PCET's Pimpri Chinchwad College of Engineering
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Machine Learning Laboratory

Mini Project Report

Universal KMeans Clustering Pipeline

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1. Introduction

Clustering is one of the most important unsupervised machine learning techniques used to group similar data points based on patterns and similarities. In this project, we have developed a Universal KMeans Clustering Pipeline that can be applied to any dataset with minimal modifications. This pipeline focuses on automating preprocessing, handling outliers, optimal cluster selection, visualization, and cluster evaluation.

2. Problem Statement

Traditional clustering tasks require manual efforts for data cleaning, outlier removal, feature scaling, and cluster selection. This becomes inefficient for real-world datasets where data quality varies. Our goal is to create a universal clustering solution that can handle any dataset end-to-end using best practices.

3. Objective

1. To design a reusable and automated KMeans Clustering Pipeline.
2. To preprocess data using appropriate imputation and scaling techniques.
3. To remove outliers effectively.
4. To automatically determine the optimal number of clusters.
5. To visualize clusters using PCA.
6. To evaluate clustering performance using Silhouette Score.

4. Literature Review

Several research studies have contributed significantly to the development of clustering techniques, dimensionality reduction, and pipeline-based machine learning systems.

Yadav and Sharma (2024) in their study *"Study Of Existing Methods & Techniques Of K-Means Clustering"* provided a detailed review of the various improvements and applications of K-Means clustering. The paper highlights that while K-Means is simple and widely used, its performance heavily depends on the choice of initial centroids and the number of clusters (K). The study also emphasizes the need for preprocessing techniques and methods to determine the optimal number of clusters.

Further, Olle Olle et al. (2024) in *"Application and Comparison of K-Means and PCA Based Segmentation Models for Alzheimer Disease Detection Using MRI"* demonstrated the use of PCA (Principal Component Analysis) for dimensionality reduction combined with K-Means clustering. Their work proved that applying PCA before clustering can significantly improve clustering performance by removing noise and reducing computational complexity.

In addition, Bagirov et al. (2023) in their research *"Finding Compact and Well-Separated Clusters: Clustering Using Silhouette Coefficients"* focused on evaluating clustering quality using the Silhouette

Score. The paper stressed that Silhouette Coefficient is a reliable metric for validating the separation and compactness of clusters formed using algorithms like K-Means.

Finally, FlyRank (2024) in *"How to Integrate K-Means Clustering in Data Pipelines"* provided a practical guide for building machine learning pipelines with integrated K-Means clustering. The article explained the importance of modular pipeline design, incorporating preprocessing steps, dimensionality reduction (like PCA), and clustering evaluation metrics (like Silhouette Score) to automate and streamline the clustering process for real-world datasets.

These studies collectively provide the foundation for building a robust machine learning pipeline combining preprocessing, dimensionality reduction using PCA, clustering with K-Means, and validation using Silhouette Score.

5. Dataset Description

The dataset used in this project is the *Iris Dataset*, a well-known benchmark dataset in machine learning. It is primarily used for classification and clustering tasks due to its clean structure, numerical features, and clear class separation.The dataset contains a total of 150 samples with 4 continuous numerical features and 1 categorical target variable.

Dataset Characteristics:

- Dataset Name: Iris Dataset
- Total Instances (Rows): 150
- Total Features (Columns): 5 (4 Input Features + 1 Target Variable)
- Data Type: Mixed — Continuous Numerical (Float) & Categorical (String)
- Missing Values: None
- File Format: CSV

Feature Description:

Feature Name	Data Type	Type of Feature	Description	Unit
SepalLengthCm	Float	Continuous	Sepal length of the flower	cm
SepalWidthCm	Float	Continuous	Sepal width of the flower	cm
PetalLengthCm	Float	Continuous	Petal length of the flower	cm
PetalWidthCm	Float	Continuous	Petal width of the flower	cm
Species	String	Categorical	Target class label (Species Name)	-

Class Distribution (Target Variable):

Species	No. of Samples

Iris-setosa	50
Iris-versicolor	50
Iris-virginica	50

6. Methodology

Algorithms Used:

- KMeans Clustering (for unsupervised learning)
- Isolation Forest (for Outlier Detection)
- PCA (for Visualization)

