Machine Learning

Principal Component Analysis

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Motivation

How to visualize this dataset?

Sepal length	**Sepal width**	**Petal length**	**Petal width**	**Class**
5.1	3.5	1.4	0.2	Setosa
4.9	3.0	1.4	0.2	Setosa
7.0	3.2	4.7	1.4	Versicolor
6.4	3.2	4.5	1.5	Versicolor
6.3	2.9	5.6	1.8	Virginica
5.9	3.0	5.1	1.8	Virginica

Pair plot of the Iris dataset

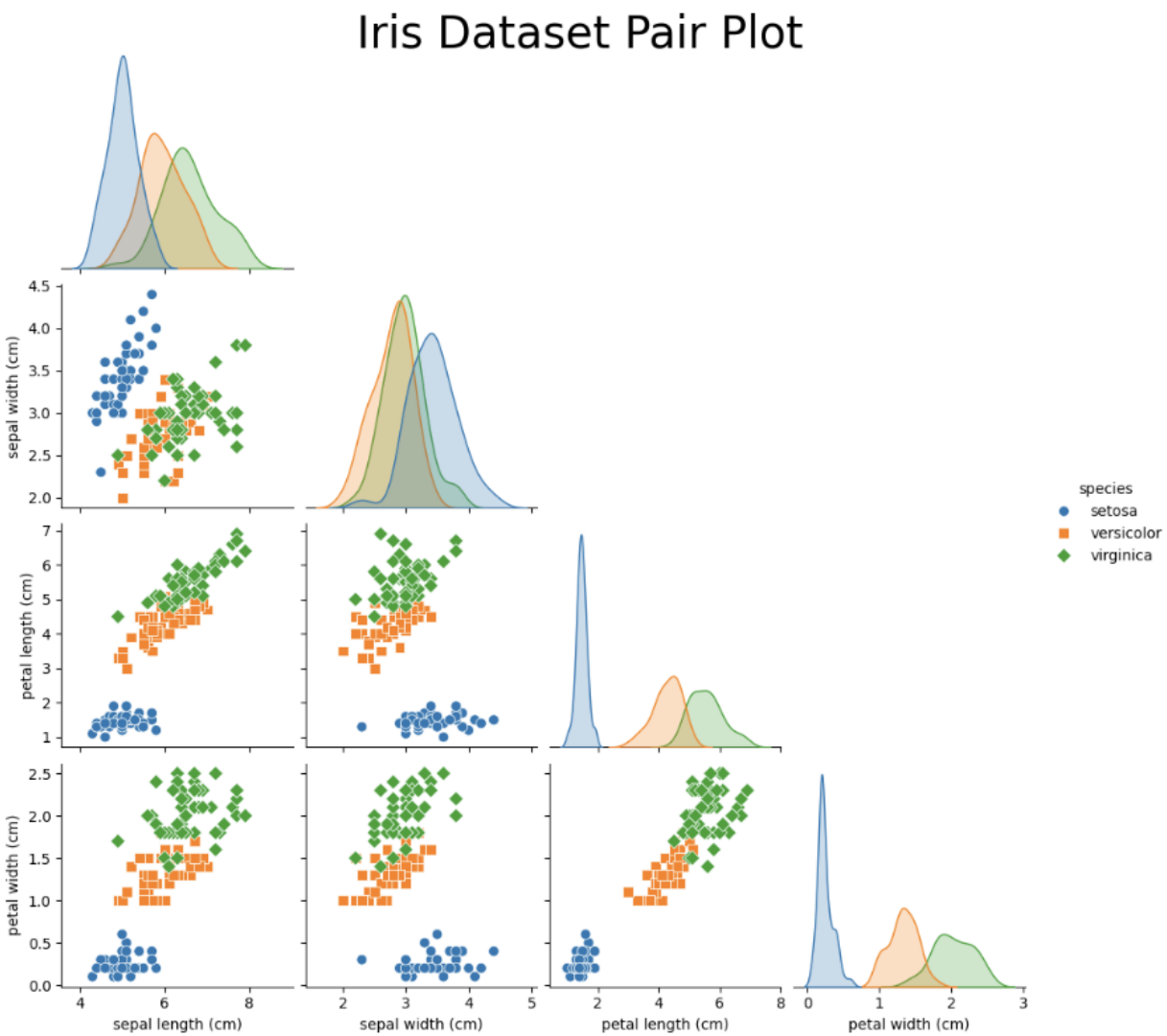


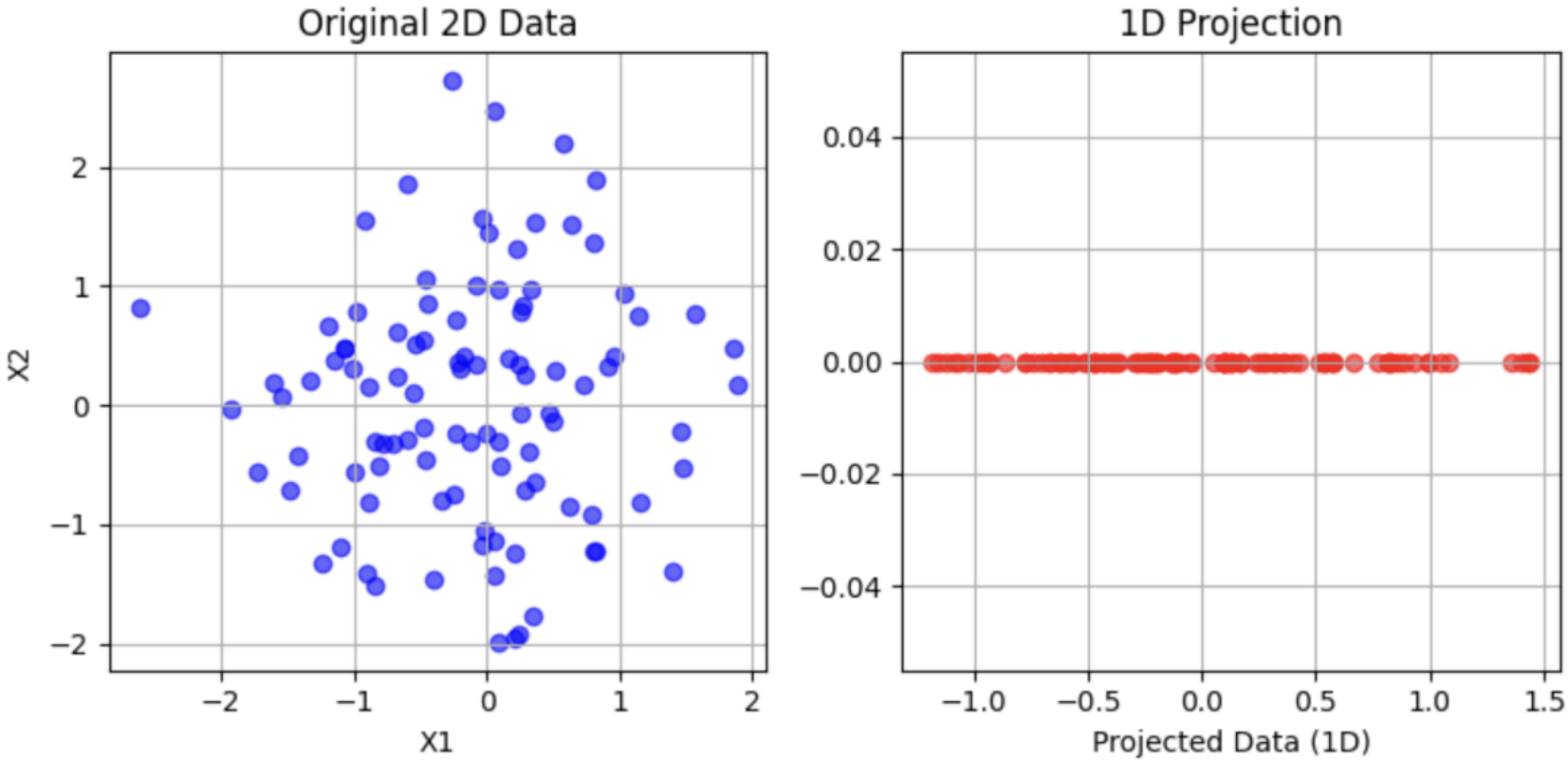
Figure: Pair plot of the iris dataset features

Pair plot of the Iris dataset

```python
import seaborn as sns
import matplotlib.pyplot as plt
from sklearn.datasets import load_iris
import pandas as pd

# Load the Iris dataset
iris = load_iris()
iris_df = pd.DataFrame(data=iris['data'], columns=iris['feature_names'])
iris_df['species'] = iris['target']

# Define the target names for the species
species_names = {i: species for i, species in enumerate(iris['target_names'])}
iris_df['species'] = iris_df['species'].map(species_names)

# Create a pair plot with adjustable font sizes
sns.pairplot(iris_df, hue='species', corner=True, markers=["o", "s", "D"],
             plot_kws={'s': 50}, diag_kws={'fill': True})

# Show plot
plt.show()
```

Methods for Reducing Dimensionality

- Visualizing a dataset with n features requires $O(n^2)$ plots, which becomes computationally expensive.
- A basic approach to reduce dimensions is by applying a random projection to the data.
- While random projections help reveal some structure, they often obscure more meaningful patterns within the data.



Dimensionality Reduction

- In Dimensionality Reduction, we represent a dataset in lower dimension without losing too much information.
- Why dimensionality reduction ?
  - Reduce the dimensions of data to 2D or 3D to visualize it precisely.
  - Help in data compressing and reducing the storage space.
  - Remove redundant features, if any.
- Some other dimension reduction methods: t-SNE, LDA,...
  - t-SNE (t-Distributed Stochastic Neighbor Embedding) is a popular machine learning algorithm primarily used for dimensionality reduction and visualization of high-dimensional data. Unlike traditional dimensionality reduction techniques like PCA, which are linear, t-SNE is a non-linear technique that excels at preserving the local structure of data, making it particularly effective for visualizing clusters or patterns in datasets.
  - Linear Discriminant Analysis (LDA) is a popular supervised learning algorithm used for classification and dimensionality reduction in machine learning and statistics. It is used to model the difference between classes by finding a linear combination of features that best separates two or more classes of data.

