



Gesture Recognition Reading Muscle Activity

Project Phase 3 - Dimensionality Reduction, Clustering and Evaluation

DS5230 / Spring 2024 Semester

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Apr 20, 2024

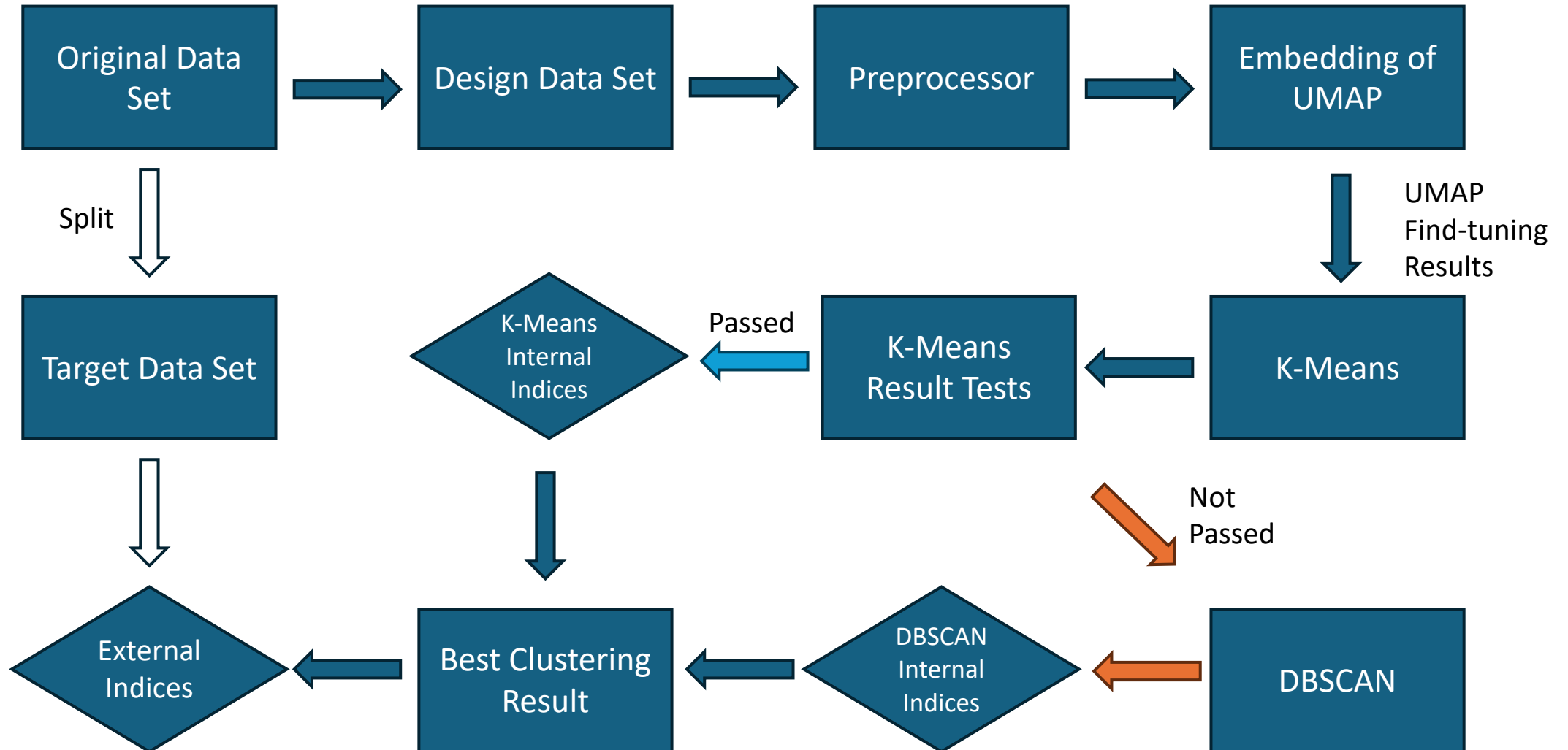
Reproducibility

All works are completed within Jupyter Notebooks and have been fully executed.

To reproduce:

- Download the **environment.yml** and recreate **project_venv** conda environment.
- Download supported python modules.
 - **processing.py**
 - **clustering.py**
 - **validation.py**
- Download Jupyter Notebooks.
 - **project_phase_3_clustering_pipeline.ipynb**
 - **project_phase_3_optimization.ipynb** (takes super long time to execute)
 - **project_phase_3_afd.ipynb** (takes long time to execute)
 - **project_phase_3_validation.ipynb**
- Open notebooks in browser, click **restart the kernel and rerun all cells** button to reproduce all works.
- HTML versions of the fully executed Jupyter Notebooks have also been provided.

