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1 Project2: Data Representations and Clustering

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```
[]: import hdbscan
     import numpy as np
     import pandas as pd
     import itertools
     import matplotlib.pyplot as plt
     import matplotlib.colors as colors
     import umap
     import umap.plot
     import time
     from sklearn.datasets import fetch_20newsgroups
     from sklearn.feature extraction import text
     from sklearn.feature_extraction.text import CountVectorizer
     from sklearn.feature_extraction.text import TfidfTransformer
     from sklearn.feature_extraction.text import TfidfVectorizer
     from sklearn.cluster import KMeans
     from sklearn.cluster import MiniBatchKMeans
     from sklearn.cluster import AgglomerativeClustering
     from sklearn.cluster import DBSCAN
     from sklearn.cluster import Birch
     from sklearn.metrics.cluster import contingency_matrix
     from sklearn.metrics.cluster import homogeneity_score, completeness_score, __
      →v_measure_score, adjusted_rand_score, adjusted_mutual_info_score
     from sklearn.metrics.cluster import rand_score
     from sklearn.decomposition import TruncatedSVD, NMF
     from sklearn.metrics import confusion_matrix
     from scipy.optimize import linear_sum_assignment
     import warnings
     warnings.filterwarnings('ignore')
     import random
```

```
np.random.seed(0)
random.seed(0)
```

2 Question 1

```
[]: class1 = ['comp.graphics', 'comp.os.ms-windows.misc', 'comp.sys.ibm.pc.

⇔hardware', 'comp.sys.mac.hardware']

class2 = ['rec.autos', 'rec.motorcycles', 'rec.sport.baseball', 'rec.sport.

⇔hockey']

dataset = fetch_20newsgroups(subset='all', categories=class1+class2, 
⇔shuffle=True, random_state=0, remove=('headers', 'footers'))
```

```
for label in dataset.target:
   if 0 <= label and label <= 3:
        data_labels.append(0)
   elif 4 <= label and label <= 7:
        data_labels.append(1)</pre>
```

```
[]: tfidf_transformer = TfidfTransformer()
  vectorizer = CountVectorizer(min_df=3, stop_words='english')

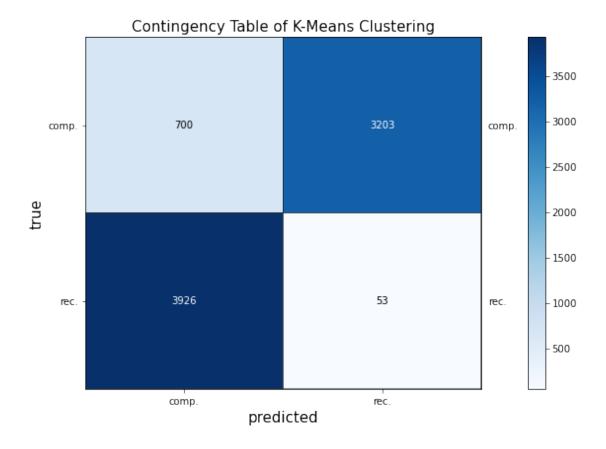
data_count = vectorizer.fit_transform(dataset.data)
  data_tfidf = tfidf_transformer.fit_transform(data_count).toarray()

print("The shape of the TF-IDF matrix is {}".format(data_tfidf.shape))
```

The shape of the TF-IDF matrix is (7882, 23522)

```
im = ax.pcolor(mat, cmap=plt.cm.Blues, linestyle='-', linewidth=0.5,_
→edgecolor=grid, vmin=vmin, vmax=vmax)
  if colorbar:
      plt.colorbar(im,fraction=0.046, pad=0.1)
  # tick marks = np.arange(len(classes))
  # Ticks
  lda_num_topics = mat.shape[0]
  nmf_num_topics = mat.shape[1]
  yticks = np.arange(lda_num_topics)
  xticks = np.arange(nmf_num_topics)
  ax.set_xticks(xticks + 0.5)
  ax.set_yticks(yticks + 0.5)
  if xticklabels is None:
      xticklabels = [str(i) for i in xticks]
  if yticklabels is None:
      yticklabels = [str(i) for i in yticks]
  ax.set_xticklabels(xticklabels)
  ax.set_yticklabels(yticklabels)
  # Minor ticks
  # ax.set xticks(xticks, minor=True);
  # ax.set_yticks(yticks, minor=True);
  # ax.set_xticklabels([], minor=True)
  # ax.set_yticklabels([], minor=True)
  # ax.grid(which='minor', color='k', linestyle='-', linewidth=0.5)
  # tick labels on all four sides
  ax.tick_params(labelright = True, labeltop = False)
  if ylabel:
      plt.ylabel(ylabel, fontsize=15)
  if xlabel:
      plt.xlabel(xlabel, fontsize=15)
  if title:
      plt.title(title, fontsize=15)
  # im = ax.imshow(mat, interpolation='nearest', cmap=plt.cm.Blues)
  ax.invert_yaxis()
  # thresh = mat.max() / 2
  def show_values(pc, fmt="%d", **kw):
      pc.update_scalarmappable()
      ax = pc.axes
```

```
for p, color, value in itertools.zip_longest(pc.get_paths(), pc.
      →get_facecolors(), pc.get_array()):
                 x, y = p.vertices[:-2, :].mean(0)
                 if np.all(color[:3] > 0.5):
                     color = (0.0, 0.0, 0.0)
                 else:
                     color = (1.0, 1.0, 1.0)
                 ax.text(x, y, fmt % value, ha="center", va="center", color=color, u
      →**kw, fontsize=10)
        if if_show_values:
             show values(im)
         # for i, j in itertools.product(range(mat.shape[0]), range(mat.shape[1])):
               ax.text(j, i, "{:.2f}".format(mat[i, j]), fontsize = 4,
                        horizontalalignment="center",
                        color="white" if mat[i, j] > thresh else "black")
        plt.tight_layout()
        if pic_fname:
            plt.savefig(pic_fname, dpi=300, transparent=True)
        plt.show()
        plt.close()
[]: | # random_state=0, max_iter>=1000, n_init>=30, n_init=200 would be better
     kmeans = KMeans(n_clusters=2, random_state=0, max_iter=1000, n_init=200).
      →fit(data_tfidf)
     plot_mat(contingency_matrix(data_labels, kmeans.labels_), size=(8, 6), __
      →xticklabels=['comp.', 'rec.'], yticklabels=['comp.', 'rec.'],□
      ⊖xlabel='predicted', ylabel='true', title='Contingency Table of K-Means⊔
```



From the plot above, the contingency matrix is square-shaped. However, it doesn't have to be square-shaped. For example, if we set KMeans(n_clusters=3, ...), the contingency matrix will not be square. And, another example is using "hdbscan", we can't expect how many clusters we will get. Thus, the contingency matrix we construct may not be square.

```
def clustering_metrics(labels_true, labels_pred):
    print("Homogeneity Score: ", homogeneity_score(labels_true, labels_pred))
    print("Completeness Score: ", completeness_score(labels_true, labels_pred))
    print("V_measure Score: ", v_measure_score(labels_true, labels_pred, beta=1.
40))
    print("Adjusted Rand Score: ", adjusted_rand_score(labels_true,
4labels_pred))
    print("Adjusted Mutual Info Score: ",
4adjusted_mutual_info_score(labels_true, labels_pred,
4average_method='arithmetic'))
    print("Rand Score: ", rand_score(labels_true, labels_pred))
    return
```

[]: clustering_metrics(data_labels, kmeans.labels_)

Homogeneity Score: 0.5905524257932604 Completeness Score: 0.6037369950642207 V_measure Score: 0.5970719337366653 Adjusted Rand Score: 0.6543270617544648

Adjusted Mutual Info Score: 0.5970346379937653

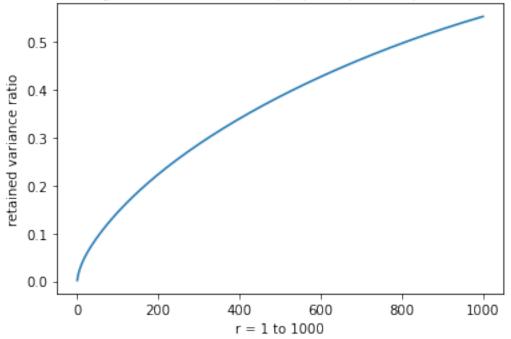
Rand Score: 0.8271633545693536

5 Question 4

```
[]: svd = TruncatedSVD(n_components=1000, random_state=0)
svd_ft = svd.fit_transform(data_tfidf)
retained_ratio = np.cumsum(svd.explained_variance_ratio_)
```

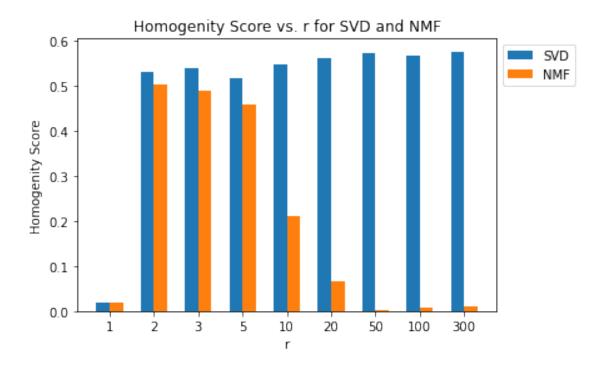
```
[]: plt.plot(np.linspace(1, 1000, num=1000), retained_ratio)
   plt.xlabel('r = 1 to 1000')
   plt.ylabel('retained variance ratio')
   plt.title('Percentage of variance that top r principal components retain')
   plt.show()
```

Percentage of variance that top r principal components retain



