07-Clustering-II

September 26, 2017

1 Clustering data with k-means

Today we'll do an extended example showing k-means clustering in practice and in the context of the python libraries **scikit-learn.**

Our goals are to learn: * How clustering is used in practice * Tools for evaluating the quality of a clustering * Tools for assigning meaning or labels to a cluster * Important visualizations * A little bit about feature extraction for text

1.1 Training wheels: Synthetic data

Generally, when learning about or developing a new unsupervised method, it's a good idea to try it out on a dataset in which you already know the "right" answer.

One way to do that is to generate synthetic data that has some known properties.

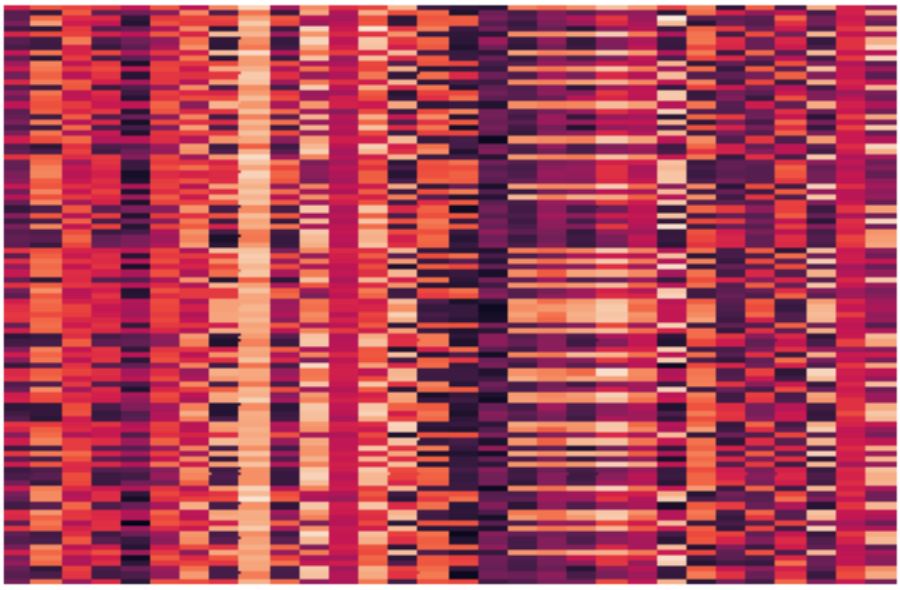
scikit-learn is the main python library for machine learning functions. It is extensive. You will use it a lot :). It is here: http://scikit-learn.org/stable/documentation.html.

Among other things, it contains tools for generating synthetic data for testing.

```
In [62]: X, y = sk_data.make_blobs(n_samples=100, centers=3, n_features=30,
                                   center_box=(-10.0, 10.0),random_state=0)
```

To get a sense of the raw data we can visualize it.

```
In [63]: _ = sns.heatmap(X, xticklabels=False, yticklabels=False, linewidths=0,cbar=False)
```



Now let's compute the pairwise distances for visualization purposes.

We can compute pairwise distances using the **sklearn.metrics** functions summarized here: http://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics

```
In [64]: euclidean_dists = metrics.euclidean_distances(X)
         # euclidean_dists
```

That plot shows all the data. These data live in a **30 dimensional** space, so we cannot directly visualize them.

This is a **big problem** that you will run into time and again!

However, there is a method that can turn a set of pairwise distances into an approximate 2-D representation **in some cases.**

1.1.1 Visualizing with MultiDimensional Scaling

The idea behind Multidimensional Scaling (MDS) is: given a dissimilarity or distance matrix, find a set of coordinates for the points that approximates those distances as well as possible.

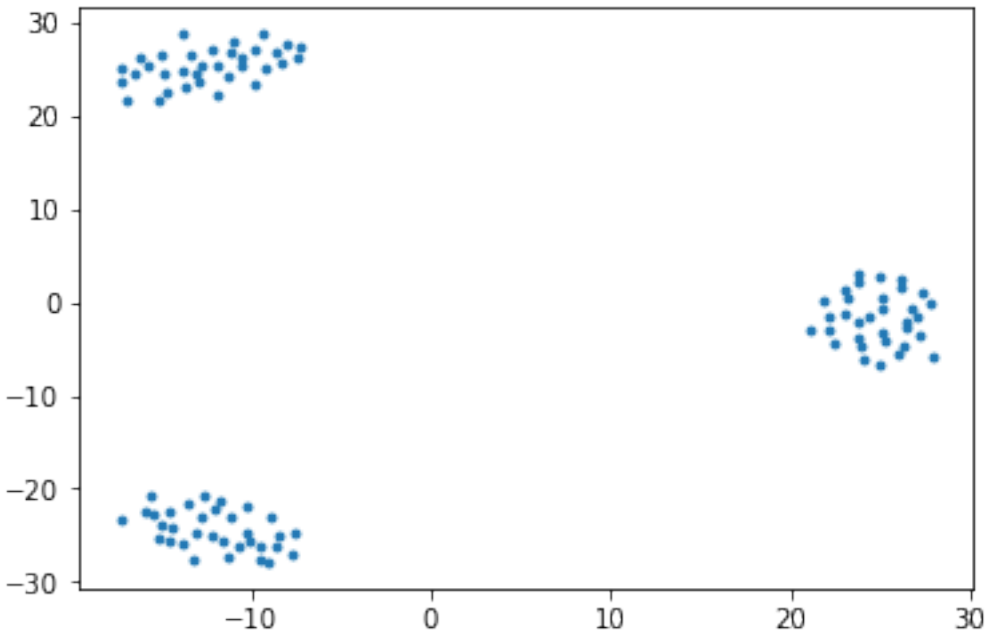
This is done by a gradient descent algorithm that starts with random positions and moves points in a way that reduces the disparity between true distance and euclidean distance.

