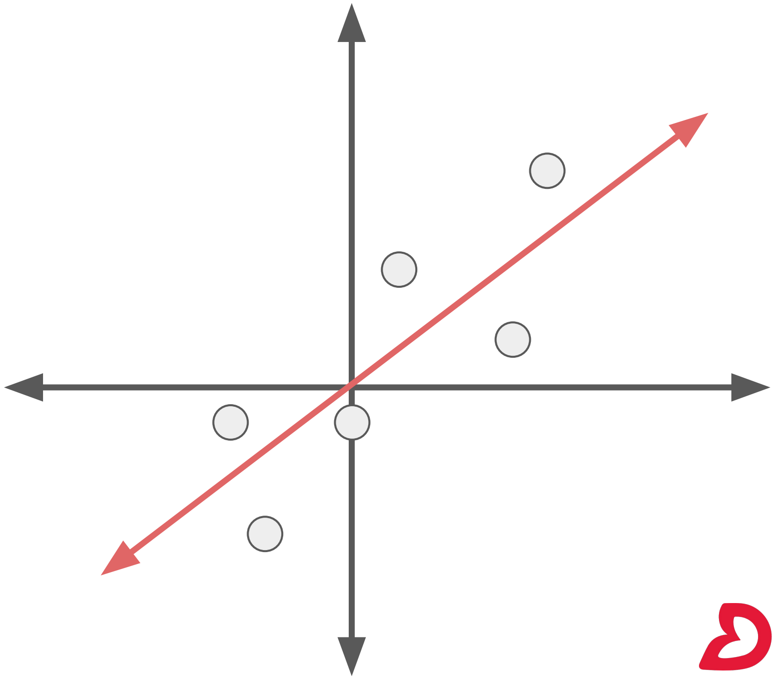
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



# Principal Component Analysis

- EigenValue measures variance explained:

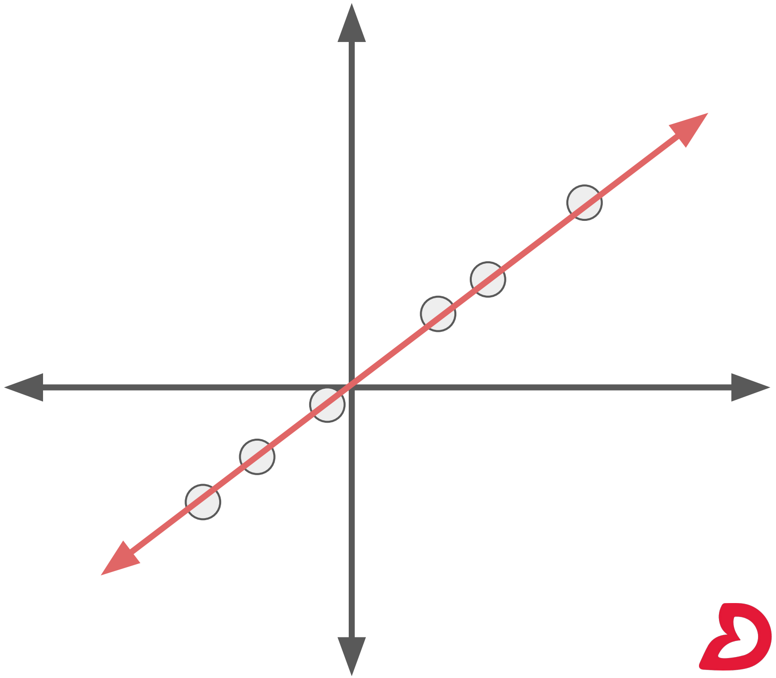
$$\begin{bmatrix} \mathrm{Var}(X) & \mathrm{Cov}(X,Y) \\ \mathrm{Cov}(X,Y) & \mathrm{Var}(Y) \end{bmatrix}$$



# Principal Component Analysis

- EigenValue measures variance explained:

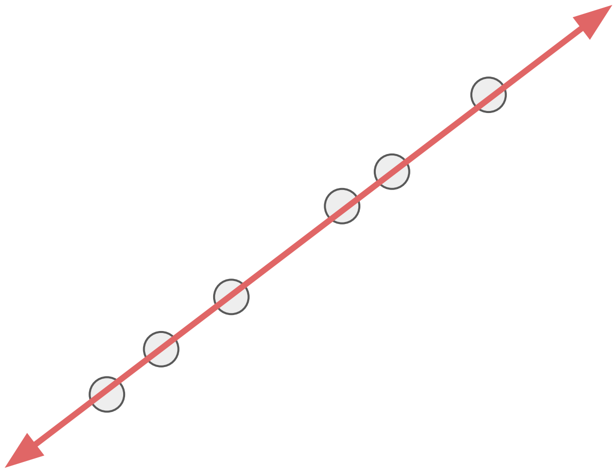
$$\begin{bmatrix} Var(X) & Cov(X,Y) \\ Cov(X,Y) & Var(Y) \end{bmatrix}$$



# Principal Component Analysis

- EigenValue measures variance explained:

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



# Principal Component Analysis

- EigenValue measures variance explained:

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

Principal Component 1

# Principal Component Analysis

- PCA Steps
  - Get original data
  - Calculate Covariance Matrix
  - Calculate EigenVectors
  - Sort EigenVectors by EigenValues
  - Choose N largest EigenValues
  - Project original data onto EigenVectors