```
[ ]: scores_svd = {}
     scores_nmf = {}
     scores_svd['h'] = []
     scores_svd['c'] = []
     scores svd['v'] = []
     scores_svd['ari'] = []
     scores_svd['ami'] = []
     scores_nmf['h'] = []
     scores_nmf['c'] = []
     scores_nmf['v'] = []
     scores_nmf['ari'] = []
     scores_nmf['ami'] = []
     rs = [1, 2, 3, 5, 10, 20, 50, 100, 300]
     kmeans = KMeans(n_clusters=2, random_state=0, max_iter=1000, n_init=200)
     for r in rs:
         print("SVD with r = {} ... ".format(r), end = '')
         svd = TruncatedSVD(n components=r, random state=0)
         svd_ft = svd.fit_transform(data_tfidf)
         kmeans_svd = kmeans.fit(svd_ft)
         scores_svd['h'].append(homogeneity_score(data_labels, kmeans_svd.labels_))
         scores_svd['c'].append(completeness_score(data_labels, kmeans_svd.labels_))
         scores_svd['v'].append(v_measure_score(data_labels, kmeans_svd.labels_))
         scores_svd['ari'].append(adjusted_rand_score(data_labels, kmeans_svd.
      →labels ))
         scores_svd['ami'].append(adjusted_mutual_info_score(data_labels, kmeans_svd.
      →labels ))
         print("Done")
     print("")
     for r in rs:
         print("NMF with r = \{\} ... ".format(r), end = '')
         nmf = NMF(n_components=r, random_state=0, init='random', max_iter=300)
         nmf_ft = nmf.fit_transform(data_tfidf)
         kmeans_nmf = kmeans.fit(nmf_ft)
         scores_nmf['h'].append(homogeneity_score(data_labels, kmeans_nmf.labels_))
         scores_nmf['c'].append(completeness_score(data_labels, kmeans_nmf.labels_))
         scores_nmf['v'].append(v_measure_score(data_labels, kmeans_nmf.labels_))
```

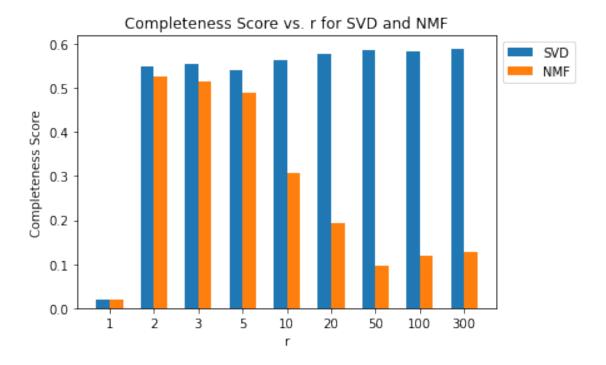
```
scores_nmf['ari'].append(adjusted_rand_score(data_labels, kmeans_nmf.
      →labels ))
         scores_nmf['ami'].append(adjusted_mutual_info_score(data_labels, kmeans_nmf.
      →labels ))
         print("Done")
     print("\nAll Done.")
    SVD with r = 1 \dots Done
    SVD with r = 2 \dots Done
    SVD with r = 3 \dots Done
    SVD with r = 5 \dots Done
    SVD with r = 10 \dots Done
    SVD with r = 20 ... Done
    SVD with r = 50 ... Done
    SVD with r = 100 \dots Done
    SVD with r = 300 \dots Done
    NMF with r = 1 \dots Done
    NMF with r = 2 \dots Done
    NMF with r = 3 \dots Done
    NMF with r = 5 ... Done
    NMF with r = 10 ... Done
    NMF with r = 20 ... Done
    NMF with r = 50 ... Done
    NMF with r = 100 \dots Done
    NMF with r = 300 \dots Done
    All Done.
[]: width = 0.3
     plt.bar(np.arange(len(rs)), scores_svd['h'], width, label='SVD')
     plt.bar(np.arange(len(rs)) + width, scores_nmf['h'], width, label='NMF')
     plt.xticks(np.arange(len(rs)) + width/2, rs)
     plt.xlabel('r')
     plt.ylabel('Homogenity Score')
     plt.title('Homogenity Score vs. r for SVD and NMF')
     plt.legend(bbox_to_anchor=(1,1), loc='upper left')
     plt.show()
     for i in np.arange(len(rs)):
         print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i],__
      ⇒scores_svd['h'][i], scores_nmf['h'][i]))
```



```
3, SVD: 0.53777 NMF: 0.48822
          5, SVD: 0.51659 NMF: 0.45739
         10, SVD: 0.54609 NMF: 0.21021
         20, SVD: 0.56097 NMF: 0.06529
         50, SVD: 0.57250
                           NMF: 0.00213
    r = 100, SVD: 0.56698 NMF: 0.00750
    r = 300, SVD: 0.57525
                           NMF: 0.01102
[]: plt.bar(np.arange(len(rs)), scores_svd['c'], width, label='SVD')
     plt.bar(np.arange(len(rs)) + width, scores_nmf['c'], width, label='NMF')
     plt.xticks(np.arange(len(rs)) + width/2, rs)
     plt.xlabel('r')
     plt.ylabel('Completeness Score')
     plt.title('Completeness Score vs. r for SVD and NMF')
     plt.legend(bbox_to_anchor=(1,1), loc='upper left')
     plt.show()
     for i in np.arange(len(rs)):
        print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i],__
      ⇔scores_svd['c'][i], scores_nmf['c'][i]))
```

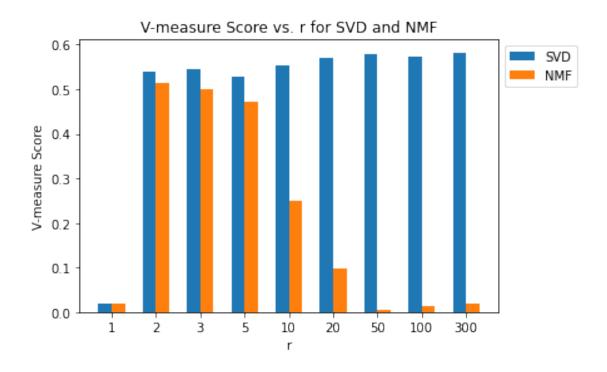
1, SVD: 0.01914 NMF: 0.01914

2, SVD: 0.53061 NMF: 0.50225



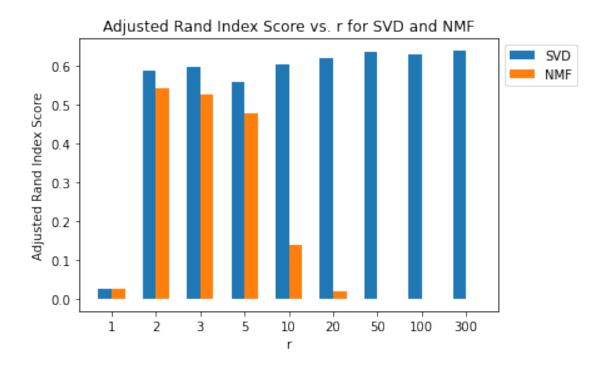
```
2, SVD: 0.54803 NMF: 0.52638
          3, SVD: 0.55428 NMF: 0.51349
          5, SVD: 0.53959 NMF: 0.49016
         10, SVD: 0.56295 NMF: 0.30644
         20, SVD: 0.57722 NMF: 0.19318
         50, SVD: 0.58691
                           NMF: 0.09591
    r = 100, SVD: 0.58220
                           NMF: 0.11960
    r = 300, SVD: 0.58965
                           NMF: 0.12823
[]: plt.bar(np.arange(len(rs)), scores_svd['v'], width, label='SVD')
     plt.bar(np.arange(len(rs)) + width, scores_nmf['v'], width, label='NMF')
     plt.xticks(np.arange(len(rs)) + width/2, rs)
     plt.xlabel('r')
     plt.ylabel('V-measure Score')
     plt.title('V-measure Score vs. r for SVD and NMF')
     plt.legend(bbox_to_anchor=(1,1), loc='upper left')
     plt.show()
     for i in np.arange(len(rs)):
        print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i],__
      ⇔scores_svd['v'][i], scores_nmf['v'][i]))
```

1, SVD: 0.01945 NMF: 0.01945



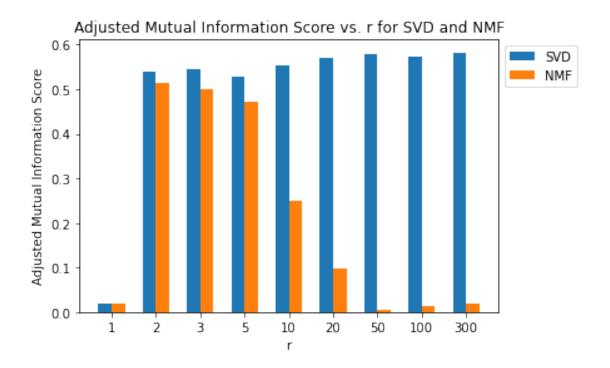
```
2, SVD: 0.53918 NMF: 0.51403
          3, SVD: 0.54590 NMF: 0.50054
          5, SVD: 0.52784 NMF: 0.47321
         10, SVD: 0.55439 NMF: 0.24936
         20, SVD: 0.56898 NMF: 0.09760
         50, SVD: 0.57962 NMF: 0.00417
    r = 100, SVD: 0.57449
                           NMF: 0.01412
    r = 300, SVD: 0.58236
                         NMF: 0.02030
[]: plt.bar(np.arange(len(rs)), scores_svd['ari'], width, label='SVD')
    plt.bar(np.arange(len(rs)) + width, scores_nmf['ari'], width, label='NMF')
    plt.xticks(np.arange(len(rs)) + width/2, rs)
    plt.xlabel('r')
    plt.ylabel('Adjusted Rand Index Score')
    plt.title('Adjusted Rand Index Score vs. r for SVD and NMF')
    plt.legend(bbox_to_anchor=(1,1), loc='upper left')
    plt.show()
    for i in np.arange(len(rs)):
        print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i],__
      ⇔scores_svd['ari'][i], scores_nmf['ari'][i]))
```

1, SVD: 0.01929 NMF: 0.01929