Dimensionality Reduction

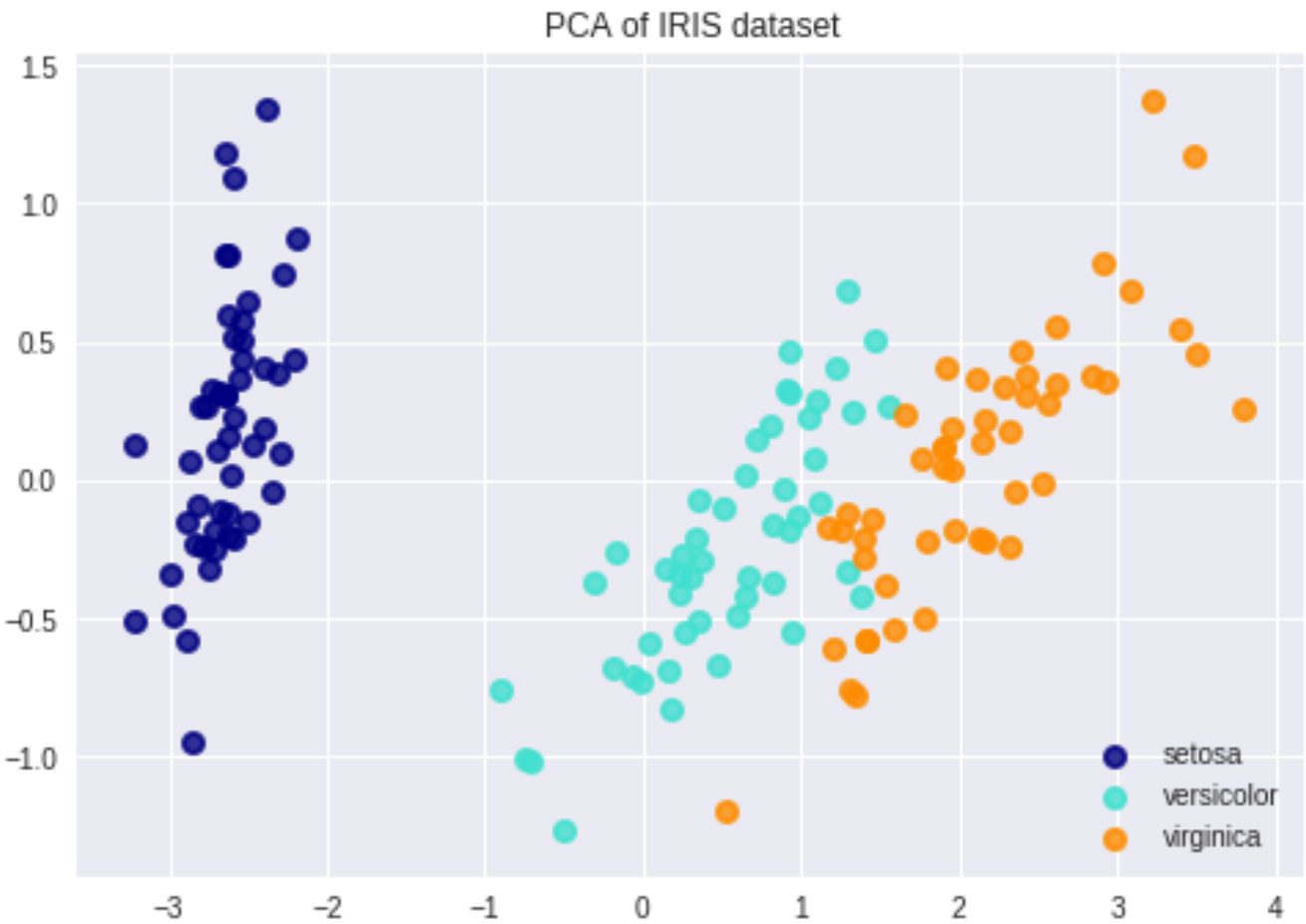


Figure: PCA of IRIS dataset, source: scikit-learn.org

Background Mathematics

Given a dataset $X \in \mathbb{R}^{N \times D}$

- Mean: $\bar{X}_i = \frac{1}{N} \sum_{j=1}^{N} X_{ji}$
- Variance: $Var(X_i) = \frac{1}{N} \sum_{j=1}^{N} (X_{ji} - \bar{X}_i)^2$
- Covariance:
  $Cov(X_i, X_k) = Cov(X_k, X_i) = \frac{1}{N} \sum_{j=1}^{N} (X_{ji} - \bar{X}_i)(X_{jk} - \bar{X}_k)$