Clustering Pipeline

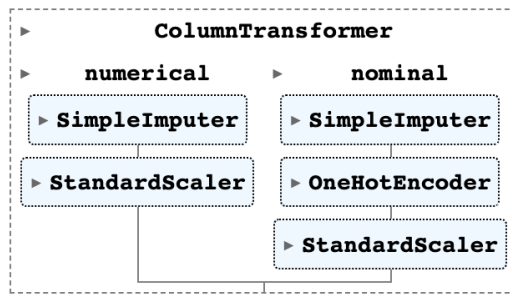


Clustering Pipeline: Updates

- This part extends the clustering pipeline from **assignment_4** and the **midterm exam**, with some errors fixed:
 - The **metric** parameter of **Trustworthiness** is now the same as **UMAP**.
 - The **metric** parameter of **Validity Index** is now the same as **DBSCAN**.
- Preprocessors such as imputers and scalers are added.

```
preprocessor = processing.get_default_preprocessor(NUMERICAL_ATTRS, NOMINAL_ATTRS)
preprocessor
```

Executed at 2024.04.21 20:33:06 in 13ms



```
twness = trustworthiness(  
    X=squareform(pdist(cap_x_df_copy)),  
    X_embedded=squareform(pdist(embedding)),  
    metric=metric  
)
```

```
validity_index = dbcv_hdbscan.validity_index(  
    X=embedding_copy.astype(np.float64),  
    labels=dbscan.labels_,  
    metric=metric  
)
```

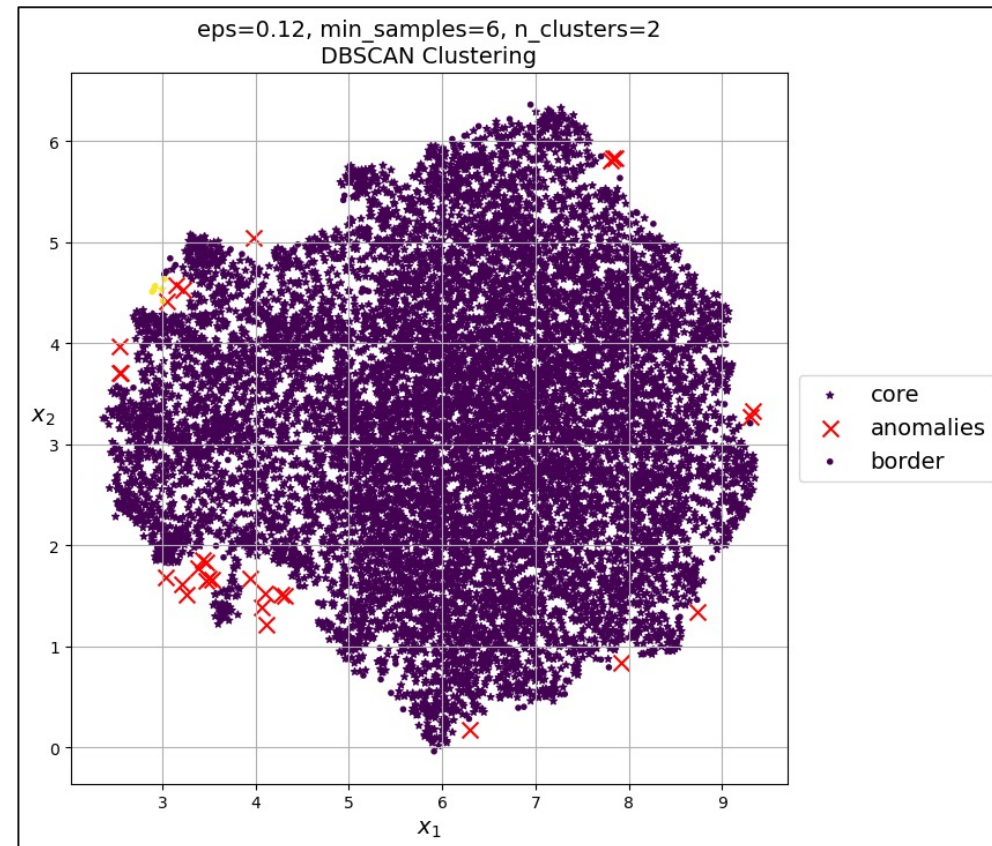
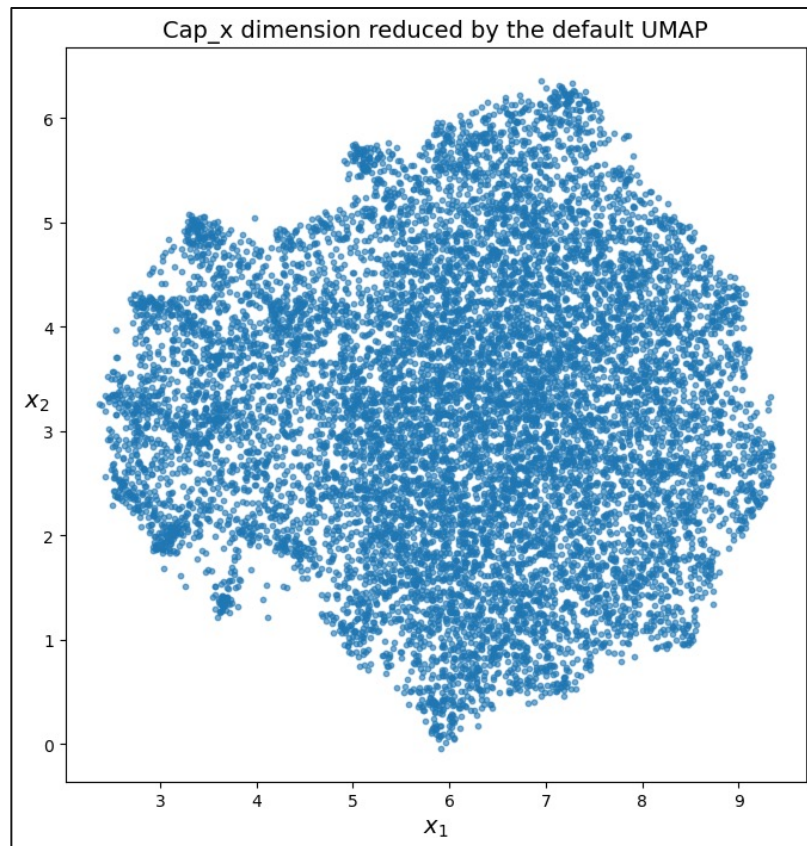
Clustering Pipeline: Default Result