```
2, SVD: 0.58717 NMF: 0.54068
    r =
          3, SVD: 0.59654 NMF: 0.52475
    r =
          5, SVD: 0.55684 NMF: 0.47558
         10, SVD: 0.60283 NMF: 0.13903
         20, SVD: 0.61790 NMF: 0.01799
         50, SVD: 0.63436
                           NMF: -0.00006
    r = 100, SVD: 0.62671
                           NMF: 0.00050
    r = 300, SVD: 0.63679
                           NMF: 0.00088
[]: plt.bar(np.arange(len(rs)), scores_svd['ami'], width, label='SVD')
     plt.bar(np.arange(len(rs)) + width, scores_nmf['ami'], width, label='NMF')
     plt.xticks(np.arange(len(rs)) + width/2, rs)
     plt.xlabel('r')
     plt.ylabel('Adjusted Mutual Information Score')
     plt.title('Adjusted Mutual Information Score vs. r for SVD and NMF')
     plt.legend(bbox_to_anchor=(1,1), loc='upper left')
     plt.show()
     for i in np.arange(len(rs)):
        print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i],__
      ⇔scores_svd['ami'][i], scores_nmf['ami'][i]))
```

1, SVD: 0.02617 NMF: 0.02617



```
2, SVD: 0.53913 NMF: 0.51399
    r =
          3, SVD: 0.54585 NMF: 0.50049
    r =
          5, SVD: 0.52780 NMF: 0.47316
         10, SVD: 0.55435 NMF: 0.24928
         20, SVD: 0.56894 NMF: 0.09748
         50, SVD: 0.57958
                           NMF: 0.00398
    r = 100, SVD: 0.57445
                           NMF: 0.01395
    r = 300, SVD: 0.58233
                          NMF: 0.02013
[]: # Calculate average scores of 5 measure scores
    scores_svd['avg'] = []
    scores_nmf['avg'] = []
    for i in np.arange(len(rs)):
         scores_svd['avg'].append((scores_svd['h'][i] + scores_svd['c'][i] +
      scores_svd['v'][i] + scores_svd['ari'][i] + scores_svd['ami'][i]) / 5)
         scores_nmf['avg'].append((scores_nmf['h'][i] + scores_nmf['c'][i] +

      scores_nmf['v'][i] + scores_nmf['ari'][i] + scores_nmf['ami'][i]) / 5)
[]: plt.bar(np.arange(len(rs)), scores_svd['avg'], width, label='SVD')
    plt.bar(np.arange(len(rs)) + width, scores_nmf['avg'], width, label='NMF')
    plt.xticks(np.arange(len(rs)) + width/2, rs)
    plt.xlabel('r')
```

1, SVD: 0.01920 NMF: 0.01920

```
plt.ylabel('Average Score of 5 Measure Scores')
plt.title('Average Score of 5 Measure Scores vs. r for SVD and NMF')
plt.legend(bbox_to_anchor=(1,1), loc='upper left')
plt.show()

for i in np.arange(len(rs)):
    print("r = {:3d}, SVD: {:.5f} NMF: {:.5f}".format(rs[i], uscores_svd['avg'][i], scores_nmf['avg'][i]))
```

Average Score of 5 Measure Scores vs. r for SVD and NMF 0.6 SVD Average Score of 5 Measure Scores NMF 0.5 0.4 0.3 0.2 0.1 0.0 2 3 5 10 20 50 100 300

```
1, SVD: 0.02065
                       NMF: 0.02065
r
      2, SVD: 0.54882
                       NMF: 0.51947
      3, SVD: 0.55607
                       NMF: 0.50550
r
      5, SVD: 0.53373
                       NMF: 0.47390
r
     10, SVD: 0.56412
                       NMF: 0.23086
r
     20, SVD: 0.57880
                       NMF: 0.09431
     50, SVD: 0.59060
                       NMF: 0.02123
 = 100, SVD: 0.58496
                       NMF: 0.03113
r = 300, SVD: 0.59328
                       NMF: 0.03611
```

- The possible values of r are 1, 2, 3, 5, 10, 20, 50, 100, 300. From the five plots of 5 different measure scores. we can see the relationship of scores and various r.
- In order to choose the best r for SVD and NMF respectively, we average the 5 different measure scores to become one score (the last plot above).
- We can discover that for SVD, the best r is 50 because the avg. scores doesn't increase much after r=50, and Kmeans doesn't perform well in high dimensions. Considering the information preservation and better performance of Kmeans in lower dimensions, the best r

for SVD is 50.

• We can obviously discover that for NMF, the best r is 2.

7 Question 6

- For SVD, we can see that with r increaces, the score basically increase, but it is disproportionate and coverages at about 0.59. If r is getting large, the amount of semantic and complex information in the data for clustering increases. Theoretically, we should get better clustering performance. However, Kmeans doesn't perform well in high dimensions because the Euclidean distance is not a good metric anymore. It causes the distances coverage to a constant value between data points and tends to be almost the same.
- For NMF, the score initially increases very high at r=2 and then decreases sharply. This is because NMF only allows positive entries in the reduced-rank feature matrix. Therefore, in higher dimensions (when r is large), SVD has better performance than NMF.

8 Question 7

Compared to the scores in Question 3, the scores on average at the best choice r are a little bit lower. (Q3: 0.60, Q5/SVD: 0.59, Q5/NMF: 0.52). The reasons why we don't get better results are discussed in the above question. It is about the trade-off between the information preservation and better performance of Kmeans in lower dimensions.

9 Question 8

- Best r for SVD = 50
- Best r for NMF = 2

We plotted the first two principal components of the feature matrix of SVD and NMF.

```
[]: # Best r for SVD = 50
# Best r for NMF = 2

kmeans = KMeans(n_clusters=2, random_state=0, max_iter=1000, n_init=200)

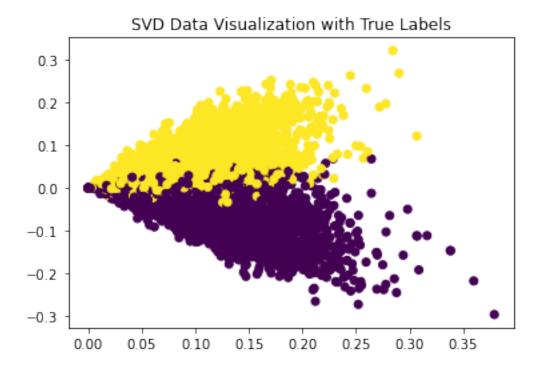
svd = TruncatedSVD(n_components=50, random_state=0)
svd_ft = svd.fit_transform(data_tfidf)
svd_labels = kmeans.fit_predict(svd_ft)

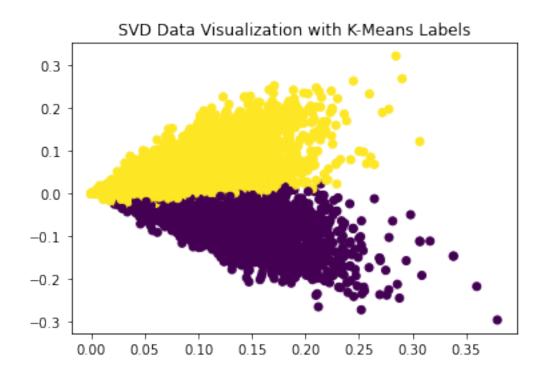
nmf = NMF(n_components=2, random_state=0, init='random', max_iter=300)
nmf_ft = nmf.fit_transform(data_tfidf)
nmf_labels = kmeans.fit_predict(nmf_ft)
```

```
[]: plt.scatter(svd_ft[:, 0], svd_ft[:, 1], c = data_labels)
  plt.title("SVD Data Visualization with True Labels")
  plt.show()

plt.scatter(svd_ft[:, 0], svd_ft[:, 1], c = svd_labels)
```

plt.title("SVD Data Visualization with K-Means Labels")
plt.show()

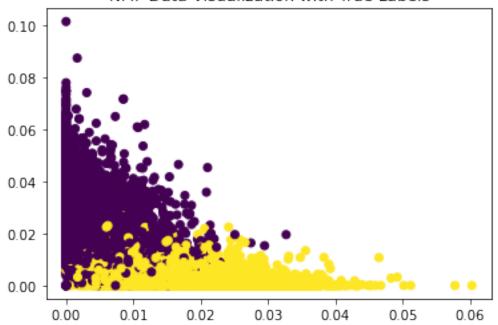


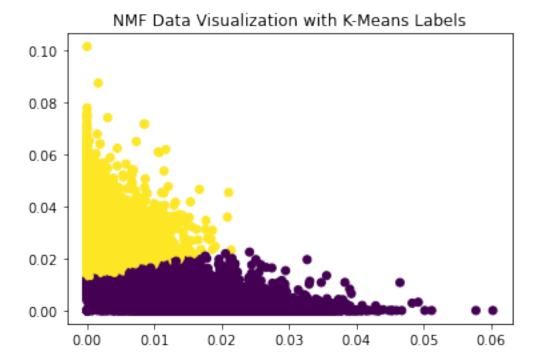


```
[]: plt.scatter(nmf_ft[:, 0], nmf_ft[:, 1], c = data_labels)
   plt.title("NMF Data Visualization with True Labels")
   plt.show()

plt.scatter(nmf_ft[:, 0], nmf_ft[:, 1], c = nmf_labels)
   plt.title("NMF Data Visualization with K-Means Labels")
   plt.show()
```

NMF Data Visualization with True Labels





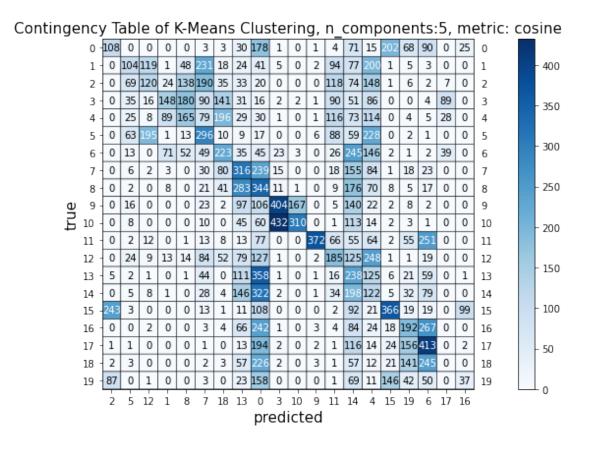
10 Question 9

- For both SVD and NMF, the distributions are not spherical on the plots. K-means assumes the clusters are convex, but the two plots are irregularly shaped, especially for NMF, the two classes have different shape.
- For both SVD and NMF, we can observe that there is a significant overlap among the two clusters, and there is no definite decision boundary between the two clusters.
- Kmeans assumes the clusters will be univariant. However, as the two plots shown, the variances are not equal for two clusters.
- Based on the above observations, the distributions of the data label for Kmeans clustering are not ideal.