Covariance

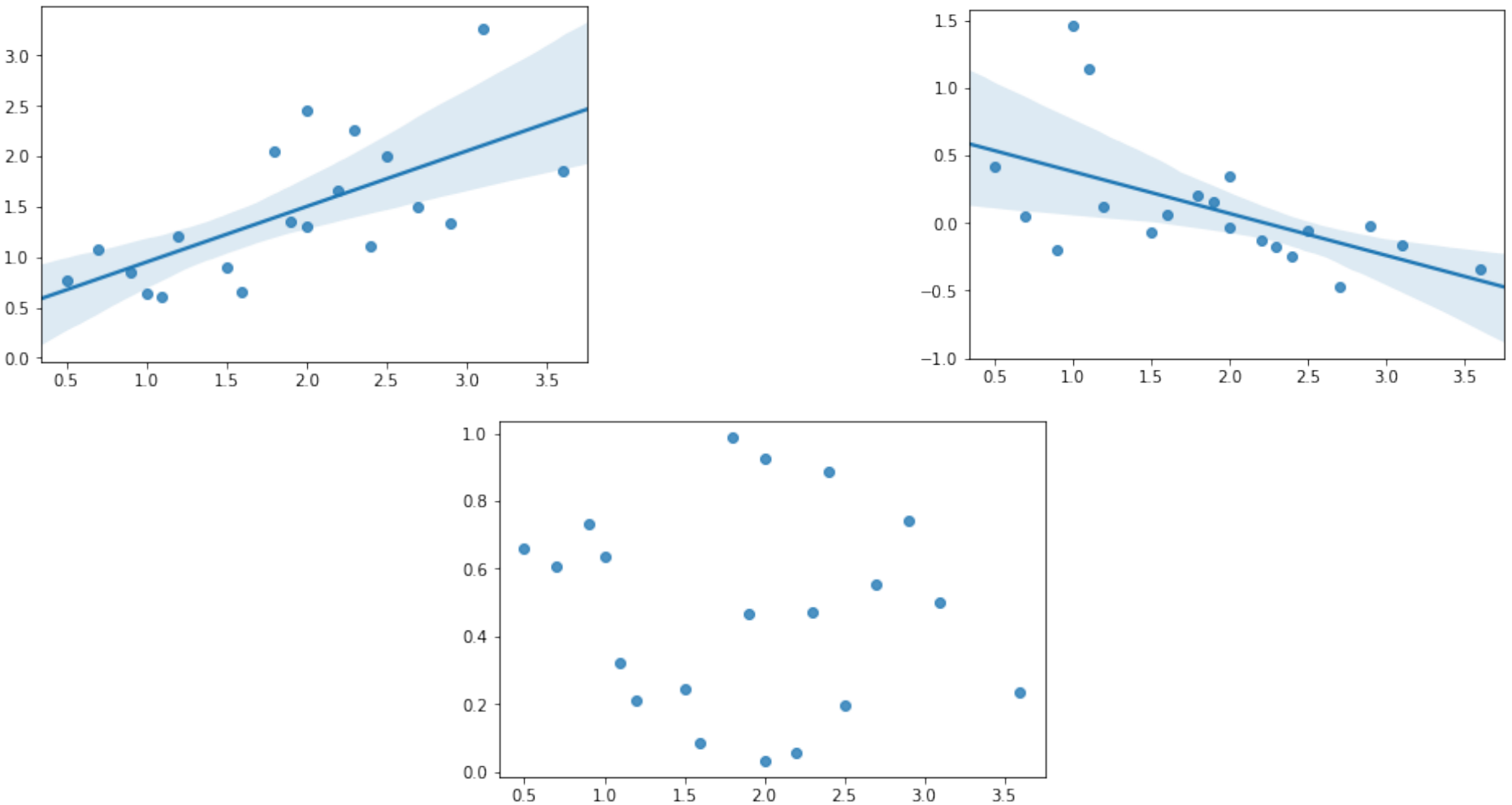


Figure: Positive, negative and zero covariance

Covariance Matrix

- Covariance matrix of $X \in \mathbb{R}^{N \times D}$

$$\Sigma = \begin{pmatrix} Var(X_1) & Cov(X_1, X_2) & \dots & Cov(X_1, X_D) \\ Cov(X_2, X_1) & Var(X_2) & \dots & Cov(X_2, X_D) \\ \vdots & \vdots & \vdots & \dots \\ Cov(X_D, X_1) & Cov(X_D, X_2) & \dots & Var(X_D) \end{pmatrix} \quad (1)$$

- For centered data: $\Sigma = \frac{1}{N} X X^T$ where X is re-constructed by subtracting every column by its mean $X_i = X_i - \bar{X}_i$.