- In the pipeline notebook, we tested the clustering with all default parameters of UMAP and K-means algorithm. This result is clearly not good, but it can at least be used as a baseline for the following pipeline optimization and validation.

silhouette_score_or_validity_index

Executed at 2024.04.21 20:37:05 in 1ms

-0.758095789387558



Clustering Pipeline Optimization: Hyperparameters

- The pipeline optimization refers to fine-tuning hyperparameters of UMAP, including several important parameters like **n_neighbors_list**, **min_dist_list**, **metric_list**, and **n_components_list**.
- We first tested a small proportion of the grid search space, to have an idea of the time consumption. It showed one hyperparameter combination takes around 3 - 5 minutes. We decided to explore a grid search space with 150 combinations, and it finally spent around 350 minutes.

11 rows 150 rows x 19 columns pd.DataFrame								
	algo	eps	dbscan_min_samples	n_clusters_found	validity_index	hopkins_statistic	umap_n_neighbors	umap_mir
47	k_means	NaN	NaN	3	NaN	0.734961	7	
48	k_means	NaN	NaN	3	NaN	0.761623	7	
38	k_means	NaN	NaN	3	NaN	0.760266	7	
39	k_means	NaN	NaN	3	NaN	0.763695	7	
37	k_means	NaN	NaN	3	NaN	0.736636	7	
...	
110	dbscan	0.115614	6.0	3	-0.736907	0.453044	42	
85	dbscan	0.152404	6.0	3	-0.743036	0.424897	17	
100	dbscan	0.096328	6.0	2	-0.752965	0.449576	42	
25	dbscan	0.473131	6.0	13	-0.773474	0.332102	3	
45	dbscan	0.271902	6.0	2	-0.797766	0.367107	7	

```
n_neighbors_list = np.logspace(0.5, 2, 5).astype(int)
n_neighbors_list
Executed at 2024.04.21 06:09:10 in 78ms

array([ 3,  7, 17, 42, 100])
```

```
min_dist_list = [0.0] + np.logspace(-5, -1, 3)
min_dist_list
Executed at 2024.04.21 06:09:10 in 75ms

array([1.e-05, 1.e-03, 1.e-01])
```

```
metric_list = ['euclidean', 'cosine']
metric_list
Executed at 2024.04.21 06:09:10 in 73ms

['euclidean', 'cosine']
```

```
n_components_list = [2, 3, 5, 10, 15]
n_components_list
Executed at 2024.04.21 06:09:10 in 70ms

[2, 3, 5, 10, 15]
```

Clustering Pipeline Optimization: Hyperparameters (continued)

- Some hyperparameters of K-Means and DBSCAN were also tuned during the optimization process.

