EE 219 Project 2
Clustering

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I. Introduction

This project focuses on performing K-means clustering on the dataset and thereby evaluate the performance of the algorithm. The performance is monitored by using different pre-processing methods. Representing the data in a way which depicts the most efficient clusters is also one of the aims of this project.

As opposed to classification which is a supervised technique for grouping data, **clustering** algorithms are **unsupervised** methods for grouping data points with similar representation in a proper space. In this method, the a priori labelling of data points is not available.

The K-means Clustering Algorithm:

K-means clustering is a simple and widely used clustering algorithm. This algorithm groups the data into k clusters or groups based on the features that are provided. It uses an iterative refinement technique to produce a final output which has each data point assigned to only one cluster. This assignment is such that the sum of the squares of the distance between each data point and the centroid of the cluster to which it belongs to is minimized.

The algorithm initially estimates the k centroids which are either generated randomly or selected randomly from the data set itself. It then iterates between the following two steps until it reaches convergence:

1. *Assigning of data point to a cluster:*

In this step, one data point is assigned/reassigned to the nearest cluster. The nearest distance is based on the squared Euclidean distance between the data point and the centroid of the cluster.

2. *Updating the centroid*

Once a data point is assigned to a cluster, all centroids are computed again. This is achieved by taking the mean of all the data points which are assigned to that centroid's cluster.

Dataset:

The dataset we have at our disposal is the '20 Newsgroups' dataset which is a collection of approximately 20,000 documents. These documents are segregated nearly evenly into 20 classes i.e. 20 newsgroups.

II. Problem Statement

1. Building the TF-IDF matrix:

Since clustering is an unsupervised technique of grouping similar data points, the class labels are not available to the algorithm. Here, we consider that the documents in each group are similar to each other than the documents in other groups/clusters. We then use the actual labels to evaluate the performance of our clustering. As such, feature extraction with the help of the TFIDF technique plays an important role here. Before applying this technique for feature extraction, we tokenize the documents into words and then exclude the stop words from them. Stop words are the words which are very commonly present in all the documents and thereby add no importance. We have used Python's NLTK library for the same.

The TFIDF measure determines the relevance of a word within a particular document. Here, TF stands for 'Term Frequency' which denotes the number of times a particular term occurs within a given document. This is used to determine the frequent words. In this project we set the threshold for frequent words using the min_df parameter. IDF stands for 'Inverse Document Frequency' which is used to specify the relevance of rare words. TFIDF of a particular word is the multiplication of the TF and IDF of that word.

After applying TFIDF transformation on the training dataset, we obtain a document – term matrix in which each row represents a document and each column a term. We have made the following observation of this TFIDF matrix by setting min_df as 3.

Number of documents	**Number of terms extracted**
7882	27805

2. Basic K-means Clustering

In this part, we apply K-means clustering with k=2 on the TFIDF data we received from the previous step.

a) We use the contingency matrix to depict how many data points belong to each cluster. Here, since we use k=2, we are grouping our data only into the broad classes of 'Computer Technology' and 'Recreational Activity'. Following is the contingency matrix observed for basic K-means clustering.

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	6	3897
Recreational Activity	1686	2293

From the above matrix, it can be clearly observed that there are a lot of incorrect assignments of data points to clusters. Once we tune the parameters and pre-process the data, the performance improves.

b) Now, we use different measures to examine the purity of the clusters with respect to the ground truth. *Homogeneity* measures the level purity of clusters. This score ranges from 0 to 1. A score of 1 signifies that each cluster contains data point from only a single class i.e. perfect clustering. *Completeness* tells us whether all data points of a particular class are indeed assigned to the same cluster. Again, this score varies from 0 to 1. *V-measure* is the harmonic mean of homogeneity and completeness. The *Adjusted Rand Index* is similar to the accuracy measure. It computes the similarity between the clustering labels and the ground truth labels. This counts all the pairs of data points that fall either in the same cluster and the same class or in different clusters and different classes. Lastly, we have the *Adjusted Mutual Information*

score which measures the mutual information between the label information of our clusters and the ground truth label distributions. The measures we observed are tabulated as follows:

Measure	Value
Homogeneity	0.246
Completeness	0.328
V-measure	0.281
Adjusted Rand Score	0.173
Adjusted Mutual Info Score	0.246

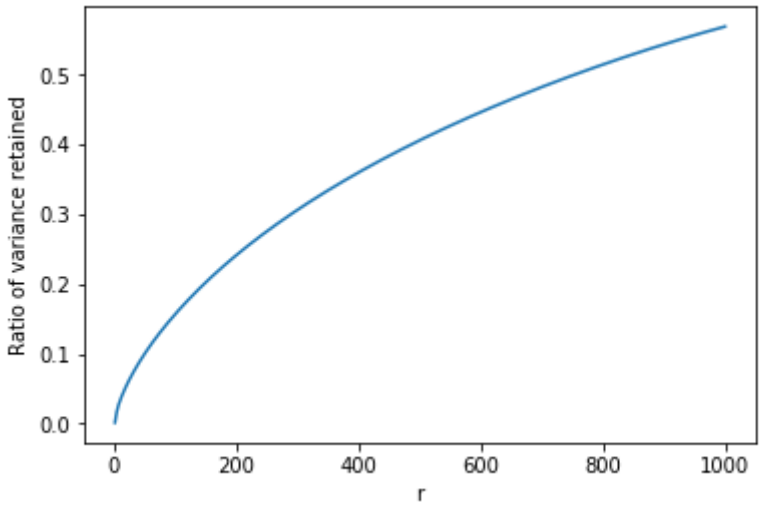
3. Pre-process the data

As observed from the above table, the metrics are not good enough when K-means is applied to a high dimensional TFIDF matrix. One of the reason for this dip in the metrics is that the Euclidean distance which is used in K-means is not a good measure in the high dimensional space. Also, K-means might fail to identity the correct clusters to which the data points belong to since it implicitly assumes that the clusters are round shaped. This is because it tries to minimize the sum of within-cluster l^2 distances. To improve the above metrics and thereby to get a better representation which suits the working of K-means algorithm, we pre-process the data before clustering.

Here, we are using the Latent Semantic Indexing (LSI) and the Non- Negative Matrix Factorization (NMF) techniques for dimensionality reduction.

i) Ratio of variance retained

Before reduction, firstly, we find the effective dimension of the data through inspection of the top singular values of the TFIDF matrix and check how many of them are significant in reconstructing the matrix with the truncated SVD representation. To do this, we sweep though different values of r from 1 to 1000 where r stands for the top principle components. And for each value of r, we plot the percent of variance it can retain after dimensionality reduction. The following plot shows the same:

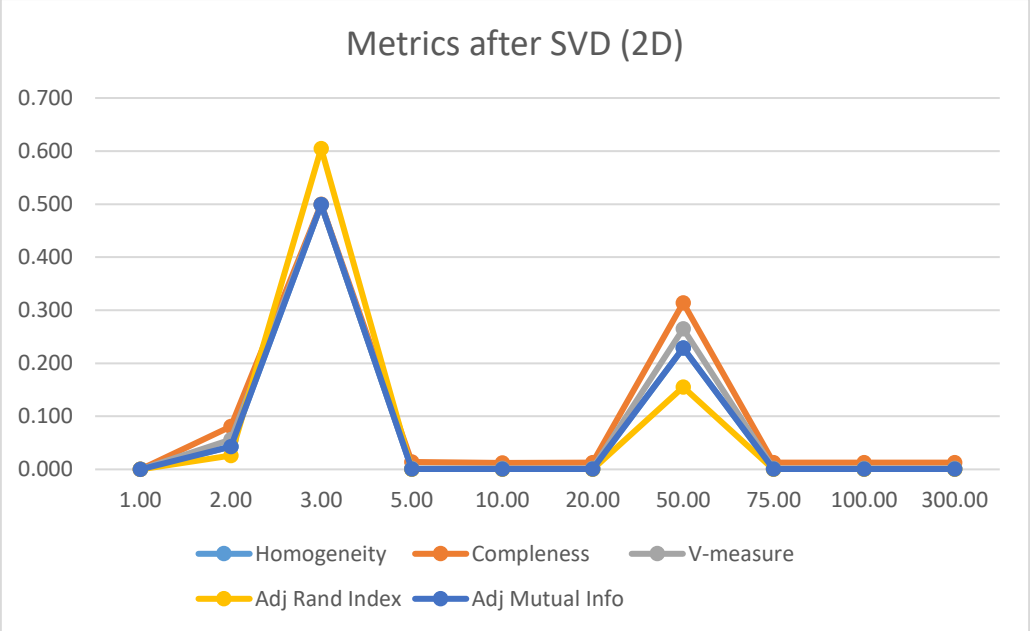


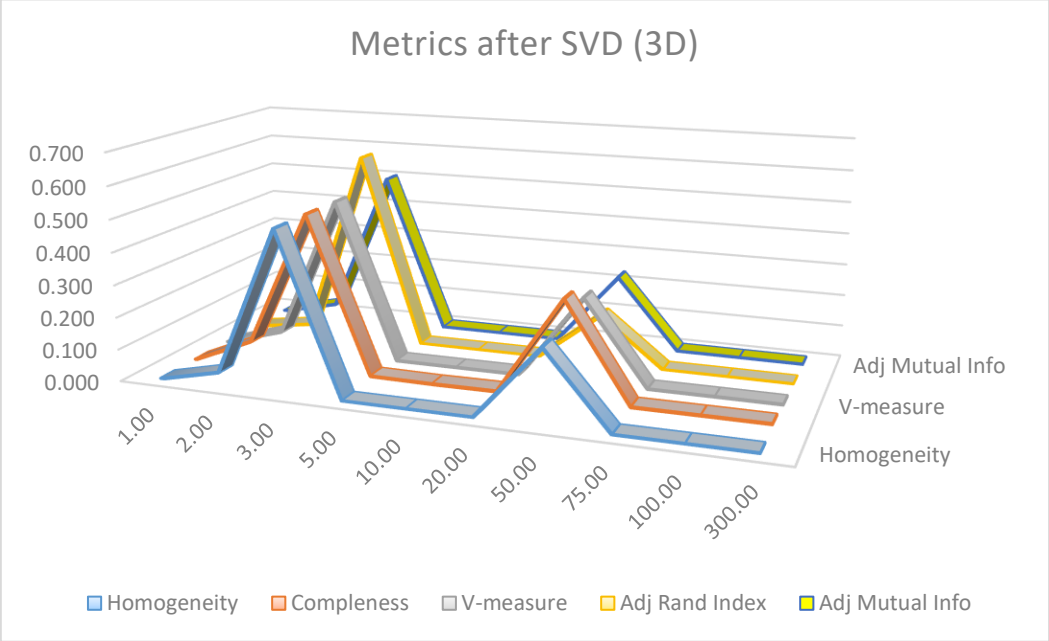
ii) Reduction of data:

We now use Truncated SVD and NMF to perform reduction on our TFIDF data. Here, we sweep over the dimension parameters and thereby get the best value of dimensional reduction. The following table denotes the different metrics we observe with different values of r (all values rounded to 3 digits after decimal point).