```
[]: import nltk
from nltk.corpus import stopwords
from string import punctuation

#Remove stopwords
stop_words_skt = text.ENGLISH_STOP_WORDS
stop_words_en = stopwords.words('english')
combined_stopwords = set.union(set(stop_words_en), set(punctuation), uset(stop_words_skt))
```

The shape of the TF-IDF matrix is (18846, 16332)

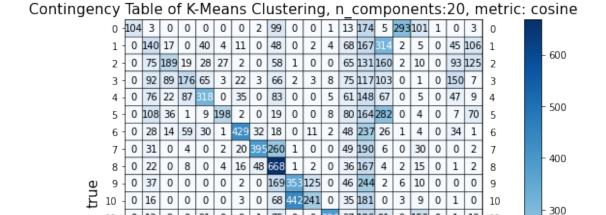


Homogeneity Score: 0.27948135941481755 Completeness Score: 0.3046329140008767 V_measure Score: 0.2915156324792342

Rand Score: 0.8911547188116486

Adjusted Rand Score: 0.0982048006382202

Adjusted Mutual Info Score: 0.28912264821974515



75 0

29 106 0

1 227 1

0 167 1

0 23 0

5 146 1

1 107 1

1 47 2 0

0 1 64

0

1

0 0

0 0

0

0 2

1

0 0

predicted

37 186 91

73 506 53

355

21 251 5

2 19 240 4

6 135 293 253

22

0

2 153

27 56

20 447

55 335

1

1 0

1

1 57

27 180 5 457 24 0

0 14 258 5 27 320 261 0

0 22 165 2 215 65 1

2 6 17 11 18 1 14 10 3 16 13 5

13

1 15

1

0 1

1 17

0 18

11

12

13

14

16

19

200

100

Homogeneity Score: 0.30930764379919023 Completeness Score: 0.3534246650819356 V_measure Score: 0.3298977549519759

0 13

0 14

15 -265 14

0 5

2 1 0 0 0 0 1

1 3 0 0 0 0

88 4

78

11

12

13

14

16

17

18

19

2 0 21

5 10 37

0 0 0 1

1 0

0 0 0

0

0 0 0 1 1

0 0 0 0

0 0 1

0

0

0

9 19

1 11

1

4

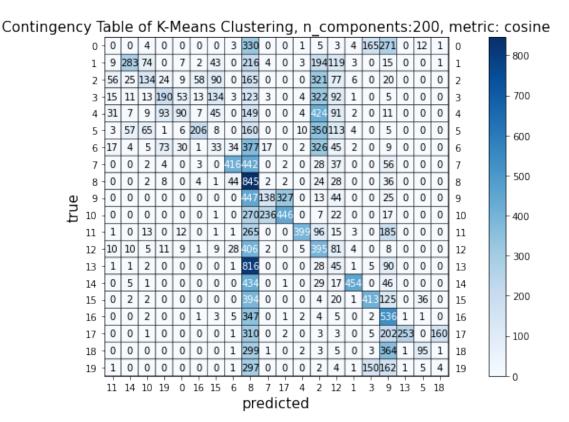
5

7 12

Rand Score: 0.8718242823153872

Adjusted Rand Score: 0.10481224693436049

Adjusted Mutual Info Score: 0.32758369956663563



Homogeneity Score: 0.30012705622977626 Completeness Score: 0.3969413975367476 V_measure Score: 0.3418110588557484

Rand Score: 0.8005061989221712

Adjusted Rand Score: 0.07586998694565665

Adjusted Mutual Info Score: 0.33937344012320975

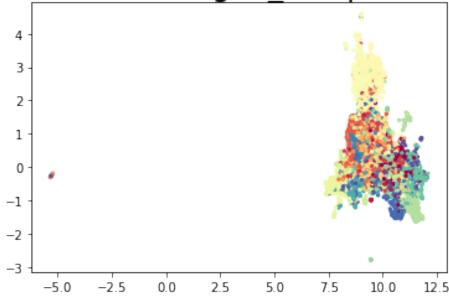
```
#Defining UMAP reduction
def umap_reduction(data, target, n_components, metric):
    map = umap.UMAP(n_components=n_components, random_state=0, metric=metric)
    embedding = map.fit_transform(data)
    plt.scatter(embedding[:, 0], embedding[:, 1], s= 5, c=target, cmap='Spectral')
    plt.title('UMAP Embedding, n_components='+str(n_components), fontsize=24)
    plt.show()
    return embedding
```

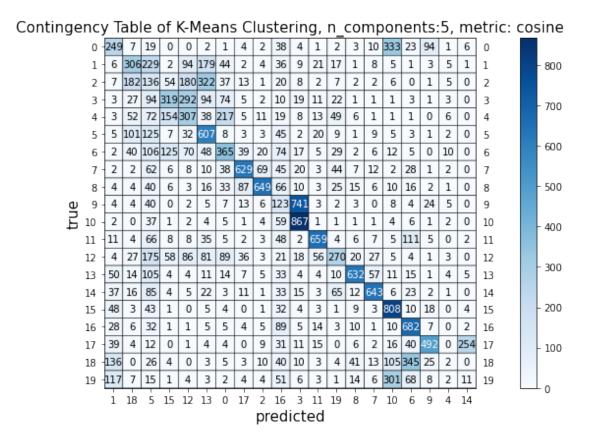
```
[]: #UMAP: Cosine
n_components=[5,20,200]
```

/usr/local/lib/python3.7/dist-packages/numba/np/ufunc/parallel.py:363:
NumbaWarning: The TBB threading layer requires TBB version 2019.5 or later i.e.,
TBB_INTERFACE_VERSION >= 11005. Found TBB_INTERFACE_VERSION = 9107. The TBB
threading layer is disabled.

warnings.warn(problem)

UMAP Embedding, n_components=5





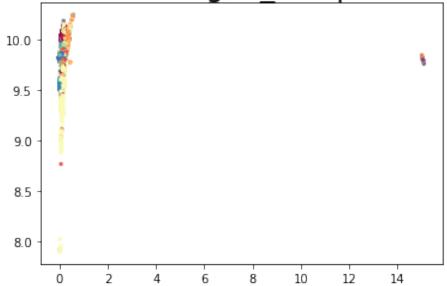
Homogeneity Score: 0.447085619390336 Completeness Score: 0.464107393138403 V_measure Score: 0.4554375164688232

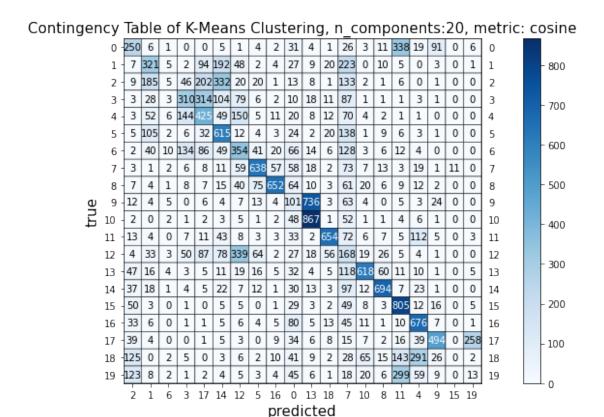
Rand Score: 0.9278027064796069

Adjusted Rand Score: 0.30991663689219257

Adjusted Mutual Info Score: 0.4536365366724623

UMAP Embedding, n_components=20





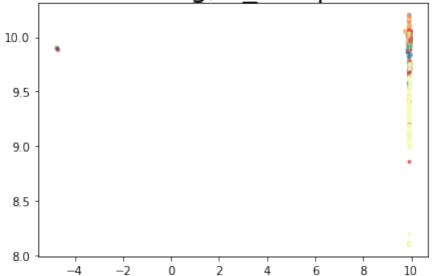
Homogeneity Score: 0.44509986552729197 Completeness Score: 0.47014668361819834 V_measure Score: 0.45728055648379706

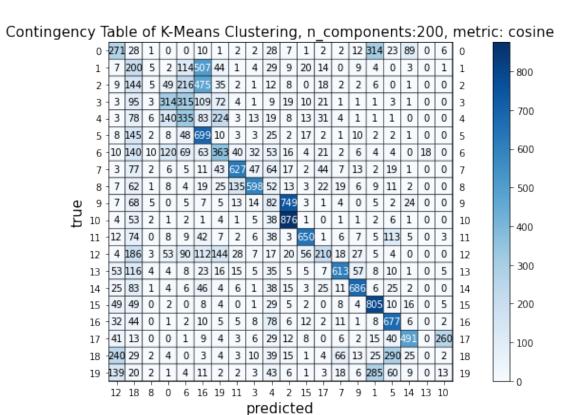
Rand Score: 0.9256836922083721

Adjusted Rand Score: 0.3075492158267226

Adjusted Mutual Info Score: 0.45546581554186527

UMAP Embedding, n_components=200





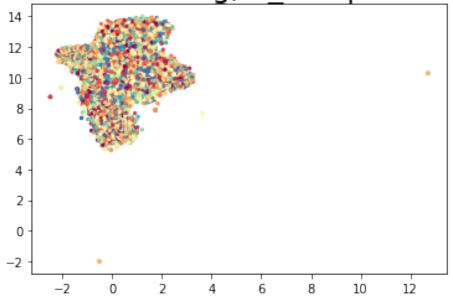
Homogeneity Score: 0.44459038442790794 Completeness Score: 0.47451675194112813 V_measure Score: 0.4590663630279601

Rand Score: 0.922751377456136

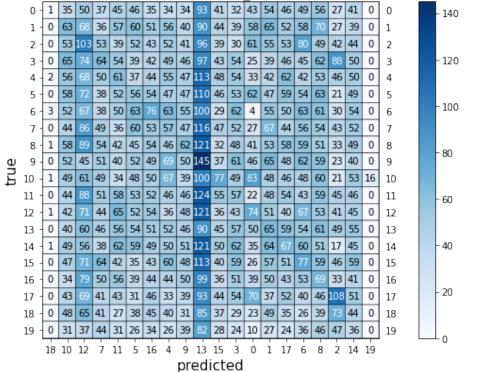
Adjusted Rand Score: 0.3033879521637711

Adjusted Mutual Info Score: 0.4572388848655579

UMAP Embedding, n_components=5







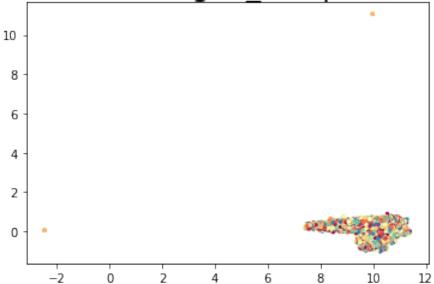
Homogeneity Score: 0.008973314227851121 Completeness Score: 0.009357410268626786 V_measure Score: 0.009161338136465087

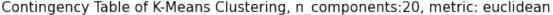
Rand Score: 0.8962586392727165

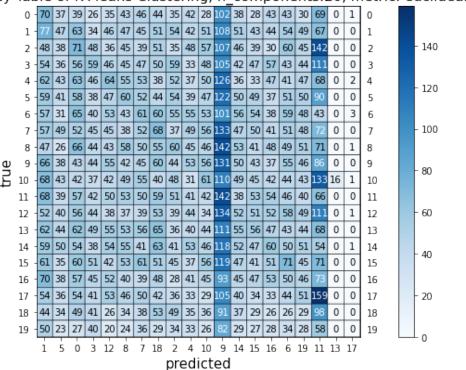
Adjusted Rand Score: 0.0014852038169070893

Adjusted Mutual Info Score: 0.005871041921772191

UMAP Embedding, n_components=20







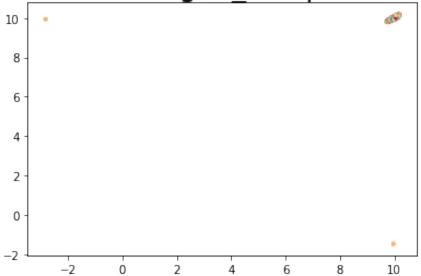
Homogeneity Score: 0.006114005577377522 Completeness Score: 0.006416903541044682 V_measure Score: 0.006261793724409466

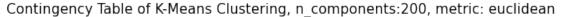
Rand Score: 0.89392734458263

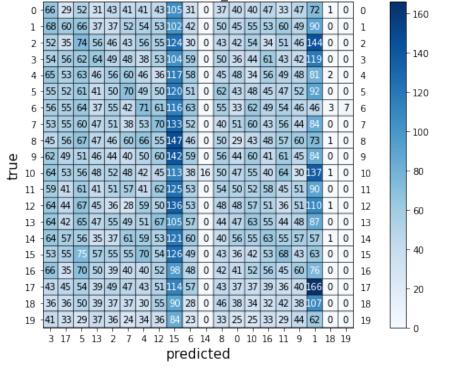
Adjusted Rand Score: 0.0010454463473835898

Adjusted Mutual Info Score: 0.002951123364435492

UMAP Embedding, n_components=200







Homogeneity Score: 0.00650516045327881 Completeness Score: 0.006957281556622199 V_measure Score: 0.006723629013395848

Rand Score: 0.8909627507726462

Adjusted Rand Score: 0.001075404452374812

Adjusted Mutual Info Score: 0.0033997930972916993

13 Question 12

UMAP reduced data with n_components=5 and k-means clustering with n_clusters=20 achieves its highest adjusted rand index for both the cosine metric and the euclidean metric (0.30991663689219257 and 0.0014852038169070893). However, this rand index is significantly higher with the cosine metric as we are dealing with text data, which doesn't rely on the lengths of each document and cosine distance is also invariant to the scalings of signals. The contingency matrix for euclidean measurements is also observed with 1 major cluster label with other points dispersed over the total 18 labels for n_components=5 as where for n_components=20, 2 major cluster labels are observed with 18 in total, and for n_components=200, 2 major cluster labels with 17 in total. The diagonal line as observed with the cosine data contingency matrices are not observed with euclidean data which indicates that the accuracies of the clustering labels compared to the target labels are much higher than that of cosine data.

14 Question 13

So far, k-Means was applied to data dimensionally reduced by UMAP, SVD, NMF indicating them to have the highest adjusted rand index (thus, accuracy in the cluster labels) in this order with UMAP creating significantly better results. Furthermore, the contingency matrix for UMAP reduced data is evenly dispersed amongst the created cluster labels with a majority of them successfully located on the diagonal, indicating that they match the labels of the target data.

15 Question 14