Preprocessing Techniques:

- KNN Imputation for float features
- Custom Integer Imputation for int features
- One Hot Encoding for categorical features
- Robust Scaler for handling outliers in numerical data

APIs / Libraries Used:

- Scikit-learn
- Pandas
- NumPy
- Matplotlib
- Seaborn
- kneed (for Elbow Method)

Performance Metrics:

- Inertia (used in Elbow Method)
- Silhouette Score (for evaluating cluster quality)

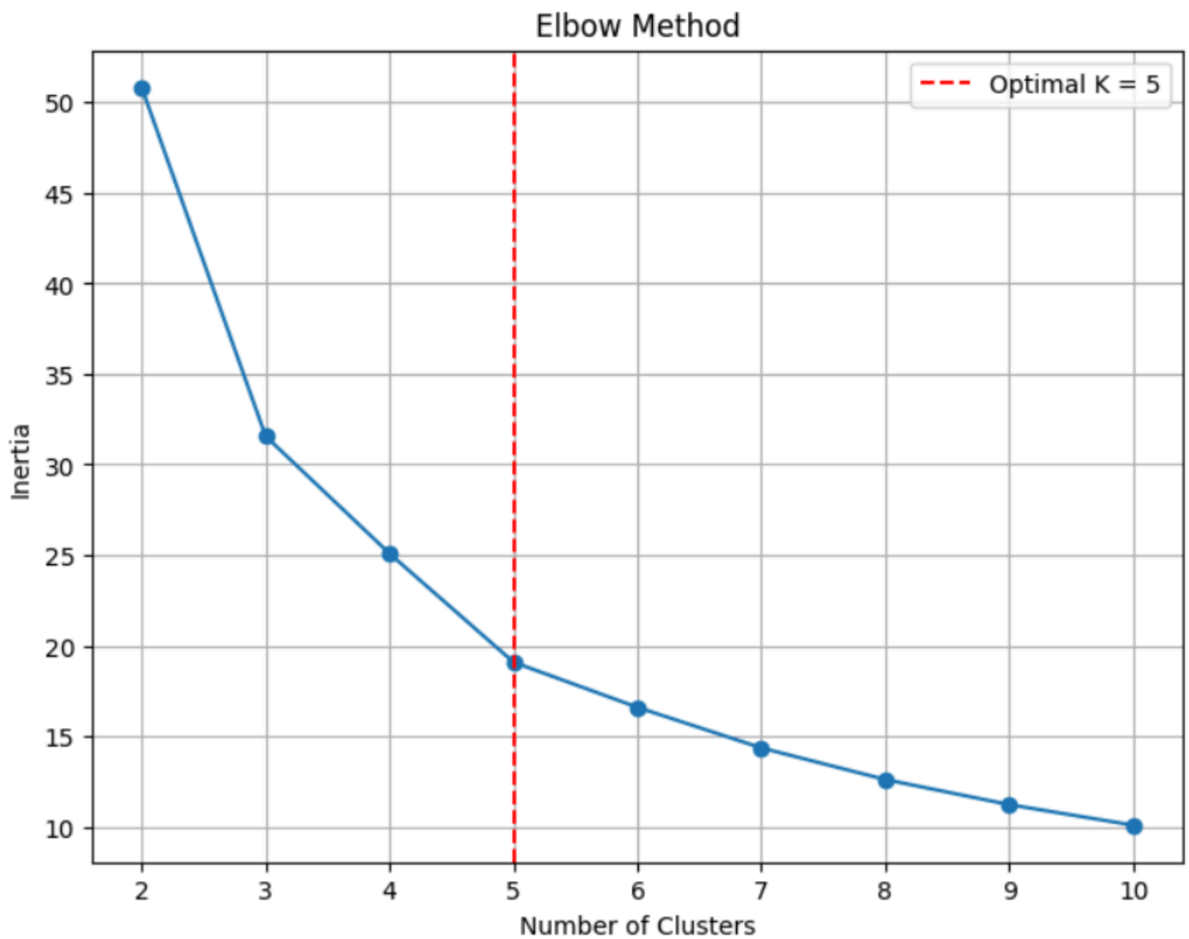
7. Results and Analysis

Outlier Removal:

Isolation Forest successfully detected and removed noisy data points, improving cluster quality.

