A3: Unsupervised learning with PCA, t-SNE, k-means, AHC and SOM

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GITHUB: https://github.com/sebastianbuzdugan/A3-NeuralNetworks

1. Environment and Language:

Programming Language: Python 3.12
Development Environment: Jupyter Notebook in Visual Studio Code This setup provides an interactive environment that's ideal for data exploration, visualization, and running machine learning algorithms.

Core Libraries and Their Uses:

- **Pandas** (pandas): Used for data manipulation and analysis. Ideal for working with structured data, like CSV or Excel files. Functions like reading data, data cleaning, and preprocessing are handled efficiently with Pandas.
- **NumPy** (numpy): Provides support for large, multi-dimensional arrays and matrices. Offers a wide range of mathematical functions to operate on these arrays. Essential for numerical operations and transformations on data.
- **Matplotlib** (matplotlib.pyplot): A comprehensive library for creating static, animated, and interactive visualizations in Python. Used for plotting a wide variety of graphs (like line, bar, scatter, histograms).
- **Seaborn** (seaborn): Based on matplotlib, it provides a high-level interface for drawing attractive and informative statistical graphics. Used for more advanced visualizations, like heatmaps and pair plots.
- **Plotly Express** (plotly.express): A high-level API for rapid data exploration and figure generation. Useful for interactive plots and advanced visualizations.

Machine Learning and Clustering Libraries:

- **Scikit-learn** (sklearn): Provides simple and efficient tools for predictive data analysis. Used for clustering algorithms like KMeans, Agglomerative Clustering, Spectral Clustering, and Affinity Propagation. Also offers tools for data preprocessing (like StandardScaler), dimensionality reduction (like PCA), and model evaluation (like classification_report).

- **SciPy** (scipy.cluster.hierarchy): Used for hierarchical clustering and generating dendrograms.
- **MiniSom** (minisom.MiniSom): An implementation of the Self-Organizing Maps (SOM). Useful for unsupervised learning and data visualization.

2. **Datasets**

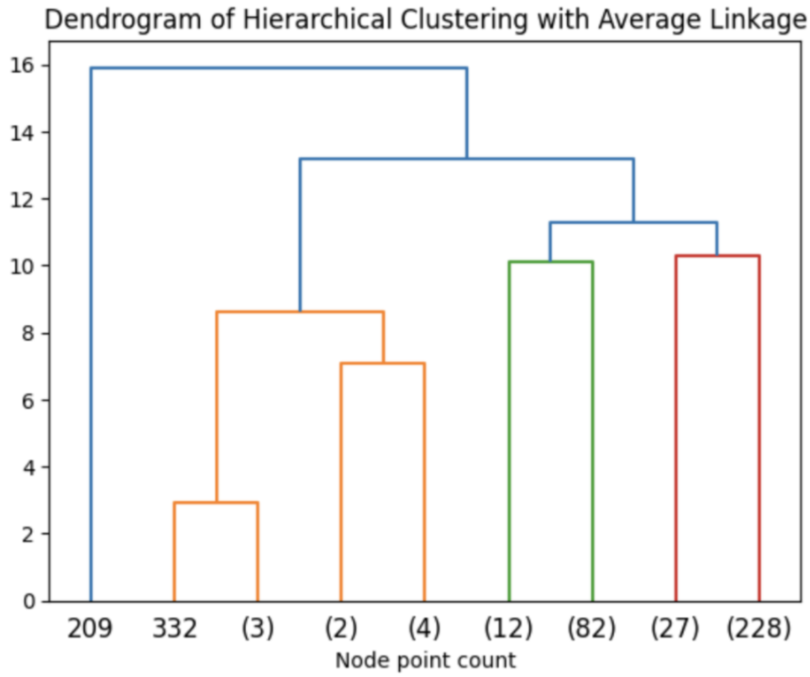
Dataset 1: Synthetic Dataset (A3-data.txt)
The Synthetic Dataset, named 'A3-data.txt', is composed of 4 variables and includes a class attribute. The dataset consists of 360 patterns, offering a rich field for applying unsupervised learning techniques. In this project, the class information is not used for the learning process itself but is crucial for identifying the classes in plots, aiding in the validation and interpretation of the clustering results. Preprocessing steps, such as normalization or standardization, might have been undertaken to prepare the data for effective clustering analysis.

Dataset 2: Dry Bean Dataset (Dry_Bean_Dataset.xlsx) -
https://www.kaggle.com/datasets/muratkokludataset/dry-bean-dataset
The Dry Bean Dataset, housed in 'Dry_Bean_Dataset.xlsx', features 16 distinct physical attributes across 13,611 patterns, categorized into 7 unique classes: 'SEKER', 'BARBUNYA', 'BOMBAY', 'CALI', 'HOROZ', 'SIRA', and 'DERMASON'. Primarily used in unsupervised learning, the class labels facilitate post-analysis validation and visualization of clustering outcomes. Standard preprocessing like normalization ensures balanced contribution from each feature, making this dataset ideal for in-depth unsupervised learning explorations.