```
[]: #Generating UMAP reduced data umap_reduced=umap_reduction(data_all_tfidf, dataset_all.target, 5, 'cosine')
```

```
[]: #Agglomerative Clustering, Linkage: None
model = AgglomerativeClustering(affinity='euclidean', n_clusters=20)
model=model.fit(umap_reduced)
print("Clustering Metrics for Agglomerative Clustering, Linkage: None")
clustering_metrics(dataset_all.target, model.labels_)
```

Clustering Metrics for Agglomerative Clustering, Linkage: None

Homogeneity Score: 0.43279752892488915 Completeness Score: 0.4638727880186545 V_measure Score: 0.44779668200528394

Rand Score: 0.9207073562435241

Adjusted Rand Score: 0.29077162437827136

Adjusted Mutual Info Score: 0.44592687704998557

None

```
[]: #Agglomerative Clustering, Linkage: Ward
    model_ward = AgglomerativeClustering(affinity='euclidean', linkage='ward',__
      ⇔n_clusters=20)
    model ward=model ward.fit(umap reduced)
    print("Clustering Metrics for Agglomerative Clustering, Linkage: Ward")
    clustering_metrics(dataset_all.target, model_ward.labels_)
    Clustering Metrics for Agglomerative Clustering, Linkage: Ward
    Homogeneity Score: 0.43279752892488915
    Completeness Score: 0.4638727880186545
    V_measure Score: 0.44779668200528394
    Rand Score: 0.9207073562435241
    Adjusted Rand Score: 0.29077162437827136
    Adjusted Mutual Info Score: 0.44592687704998557
[]: #Agglomerative Clustering, Linkage: Single
    model_single = AgglomerativeClustering(affinity='euclidean', linkage='single', u
      on clusters=20)
    model_single=model_single.fit(umap_reduced)
    print("Clustering Metrics for Agglomerative Clustering, Linkage: Single")
    clustering_metrics(dataset_all.target, model_single.labels_)
    Clustering Metrics for Agglomerative Clustering, Linkage: Single
    Homogeneity Score: 0.013598525247829195
    Completeness Score: 0.2777544298099884
    V measure Score: 0.025927663069132023
    Rand Score: 0.08491816495809255
    Adjusted Rand Score: 5.355236296715627e-06
    Adjusted Mutual Info Score: 0.019862105241847384
    16
         Question 15
[]: #DBSCAN Clustering Metrics
    model_db = DBSCAN(eps=0.5, min_samples=60).fit(umap_reduced)
    print("Clustering Metrics for DBSCAN, eps=0.5, min_samples=60")
    clustering_metrics(dataset_all.target, model_db.labels_)
    Homogeneity Score: 0.3586719257511675
    Completeness Score: 0.4819452307177034
    V_measure Score: 0.4112697978571667
    Rand Score: 0.8358446885139912
    Adjusted Rand Score: 0.15255361129593412
    Adjusted Mutual Info Score: 0.4089047901263241
[]: print("Number of Noise Points: ", sum(model_db.labels_==-1)," out of_
```

Number of Noise Points: 5015 out of 18846

→",len(model_db.labels_))