- **n_clusters** of K-Means
- **eps** of DBSCAN
- **min_samples** of DBSCAN
- **metric** of DBSCAN

```
n_clusters_list = list(np.arange(2, 16))
```

```
k_list = [3, 4, 5, 6]
```

```
eps_factor_list = list(np.arange(0.5, 1.8, 0.2))
```

```
eps_k_df = get_eps_k_df(embedding, k_list)
max_eps = eps_k_df['eps'].values.max()
min_samples = eps_k_df.loc[eps_k_df.eps == max_eps, 'k'].values[0]
```

```
metric=umap_results_dict['metric']
```

Clustering Pipeline Optimization: Results

- Internal indices are used to select the best results during the pipeline optimization, includes:
 - **Silhouette Score** of K_Means
 - **Validity Index** of DBSCAN
- The result of pipeline optimization is a DataFrame of shape **(150, 19)**, including hyperparameter combinations, their resulting internal indices, UMAP embeddings, and fitted models.
- It was saved into an **optimization_results.pkl** file for the access of the following False Discovery Checking and Validation processes.

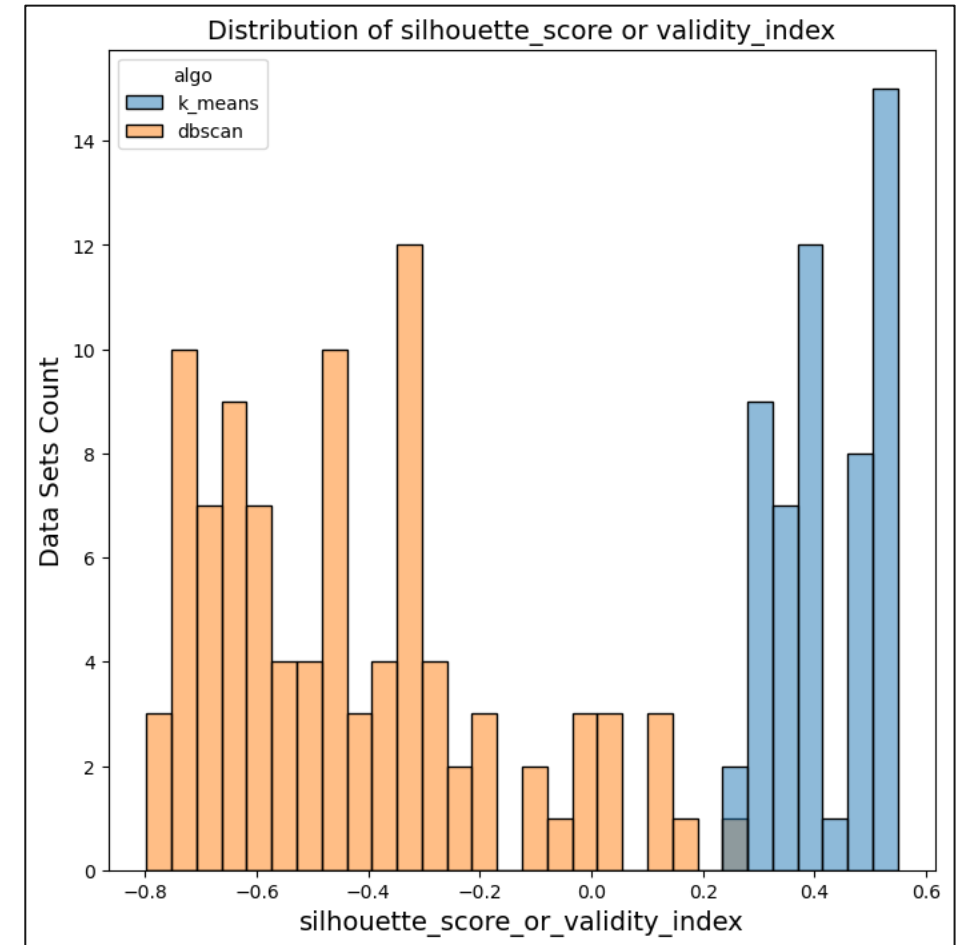
```
SOLUTION_PICKLE_FILE_PATH = 'data/optimization_results.pkl'
```

```
clustering_results_df.to_pickle(SOLUTION_PICKLE_FILE_PATH)
```

Executed at 2024.04.21 11:43:07 in 1s 193ms

Avoid False Discovery: Internal Indices Distribution

- As the optimization takes quite a long time, we put all results analysis and false discovery checking content in the **afd** notebook.
- Among the 150 clustering results, we put the **silhouette_score** of K_means and **validity_index** of DBSCAN together as the rank of results.
 - 1 means best clustering
 - 0 means overlapping clusters
 - -1 means worst clustering
- The distribution of **silhouette_score** or **validity_index** among the 150 results shows that **K_means performs better than DBSCAN** in general. And most DBSCAN have negative validity indices.