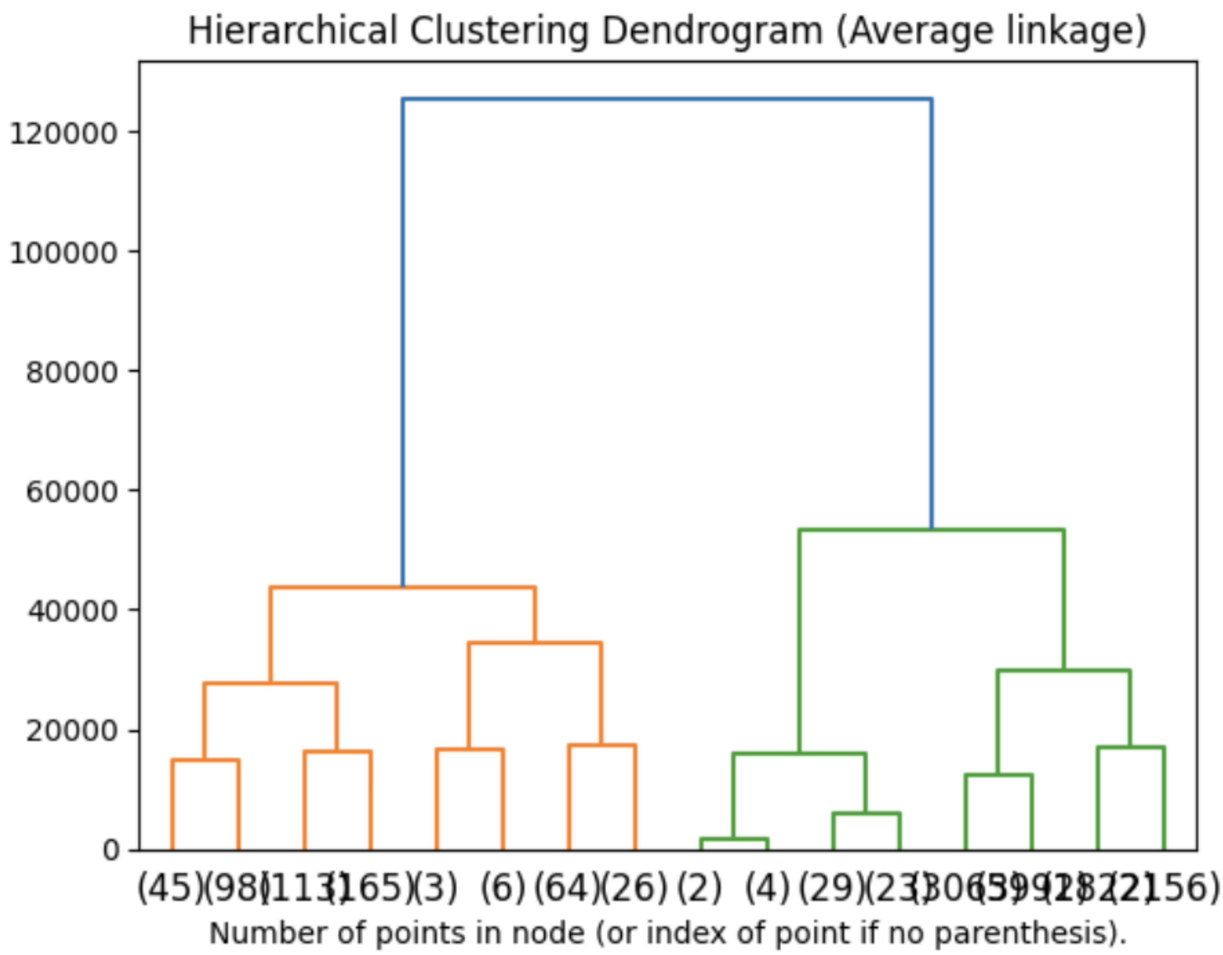
3. **Comparing unsupervised learning algorithms**

Agglomerative Hierarchical Clustering (AHC) is a method of cluster analysis which seeks to build a hierarchy of clusters. It's a "bottom-up" approach: each observation starts as its own cluster, and pairs of clusters are merged as one moves up the hierarchy. This method builds a dendrogram, representing the nested levels of clusters, which aids in understanding the data's structure and deciding the number of clusters by cutting the dendrogram at a suitable level.

Dataset A3-data.txt plot for the average linkage:

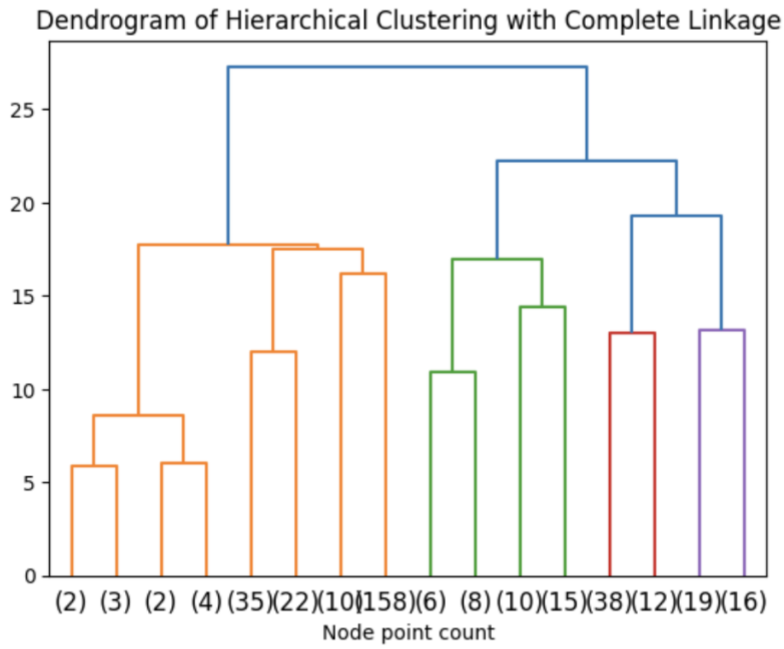


Dataset Dry_Bean_data for the average linkage:

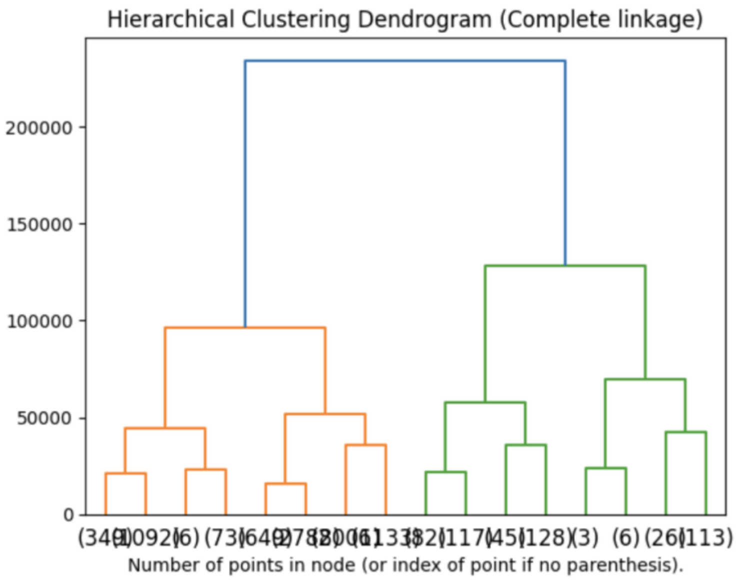


In AHC with average linkage, the Synthetic Dataset (A3-data) demonstrates uniform clustering with merge distances ranging from about 8.03 to 15.91, indicating closely related groups. In contrast, the Dry Bean Dataset exhibits a more complex pattern, with merge distances spanning from approximately 16,247 to 125,455, suggesting a diverse and heterogeneous cluster formation. This comparison highlights the Synthetic Dataset's relative homogeneity and the Dry Bean Dataset's intricate clustering complexity.

Dataset A3-data.txt plot for the complete linkage:



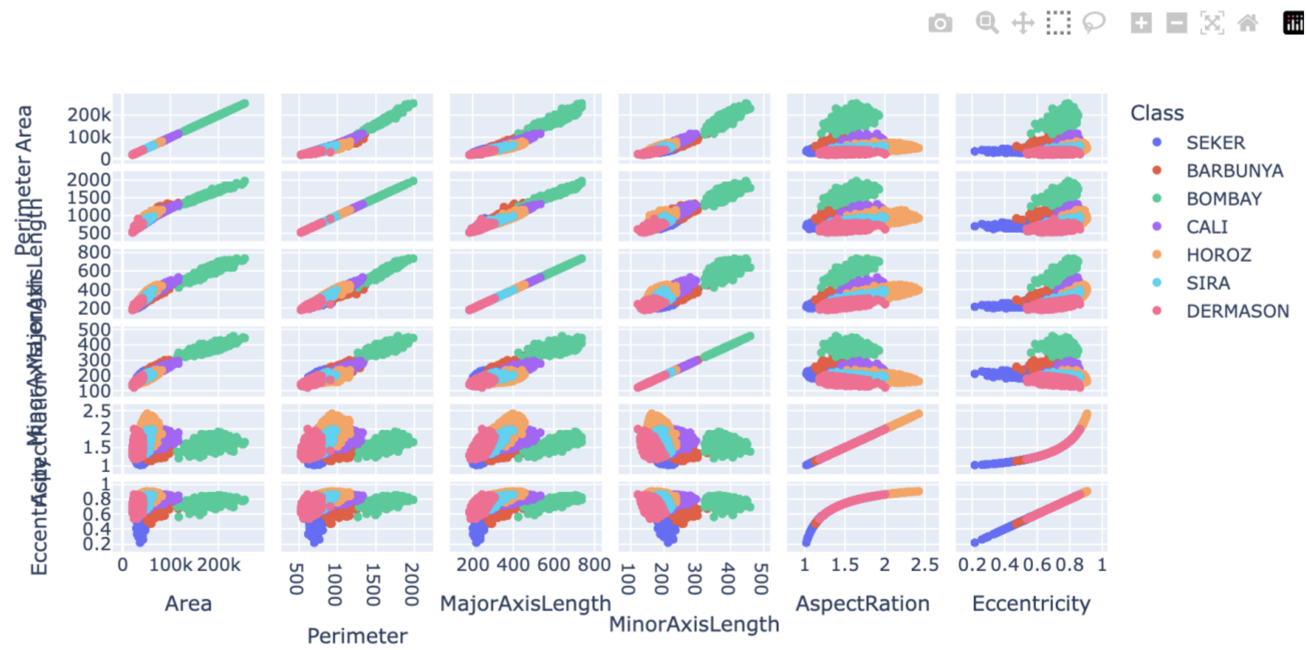
Dataset Dry_Bean_data for the complete linkage:

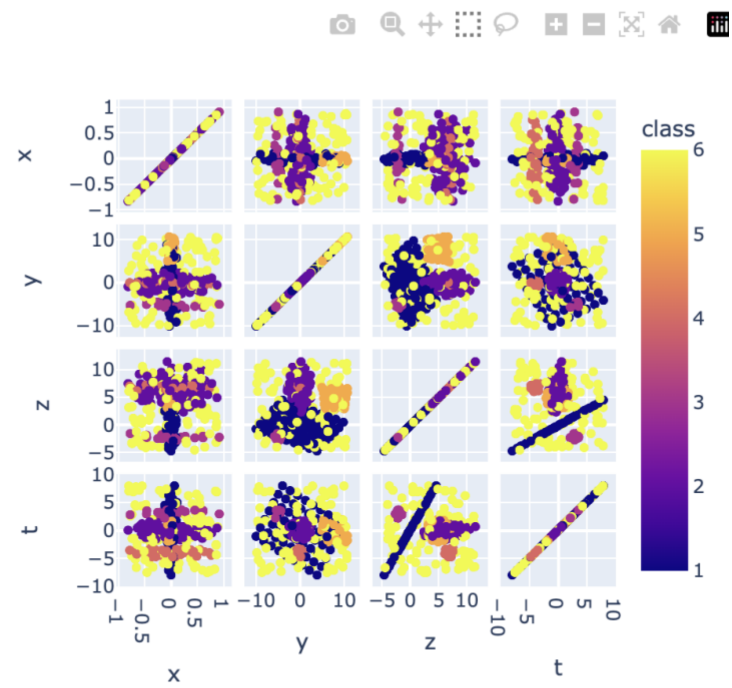


In Agglomerative Hierarchical Clustering with complete linkage, the Synthetic Dataset (A3-data) presents a relatively homogeneous clustering, evident from its merge distances ranging from about 13.15 to 27.31. This range suggests tighter groupings and more similarity within clusters. On the other hand, the Dry Bean Dataset displays a starkly different clustering behavior with merge distances extending from approximately 35,835 to 234,201. These wider merge distances underscore a highly varied and complex data structure, indicating a significant disparity within clusters. This juxtaposition of the Synthetic Dataset's cohesive clustering against the Dry Bean Dataset's diverse and intricate cluster formations accentuates the unique characteristics inherent in each dataset.

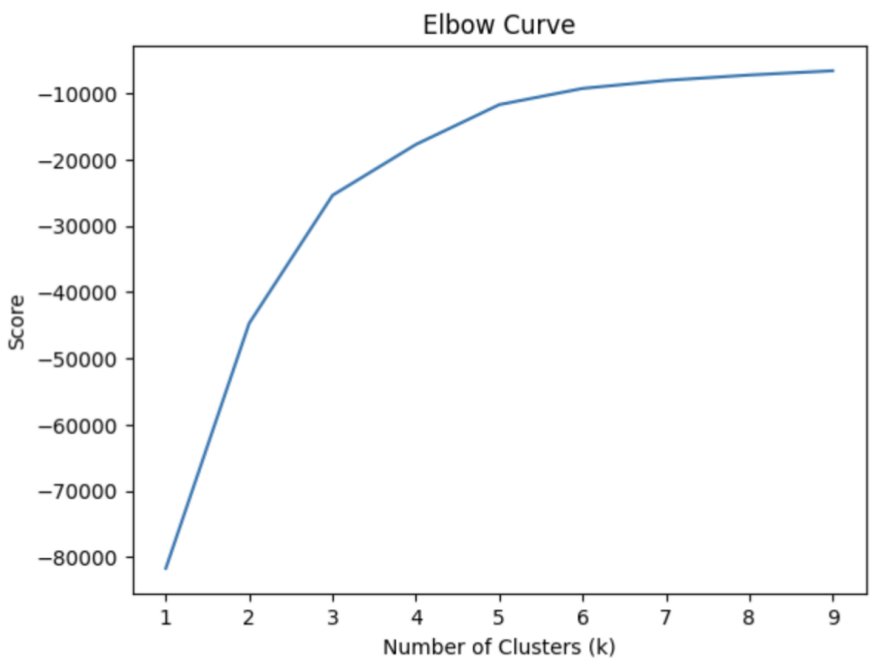
The **K-means** algorithm is a popular unsupervised machine learning technique used for cluster analysis in data mining and statistics. It aims to partition a set of observations into 'k' clusters, where each observation belongs to the cluster with the nearest mean, serving as a prototype of the cluster.

K-means datasets (Dry-Bean vs A3 synthetic):