```
[]: #DBSCAN Clustering Metrics (noise removed)
     cluster_labels=model_db.labels_
     predicted_labels=dataset_all.target
     predicted_labels_new=[]
     cluster_labels_new=[]
     count=0
     while count<len(cluster_labels):</pre>
       if cluster labels[count]!=-1:
         cluster_labels_new.append(cluster_labels[count])
        predicted labels new.append(predicted labels[count])
       count+=1
     clustering_metrics(predicted_labels_new, cluster_labels_new)
    Homogeneity Score: 0.48079524748857516
    Completeness Score: 0.6391075149226085
    V measure Score: 0.5487616713212515
    Rand Score: 0.8542255226072945
    Adjusted Rand Score: 0.26664323875190493
    Adjusted Mutual Info Score: 0.5464103799059666
[]: #HDBSCAN Clustering Metrics
     model_hdb = hdbscan.HDBSCAN(min_cluster_size=100)
     model hdb.fit(umap reduced)
     clustering_metrics(dataset_all.target, model_hdb.labels_)
    Homogeneity Score: 0.3190189662404249
    Completeness Score: 0.4856133870937405
    V_measure Score: 0.385069976620286
    Rand Score: 0.7772166222393191
    Adjusted Rand Score: 0.09715093779643687
    Adjusted Mutual Info Score: 0.38342299260397267
[]: print("Number of Noise Points: ",sum(model_hdb.labels_==-1)," out ofu
      →",len(model_hdb.labels_))
    Number of Noise Points: 7488 out of 18846
[]: #HDBSCAN Clustering Metrics (noise removed)
     cluster_labels=model_hdb.labels_
     predicted_labels=dataset_all.target
     predicted_labels_new=[]
     cluster_labels_new=[]
     count=0
     while count<len(cluster_labels):</pre>
       if cluster_labels[count]!=-1:
         cluster_labels_new.append(cluster_labels[count])
```

```
predicted_labels_new.append(predicted_labels[count])
count+=1
clustering_metrics(predicted_labels_new, cluster_labels_new)
```

Homogeneity Score: 0.5168356886472298 Completeness Score: 0.7138041636497449 V_measure Score: 0.5995571584823813

Rand Score: 0.8598484786818267

Adjusted Rand Score: 0.305613372008265

Adjusted Mutual Info Score: 0.59795787553628

```
[]: #Contingency Matrix of HDBSCAN, noise removed (Best Model)

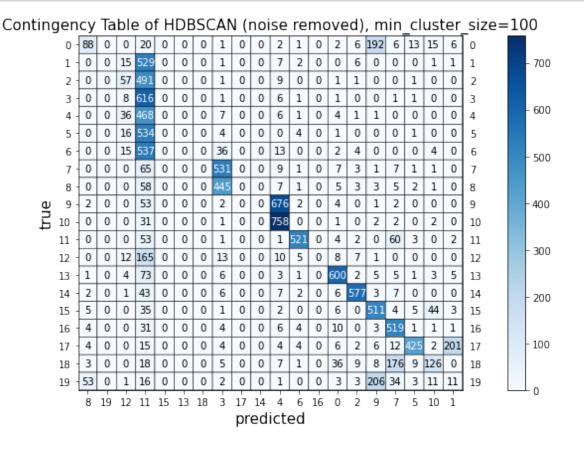
cm = confusion_matrix(predicted_labels_new, cluster_labels_new)

rows, cols = linear_sum_assignment(cm, maximize=True)

plot_mat(cm[rows[:, np.newaxis], cols], xticklabels=cols, yticklabels=rows,__

size=(8,6), xlabel='predicted', ylabel='true', title='Contingency Table of__

HDBSCAN (noise removed), min_cluster_size=100')
```



Approximately 13 clusters were created in HDBSCAN with 9 of them being major clusters. "-1" is the cluster label of the points that do not fall under the main clusters. Although the data points labeled as noise have been removed for the best model, the contingency matrix lacks the smoothness of the diagonalized contingency matrix created earlier by applying k-Means clustering on UMAP data.

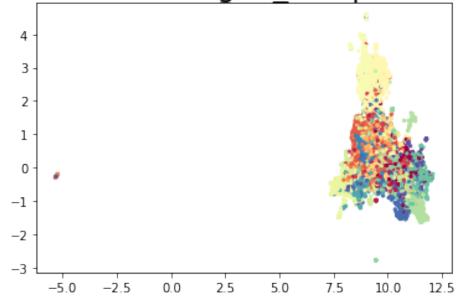
```
[]: #Hyperparameter Tuning
     n_{\text{components}}=[5,20,200]
     k_values = [10, 20, 50]
     cluster values = [20]
     eps values=[0.5,5]
     min_cluster_values = [100,200]
     adjusted_rand_score_values=[]
     highest_tracker_values=[]
     for component in n_components:
       reduction_methods=(umap_reduction(data_all_tfidf, dataset_all.target,_
      →component, 'cosine'), TruncatedSVD(n_components=component, random_state=42).
      ofit_transform(data_all_tfidf), NMF(n_components=component, init='random', ⊔
      →random_state=0, max_iter=500).fit_transform(data_all_tfidf))
       for reduced data in reduction methods:
         adjusted_rand_score_highest=0
         highest_tracker=0
         for k in k_values:
           kmeans = KMeans(n_clusters=k, random_state=0, max_iter=1000, n_init=200).
      →fit(reduced data)
           if adjusted_rand_score(dataset_all.target, kmeans.labels_) > __
      ⇒adjusted_rand_score_highest:
             adjusted_rand_score_highest=adjusted_rand_score(dataset_all.target,_
      ⇔kmeans.labels )
             highest_tracker="n_components="+str(component)+", k="+str(k)
           else:
             pass
         for n_clusters in cluster_values:
           model = AgglomerativeClustering(affinity='euclidean', __
      →n_clusters=n_clusters)
           model=model.fit(reduced_data)
           if adjusted_rand_score(dataset_all.target, model.labels_) >_
      ⇒adjusted_rand_score_highest:
             adjusted_rand_score_highest=adjusted_rand_score(dataset_all.target,_
      →model.labels )
             highest_tracker="n_components="+str(component)+", __
      →n_clusters="+str(n_clusters)
           else:
```

```
pass
    for eps in eps_values:
      model_db = DBSCAN(eps=eps, min_samples=60).fit(reduced_data)
      cluster_label = model_db.labels_
      if adjusted_rand_score(dataset_all.target, model_db.labels_) > ___
 →adjusted_rand_score_highest:
        adjusted_rand_score_highest=adjusted_rand_score(dataset_all.target,_
 →model_db.labels_)
        highest_tracker="n_components="+str(component)+", eps="+str(eps)
      else:
        pass
    for min cluster in min cluster values:
      model_hdb = hdbscan.HDBSCAN(min_cluster_size=min_cluster)
      model_hdb.fit(reduced_data)
      if adjusted_rand_score(dataset_all.target, model_hdb.labels_) >__
 →adjusted_rand_score_highest:
        adjusted_rand_score_highest=adjusted_rand_score(dataset_all.target,__
 →model_hdb.labels_)
        highest_tracker="n_components="+str(component)+", __
 →min cluster size="+str(min cluster)
      else:
        pass
    adjusted_rand_score_values.append(adjusted_rand_score_highest)
    highest_tracker_values.append(highest_tracker)
highest_adj rand=list(zip(highest_tracker_values, adjusted_rand_score_values))
print("UMAP Reduced Data: ", highest_adj_rand[:3])
print("SVD Reduced Data: ", highest_adj_rand[3:6])
print("NMF Reduced Data: ", highest_adj_rand[6:9])
```

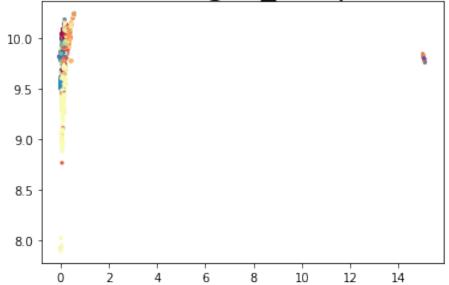
/usr/local/lib/python3.7/dist-packages/numba/np/ufunc/parallel.py:363:
NumbaWarning: The TBB threading layer requires TBB version 2019.5 or later i.e.,
TBB_INTERFACE_VERSION >= 11005. Found TBB_INTERFACE_VERSION = 9107. The TBB
threading layer is disabled.

warnings.warn(problem)

UMAP Embedding, n_components=5



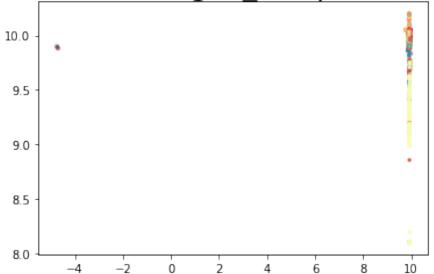
UMAP Embedding, n_components=20



/usr/local/lib/python3.7/dist-packages/sklearn/decomposition/_nmf.py:1641: ConvergenceWarning: Maximum number of iterations 500 reached. Increase it to improve convergence.

ConvergenceWarning,

UMAP Embedding, n_components=200