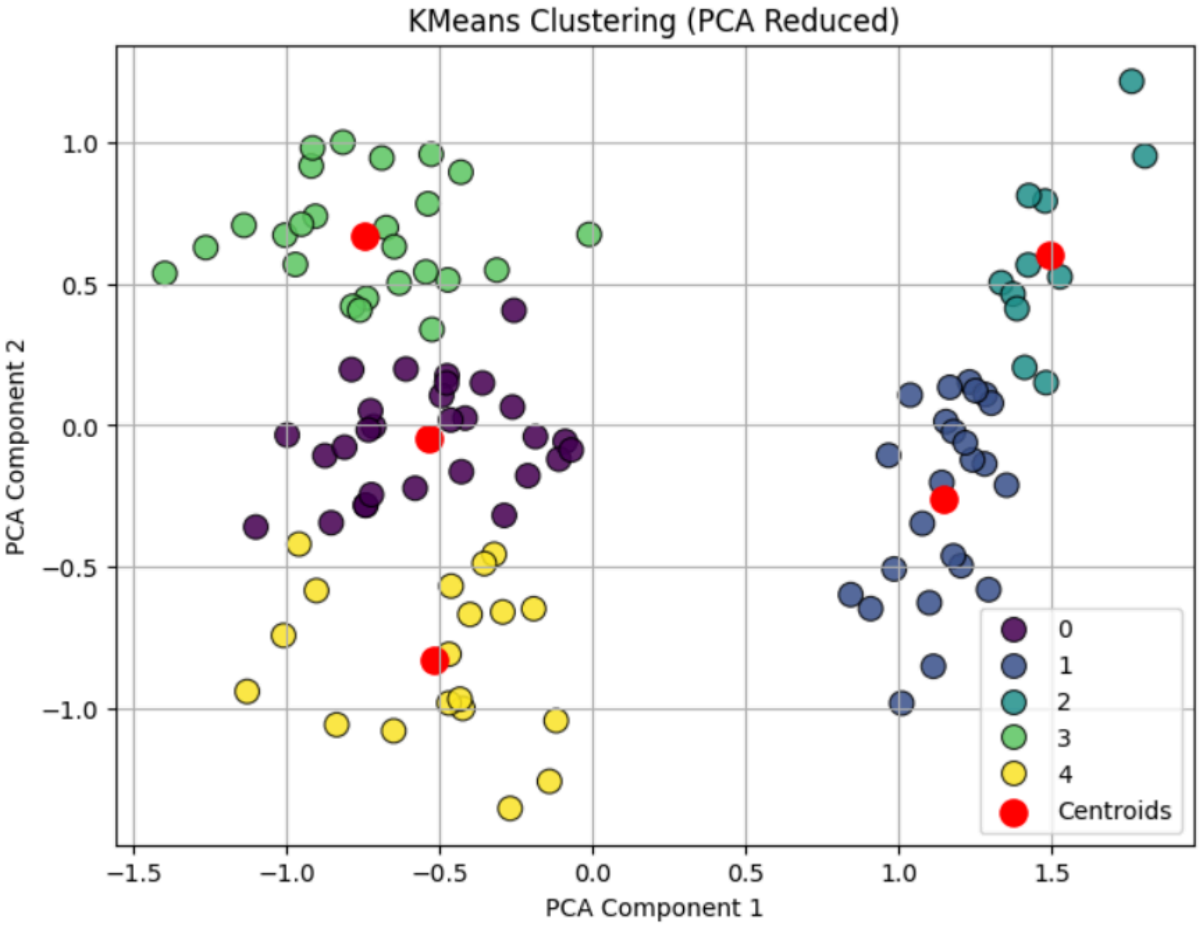
Optimal K Selection:

The Elbow Method was used to find the optimal number of clusters (K) by plotting the WCSS values for different K. The *KneeLocator* library was used to automatically detect the elbow point. Based on this analysis, the optimal number of clusters was found to be $K = 5$.