Note that there are many ways that this can fail!

- Perhaps the dissimilarities are not well modeled as euclidean distances
- It may be necessary to use more than 2 dimensions to capture any clustering via euclidean distances

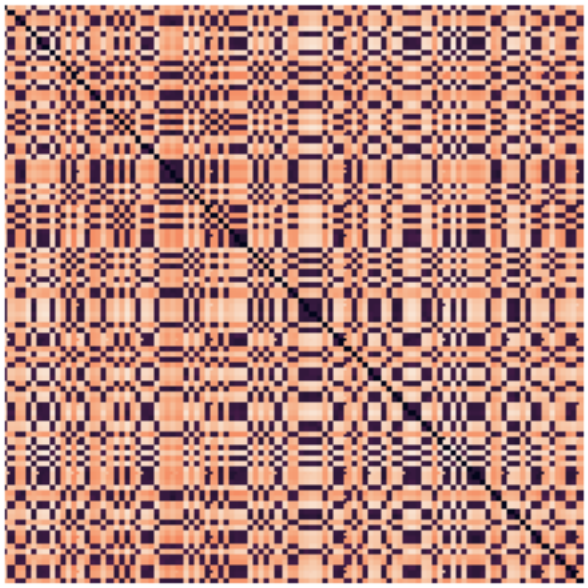
```
In [65]: import sklearn.manifold
         mds = sklearn.manifold.MDS(n_components=2, max_iter=3000, eps=1e-9, random_state=0,
                                    dissimilarity="precomputed", n_jobs=1)
```

```
fit = mds.fit(euclidean_dists)
pos = fit.embedding_
_ = plt.scatter(pos[:, 0], pos[:, 1], s=8)
```



A second way to visualize the data is by using a heatmap on the set of pairwise distances.

```
In [66]: _ = sns.heatmap(euclidean_dists, xticklabels=False, yticklabels=False, linewidths=0,
                         square=True,cbar=False)
```



1.2 Applying k-means

The Python package `scikit-learn` has a huge set of tools for unsupervised learning generally, and clustering specifically.

These are in `sklearn.cluster`.
(http://scikit-learn.org/stable/modules/clustering.html)
There are 3 functions in all the clustering classes,

- `fit()`,
- `predict()`, and
- `fit_predict()`.

`fit()` builds the model from the training data (e.g. for kmeans, it finds the centroids),
`predict()` assigns labels to the data after building the model, and
`fit_predict()` does both at the same data (e.g in kmeans, it finds the centroids and assigns the labels to the dataset).

```
In [67]: from sklearn.cluster import KMeans
         kmeans = KMeans(init='k-means++', n_clusters=3, n_init=100)
         kmeans.fit_predict(X)
```

```
Out[67]: array([1, 2, 0, 0, 2, 1, 2, 2, 1, 2, 0, 1, 0, 1, 2, 0, 0, 1, 0, 2, 0, 2, 0,
                1, 2, 2, 1, 0, 0, 0, 0, 1, 0, 1, 0, 2, 0, 2, 0, 2, 2, 2, 1, 0, 1, 0,
                1, 2, 1, 0, 0, 1, 1, 1, 1, 0, 1, 2, 2, 0, 1, 0, 2, 1, 1, 2, 0, 1, 1,
                2, 2, 2, 1, 1, 0, 1, 2, 1, 2, 1, 2, 2, 2, 1, 0, 0, 2, 1, 1, 0, 1, 2,
                2, 0, 1, 0, 0, 2, 2, 0], dtype=int32)
```

All the tools in `scikit-learn` are implemented as python objects.
Thus, the general sequence for using a tool from `scikit-learn` is:

- Create the object, probably with some parameter settings or intialization,
- Run the method, generally by using the `fit()` function, and
- Examine the results, which are generally instance variables of the object.

```
In [68]: centroids = kmeans.cluster_centers_
         labels = kmeans.labels_
         error = kmeans.inertia_
```

```
In [69]: print("The total error of the clustering is: {}.".format(error))
         print('\nCluster labels:')
         print(labels)
         print('\nCluster centroids:')
         print(centroids)
```

```
The total error of the clustering is: 2733.8430818977895.
```