Example Dataset

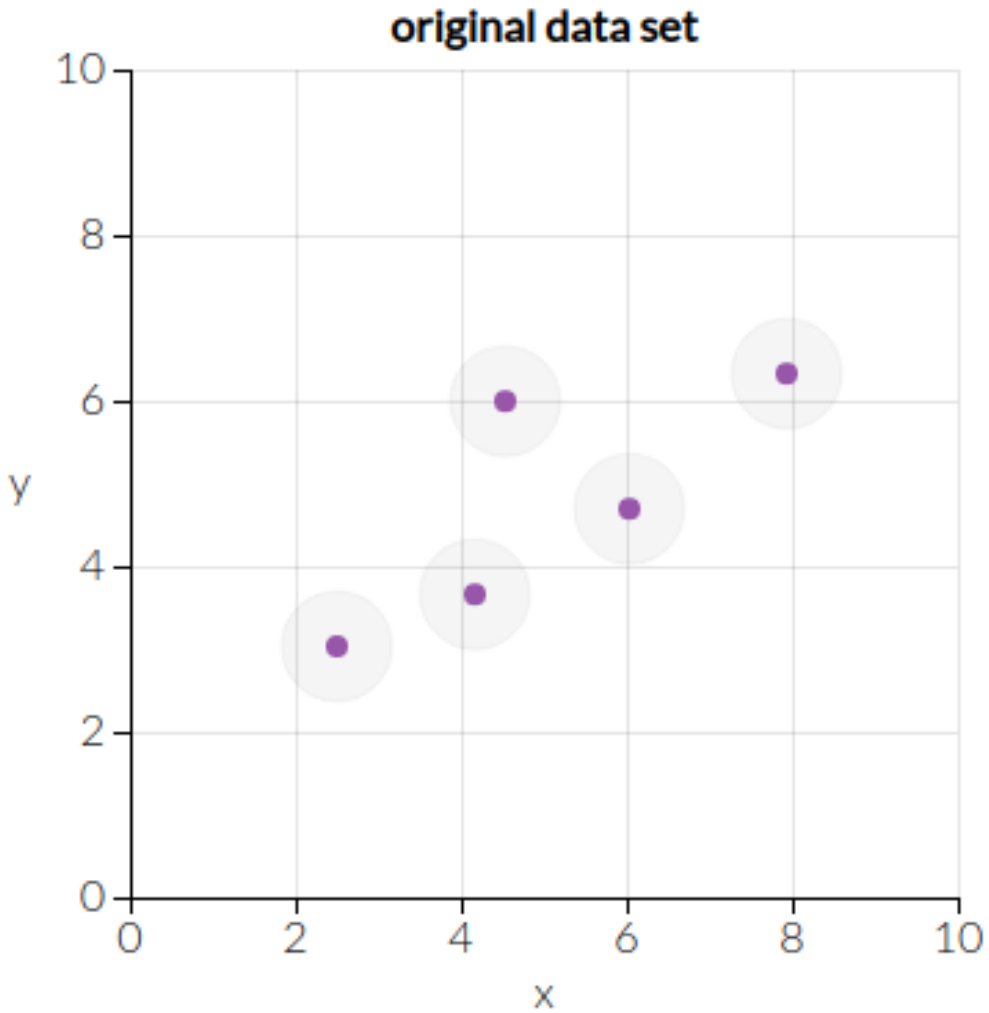


Figure: Sample data points in 2D

Example Dataset - X, Y coordinates

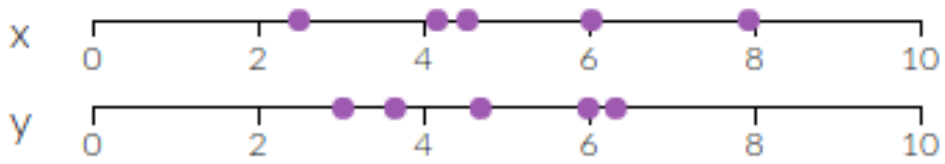


Figure: Sample data points in 2D

Example Dataset - Projections

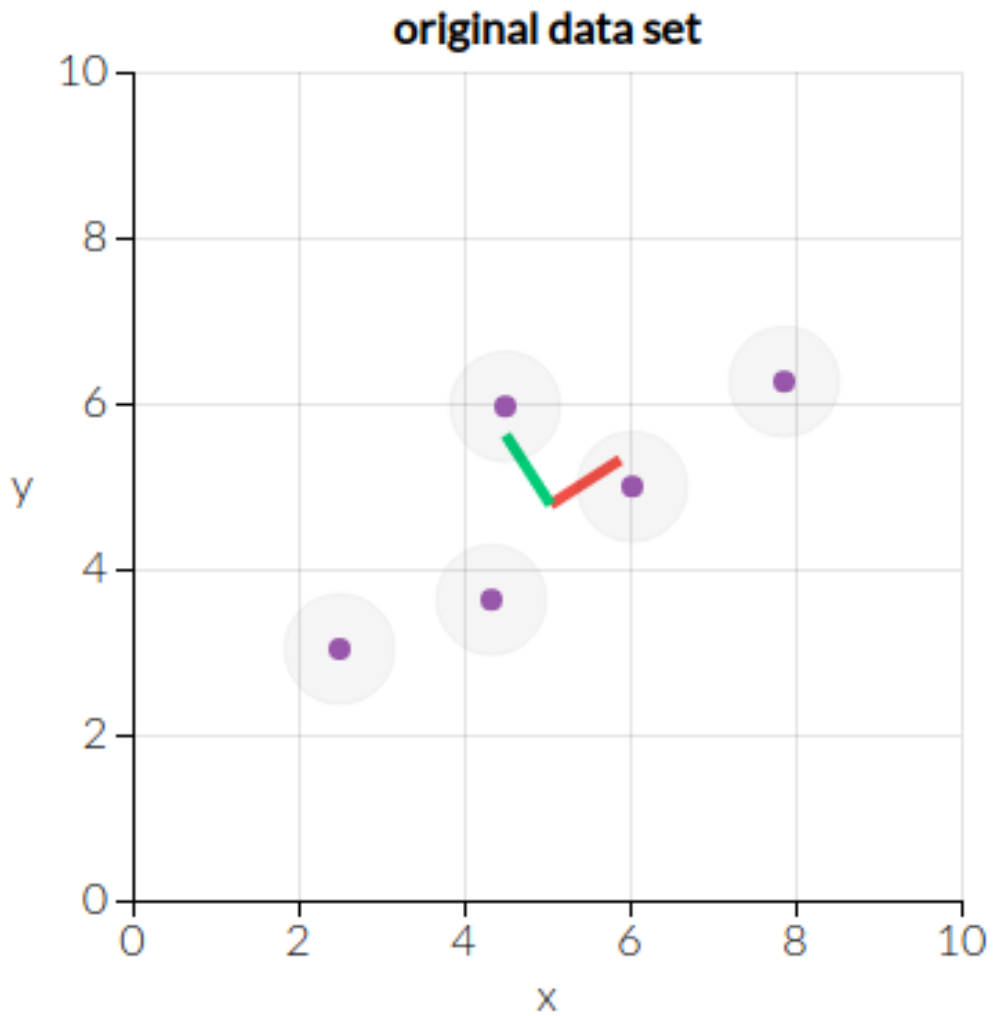


Figure: PCA of sample data points in 2D

Principal Component Analysis (PCA)