```
[0.30991663689219257, 0.0982048006382202, 0.08568625308577832, 0.3075492158267226, 0.11465978927950503, 0.09327638757247968, 0.3033879521637711, 0.08589556346009504, 0.038359243575845525]
['reduction= n_components=5 k=20', 'reduction= n_components=5 k=20', 'reduction= n_components=20 k=20', 'reduction= n_components=20 k=20', 'reduction= n_components=200 k=20', 'reduction= n_components=200 k=20', 'reduction= n_components=200 k=20']
```

The adjusted rand scores for each of the clustering methods were computed for each type of the dimensionally reduced data, and the highest adjusted rand scores for each of the dimensionally reduced data were recorded.

 $\begin{tabular}{ll} \bf UMAP: * n_components=5, Adjusted Rand Score: 0.30991663689219257, clustering: k-means, k=20 \end{tabular}$

- n_components=20, Adjusted Rand Score: 0.3075492158267226, clustering: k-means, k=20
- n components=200, Adjusted Rand Score: 0.3033879521637711, clustering: k-means, k=20

SVD: * n components=5, Adjusted Rand Score: 0.0982048006382202, clustering: k-means, k=20

- n_components=20, Adjusted Rand Score: 0.11465978927950503, clustering: k-means, k=50
- n_components=200, Adjusted Rand Score: 0.08589556346009504, clustering: k-means, k=50

 $\mathbf{NMF:}$ * n_components=5, Adjusted Rand Score: 0.08568625308577832, clustering: k-means, k=20

- n components=20, Adjusted Rand Score: 0.09327638757247968, clustering: k-means, k=20
- n_components=200, Adjusted Rand Score: 0.038359243575845525, clustering: k-means, k=20

Overall, dimensional reduction by UMAP with n_components=5 and clustering by k-means with k=20 is shown to have the highest adjusted rand score of: 0.30991663689219257.

19 Question 18

Here, other clustering methods are investigated.

OPTICS (Ordering Points To Identify the Clustering Structure)

This method works similar to DBSCAN however, it covers for its weakness of missing meaningful clusters by ordering the points so that spatially close points become neighbors in the ordering.

Clustering Metrics for OPTICS (min_samples=45) Homogeneity Score: 0.36344959261821275

Completeness Score: 0.5098003223115815 V_measure Score: 0.42436126541317587

Rand Score: 0.8248936296080052

Adjusted Rand Score: 0.17786198292594774

Adjusted Mutual Info Score: 0.4215621018845384

Clustering Metrics for OPTICS (min_samples=50)

Homogeneity Score: 0.37572126549136575 Completeness Score: 0.5048428929098785 V_measure Score: 0.4308151968002098

Rand Score: 0.8391631862639882

Adjusted Rand Score: 0.1835003136411546

Adjusted Mutual Info Score: 0.4283783410386442

Clustering Metrics for OPTICS (min_samples=55)

Homogeneity Score: 0.3693428022289645 Completeness Score: 0.5036767314269334 V_measure Score: 0.42617460029496407

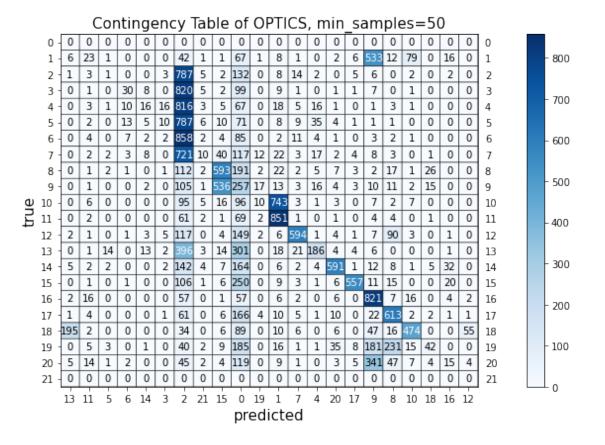
Rand Score: 0.8367510531450865

Adjusted Rand Score: 0.17634616112065196

Adjusted Mutual Info Score: 0.42399544740995004

Adjusted Rand Index is observed at its highest (0.1835003136411546) when min_samples=50.

Below is the observed contingency matrix.



Computing Time: 122.41429615020752

BIRCH

Birch is an alternative algorithm to MiniBatchKMeans, but is more memory efficient. It creates a Clustering Tree for specified data.

```
model_birch = Birch(n_clusters=20)
model_birch.fit(umap_reduced)
cm = confusion_matrix(dataset_all.target, model_birch.labels_)
rows, cols = linear_sum_assignment(cm, maximize=True)
clustering_metrics(dataset_all.target, model_birch.labels_)
plot_mat(cm[rows[:, np.newaxis], cols], xticklabels=cols, yticklabels=rows,u
size=(8,6), xlabel='predicted', ylabel='true', title='Contingency Table ofu
sBIRCH, n_clusters=20')
end = time.time()
print("Computing Time: "+str(end - start))
```

Homogeneity Score: 0.42877938803631793 Completeness Score: 0.46450175808487426 V_measure Score: 0.44592630313145504

Rand Score: 0.9221120921816005

Adjusted Rand Score: 0.3080960592930424

Adjusted Mutual Info Score: 0.44404519632825534

Contingency Table of BIRCH, n clusters=20 0 206 10 328 20 139 43 13 7 330 0 141 370 17 - 700 3 113 28 11 35 191 10 359 46 - 600 - 500 78 776 5 43 886 2 9 651 2 138 184 164 52 21 116 23 23 9 | 16 17 | 52 84 22 30 11 27 | 15 33 | 17 | 19 21 | 11 207 7 28 18 21 302 138 15 22 | 12 24 277 predicted

Computing Time: 4.58010721206665

BIRCH and OPTICS both use euclidean distance/distance between the points for its metrics but the computing time for a single iteration is much faster with BIRCH as compared to OPTICS (4.58010721206665 [s] vs 122.41429615020752 [s]). The adjusted rand index is also much higher with BIRCH (0.3080960592930424 vs 0.1835003136411546).

Mini Batch K-Means

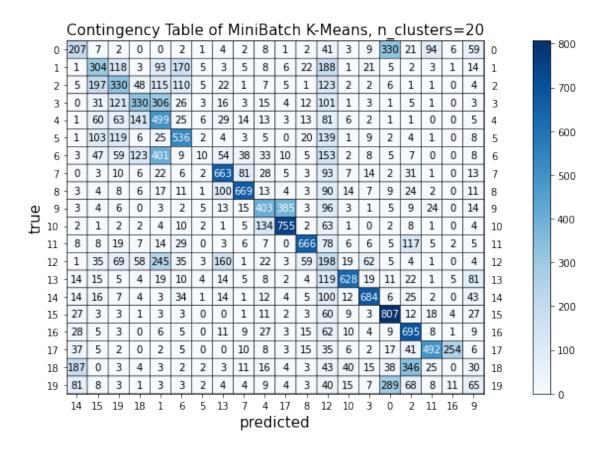
K-Means updated for smaller batch sizes rather than the whole data, better than K-Means if the dataset is large.

Homogeneity Score: 0.444457604564184 Completeness Score: 0.46340988995960514 V_measure Score: 0.4537359270271818

Rand Score: 0.9253614929255675

Adjusted Rand Score: 0.2948513024051965

Adjusted Mutual Info Score: 0.45192515032380415



Computing Time: 4.775979042053223

K-Means on UMAP reduced data using these same parameters has an adjusted rand index of 0.30991663689219257 as where this Mini Batch K-Means provides a score of 0.2948513024051965, creating little difference. However, the computing time is observed to be better with Mini Batch K-Means(4.775979042053223 [s] vs 74.41381978988647 [s]).

From the above, either BIRCH or Mini Batch K-Means may be a better method to enhance the clustering performance.

```
[]: import torch
import torch.nn as nn
from torchvision import transforms, datasets
from torch.utils.data import DataLoader, TensorDataset
import seaborn as sns
import umap

from tqdm import tqdm
import requests
```

```
import os
import tarfile

from sklearn.base import TransformerMixin
from sklearn.model_selection import train_test_split
```

```
[]: filename = './flowers_features_and_labels.npz'
     if os.path.exists(filename):
        file = np.load(filename)
         f all, y all = file['f all'], file['y all']
     else:
         if not os.path.exists('./flower_photos'):
             # download the flowers dataset and extract its images
             url = 'http://download.tensorflow.org/example_images/flower_photos.tgz'
             with open('./flower_photos.tgz', 'wb') as file:
                 file.write(requests.get(url).content)
             with tarfile.open('./flower_photos.tgz') as file:
                 file.extractall('./')
             os.remove('./flower_photos.tgz')
         class FeatureExtractor(nn.Module):
             def __init__(self):
                 super().__init__()
                 vgg = torch.hub.load('pytorch/vision:v0.10.0', 'vgg16',
      →pretrained=True)
                 # Extract VGG-16 Feature Layers
                 self.features = list(vgg.features)
                 self.features = nn.Sequential(*self.features)
                 # Extract VGG-16 Average Pooling Layer
                 self.pooling = vgg.avgpool
                 # Convert the image into one-dimensional vector
                 self.flatten = nn.Flatten()
                 # Extract the first part of fully-connected layer from VGG16
                 self.fc = vgg.classifier[0]
             def forward(self, x):
                 # It will take the input 'x' until it returns the feature vector\Box
      ⇔called 'out'
                 out = self.features(x)
                 out = self.pooling(out)
                 out = self.flatten(out)
                 out = self.fc(out)
                 return out
```

```
# Initialize the model
  assert torch.cuda.is_available()
  feature_extractor = FeatureExtractor().cuda().eval()
  dataset = datasets.ImageFolder(root='./flower_photos',
                                  transform=transforms.Compose([transforms.
→Resize(224),
                                                                 transforms.
→CenterCrop(224),
                                                                 transforms.
→ToTensor(),
                                                                 transforms.
Normalize(mean=[0.485, 0.456, 0.406], std=[0.229, 0.224, 0.225])]))
  dataloader = DataLoader(dataset, batch_size=64, shuffle=True)
  # Extract features and store them on disk
  f_{all}, y_{all} = np.zeros((0, 4096)), np.zeros((0,))
  for x, y in tqdm(dataloader):
      with torch.no grad():
          f_all = np.vstack([f_all, feature_extractor(x.cuda()).cpu()])
          y all = np.concatenate([y all, y])
  np.savez(filename, f_all=f_all, y_all=y_all)
```

```
[]: print(f_all.shape, y_all.shape)
num_features = f_all.shape[1]
```

```
(3670, 4096) (3670,)
```

VGG network is trained by large amount of data, and has high accuracy on ImageNet. Therefore, it should have a great constructure about how to extract features of images. For any custom dataset, VGG still can get the suitable features. Hence, the performance will still be good.

21 Question 20

First, we transform the image to (224, 224, 3) data. The class, FeatureExtractor, extracts the feature layers of the VGG, but we don't get all layers. Since we don't need the output of VGG, we get layers until the first part of fully-connected layer from VGG16. And the data would be transformed to (1, 1, 4096) in this layer. That's the reason that we have 4096 features.