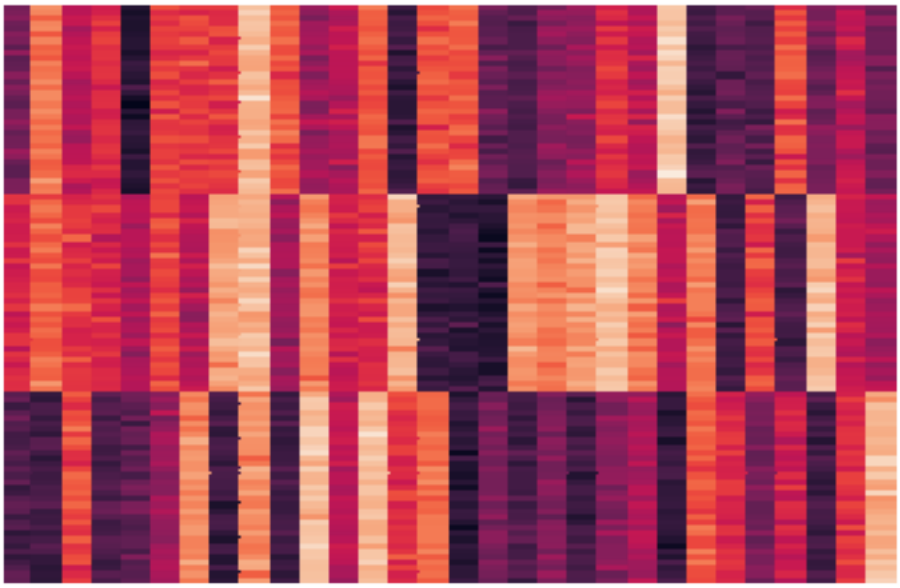
```
Cluster labels:
[1 2 0 0 2 1 2 2 1 2 0 1 0 1 2 0 0 1 0 2 0 2 0 1 2 2 1 0 0 0 0 1 0 1 0 2 0
 2 0 2 2 2 1 0 1 0 1 2 1 0 0 1 1 1 1 0 1 2 2 0 1 0 2 1 1 2 0 1 1 2 2 2 1 1
 0 1 2 1 2 1 2 2 2 1 0 0 2 1 1 0 1 2 2 0 1 0 0 2 2 0]

Cluster centroids:
[[-4.7833887   5.32946939 -0.87141823  1.38900567 -9.59956915  2.35207348
   2.22988468  2.03394692  8.9797878   3.67857655 -2.67618716 -1.17595897
   3.76433199 -8.46317271  3.28114395  3.73803392 -5.73436869 -7.0844462
  -3.75643598 -3.07904369  1.36974653 -0.95918462  9.91135428 -8.17722281
  -5.8656831  -6.76869078  3.12196673 -4.85745245 -0.70449349 -4.94582258]
 [ 0.88697885  4.29142902  1.93200132  1.10877989 -1.55994342  2.80616392
  -1.11495818  7.74595341  8.92512875 -2.29656298  6.09588722  0.47062896
   1.36408008  8.63168509 -8.54512921 -8.59161818 -9.64308952  6.92270491
   5.65321496  7.29061444  9.58822315  5.79602014 -0.84970449  5.46127493
  -7.77730238  2.75092191 -7.17026663  9.07475984  0.04245798 -1.98719465]
 [-7.0489904  -7.92501873  2.89710462 -7.17088692 -6.01151677 -2.66405834
   6.43970052 -8.20341647  6.54146052 -7.92978843  9.56983319 -0.86327902
   9.25897119  1.73061823  4.84528928 -9.26418246 -4.54021612 -7.47784575
  -4.15060719 -7.85665458 -3.76688414 -1.6692291  -8.78048843  3.78904162
   1.24247168 -4.73618733  0.27327032 -7.93180624  1.59974866  8.78601576]]
```

1.2.1 Visualizing the results of clustering

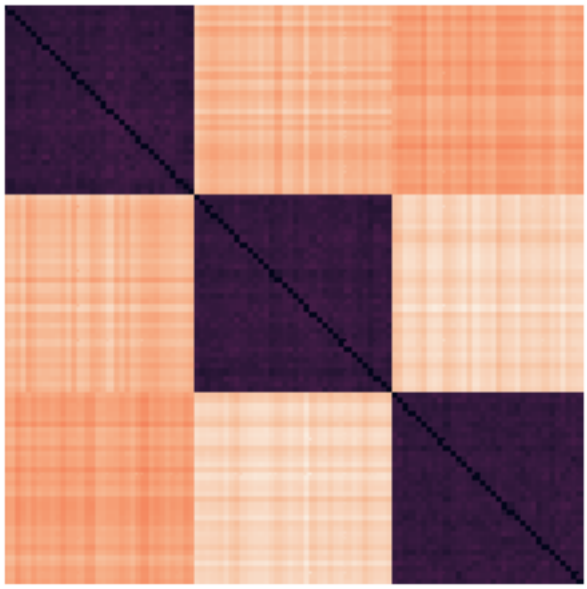
Let's visualize the results. We'll do that by reording the data items according to their cluster.

```
In [70]: idx = np.argsort(labels)
         rX = X[idx,:]
         _ = sns.heatmap( rX,xticklabels=False, yticklabels=False, linewidths=0,cbar=False)
```



```
In [71]: rearranged_dists = euclidean_dists[idx,:][:,idx]
         sns.heatmap(rearranged_dists, xticklabels=False, yticklabels=False, linewidths=0, squar

Out[71]: <matplotlib.axes._subplots.AxesSubplot at 0x119faf668>
```



1.3 Deciding on the number of clusters

So far, we have assumed that the number of clusters is given or known in advance. Of course that's almost never the case.

In practice, to use k-means or most other clustering methods, one must choose k, the number of clusters, via some other process.

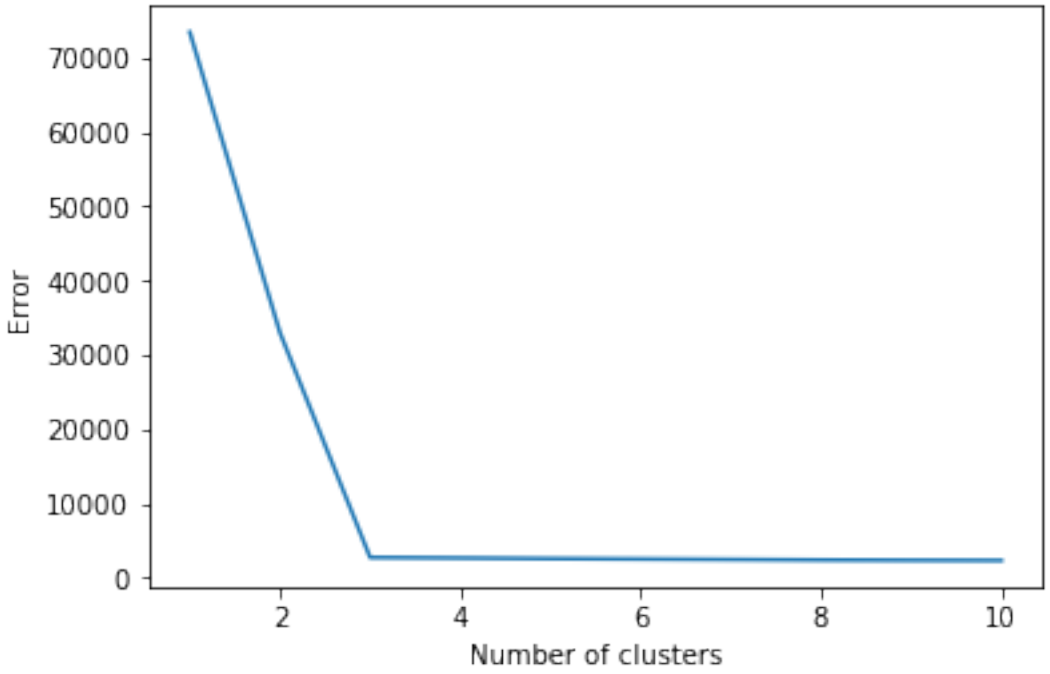
1.3.1 Inspecting Clustering Error

The first thing you might do is to look at the k-means objective function (which is considered the clustering "error") and see if it levels off after a certain point.