Avoid False Discovery: Latent Manifold Details

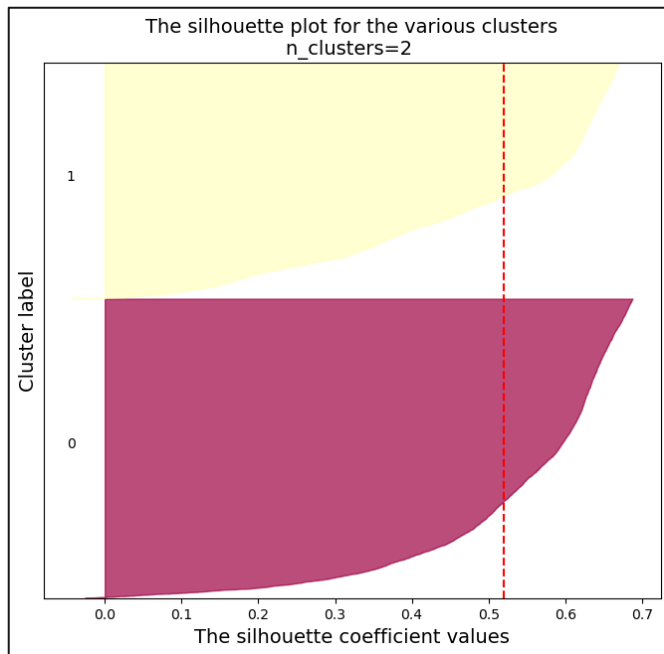
- The best result was chosen as the Latent Manifold and here is the hyperparameters and internal indices:

number of classes in data set	UMAP n_components	UMAP min_dist	UMAP n_neighbors	UMAP metric	trustworthiness	clustering algorithm	number of clusters found	validity index or silhouette score
4	5	0.001	7	cosine	0.823645	k_means	3	0.549104

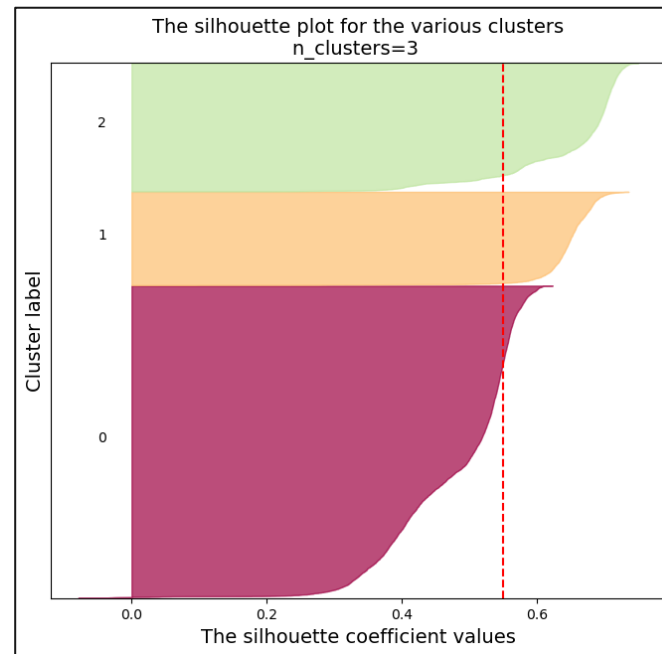
- It shows the highest validity_index or silhouette_score is **0.55**, which is not very high. We will discuss this in detail in the validation part.