```
[]: from PIL import Image
ans = 0
path = './flower_photos/'
for fl in ['daisy/', 'dandelion/', 'roses/', 'sunflowers/', 'tulips/']:
    for i in os.listdir(path+fl):
```

```
im = Image.open(path+fl+i)
    ans += np.array(im).shape[0] * np.array(im).shape[1]
print('There are {} pixels in the original images.'.format(ans))
```

There are 382129582 pixels in the original images.

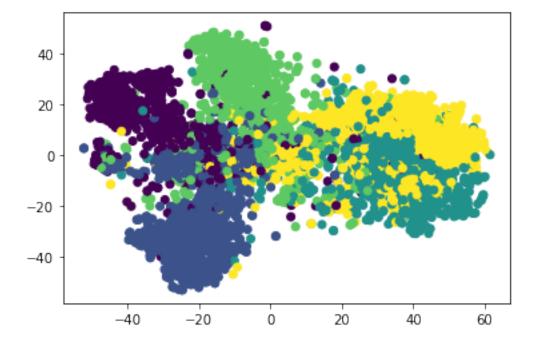
VGG extract 4096 features per image.

23 Question 22

```
[]: print('number of 0 of features in text: {}'.format(np.sum(data_tfidf==0)))
print('number of 0 of features in image: {}'.format(np.sum(f_all==0)))
```

number of 0 of features in text: 184877742 number of 0 of features in image: 0

The extracted features of image are denser than features in text.



We can see that for the data of the same label clustering. For the two labels at right-middle, they are overlap a bit. For the other three labels, it's good for implementing unsupervised learning.

```
[]: class Autoencoder(torch.nn.Module, TransformerMixin):
         def __init__(self, n_components):
             super().__init__()
             self.n_components = n_components
             self.n_features = None # to be determined with data
             self.encoder = None
             self.decoder = None
         def _create_encoder(self):
             return nn.Sequential(
                 nn.Linear(4096, 1280),
                 nn.ReLU(True),
                 nn.Linear(1280, 640),
                 nn.ReLU(True), nn.Linear(640, 120), nn.ReLU(True), nn.Linear(120, un.ReLU(True))
      ⇒self.n_components))
         def _create_decoder(self):
             return nn.Sequential(
                 nn.Linear(self.n_components, 120),
                 nn.ReLU(True),
                 nn.Linear(120, 640),
                 nn.ReLU(True),
                 nn.Linear(640, 1280),
                 nn.ReLU(True), nn.Linear(1280, 4096))
         def forward(self, X):
             encoded = self.encoder(X)
             decoded = self.decoder(encoded)
             return decoded
         def fit(self, X):
             X = torch.tensor(X, dtype=torch.float32, device='cuda')
             self.n_features = X.shape[1]
             self.encoder = self._create_encoder()
             self.decoder = self._create_decoder()
             self.cuda()
             self.train()
             criterion = nn.MSELoss()
             optimizer = torch.optim.Adam(self.parameters(), lr=1e-3,__
      ⇒weight_decay=1e-5)
```

```
dataset = TensorDataset(X)
            dataloader = DataLoader(dataset, batch_size=128, shuffle=True)
            for epoch in tqdm(range(100)):
                for (X_,) in dataloader:
                    X_ = X_ . cuda()
                    # =======forward==========
                    output = self(X)
                    loss = criterion(output, X )
                    optimizer.zero_grad()
                    loss.backward()
                    optimizer.step()
            return self
        def transform(self, X):
            X = torch.tensor(X, dtype=torch.float32, device='cuda')
            self.eval()
            with torch.no_grad():
                return self.encoder(X).cpu().numpy()
[]: np.random.seed(42)
    random.seed(42)
    #dimensionality reduction
    f_svd = TruncatedSVD(n_components=50, random_state=42).fit_transform(f_all)
    f_umap = umap.UMAP(n_components=50, random_state=42).fit_transform(f_all)
    f_auto = Autoencoder(50).fit_transform(f_all)
[]: d = {0: 'None', 1: 'SVD', 2: 'UMAP', 3: 'Autoencoder'}
    for i, f in enumerate([f_all, f_svd, f_umap, f_auto]):
        kmeans = KMeans(n_clusters=5, random_state=42).fit(f)
        print('DR: '+d[i]+', Clustering: Kmeans, rand_score = {}'.

¬format(rand_score(kmeans.labels_, y_all)))

        clustering = AgglomerativeClustering(n_clusters=5).fit(f)
        print('DR: '+d[i]+', Clustering: Agglomerative, rand_score = {}'.
      →format(rand_score(clustering.labels_, y_all)))
        hdbs = hdbscan.HDBSCAN(min_cluster_size=90,min_samples=20).fit(f)
        print('DR: '+d[i]+', Clustering: HDBSCAN, rand_score = {}'.

¬format(rand_score(hdbs.labels_, y_all)))
    DR: None, Clustering: Kmeans, rand_score = 0.704367025294035
    DR: None, Clustering: Agglomerative, rand_score = 0.6862000871875192
    DR: None, Clustering: HDBSCAN, rand_score = 0.20358404572368982
    DR: SVD, Clustering: Kmeans, rand_score = 0.7029640043281845
    DR: SVD, Clustering: Agglomerative, rand_score = 0.6780956582249245
    DR: SVD, Clustering: HDBSCAN, rand_score = 0.20358404572368982
```

```
DR: UMAP, Clustering: Kmeans, rand_score = 0.7954023807985456

DR: UMAP, Clustering: Agglomerative, rand_score = 0.7875960529452524

DR: UMAP, Clustering: HDBSCAN, rand_score = 0.7894305555864994

DR: Autoencoder, Clustering: Kmeans, rand_score = 0.7047682067072006

DR: Autoencoder, Clustering: Agglomerative, rand_score = 0.7201393515001229

DR: Autoencoder, Clustering: HDBSCAN, rand_score = 0.20358404572368982
```

```
[]: class MLP(torch.nn.Module):
       def __init__(self, num_features):
         super().__init__()
         self.model = nn.Sequential(
             nn.Linear(num_features, 1280),
             nn.ReLU(True),
             nn.Linear(1280, 640),
             nn.ReLU(True),
             nn.Linear(640, 5),
             nn.LogSoftmax(dim=1)
         self.cuda()
       def forward(self, X):
         return self.model(X)
       def train(self, X, y):
         X = torch.tensor(X, dtype=torch.float32, device='cuda')
         y = torch.tensor(y, dtype=torch.int64, device='cuda')
         self.model.train()
         criterion = nn.NLLLoss()
         optimizer = torch.optim.Adam(self.parameters(), lr=1e-3, weight_decay=1e-5)
         dataset = TensorDataset(X, y)
         dataloader = DataLoader(dataset, batch_size=128, shuffle=True)
         for epoch in tqdm(range(100)):
           for (X_, y_) in dataloader:
             optimizer.zero_grad()
             X_{, y_{-}} = X_{.to('cuda')}, y_{.to('cuda')}
             pred = self.forward(X_)
             loss = criterion(pred, y_)
             loss.backward()
             optimizer.step()
         return self
```

```
def eval(self, X_test, y_test):
    X_test = torch.tensor(X_test, dtype=torch.float32, device='cuda')
    y_test = torch.tensor(y_test, dtype=torch.int64, device='cuda')
    self.model.eval()
    X_test, y_test = X_test.to('cuda'), y_test.to('cuda')
    pred = self.forward(X_test)
    pred = torch.argmax(pred, dim=1)
    acc = 0
    for i in range(pred.size()[0]):
        if pred[i] == y_test[i]:
            acc += 1
        print('accuracy: {}'.format(acc/pred.size()[0]))
```

```
[]: mlp.eval(X_test, y_test)
```

accuracy: 0.9087193460490464

```
[]: #dimensional reduction features by umap

X_train, X_test, y_train, y_test = train_test_split(f_umap, y_all, test_size=0.

→2, random_state=42)

mlp = MLP(50)

mlp.train(X_train, y_train)
```

```
[]: mlp.eval(X_test, y_test)
```

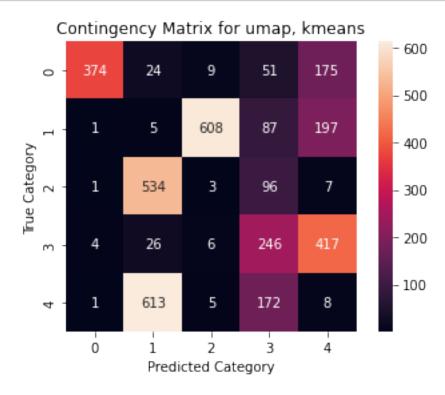
accuracy: 0.8474114441416893

The accuracy of the MLP classifier on the original VGG features is about 90.8%(4096 features), and 84.7%(50 features) for the data after dimensinality reduction by UMAP. We can see there is about 6.1% difference after we reduct the dimension.

We choose our best model (umap, kmeans) to see our accuracy.

```
[]: def plt_contingency_matrix(pred_test, txt):
    cmx_data = confusion_matrix(y_all, pred_test)
    df_cmx = pd.DataFrame(cmx_data)
    sns.heatmap(df_cmx, fmt='d', annot=True, square=True)
    plt.title('Contingency Matrix for '+txt)
    plt.xlabel('Predicted Category')
    plt.ylabel('True Category')
    plt.show()
```

[]: kmeans = KMeans(n_clusters=5, random_state=42).fit(f_umap)
plt_contingency_matrix(kmeans.labels_,'umap, kmeans')



By the contingency matrix, our accuracy is (374+613+608+96+417)/3670=0.5743

The performance is better of the MLP classifier compared to our best unsupervised model(UMAP, kmeans). Since MLP classifier is supervised learning, knowing exactly every label in the training data. On the contrary, unsupervised models group only have information about features and try to group them.