This would suggest that the clustering is not improving as the number of clusters is increased.

```
In [72]: error = np.zeros(11)
         for k in range(1,11):
             kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10)
             kmeans.fit_predict(X)
             error[k] = kmeans.inertia_
```

```
In [73]: plt.plot(range(1,len(error)),error[1:])
         plt.xlabel('Number of clusters')
         dummy = plt.ylabel('Error')
```



Warning: This synthetic data is not at all typical. You will almost never see such a sharp change in the error function as we see here.

Let's create a function for later use.

```
In [74]: def evaluate_clusters(X,max_clusters):
             error = np.zeros(max_clusters+1)
             error[0] = 0;
             for k in range(1,max_clusters+1):
                 kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10)
                 kmeans.fit_predict(X)
                 error[k] = kmeans.inertia_

             plt.plot(range(1,len(error)),error[1:])
             plt.xlabel('Number of clusters')
             plt.ylabel('Error')
```

1.3.2 Adjusted Rand Index

The Rand Index is a simple similarity measure for clusterings. We can use it to compare two clusterings for similarity.

Or, if we are testing an algorithm on data for which we know ground truth, we can use it to assess the algorithm's accuracy.

If T is a ground truth label assignment and C the clustering.

Let a be: the number of pairs of elements that have the same label in T and the same label in C.

Also let b be: the number of pairs of elements that have different labels in T and different labels in C.

Then the Rand Index is:

$$\mathrm{RI}(T, C) = \frac{a + b}{\binom{n}{2}}$$

However the RI score does not guarantee that random label assignments will get a value close to zero

(especially if the number of clusters is in the same order of magnitude as the number of samples).

To counter this effect we can use the expected RI $E[\mathrm{RI}]$ of random labelings to define the adjusted Rand index as follows:

$$\mathrm{ARI} = \frac{\mathrm{RI} - E[\mathrm{RI}]}{\max(\mathrm{RI}) - E[\mathrm{RI}]} \tag{1}$$

The computation of the expected RI is simple combinatorics (and left as an exercise for you :).

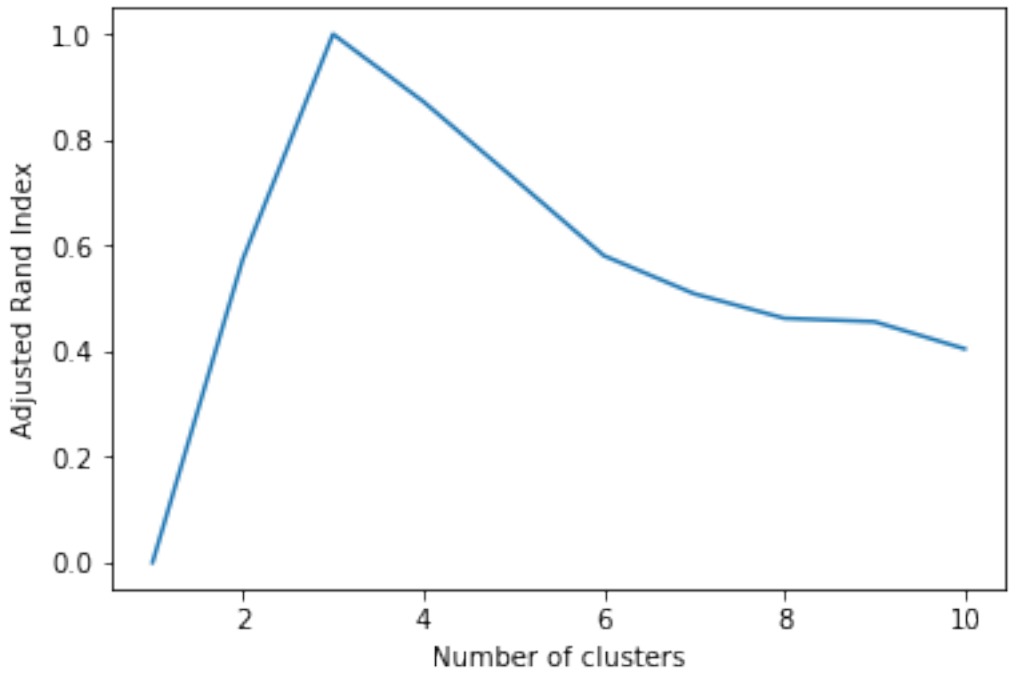
```
In [75]: ri = metrics.adjusted_rand_score(labels,y)
         print(ri)
```

```
1.0
```

Again, we'll create a function to evaluate clusterings.

```
In [76]: def ri_evaluate_clusters(X,max_clusters,ground_truth):
             ri = np.zeros(max_clusters+1)
             ri[0] = 0;
             for k in range(1,max_clusters+1):
                 kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10)
                 kmeans.fit_predict(X)
                 ri[k] = metrics.adjusted_rand_score(kmeans.labels_,ground_truth)
             plt.plot(range(1,len(ri)),ri[1:])
             plt.xlabel('Number of clusters')
             plt.ylabel('Adjusted Rand Index')

         ri_evaluate_clusters(X,10,y)
```



1.3.3 Silhouette Coefficient

Of course, normally, the ground truth labels are not known.