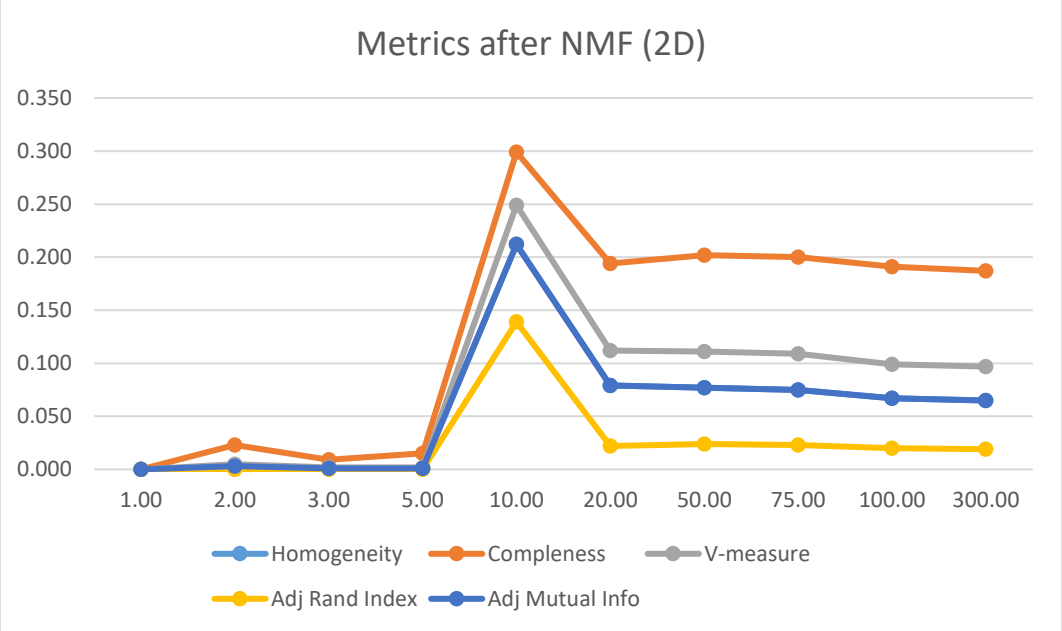
Dimension Parameter	Type	Homogeneity	Completeness	V-measure	Adjusted Rand Score	Adjusted Mutual Info Score
1	LSI	0.000	0.000	0.000	0.000	0.000
	NMF	0.000	0.000	0.000	0.000	0.000
2	LSI	0.043	0.081	0.056	0.026	0.043
	NMF	0.003	0.023	0.005	0.000	0.003
3	LSI	0.499	0.500	0.499	0.605	0.499
	NMF	0.001	0.009	0.002	0.000	0.001
5	LSI	0.001	0.014	0.002	0.000	0.001
	NMF	0.001	0.015	0.002	0.000	0.001
10	LSI	0.001	0.012	0.002	0.000	0.001
	NMF	0.212	0.299	0.249	0.139	0.212
20	LSI	0.001	0.013	0.002	0.000	0.001
	NMF	0.079	0.194	0.112	0.022	0.079
50	LSI	0.229	0.314	0.265	0.155	0.229
	NMF	0.077	0.202	0.111	0.024	0.077
75	LSI	0.001	0.013	0.002	0.000	0.001
	NMF	0.075	0.200	0.109	0.023	0.075
100	LSI	0.001	0.013	0.002	0.000	0.001
	NMF	0.067	0.191	0.099	0.020	0.067
300	LSI	0.001	0.013	0.002	0.000	0.001
	NMF	0.065	0.187	0.097	0.019	0.065

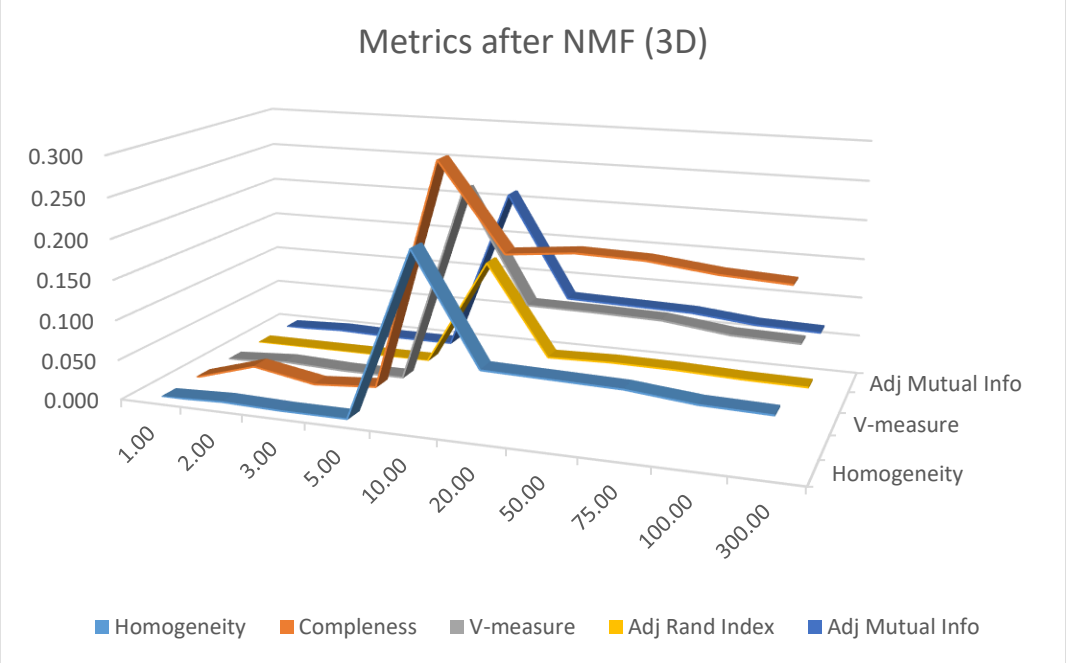
Thus, the best r value for LSI is 3, and that for NMF is 10. This can also be observed from the graphs shown below. The values of the five metrics were first exported to excel and then plotted.





The 3D version of the graph was plotted to clearly depict the values of different metrics overlapping at the same score for the same value of r.





The contingency matrices for each of the rows of the above table are as follows:

- r=1; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	2472	1431
Recreational Activity	2525	1454

- r=1; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	2472	1431
Recreational Activity	2525	1454

- r=2; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3128	775
Recreational Activity	3802	177

- r=2; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3871	32
Recreational Activity	3887	92

- r=3; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	519	3384
Recreational Activity	3623	356

- r=3; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3843	60
Recreational Activity	3867	112

- r=5; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3854	49

Recreational Activity	3957	22

- r=5; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3854	49
Recreational Activity	3958	21

- r=10; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3852	51
Recreational Activity	3955	24

- r=10; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	10	3893
Recreational Activity	1517	2462

- r=20; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3853	50
Recreational Activity	3956	23

- r=20; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3897	6
Recreational Activity	3346	633

- r=50; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3896	7
Recreational Activity	2381	1598

- r=50; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3322	581
Recreational Activity	3977	2

- r=75; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	50	3853
Recreational Activity	23	3956

- r=75; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3335	568
Recreational Activity	3977	2

- r=100; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	50	3853
Recreational Activity	23	3956

- r=100; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3386	517

Recreational Activity	3976	3

- r=300; LSI

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	50	3853
Recreational Activity	23	3956

- r=300; NMF

Actual	**Predicted**	
	Computer Technology	Recreational Activity
Computer Technology	3393	510
Recreational Activity	3975	4

Question: How do you explain the non-monotonic behaviour of the measures as r increases?

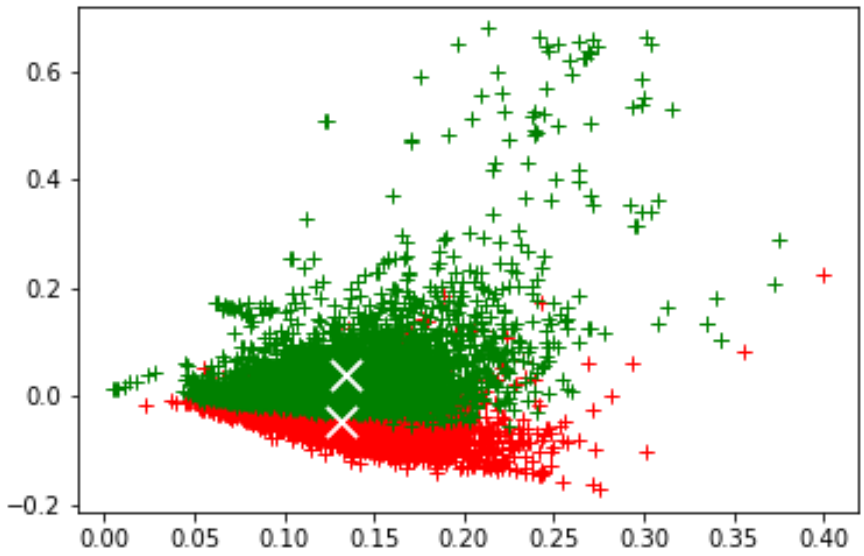
From the plots above, we observe that as the value of r increases, the non-monotonicity in the behavior of the metrics becomes evident. The reason for this is two things that balance each other's effect. One is information retention which happens at high dimensions i.e. high value of r and the other is performance of k-means algorithm. It is widely known that k-means performs bad in high dimensions. This is the reason that we don't get the best values of the measures at the highest value of r. Thus, as we increase r, the performance improves up to a certain point after which it starts degrading. This justifies the non-monotonic behavior of the measures.