Avoid False Discovery: Silhouette Analysis

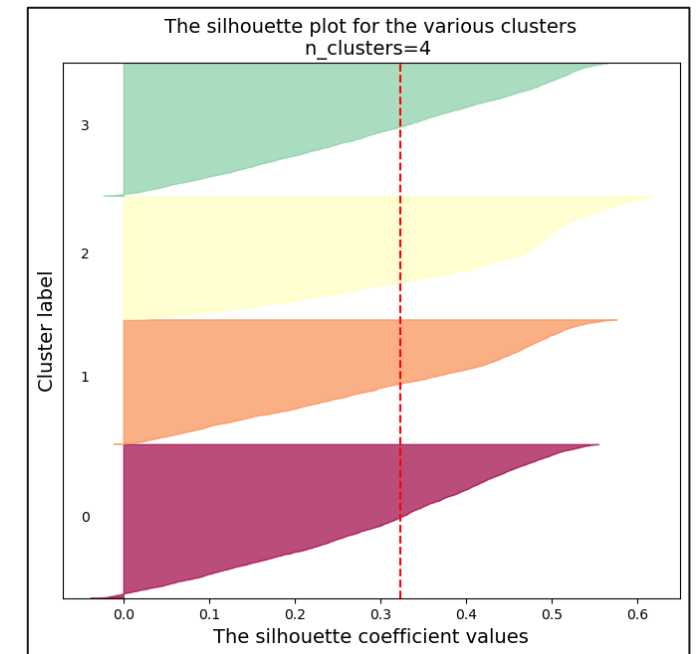
- Although we have chosen the latent manifold with the highest silhouette_score, we also did some exploration using the silhouette_score plots.
- Among the 150 clustering results, all ones using **k_means** algorithm have the following **n_clusters_found**: **2, 3, and 4**. For each of them, we select the best one result with the highest **silhouette_score** to analyze.



best_index for n_clusters: 2 is 12
the average silhouette_score is 0.5192729830741882



best_index for n_clusters: 3 is 0
the average silhouette_score is 0.5491037368774414



best_index for n_clusters: 4 is 43
the average silhouette_score is 0.32299160957336426

Avoid False Discovery: Silhouette Analysis (continued)

- The 3 silhouette_score plots show that although `n_clusters=3` has the highest silhouette_score, `n_clusters=2` and `n_clusters=4` also have some meaningful results.
 - Width of the silhouette plot (y-axis) represents **the number of points in each cluster**. A wider silhouette indicates more points in the cluster.
 - Height of the silhouette plot (x-axis) represents **the silhouette score**. A silhouette that reaches closer to 1 indicates better clustering.
 - The red dashed line represents **the average silhouette score across all samples**. The closer the silhouette's height is to this line (or beyond), the better it is considered for the clustering.
- Although `n_clusters=3` has the highest overall average silhouette score, indicating better average separation and cohesion, `n_clusters=2` and `n_clusters=4` also show that **the additional clusters' silhouettes are above the average line**. This means the existence of one extra cluster doesn't deteriorate the overall structure, and the additional clusters also hold statistically meaningful cohesion and separation.

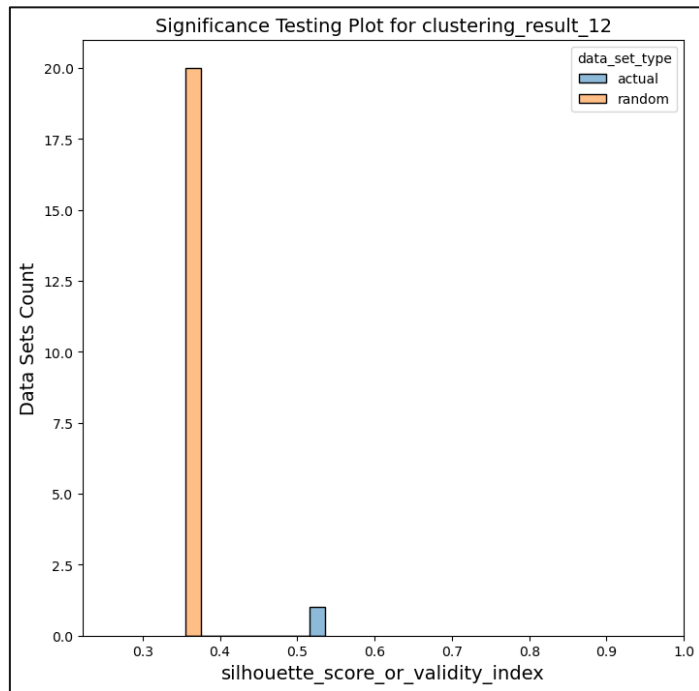
Avoid False Discovery: Checking Sets

- Although we choose `silhouette_score` as the standard to rank clustering results, other clustering results may also be meaningful. Thus, in the False Discovery Checking part, we continue to check false discoveries for all the above 3 clustering results.
- For each clustering result, we use its UMAP embedding to generate randomly distributed data sets, and calculate their silhouette scores. **For a true discovery, its silhouette score should separate clearly from those of randomly distributed data sets.**
- The number of generated random sets (**`random_data_sets_num`**) can be declared and assigned to the AFD function. Also, we use one parameter **`afd_check_indices`** to determine which indices we are going to check. (here is the 3 results above)