In that case, evaluation must be performed using the model itself.

The Silhouette Coefficient is an example of such an evaluation, where a higher Silhouette Coefficient score relates to a model with "better defined" clusters.

(`sklearn.metrics.silhouette_score`)

Let a be the mean distance between a data point and all other points in the same cluster.

Let b be the mean distance between a data point and all other points in the next nearest cluster.

Then the **Silhouette Coefficient** for a clustering is:

$$s = \frac{b - a}{\max(a, b)}$$

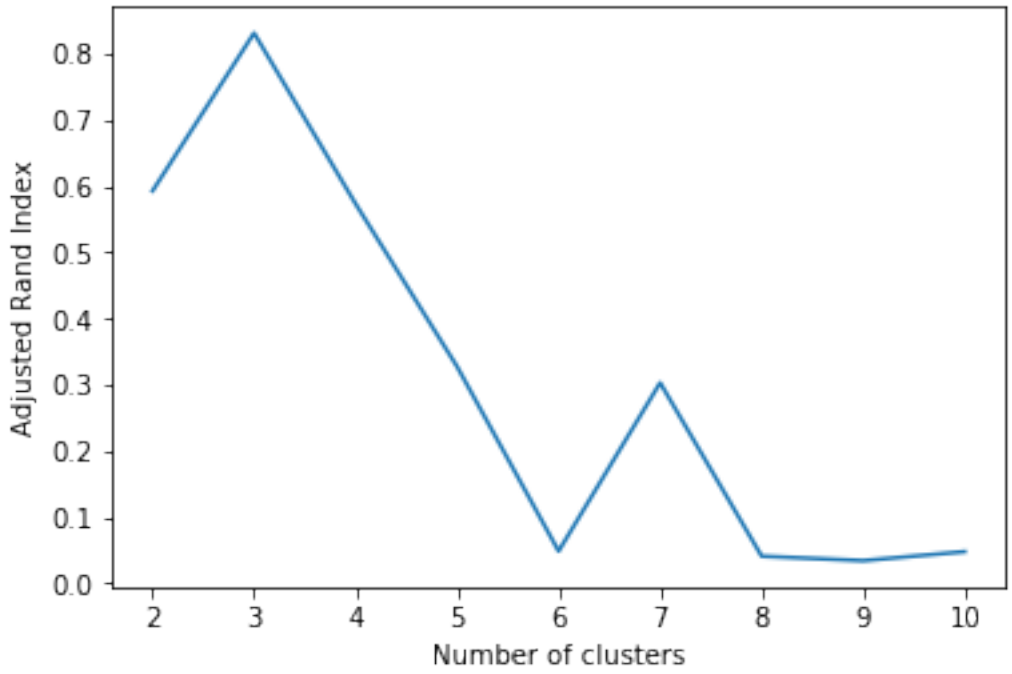
```
In [77]: sc = metrics.silhouette_score(X, labels, metric='euclidean')
         print(sc)
```

```
0.83193488414
```

```
In [78]: def sc_evaluate_clusters(X,max_clusters):
             s = np.zeros(max_clusters+1)
             s[0] = 0;
             s[1] = 0;
             for k in range(2,max_clusters+1):
```

```
            kmeans = KMeans(init='k-means++', n_clusters=k, n_init=10)
            kmeans.fit_predict(X)
            s[k] = metrics.silhouette_score(X,kmeans.labels_,metric='euclidean')
        plt.plot(range(2,len(s)),s[2:])
        plt.xlabel('Number of clusters')
        plt.ylabel('Adjusted Rand Index')

sc_evaluate_clusters(X,10)
```



Again, these results are more perfect than typical. But the general idea is to look for a local maximum in the Silhouette Coefficient as the potential number of clusters.

1.4 Working with real data

As a "real world" example, we'll use the "20 Newsgroup" data provided as example data in sklearn. (http://scikit-learn.org/stable/datasets/twenty_newsgroups.html).

```
In [79]: from sklearn.datasets import fetch_20newsgroups

        """
        categories = [
         'comp.windows.x',
         'misc.forsale',
         'rec.autos',
         'rec.motorcycles',
         'rec.sport.baseball',
```

```
 'rec.sport.hockey',
 'talk.religion.misc',
 'comp.graphics',
 'sci.space',
 'rec.autos',
 'rec.sport.baseball'
]
"""
categories = ['comp.os.ms-windows.misc', 'sci.space','rec.sport.baseball']
news_data = fetch_20newsgroups(subset='train', categories=categories)
print(news_data.target, len(news_data.target))
print(news_data.target_names)
```

```
[2 0 0 ..., 2 1 2] 1781
['comp.os.ms-windows.misc', 'rec.sport.baseball', 'sci.space']
```

```
In [80]: news_data.data[0]
```

```
Out[80]: 'From: aws@iti.org (Allen W. Sherzer)\nSubject: Re: DC-X update???\nOrganization: Evil
```

1.4.1 Feature Extraction

We've discussed a bit the challenges of feature engineering. One of the most basic issues concerns how to encode categorical or text data in a form usable by algorithms that expect numeric input.

As we've discussed already, one can encode a set using a binary vector with one component for each potential set member.

The so-called *bag of words* encoding for a document is to treat the document as a **multi**set of words.

That is, we simply count how many times each word occurs. It is a "bag" because all the order of the words in the document is lost.

Surprisingly, we can still tell a lot about the document even without knowing its word ordering.

Counting the number of times each word occurs in a document yields a vector of **term frequencies.**

However, simply using the "bag of words" directly has a number of drawbacks. First of all, large documents will have more words than small documents. Hence it often makes sense to normalize the frequency vectors.