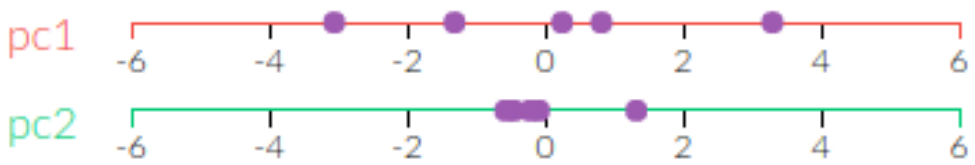


Figure: PCA of sample data points in 2D

Principal Component Analysis (PCA)

- Algebraically, principal components are particular linear combinations of the p random variables $X_1, X_2, ..., X_D$.
- Geometrically, these linear combinations represent the selection of a new coordinate system obtained by rotating the original system.

Principal Component Analysis (PCA)

- Let $X \in \mathbb{R}^{N \times D}$ is the original data matrix with N samples and D measurements.
- Consider the linear combinations:

$$\begin{aligned} Y_1 = w_1^T X \quad &= w_{11}X_1 + w_{12}X_2 + ... + w_{1D}X_D \\ Y_2 = w_2^T X \quad &= w_{21}X_1 + w_{22}X_2 + ... + w_{2D}X_D \\ &\vdots \\ Y_D = w_D^T X \quad &= w_{D1}X_1 + w_{D2}X_2 + ... + w_{DD}X_D \end{aligned} \tag{2}$$

where $w \in \mathbb{R}^{D \times D}$

Principal Component Analysis (PCA)

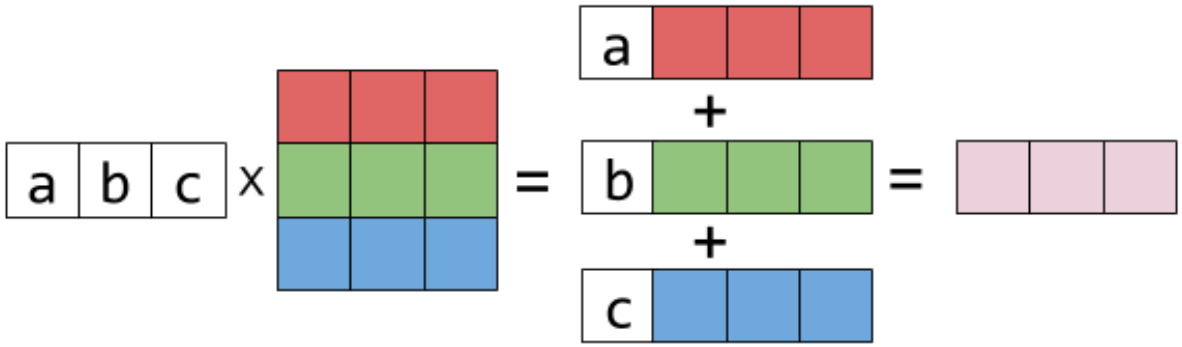


Figure: Matrix multiplication visualization, source: eli.thegreenplace.net

Principal Component Analysis (PCA)

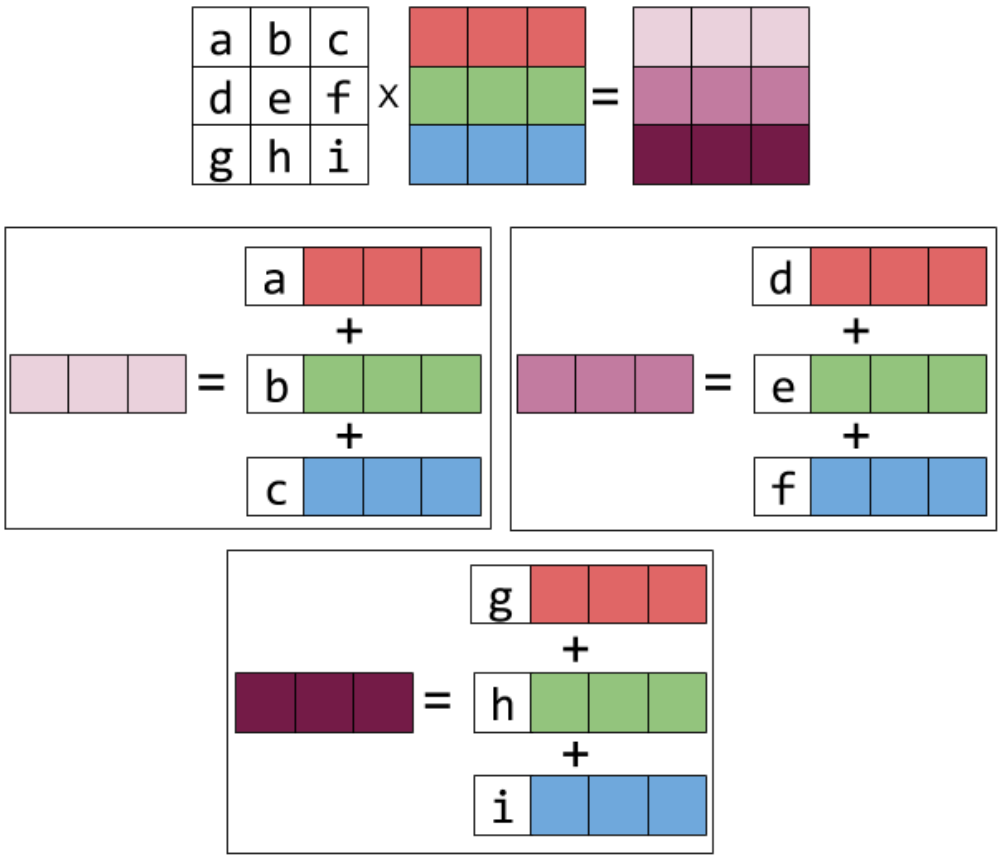


Figure: Matrix multiplication visuallization, source: eli.thegreenplace.net

The important point to note is that the variance of any linear combination can be computed using the covariance matrix of the data:

$$
\begin{aligned}
Var(Y_i) &= \frac{1}{N}\left(\sum_j X_j w_i\right)^2 \\
&= \frac{1}{N}(Xw_i)^T(Xw_i) \\
&= \frac{1}{N} w_i{}^T X^T X w_i \\
&= w_i{}^T \frac{X^T X}{N} w_i \\
&= w_i{}^T \Sigma w_i
\end{aligned}
\tag{3}
$$

Principal Component Analysis (PCA)

- Principal components are those linear combinations $Y_1, Y_2, ..., Y_D$ whose variances are as large as possible.
- First principal component: Linear combination $w_1^T X$ that maximize $Var(w_1^T X)$ subject to $||w_1||_2^2 = 1$
- Second principal component: Linear combination $w_2^T X$ that maximize $Var(w_2^T X)$ subject to $||w_2||_2^2 = 1$ and $w_2^T w_1 = 0$
- ith principal component: Linear combination $w_i^T X$ that maximize $Var(w_i^T X)$ subject to $||w_i||_2^2 = 1$ and $w_i^T w_k = 0$ for $k < i$

First Principal Component Analysis (PC1)

For the first principal component, we maximize:

$$Var(Y_1) = w_1^T \Sigma w_1 \tag{4}$$

subject to:

$$w_1^T w_1 = 1 \tag{5}$$

First Principal Component Analysis (PC1)

Using the Lagrange function:

$$\mathcal{L} = w_1^T \Sigma w_1 + \lambda_1 (1 - w_1^T w_1) \tag{6}$$

Taking the partial derivative of $\mathcal{L}$ with respect to w_1, λ_1:

$$\frac{\partial}{\partial w_1} \mathcal{L}(w_1, \lambda_1) = 2\Sigma w_1 - 2\lambda_1 w_1 = 0 \tag{7}$$

$$\frac{\partial}{\partial \lambda_1} \mathcal{L}(w_1, \lambda_1) = 1 - w_1^T w_1 = 0 \tag{8}$$

First Principal Component (PC1)

From Eq (7), we get that:

$$\Sigma w_1 = \lambda_1 w_1 \tag{9}$$

This implies w_1 is an eigenvector of Σ and λ_1 is the corresponded eigenvalue.
Multiply each side of 9 to w_1^T, we've got:

$$w_1^T \Sigma w_1 = Var(w_1^T X) = \lambda_1 w_1^T w_1 = \lambda_1 \tag{10}$$

So $Var(w_1^T X)$ is maximized when λ_1 is the largest eigenvalue of Σ.

Second Principal Component (PC2)

For the second principal component, we maximize:

$$Var(Y_2) = w_2^T \Sigma w_2 \tag{11}$$

subject to:

$$w_2^T w_2 = 1 \tag{12}$$

$$w_1^T w_2 = 0 \tag{13}$$

Second Principal Component (PC2)

Lagrangian of the problem 11:

$$\mathcal{L} = w_2^T \Sigma w_2 + \lambda_2(1 - w_1^T w_1) + \beta w_1^T w_2 \tag{14}$$

Taking the partial derivative of $\mathcal{L}$ with respect to w_1, λ_1, β:

$$\frac{\partial}{\partial w_2}\mathcal{L}(w_2, \lambda_2, \beta) = 2\Sigma w_2 - 2\lambda_2 w_2 + \beta w_1 = 0 \tag{15}$$

$$\frac{\partial}{\partial \lambda_2}\mathcal{L}(w_2, \lambda_2, \beta) = 1 - w_2^T w_2 = 0 \tag{16}$$

$$\frac{\partial}{\partial \beta}\mathcal{L}(w_2, \lambda_2, \beta) = w_1^T w_2 = 0 \tag{17}$$

Second Principal Component

Multiply each side of (15) with w_1^T:

$$\begin{aligned} 2w_1^T \Sigma w_2 + \beta &= 0 \\ \leftrightarrow 2w_1^T \Sigma w_2 + \beta &= 0 \\ \leftrightarrow 2(\Sigma w_1)^T w_2 + \beta &= 0 \\ \leftrightarrow 2\lambda_1 w_1^T w_2 + \beta &= 0 \\ \rightarrow \beta &= 0 \end{aligned} \tag{18}$$

Second Principal Component (PC2)

- Equation (15) now becomes:

$$\Sigma w_2 = \lambda_2 w_2 \tag{19}$$

- This implies w_2 is an eigenvector of Σ and λ_2 is the corresponded eigenvalue.
- Multiply each side of Eq (9) to w_2^T, we get that:

$$w_2^T \Sigma w_2 = Var(w_2^T X) = \lambda_2 w_2^T w_2 = \lambda_2 \tag{20}$$

- So $Var(w_2^T X)$ is maximized when λ_2 is the second largest eigenvalue of Σ.
- The ith principal component turns out to be obtained by the ith largest eigenvector of Σ.