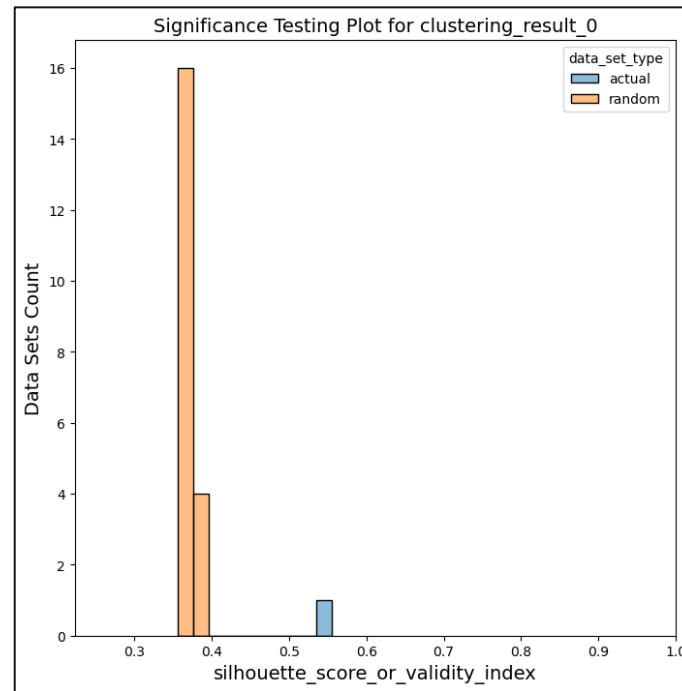
```
# For comparison, select different entries across the clustering results
afd_results_df = validation.clustering_randomly_distributed_data(
    clustering_results_df=clustering_results_df,
    afd_check_indices=best_index_list,
    random_data_sets_num=RANDOM_DATA_SETS_NUM,
    random_state=RANDOM_SEED
)
```

Avoid False Discovery: Checking Results

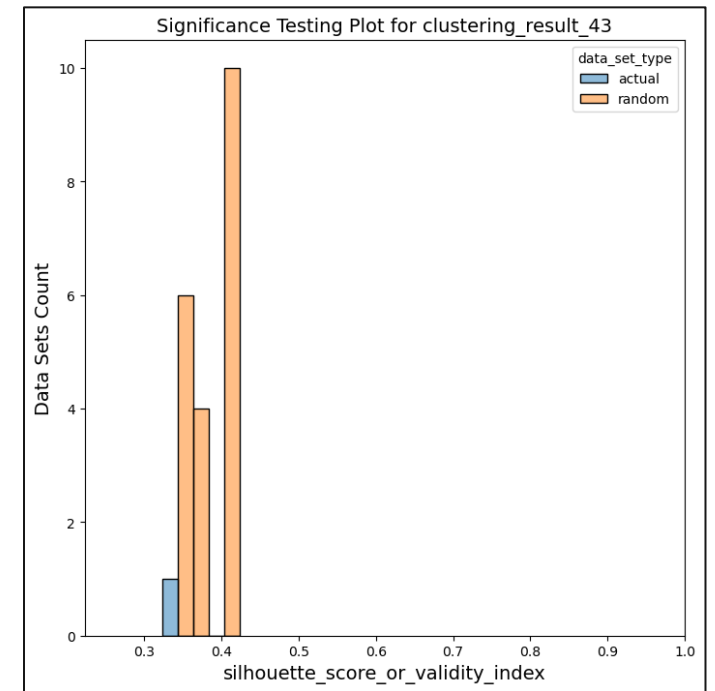
- The false discovery checking results are shown in the 3 plots below. It shows that **both $n_clusters=2$ and $n_clusters=3$ have a good separation with random data sets**, while $n_clusters=4$ has much overlapped with random sets.
- Considering the high silhouette score, **it seems $n_clusters=3$ is a good clustering result**.



best_index for n_clusters: 2 is 12
the average silhouette_score is 0.5192729830741882



best_index for n_clusters: 3 is 0
the average silhouette_score is 0.5491037368774414



best_index for n_clusters: 4 is 43
the average silhouette_score is 0.32299160957336426

Clustering Validation: External Indices

■ In this part, we read back the pre-separated **target file** and **design file** in project phase 1, merge them back by **id**, add the **predicted label** from the best clustering result (the latent manifold), and calculate its external indices.