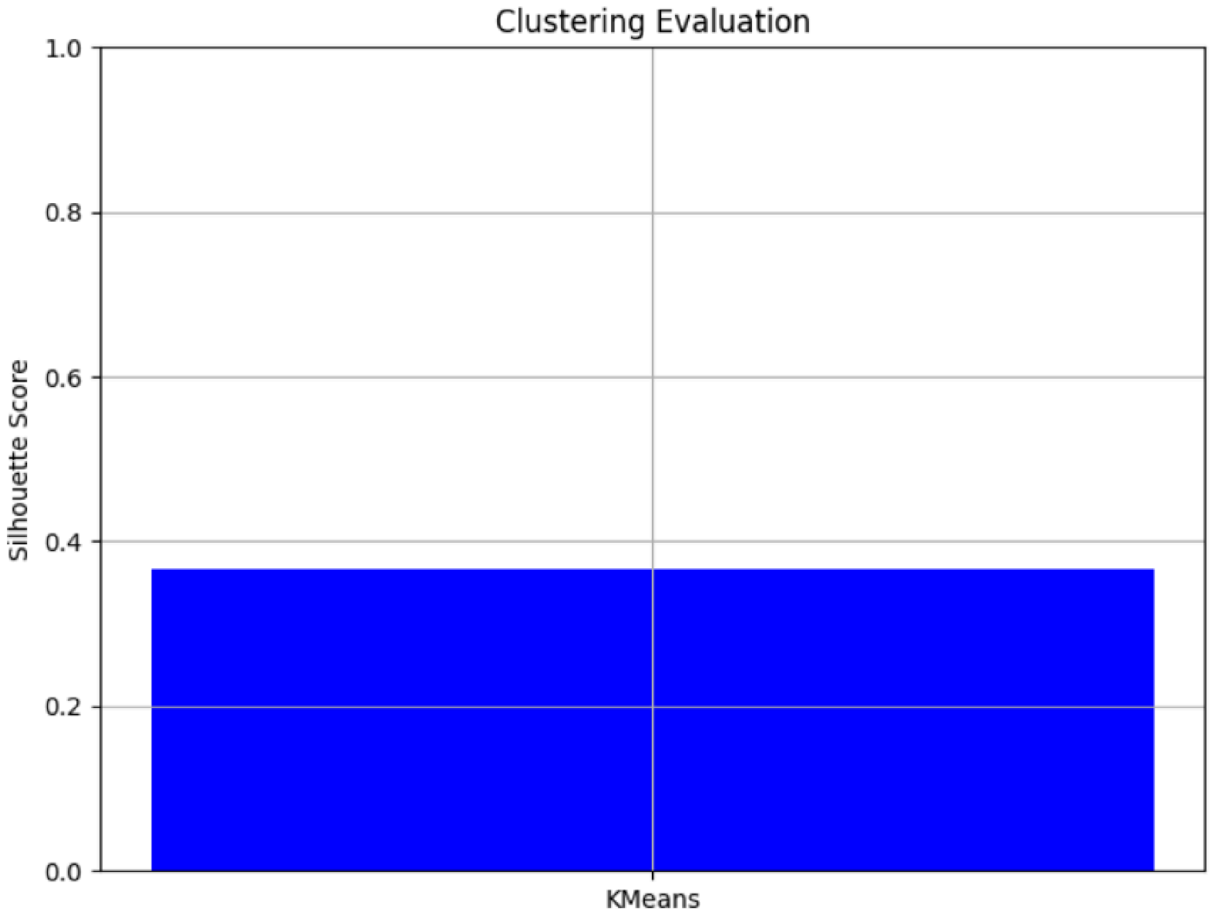
Clustering Visualization:

PCA was applied to reduce the dataset's dimensionality for cluster visualization. The resulting PCA plot showed well-separated and distinct clusters.



Silhouette Score:

Since our score is 0.367, the clustering structure is acceptable but not very strong — which is expected from small or simple datasets like Iris.



8. Conclusion

We successfully built a Universal KMeans Clustering Pipeline capable of handling any dataset in a modular and automated manner. The project highlights the importance of preprocessing, outlier handling, and optimal cluster selection in unsupervised learning tasks.This pipeline can be extended to larger real-world datasets where clustering is required. The methodology ensures minimal manual intervention and can be reused in multiple scenarios.

9. References

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5. Scikit-learn Documentation. *Machine Learning in Python*.
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