4. Visualization of clusters

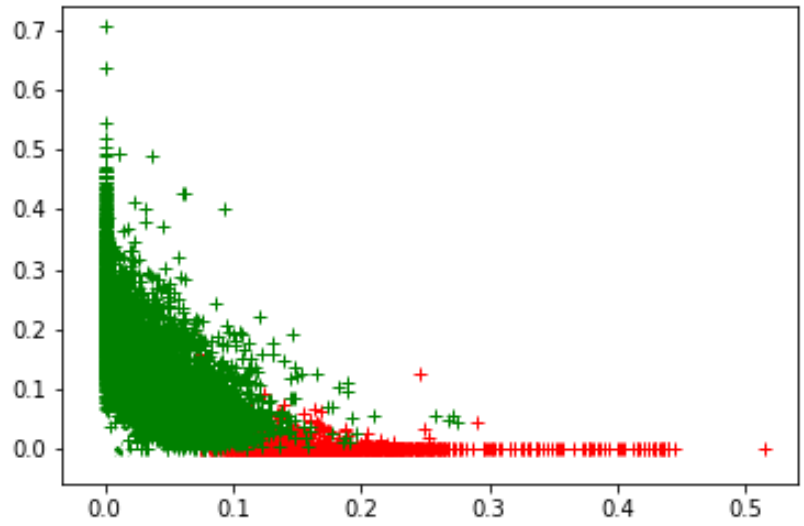
a) Visualizing in 2D with best r

We now use the best value of r as received from the above part to visualize the clusters. Since our **best value r is 3 and 10 for LSI and NMF** respectively and we need to project the final data vectors onto a 2D plane, we convert the matrix obtained after reduction into a two dimensional matrix. We use **SVD** to do so.

- After LSI decomposition



- After NMF Decomposition

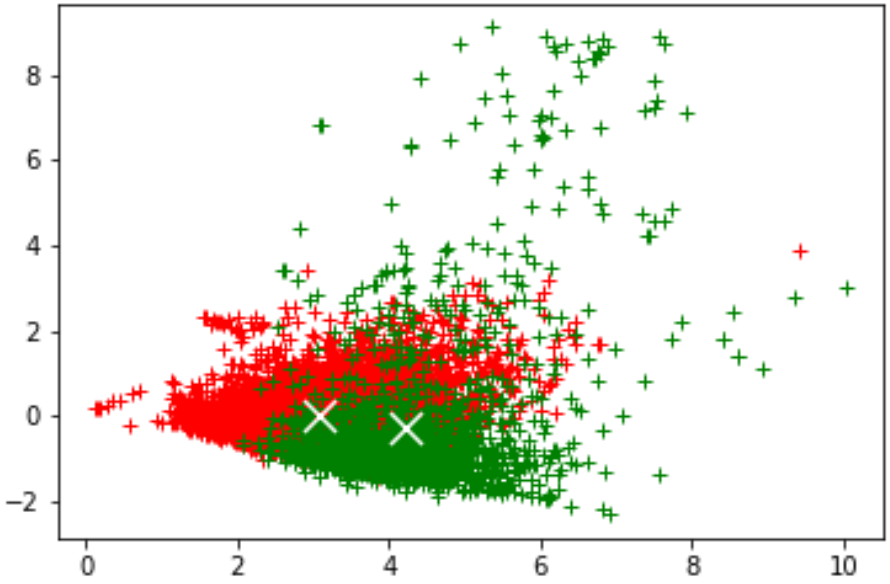


b) Visualizing in 2D with best r value after applying transformations

Now, we try different methods as below and test whether they increase the clustering performance (with the same best values of r). These visualizations are also on a 2D plane after applying SVD to the LSI and NMF matrices respectively.

i. Normalizing the features

- *After LSI Decomposition*

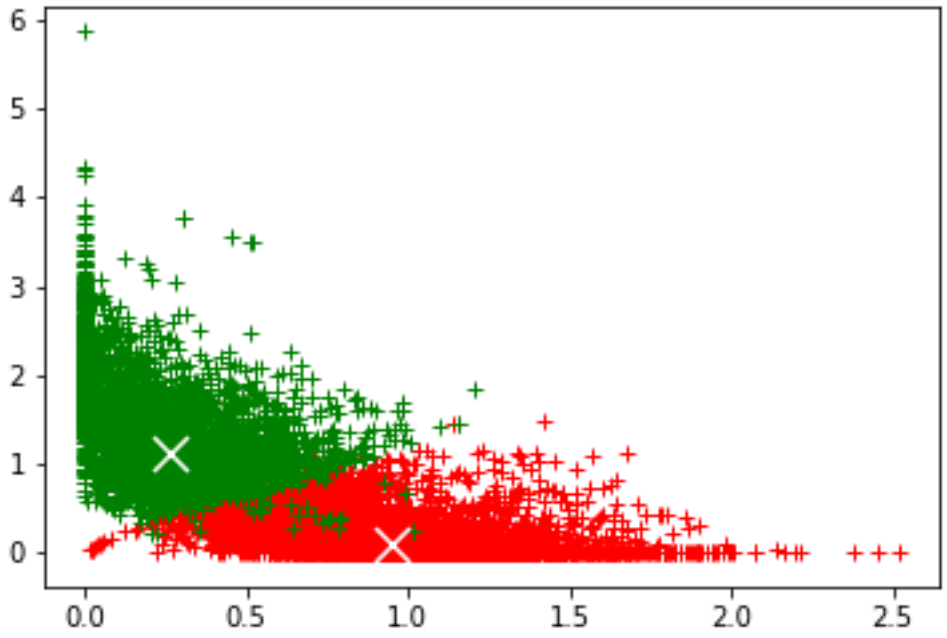


Metric	Value
Homogeneity	0.164
Completeness	0.214
V-measure	0.186
Adjusted Rand Index	0.135
Adjusted Mutual Info Score	0.164

	Predicted	
Actual	Computer Technology	Recreational Activity
Computer Technology	3761	142
Recreational Activity	2350	1629

As seen from the above measures, we notice that normalizing the LSI matrix, degrades its purity. That is normalizing features does not really help in improving the performance after LSI decomposition.

- *After NMF Decomposition*

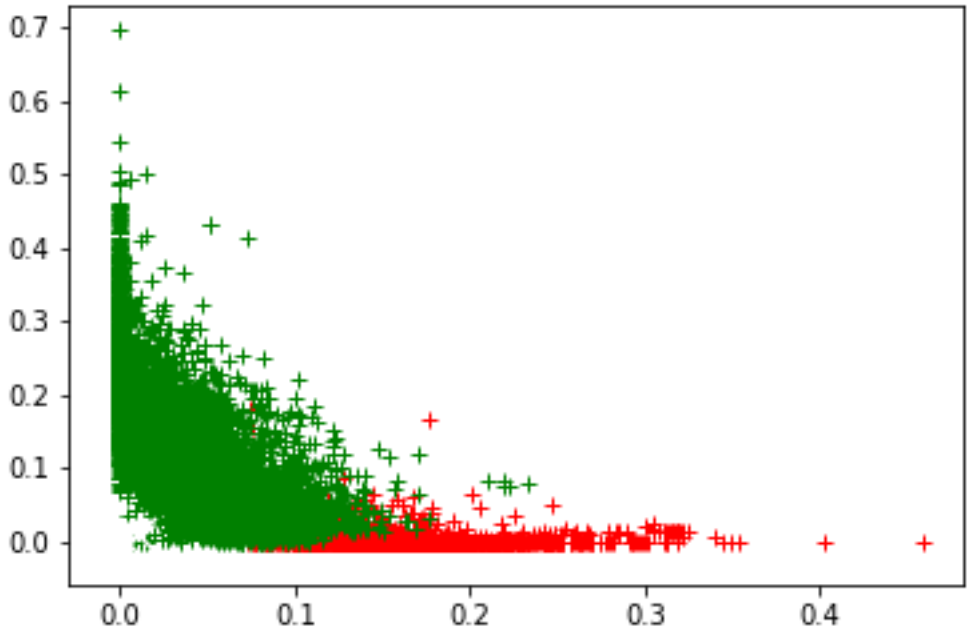


Metric	Value
Homogeneity	0.490
Completeness	0.505
V-measure	0.497
Adjusted Rand Index	0.558
Adjusted Mutual Info Score	0.490

	Predicted	
Actual	Computer Technology	Recreational Activity
Computer Technology	875	3028
Recreational Activity	3856	123

We can see from the above statistics that there is a significant improvement in the performance after we normalize the features and feed it to NMF decomposition.

ii. Non-linear (logarithmic) transformation after NMF



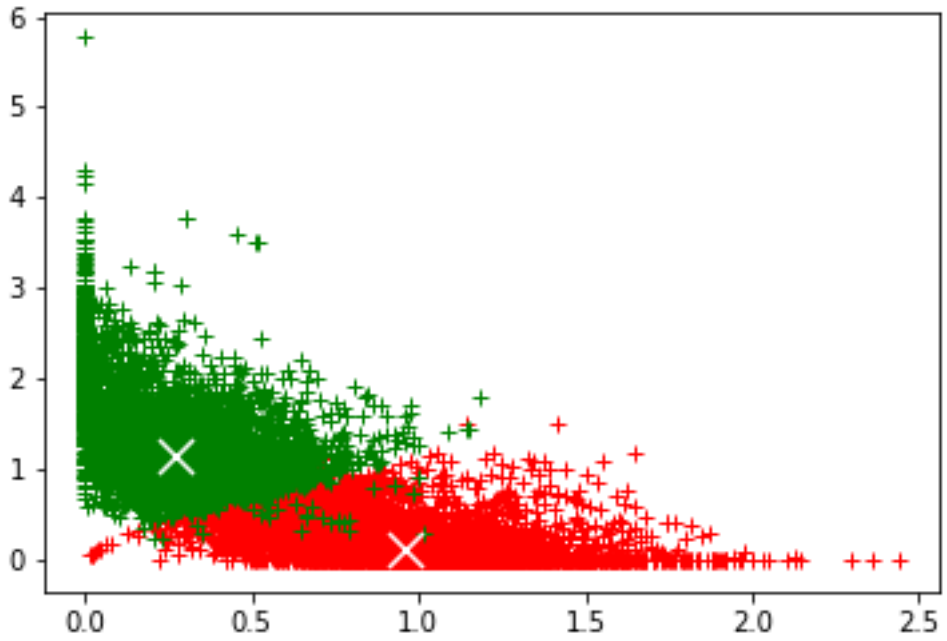
Metric	Value
Homogeneity	0.218
Completeness	0.305
V-measure	0.254
Adjusted Rand Index	0.142
Adjusted Mutual Info Score	0.218

Actual	Predicted	
	Computer Technology	Recreational Activity
Computer Technology	7	3896
Recreational Activity	1532	2447

Question: Can you justify why logarithm transformation may increase the clustering results?