ℓ_1 or ℓ_2 normalization are common.

Next, as noted in **scikit-learn**:

> In a large text corpus, some words will be very [frequent] (e.g. "the", "a", "is" in English) hence carrying very little meaningful information about the actual contents of the document.
>
> If we were to feed the direct count data directly to a classifier those very frequent terms would shadow the frequencies of rarer yet more interesting terms.
>
> In order to re-weight the count features into floating point values suitable for usage by a classifier it is very common to use the tf–idf transform.

Tf means **term-frequency** while **tf–idf** means **term-frequency times inverse document-frequency.**

This is a originally a term weighting scheme developed for information retrieval (as a ranking function for search engines results), that has also found good use in document classification and clustering.

The idea is that rare words are more informative than common words. (This has connections to information theory).

Hence, the definition of tf-idf is as follows.

First:

$$\text{tf}(t,d) = \text{Number of times term } t \text{ occurs in document } d$$

Next, if N is the total number of documents in the corpus D then:

$$\text{idf}(t,D) = \frac{N}{|\{d \in D : t \in d\}|}$$

where the denominator is the number of documents in which the term t appears.

And finally:

$$\text{tf-idf}(t,d) = \text{tf}(t,d) \times \text{idf}(t,D)$$

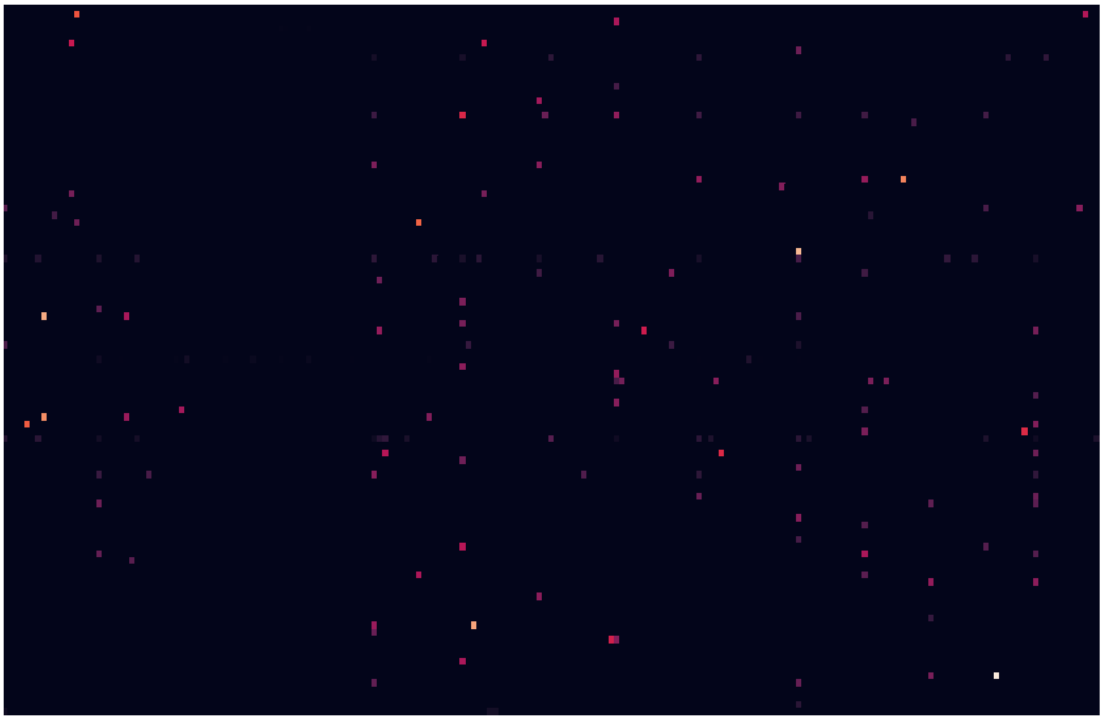
```
In [81]: from sklearn.feature_extraction.text import TfidfVectorizer
         vectorizer = TfidfVectorizer(stop_words='english', min_df=4, max_df=0.8)
         data = vectorizer.fit_transform(news_data.data)
```

1.4.2 Getting to know the Data

```
In [82]: print(type(data), data.shape)
```

```
<class 'scipy.sparse.csr.csr_matrix'> (1781, 9409)
```

```
In [83]: fig, ax1 = plt.subplots(1,1,figsize=(15,10))
         dum = sns.heatmap(data[1:100,1:200].todense(), xticklabels=False, yticklabels=False,
                           linewidths=0, cbar=False, ax=ax1)
```

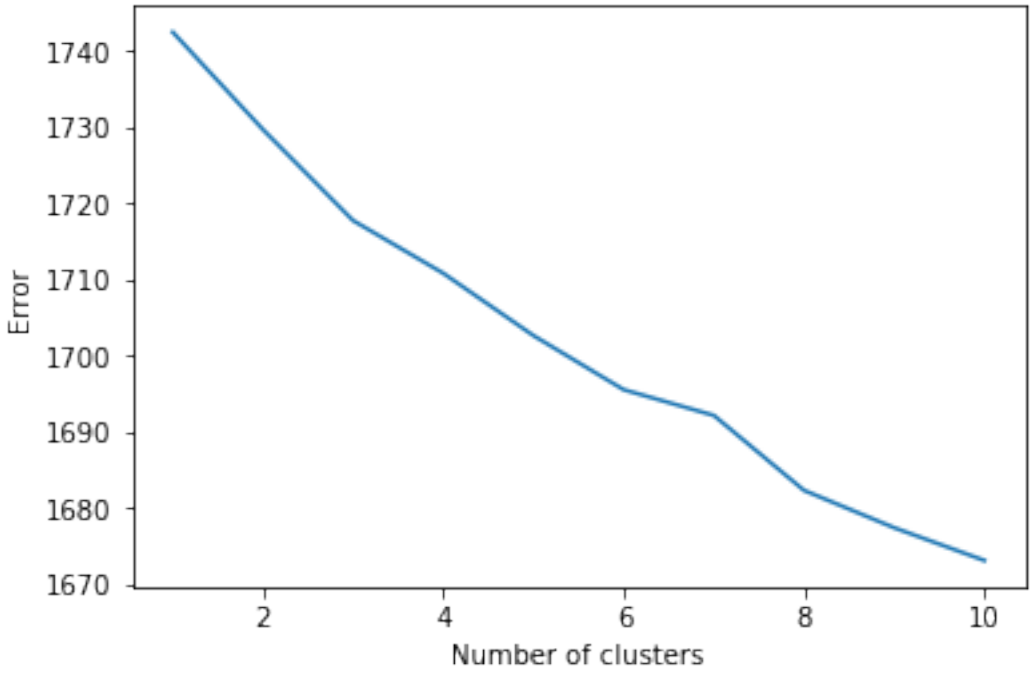


```
In [84]: print(news_data.target)
         print(news_data.target_names)
```