- **rand_score**: [0, 1], 1 means perfect clustering
- **adjusted_rand_score**: [-1, 1], 1 means perfect clustering
- **fowlkes_mallows_score**: [0, 1], 1 means perfect clustering
- **normalized_mutual_info_score**: [0, 1], 1 means perfect clustering
- **jaccard_score**: scores for each label. [0, 1], 1 means perfect clustering
- **f1_score**: scores for each label. [0, 1], 1 means perfect clustering
- **purity_score**: [0, 1], 1 means perfect clustering
- contingency_matrix

```
cap_x_df = pd.read_csv(TARGET_FILE_PATH)
y_df = pd.read_csv(DESIGN_FILE_PATH)
Executed at 2024.04.21 21:51:57 in 64ms

merged_df = pd.merge(cap_x_df, y_df, on='id', how='left')
merged_df['pred_labels'] = clustering_results_df.loc[best_index, 'cluster_labels']
merged_df.rename(columns={TARGET_ATTR: 'target'}, inplace=True)
```

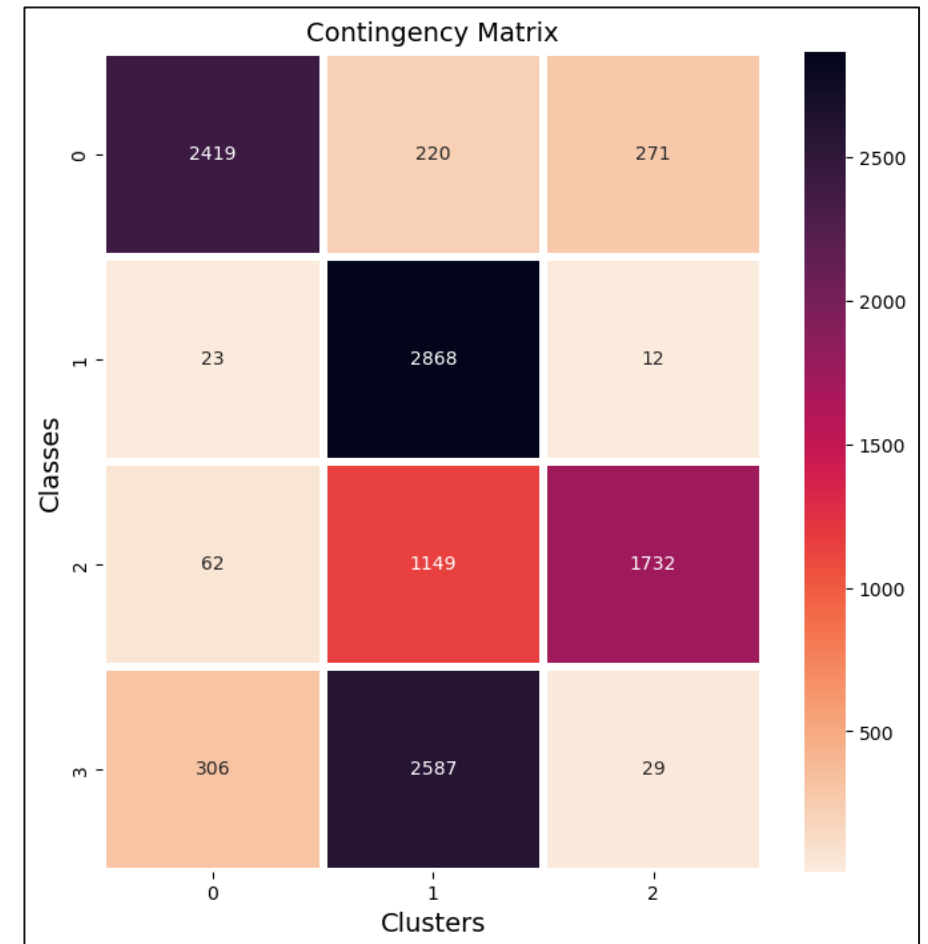
```
external_indices_df = validation.get_external_indices(
    merged_df,
    clustering_results_df.loc[best_index, 'algo']
)
```

Clustering Validation: External Indices Results

- The external indices results and the contingency matrix are generated in a data frame, they are also shown in the below table and the matrix plot.

rand_score	adjusted_rand_score	fowlkes_mallows_score	normalized_mutual_info_score
0.691157	0.335773	0.565941	0.436435

jaccard_score	f1_score	purity_score
[0.02312381753205802, 0.0024316109422492403, 0.010894394658232297, 0.0]	[0.04520238339839737, 0.0048514251061249234, 0.021553971840778726, 0.0]	0.601045



Discussion of Performance

- The number of clusters in our result (3) is different from the true number of classes (4). Specifically, the class 3 is not recognized and is mixed up with cluster 1.
- The external indices show some relatively good results, but not that good enough due to the different number of clusters with the true label numbers. Notice that `jaccard_score` and `f1_score` are label-based, which shows 0 score for the missing label.
- As the time limit, we can only perform current hyperparameter searching and get our current best result. For future research, maybe a broader search space, or different algorithms such as deep learnings can be applied to improve the performance.