It should be noted that as the frequency of a term increases, it does not indicate that the relevance of the term should increase by an equivalent amount. To mitigate this issue, we apply non-linear transformation to our data. We particularly use logarithmic function because it does a great job of amortizing the influence of rare or frequent words thus, assigning appropriate weights to each term and improving the clustering performance.

iii. Logarithmic Transformation + Normalization on NMF

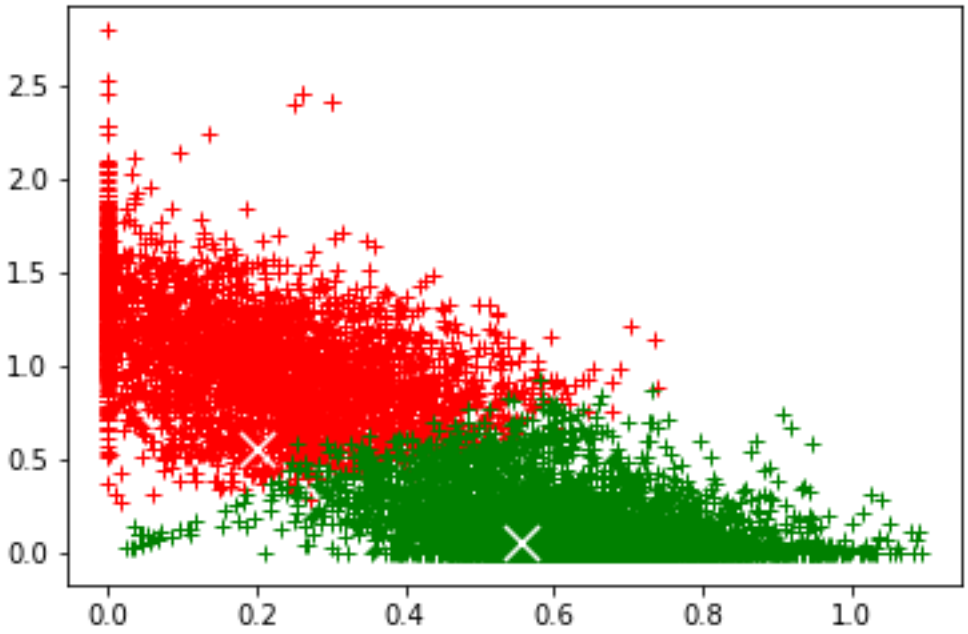


Metric	Value
Homogeneity	0.493
Completeness	0.507
V-measure	0.500
Adjusted Rand Index	0.561
Adjusted Mutual Info Score	0.493

Actual	Predicted	
	Computer Technology	Recreational Activity
Computer Technology	866	3037
Recreational Activity	3856	123

We can see from the above statistics that there is a pretty good improvement in the performance if we apply logarithmic transformation and then normalize the features for NMF.

iv. Normalization + Logarithmic Transformation on NMF



Metric	Value
Homogeneity	0.649
Completeness	0.653
V-measure	0.651
Adjusted Rand Index	0.739
Adjusted Mutual Info Score	0.649

Actual	Predicted	
	Computer Technology	Recreational Activity
Computer Technology	3460	443
Recreational Activity	110	3869

We can see from the above statistics that the **best improvement in the** performance is obtained after we normalize the features and then apply logarithmic transformation to the NMF reduced data.

5. Expand Dataset into 20 categories

In this part, we have grouped the data-points into 20 clusters which correspond to the 20 original classes in the 20 Newsgroups dataset. We then examine the purity of the clusters using the same 5 measures we used in the previous parts, namely: Homogeneity, Completeness, V-Measure, Adjusted Rand Index and Adjusted Mutual Information Score. The steps taken are as follows:

- Apply TFIDF Transformation
- Reduce the dimensions of TFIDF matrix using Truncated SVD and NMF. The results have been compared for both these reduction techniques.
- Sweep through different values of r (dimension parameter) and record the best value for LSI and NMF decomposition respectively.
- Apply different transformations such as Normalization on LSI and NMF decomposed data, Logarithmic Transformation on only NFM decomposed data. We have also tried the combinations of Normalization + Logarithmic Transformation as well as Logarithmic Transformation + Normalization on NMF decomposed data.
- Visualize the 20 clusters in 2D plane after applying the above mentioned transformations.

a) Apply TFIDF Transformation

After applying the TFIDF transformation for 20 classes on the entire dataset, we get the following results:

Number of documents	Number of terms extracted
18846	52333

These results were obtained by applying the same parameters as in part 1 of this project.

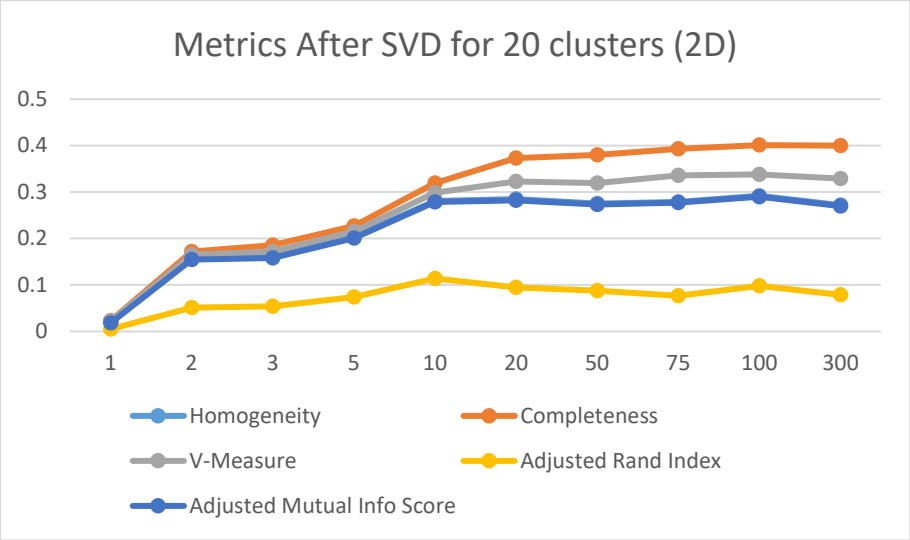
b) Choosing Best Value of dimension parameter (r)

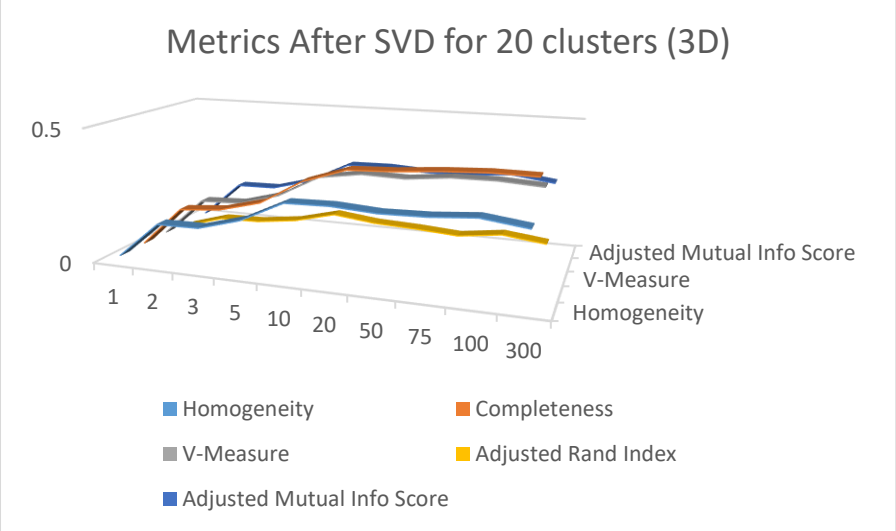
We decomposed the TFIDF matrix as received above using LSI and NMF decomposition. A comparison was drawn for the 5 measures as described above. It is stated in the following table:

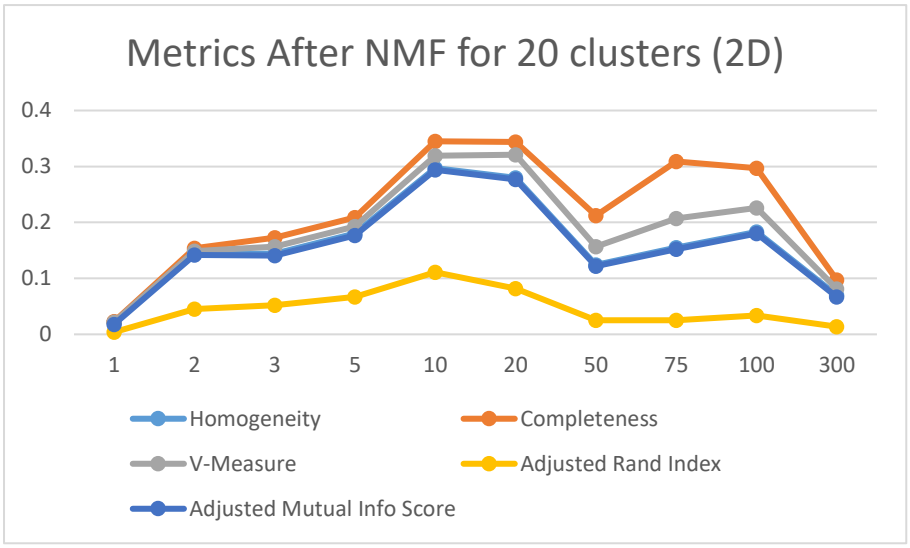
Dimension Parameter	Decomposition	Homogeneity	Completeness	V-measure	Adj Rand Index	Adj Mutual Info Score
1	LSI	0.022	0.023	0.022	0.005	0.018
1	NMF	0.022	0.023	0.022	0.004	0.018
2	LSI	0.158	0.172	0.165	0.051	0.155
2	NMF	0.144	0.154	0.149	0.045	0.142
3	LSI	0.160	0.186	0.172	0.054	0.158
3	NMF	0.144	0.173	0.157	0.052	0.141
5	LSI	0.204	0.227	0.215	0.074	0.201
5	NMF	0.180	0.209	0.193	0.067	0.177
10	LSI	0.281	0.319	0.299	0.114	0.279
10	NMF	0.297	0.345	0.319	0.111	0.294

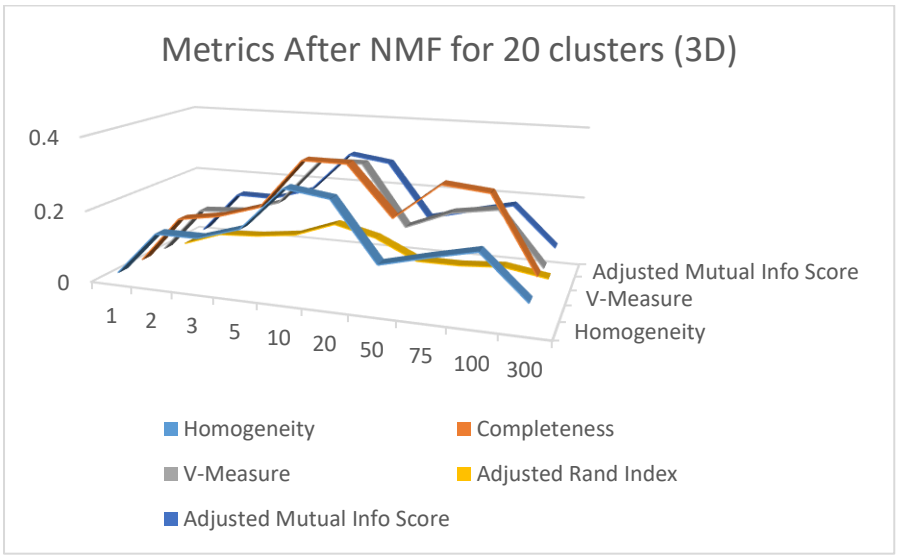
20	LSI	0.285	0.373	0.323	0.095	0.282
20	NMF	0.280	0.344	0.321	0.082	0.277
50	LSI	0.275	0.380	0.319	0.088	0.273
50	NMF	0.124	0.212	0.157	0.025	0.122
75	LSI	0.279	0.393	0.336	0.077	0.277
75	NMF	0.155	0.309	0.207	0.025	0.152
100	LSI	0.292	0.401	0.338	0.098	0.290
100	NMF	0.183	0.297	0.226	0.034	0.180
300	LSI	0.272	0.400	0.329	0.079	0.270
300	NMF	0.070	0.097	0.081	0.014	0.067

As observed from the table above, it is clear that **the best value for r is 100 for LSI decomposition and is 10 for NMF decomposition.** This can be seen from the plot of all the measures for different values of r which is as follows:



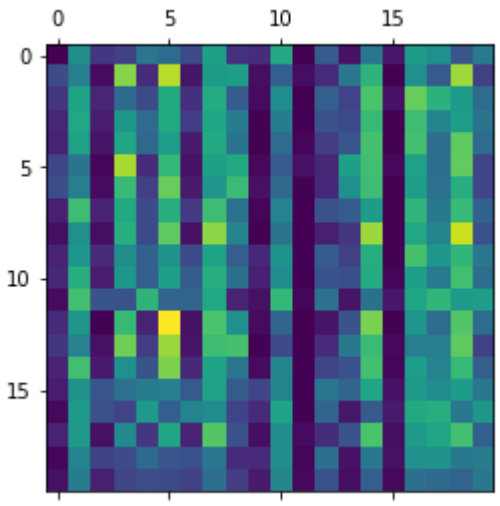



Metrics After NMF for 20 clusters (2D)
0.4
0.3
0.2
0.1
0
1
2
3
5
10
20
50
75
100
300
Homogeneity
Completeness
V-Measure
Adjusted Rand Index
Adjusted Mutual Info Score

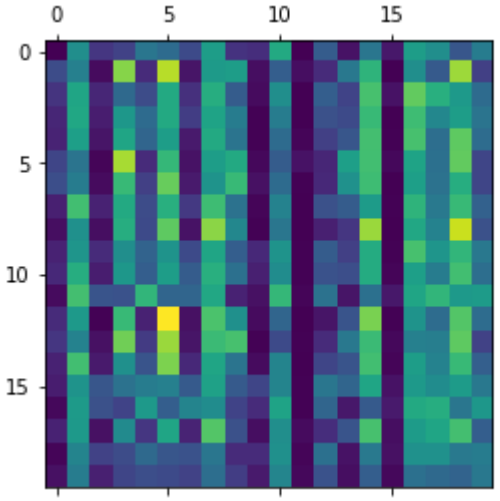

Metrics After NMF for 20 clusters (3D)
0.4
0.2
0
1
2
3
5
10
20
50
75
100
300
Adjusted Mutual Info Score
V-Measure
Homogeneity
Homogeneity
Completeness
V-Measure
Adjusted Rand Index
Adjusted Mutual Info Score

We have visualized the contingency matrices as follows:

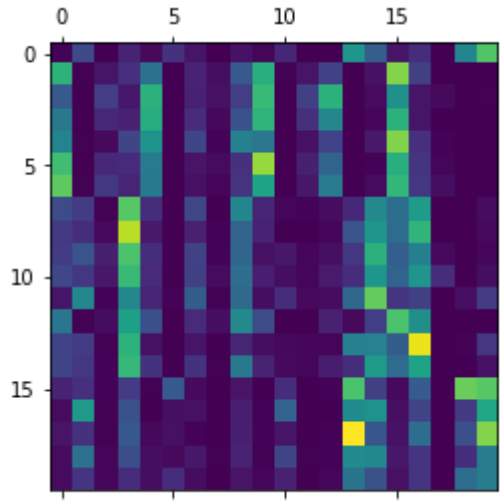
- **r=1; with LSI decomposition**



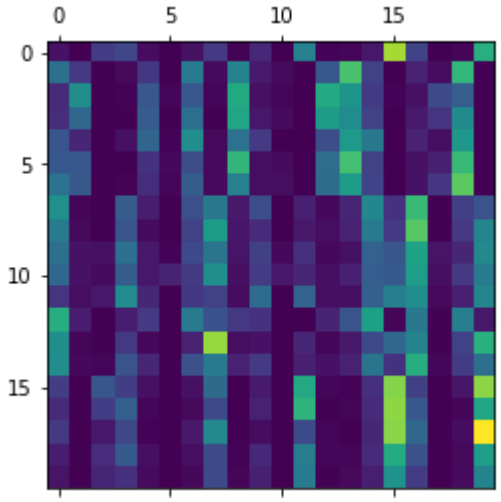
- **r=1; with NMF decomposition**



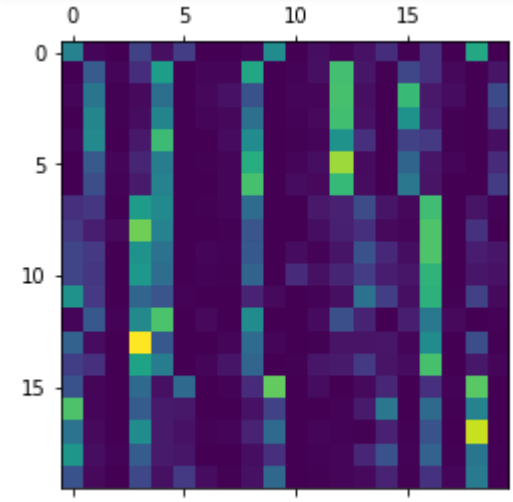
- r=2; **with LSI decomposition**



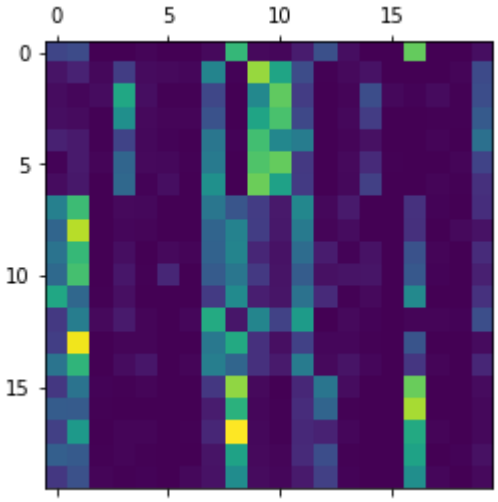
- r=2; **with NMF decomposition**



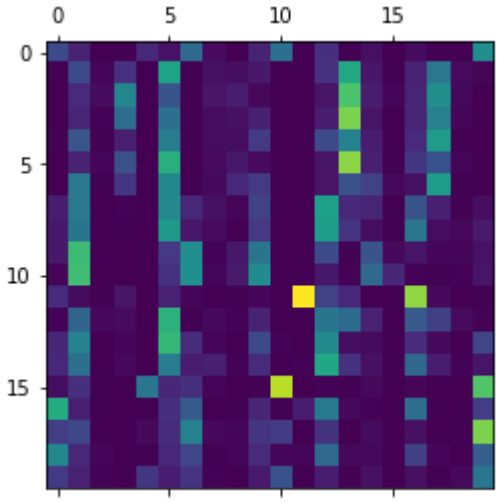
- r=3; **with LSI decomposition**



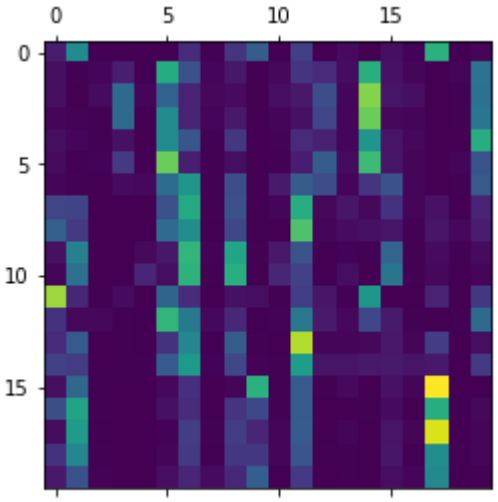
- r=3; **with NMF decomposition**



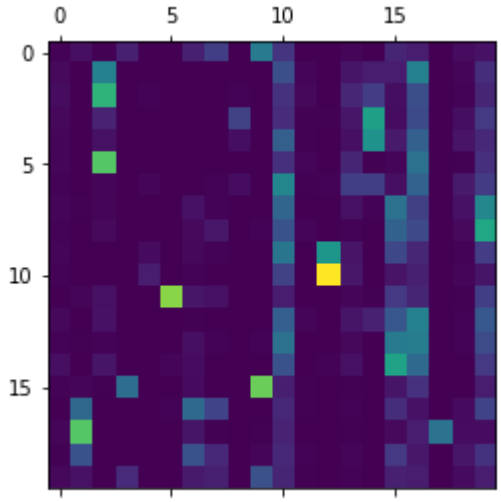
- r=5; **with LSI decomposition**



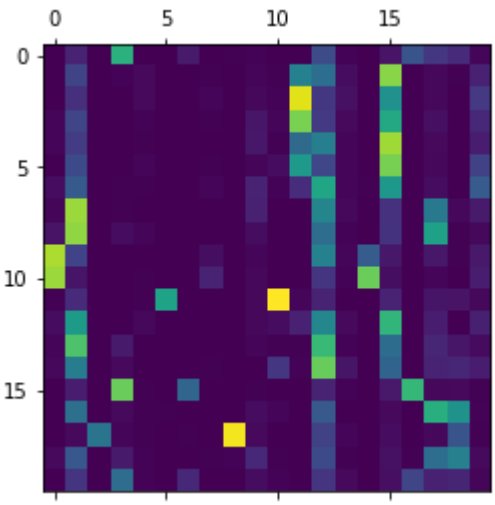
- r=5; **with NMF decomposition**



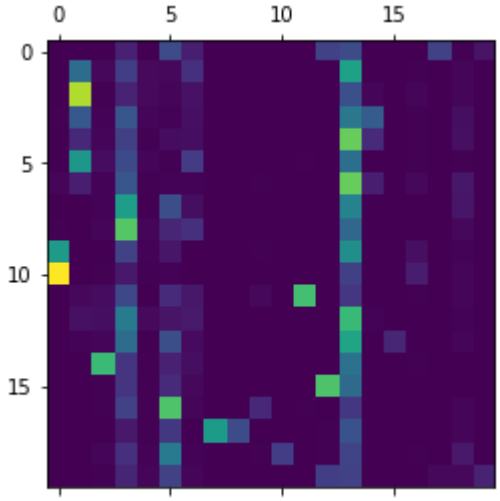
- r=10; **with LSI decomposition**



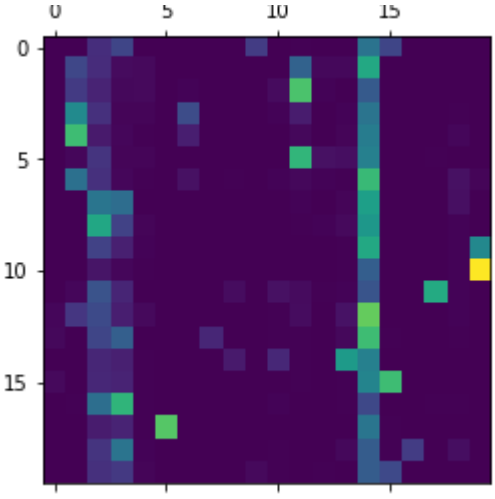
- r=10; **with NMF decomposition**



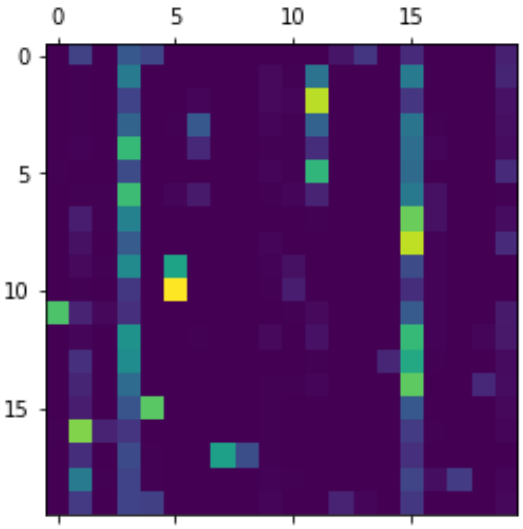
- r=20; **with LSI decomposition**



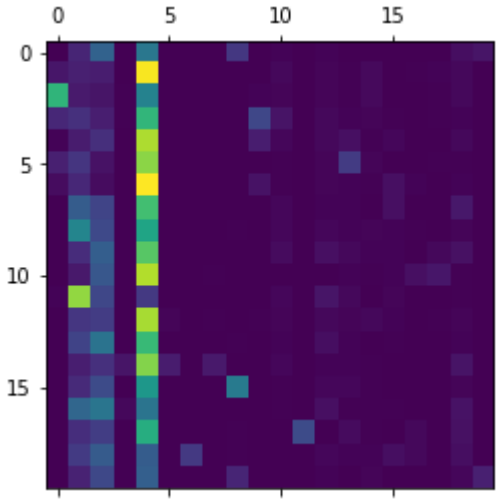
- r=20; **with NMF decomposition**



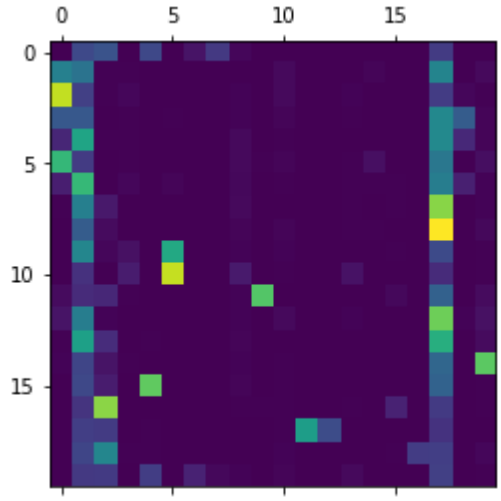
- r=50; **with LSI decomposition**



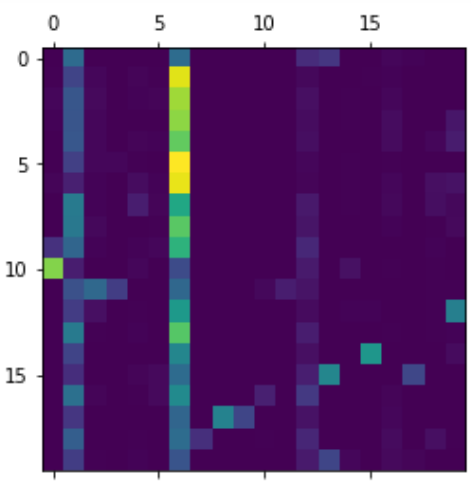
- r=50; **with NMF decomposition**



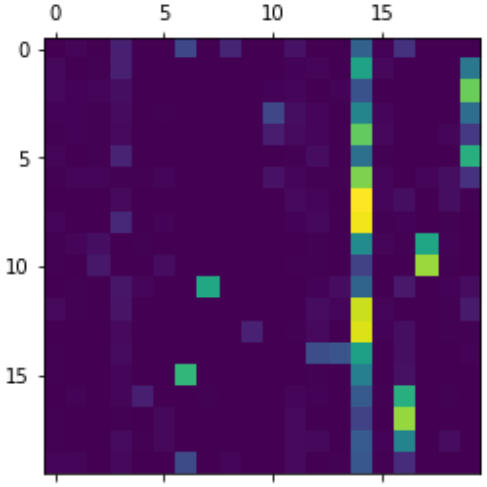
- r=100; **with LSI decomposition**