PCA step by step

1. Compute mean of each column:

$$\bar{X}_i = \frac{1}{N}\sum_{j=1}^{N} X_{ij} \tag{21}$$

2. Subtract mean:

$$X_i = X_i - \bar{X}_i \tag{22}$$

3. Compute covariance matrix:

$$\Sigma = \frac{1}{N} X X^T \tag{23}$$

4. Compute eigenvectors and eigenvalues of Σ: $(\lambda_1, w_1), .., (\lambda_D, w_D)$, $\lambda_1 > \lambda_2 > ... > \lambda_D$
5. Pick K eigenvectors with highest eigenvalues as a matrix: U_K
6. Project original data to selected eigenvectors:

$$\tilde{X} = U_K^T X \tag{24}$$

PCA step by step

PCA procedure

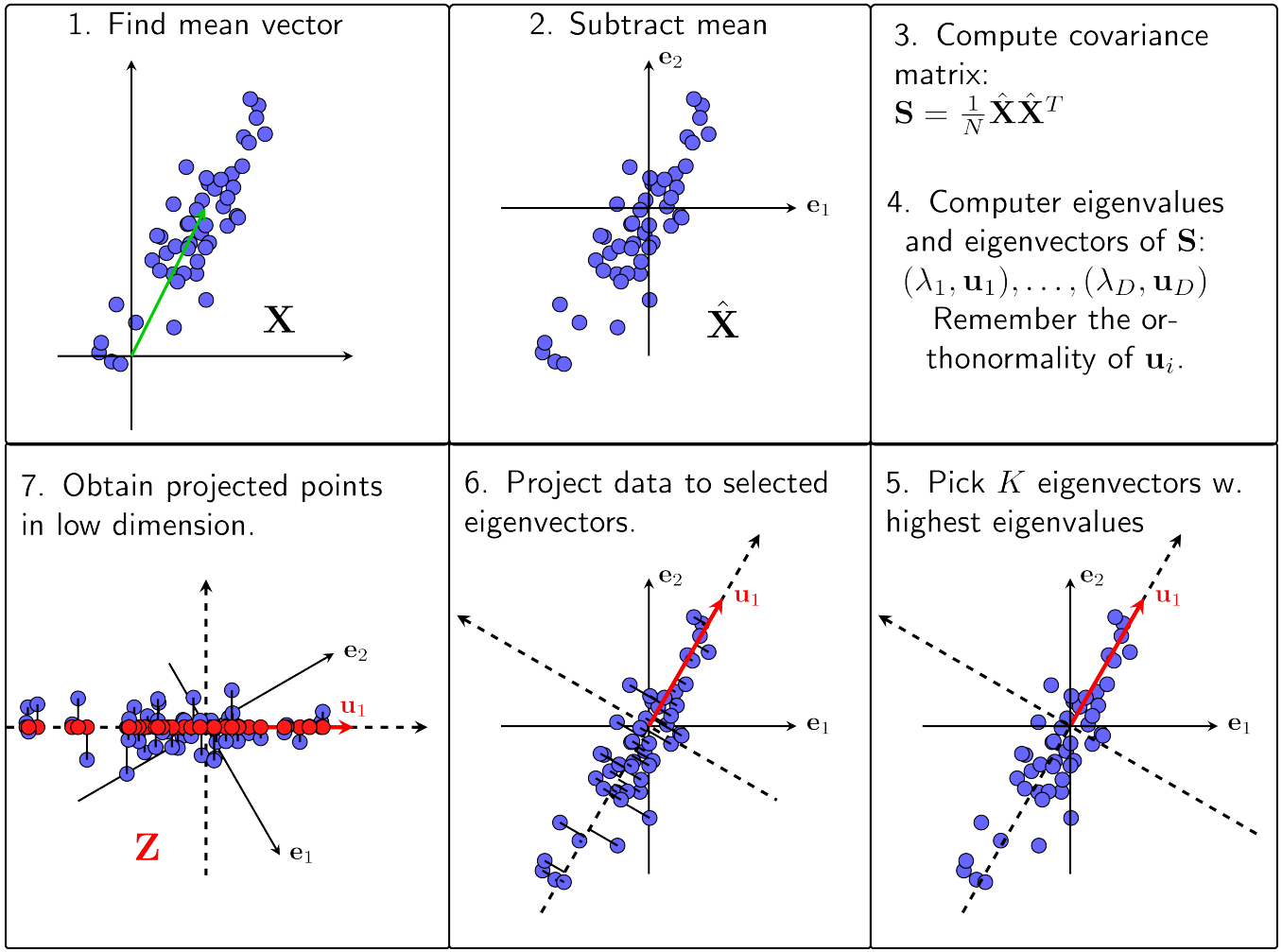


Figure: PCA procedure, source: machinelearningcoban.com

References

[1] Richard Johnson et al, Applied Multivariate Statistical Analysis 6th Edition.
[2] Tiep H. Vu, Principal Component Analysis, https://machinelearningcoban.com/2017/06/15/pca/
[3] OpenAI. (2024). ChatGPT (September 10 Version) [Large language model]. https://chat.openai.com/