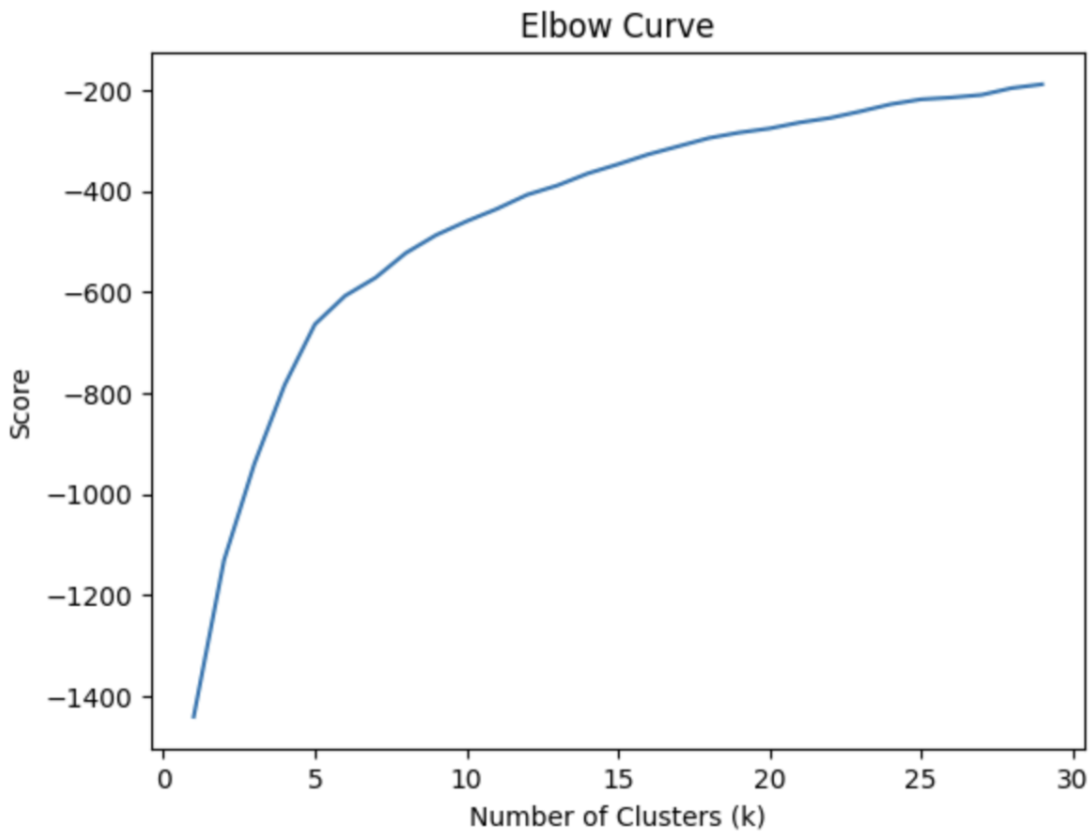




When comparing the K-means clustering results of the Dry Bean Dataset with those of the Synthetic A3 Dataset, several notable differences emerge. The Dry Bean Dataset below, characterized by its physically measured features such as 'Area' and 'Perimeter', exhibits centroids with larger values in a six-dimensional space, indicating a complex clustering pattern reflective of the diverse physical attributes of beans.