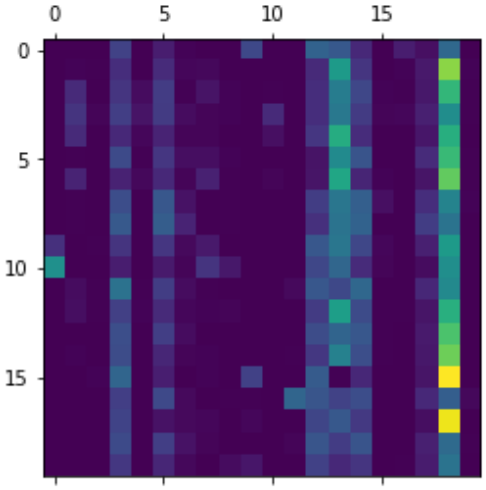
- r=100; **with NMF decomposition**



- r=300; **with LSI decomposition**



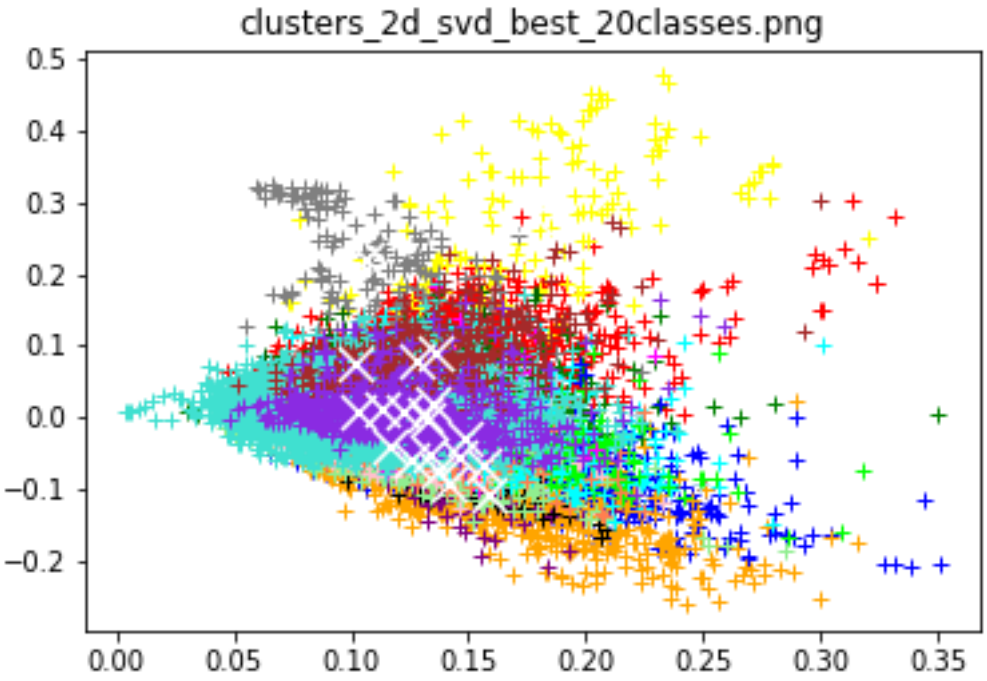
- r=300; **with NMF decomposition**



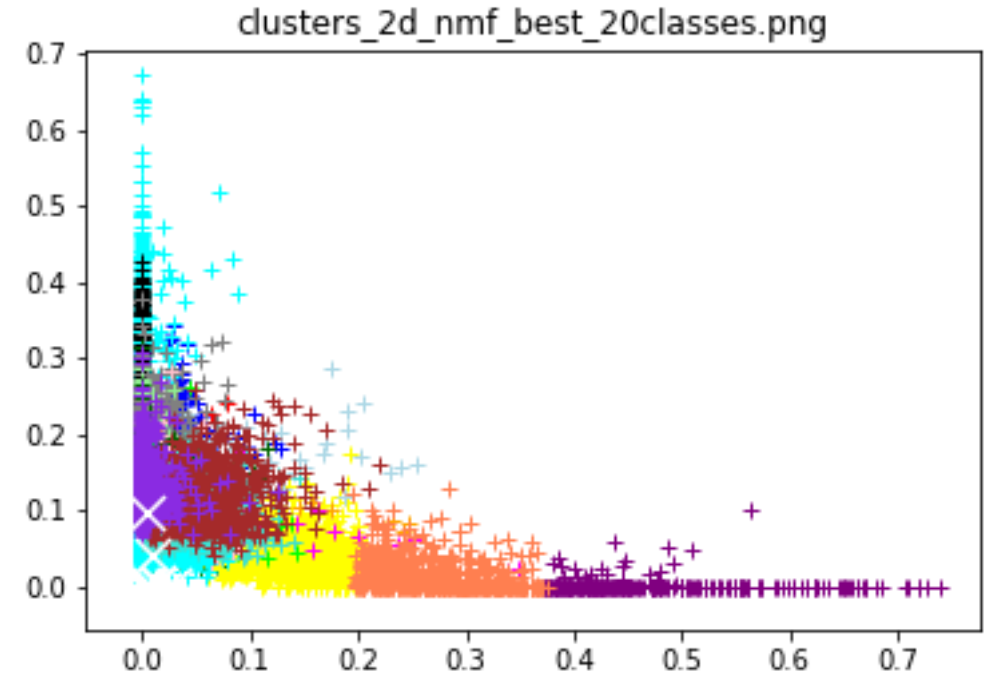
c) Visualization in 2D with best r:

We then visualized both the LSI reduced and the NMF reduced matrix in 2D after applying K-means. For visualizing, we used SVD to convert the matrix with best r in two dimensional and then plot the clusters

- **After LSI Decomposition**



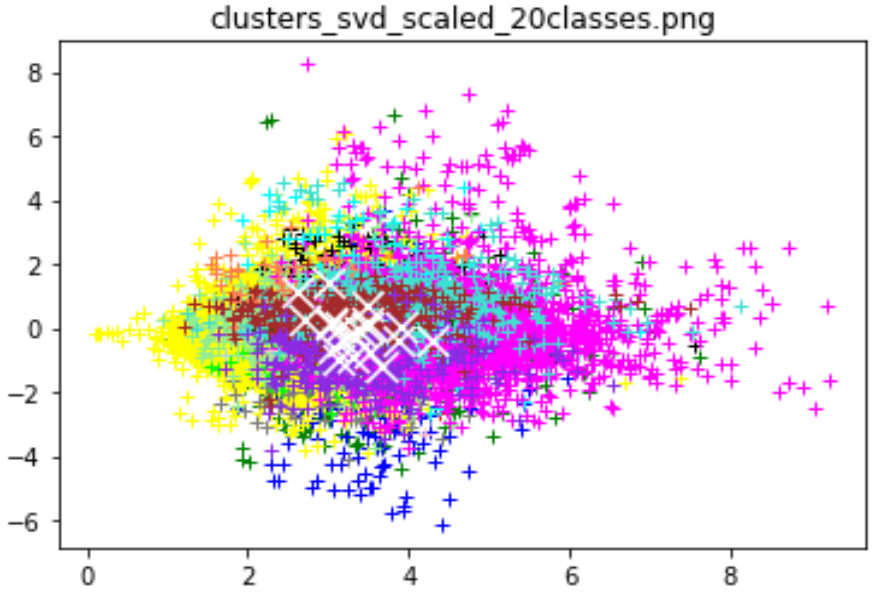
- **After NMF Decomposition**



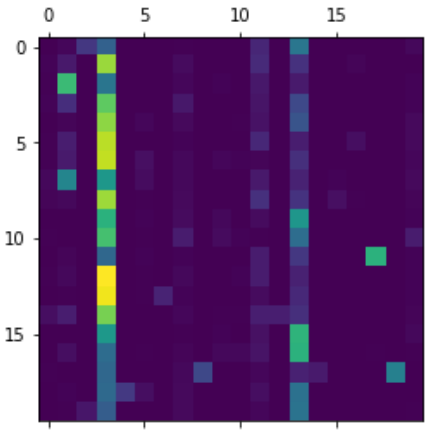
d) Applying transformations and visualizing in 2D with best r:

Now, we have applied some transformations on the LSI and NMF decomposed data as in part 4b. Following section shows the visualization and the contingency matrix for for LSI decomposed data (r=100) and NMF decomposed data (r=10) after applying transformations.

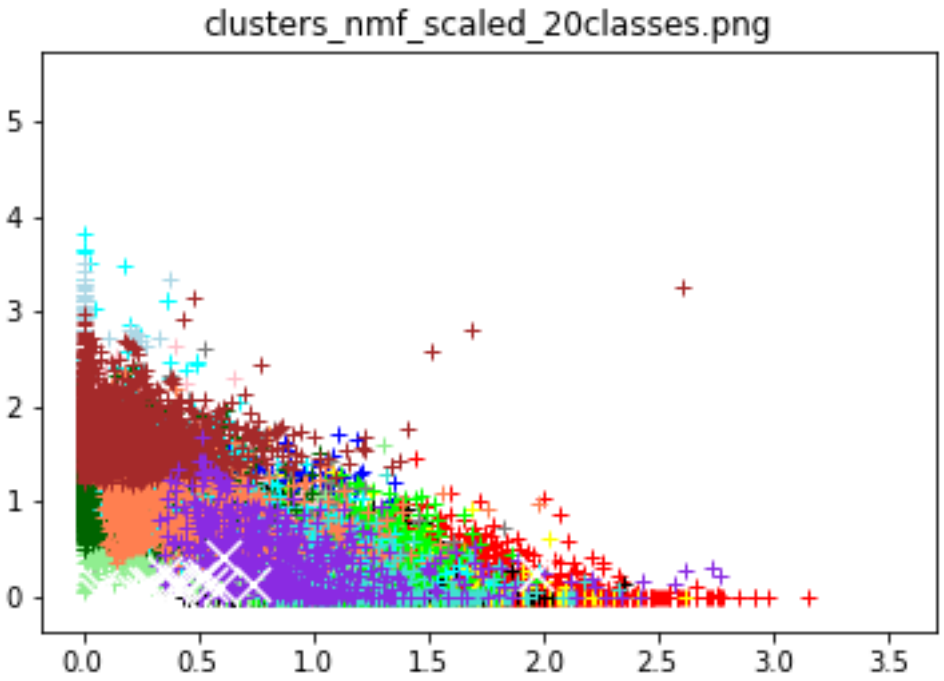
- ***Normalization on LSI Decomposed Matrix***



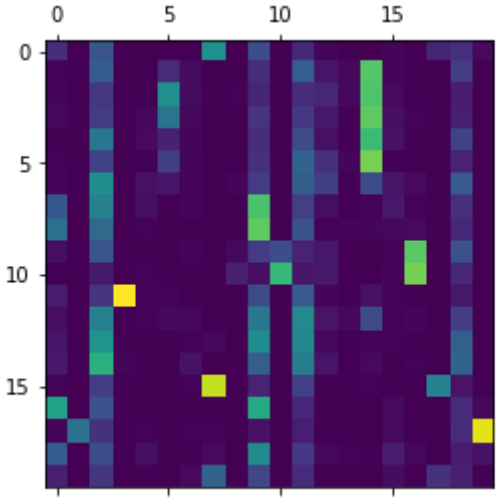
Metric	Value
Homogeneity	0.148
Completeness	0.270
V-measure	0.191
Adjusted Rand Index	0.031
Adjusted Mutual Info Score	0.145