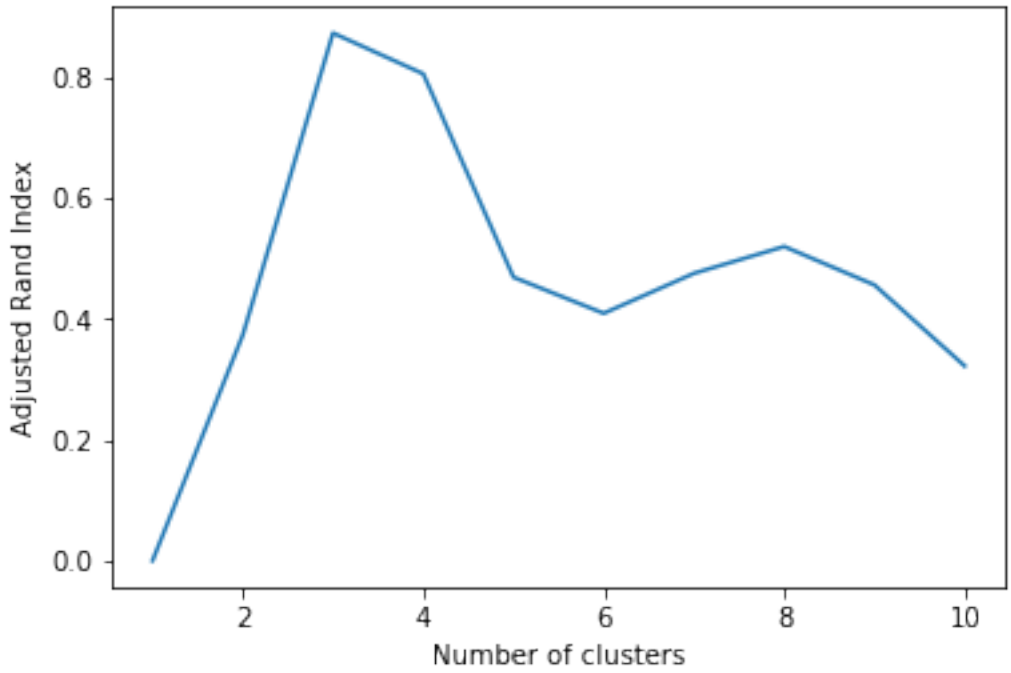
```
[2 0 0 ..., 2 1 2]
['comp.os.ms-windows.misc', 'rec.sport.baseball', 'sci.space']
```

1.4.3 Selecting the Number of Clusters

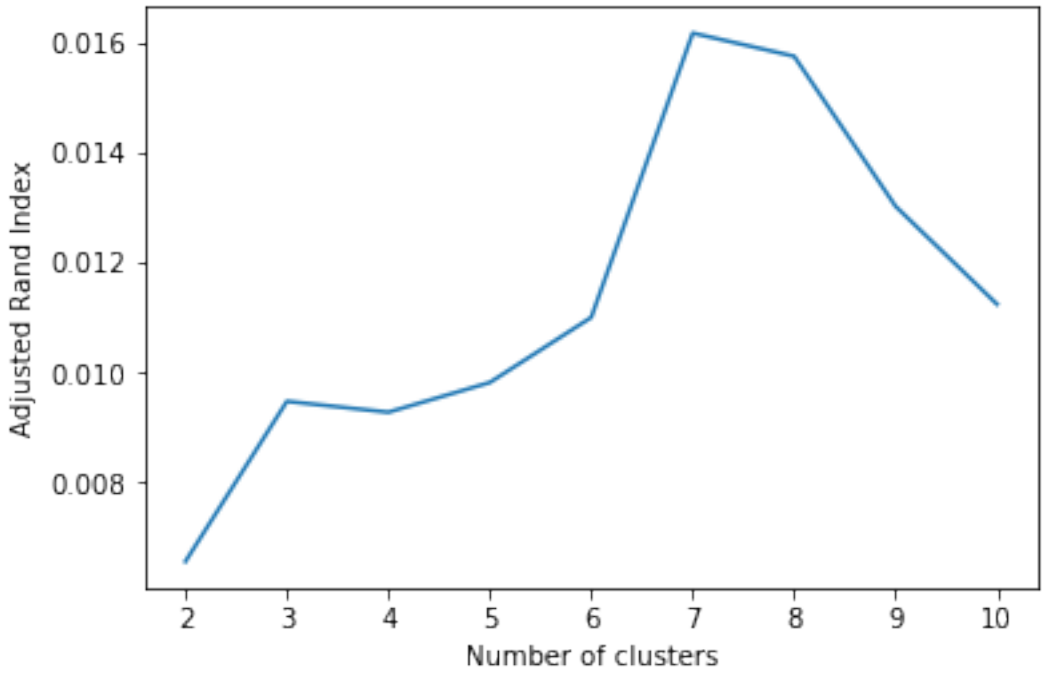
```
In [85]: evaluate_clusters(data, 10)
```