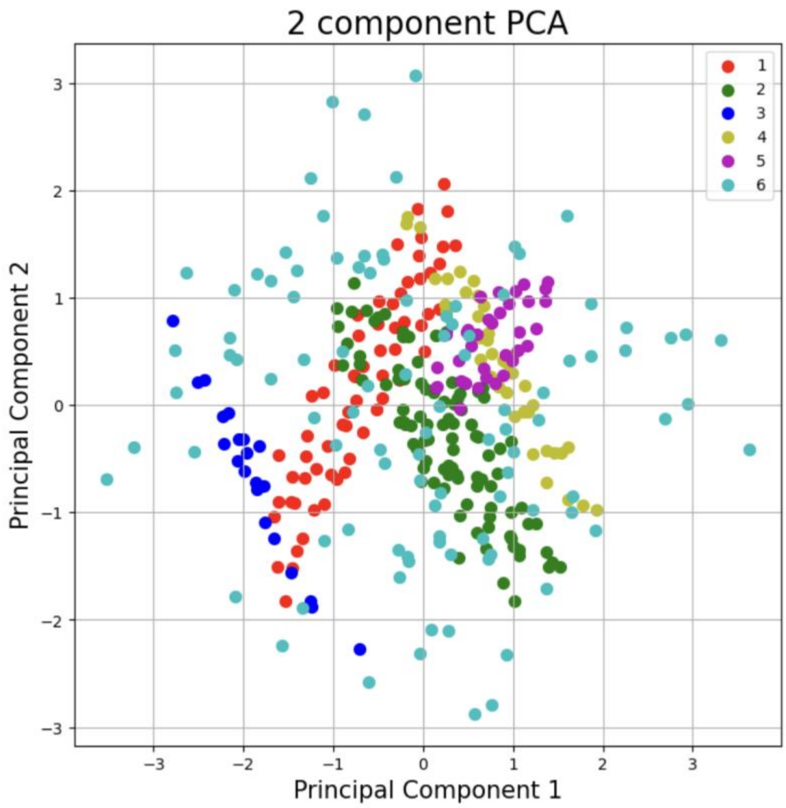


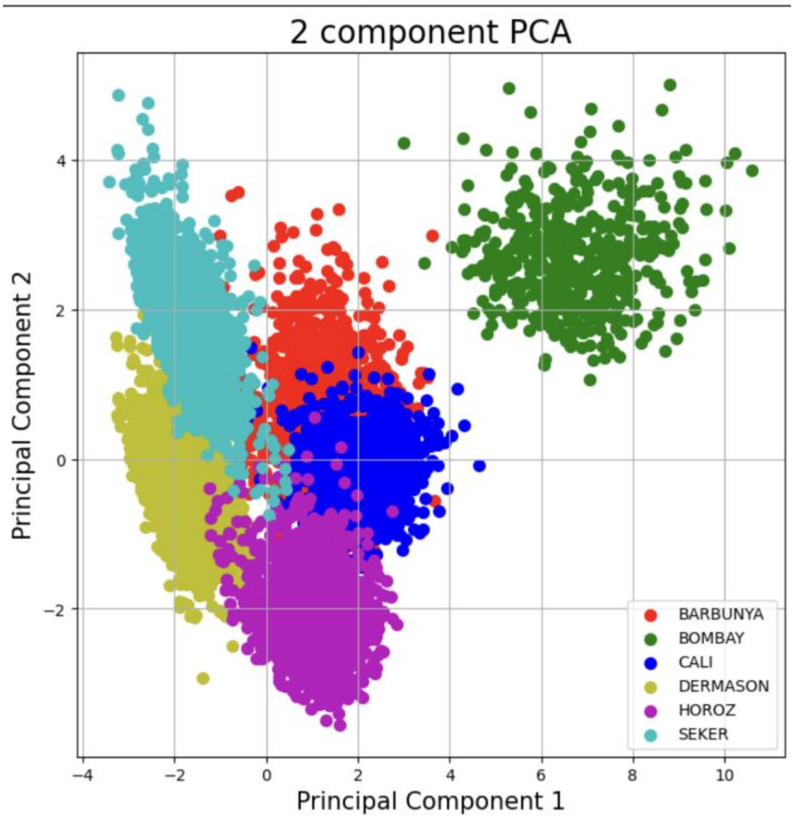
In contrast, the Synthetic A3 Dataset's centroids as can be seen in the figure below, spread across four dimensions, are smaller, suggesting a more normalized or abstract feature space. This difference in scale and dimensionality underlines the distinct nature of the datasets: the Dry Bean Dataset captures real-world physical variations in beans, while the Synthetic A3 Dataset seems to represent synthesized or categorical groupings. The clustering in the Dry Bean Dataset is likely identifying different bean types based on physical traits, whereas in the Synthetic A3 Dataset, it discerns patterns within a more conceptual feature space. Despite these differences, both datasets share a common aspect in the clustering process, where the number of clusters is determined by the unique classes present, providing a structured approach to uncovering inherent groupings in each dataset.



Principal Component Analysis (PCA) is a statistical technique used in the field of machine learning and data analysis to emphasize variation and bring out strong patterns in a dataset. It's often used as a tool in exploratory data analysis and for making predictive models. PCA is commonly used for dimensionality reduction by transforming a large set of variables into a smaller one that still contains most of the information in the large set.

2D Projection of the A3-data vs Dry_Bean_Dataset:

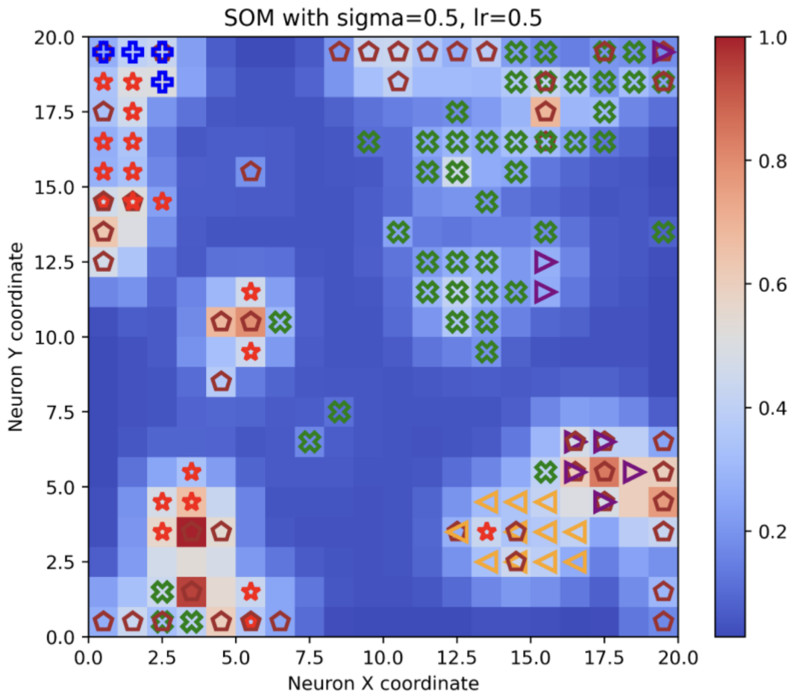


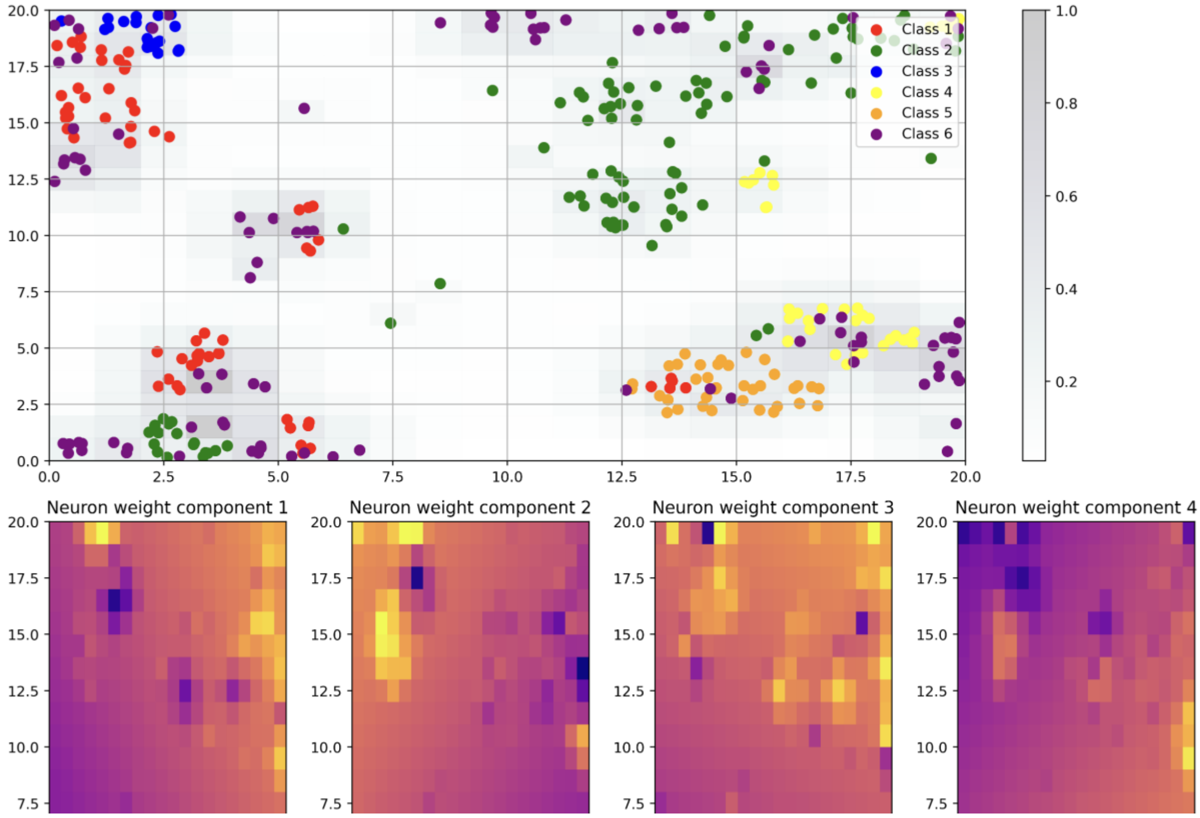


- **Dataset Complexity and Scale:** The Dry Bean Dataset (2nd one) is substantially larger and more complex, with a higher number of classes and a broader range of features compared to the Synthetic A3 Dataset (1st one).
- **PCA Distribution:** The spread of PCA values in the Dry Bean Dataset might be more dispersed due to the dataset's complexity and the variety of physical characteristics of beans. In contrast, the Synthetic A3 Dataset, with fewer data points and classes, might show a more compact distribution in the PCA-transformed space.
- **Insights Gained:** PCA effectively reduces the dimensionality of both datasets while retaining the essential variance. For the Synthetic A3 Dataset, this could mean capturing synthesized or transformed features, while for the Dry Bean Dataset, it involves distilling key physical attributes of different bean types.

Self-Organizing Maps (SOM), also known as Kohonen maps, are a type of unsupervised neural network algorithm used for data visualization and dimensionality reduction. Developed by Teuvo Kohonen in the 1980s, SOMs enable the visualization of complex, high-dimensional data in a lower-dimensional (typically two-dimensional) space. They are particularly useful for identifying inherent patterns, clustering, and feature mapping in the data.

SOM plots for A3-text compared to the Dry_Bean_Dataset:

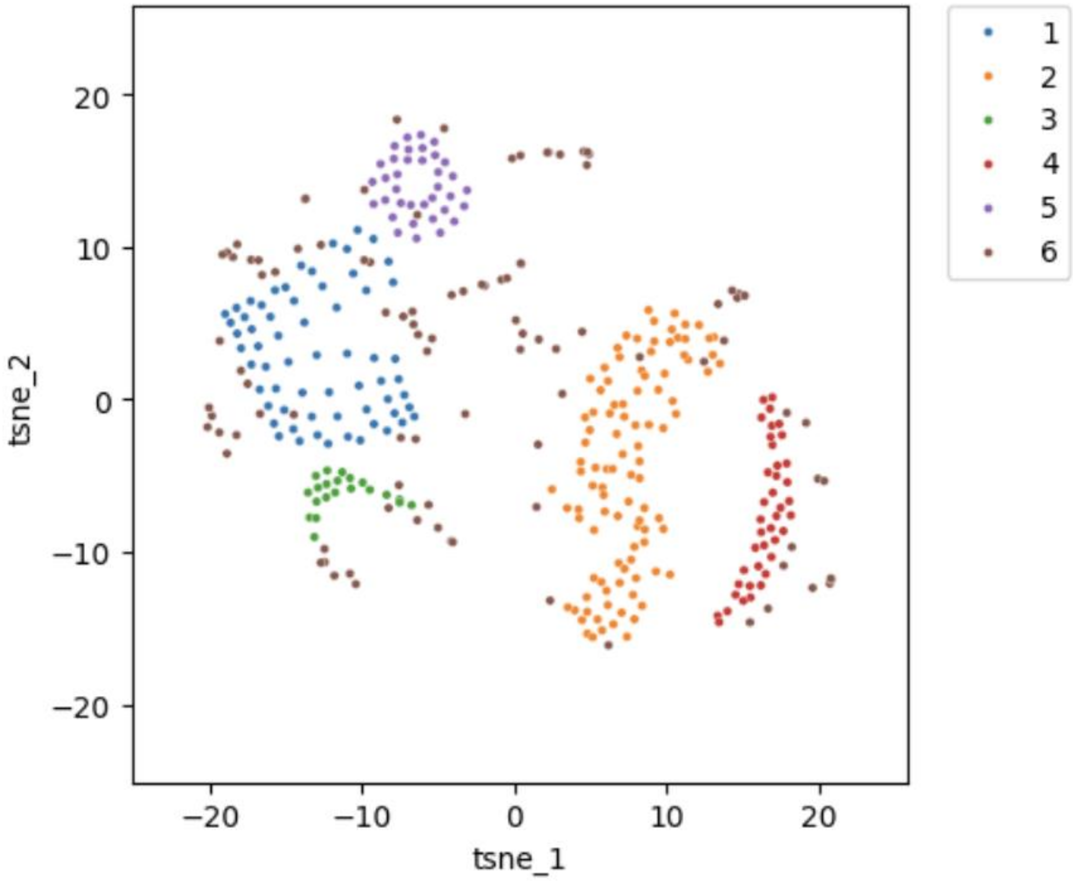


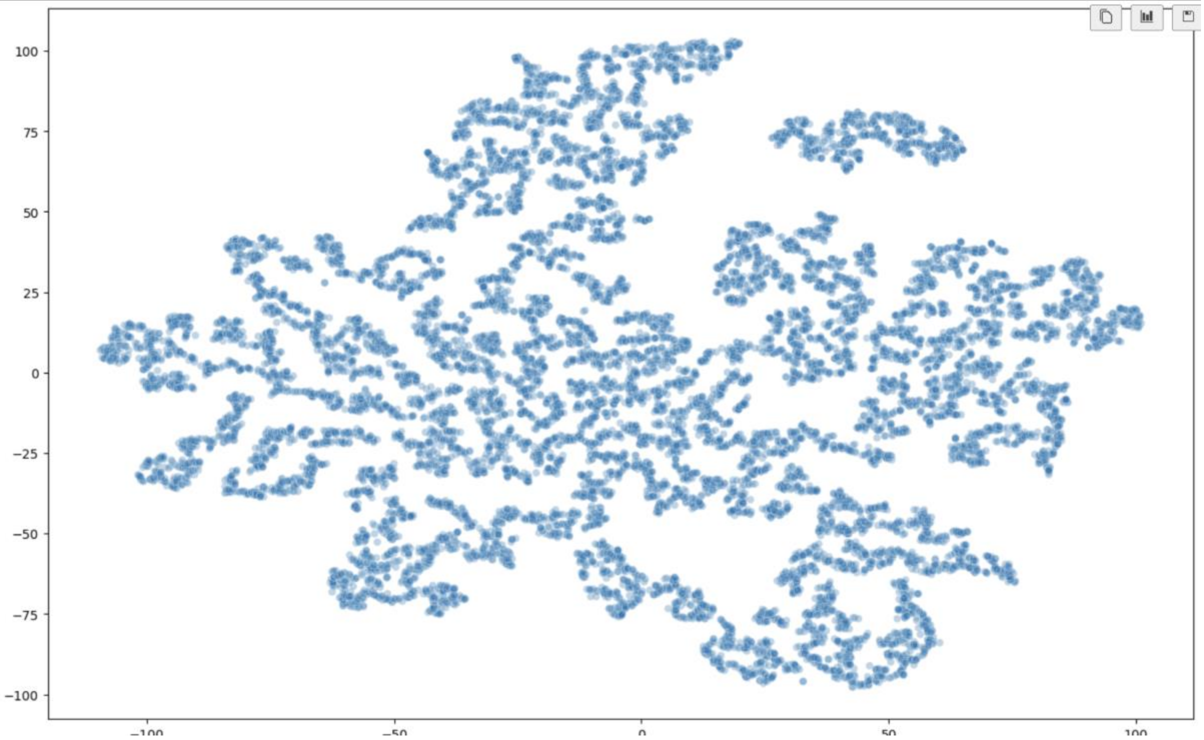


t-SNE (t-Distributed Stochastic Neighbor Embedding) is known for being computationally intensive and sometimes slow, especially on large datasets. However, if you're experiencing an unusually long or seemingly endless loop, it might be due to the size of the dataset or the specific parameters of t-SNE.

Computation Time: The dry bean dataset takes significantly longer (around 61 seconds) to process with t-SNE compared to the A3-text synthetic dataset (around 0.96 seconds). This difference is largely due to the difference in the number of samples.
Mean Sigma: The mean sigma (bandwidth) for the dry bean dataset is 0.066541, much smaller than the mean sigma for the A3-text synthetic dataset, which is 0.692581. A smaller sigma in the dry bean dataset suggests that the data points are more densely packed or that there's less variability in the distances between points.
KL Divergence: The final KL divergence after 1000 iterations for the dry bean dataset is 0.858700, and for the A3-text dataset, it is 0.481037. A lower KL divergence indicates a better fit of the t-SNE model to the data. This suggests that t-SNE may have been able to find a more coherent structure in the A3-text dataset than in the dry bean dataset.
Visualization and Interpretation: The final aspect, which is crucial for t-SNE, is how the data is visually represented in the 2D space and how well the t-SNE results capture the underlying structure of the data. Different datasets can lead

to very different visualizations, with some showing clear clusters while others might display more overlap or less distinct groupings.





It's important to note that t-SNE is a stochastic algorithm, meaning it can produce slightly different results every time it's run, especially if the perplexity and learning rate parameters are changed. The interpretation of t-SNE results relies heavily on visual inspection and should be done with an understanding of the dataset's characteristics and the algorithm's nature.