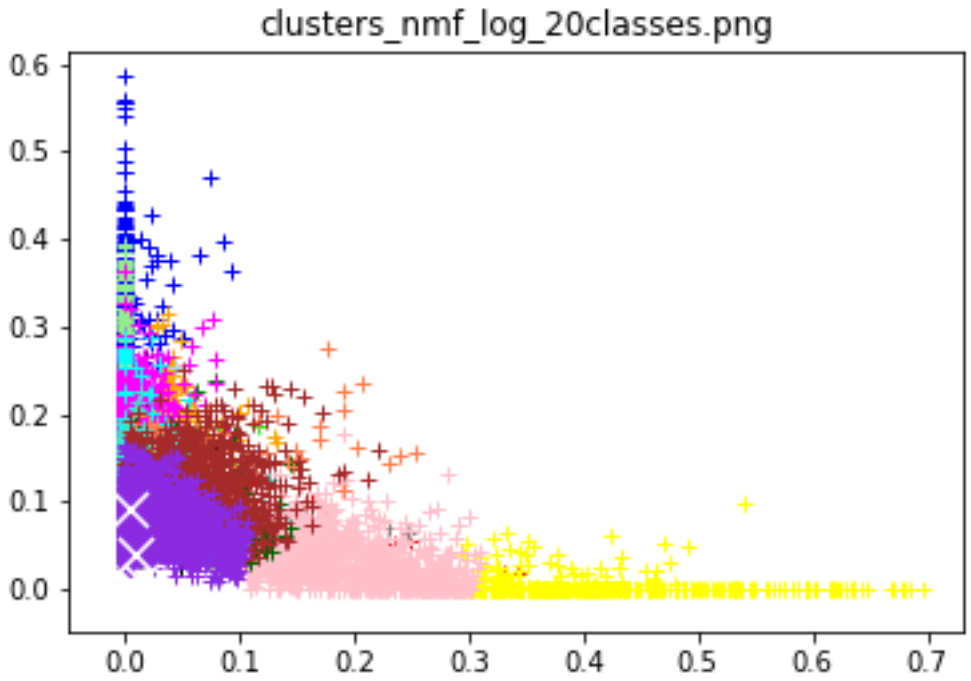
- ***Normalization on NMF Decomposed Matrix***



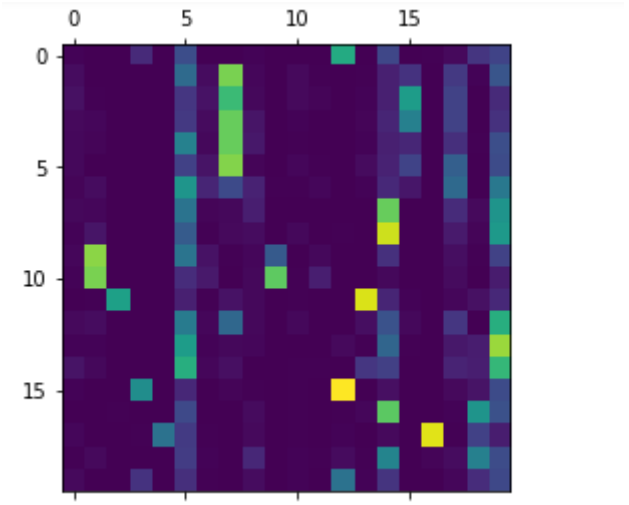
Metric	Value
Homogeneity	0.260
Completeness	0.302
V-measure	0.279
Adjusted Rand Index	0.099
Adjusted Mutual Info Score	0.257



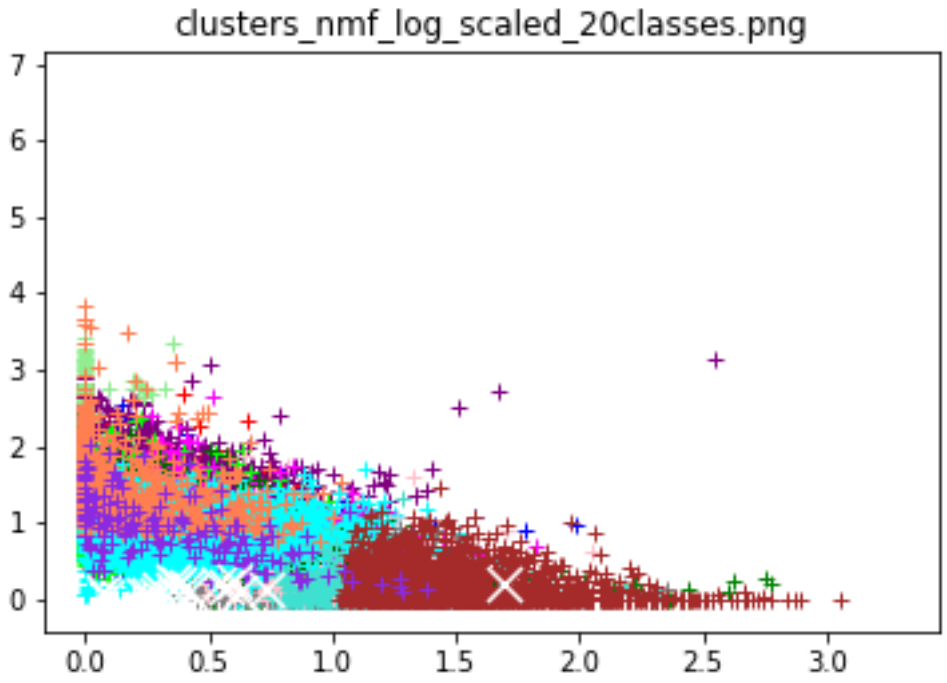
- ***Non-linear (logarithmic) transformation on NMF Decomposed matrix***



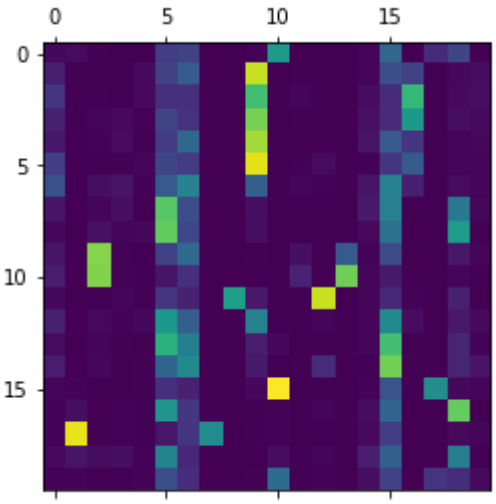
Metric	Value
Homogeneity	0.294
Completeness	0.342
V-measure	0.316
Adjusted Rand Index	0.114
Adjusted Mutual Info Score	0.292



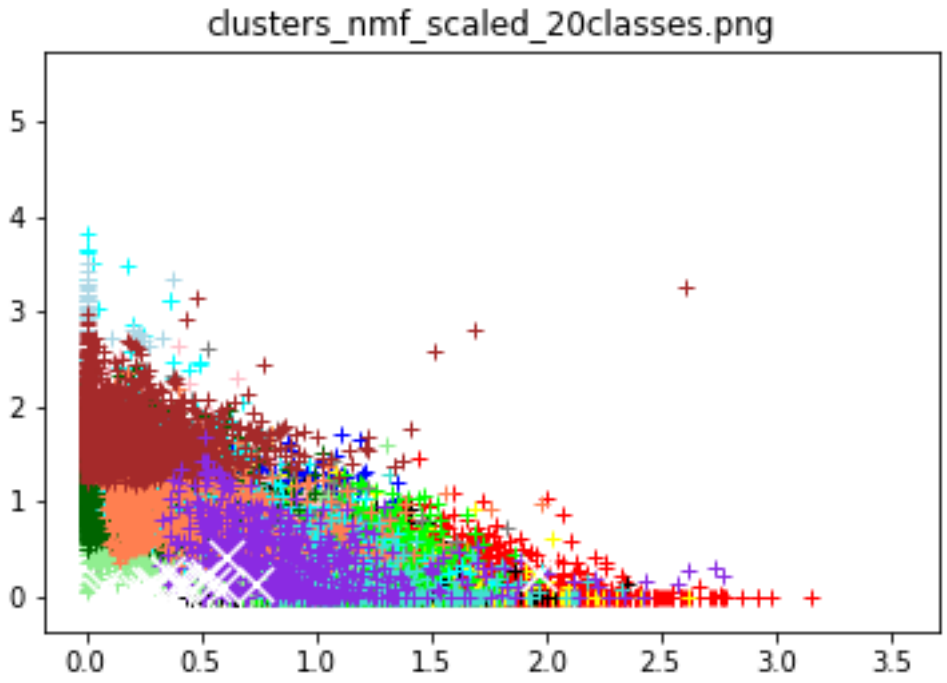
- ***Non-linear (logarithmic) transformation + Normalization on NMF Decomposed matrix***



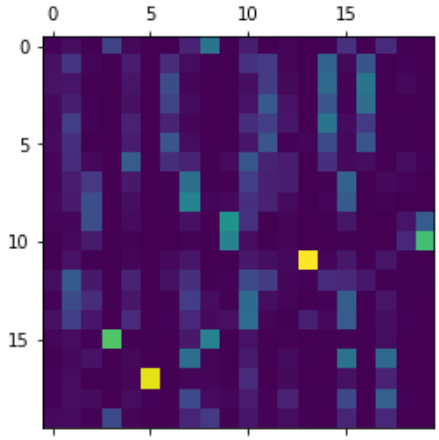
Metric	Value
Homogeneity	0.276
Completeness	0.323
V-measure	0.297
Adjusted Rand Index	0.105
Adjusted Mutual Info Score	0.273



- ***Normalization + Non-linear (logarithmic) transformation on NMF Decomposed matrix***



Metric	Value
Homogeneity	0.318
Completeness	0.330
V-measure	0.324
Adjusted Rand Index	0.151
Adjusted Mutual Info Score	0.316



Thus, we see that normalization to LSI decomposed data does not increase the purity. While, for NMF decomposed data, the purity is increased by first normalizing and then applying logarithmic transformation.