In [86]: `ri_evaluate_clusters(data,10,news_data.target)`



```
In [87]: sc_evaluate_clusters(data,10)
```



1.4.4 Looking into the clusters

```
In [88]: k=3
         kmeans = KMeans(n_clusters=k, init='k-means++', max_iter=100, n_init=1)
         kmeans.fit_predict(data)

Out[88]: array([2, 1, 1, ..., 2, 0, 2], dtype=int32)

In [89]: print("Top terms per cluster:")
         asc_order_centroids = kmeans.cluster_centers_.argsort()#[:, ::-1]
         order_centroids = asc_order_centroids[:,::-1]
         terms = vectorizer.get_feature_names()
         for i in range(k):
             print("Cluster {}:".format(i))
             for ind in order_centroids[i, :10]:
                 print(' {}'.format(terms[ind]))
             print('')

Top terms per cluster:
Cluster 0:
 edu
 com
 baseball
```

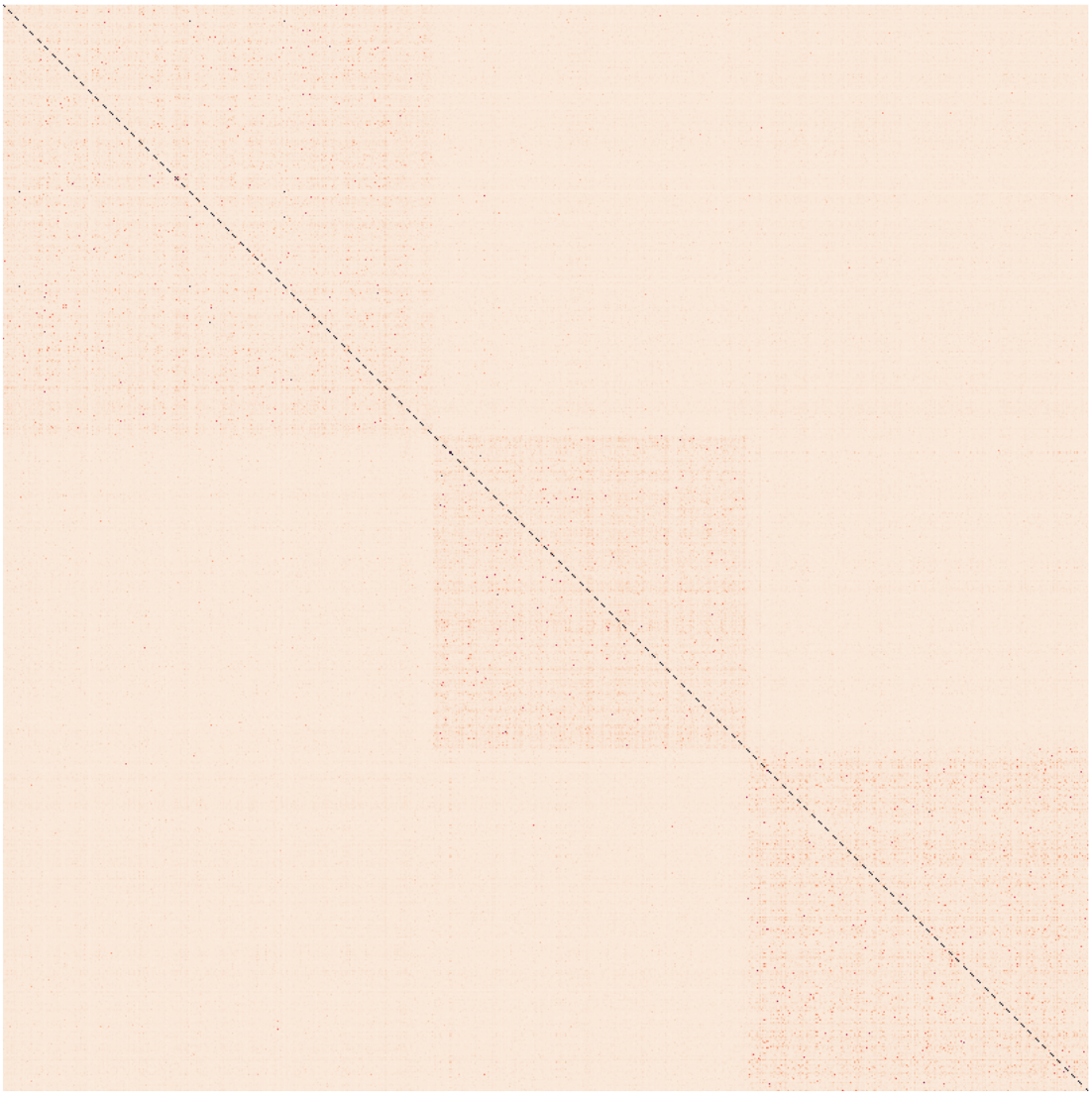
```
 year
 team
 game
 article
 writes
 cs
 players

Cluster 1:
 windows
 edu
 file
 dos
 files
 com
 driver
 card
 use
 drivers

Cluster 2:
 space
 nasa
 edu
 henry
 access
 com
 gov
 alaska
 moon
 digex
```

```
In [90]: kmeans?
```

```
In [91]: euclidean_dists = metrics.euclidean_distances(data)
         labels = kmeans.labels_
         idx = np.argsort(labels)
         clustered_dists = euclidean_dists[idx][:,idx]
         fig, ax1 = plt.subplots(1,1,figsize=(15,15))
         dum = sns.heatmap(clustered_dists, xticklabels=False, yticklabels=False, linewidths=0,
```



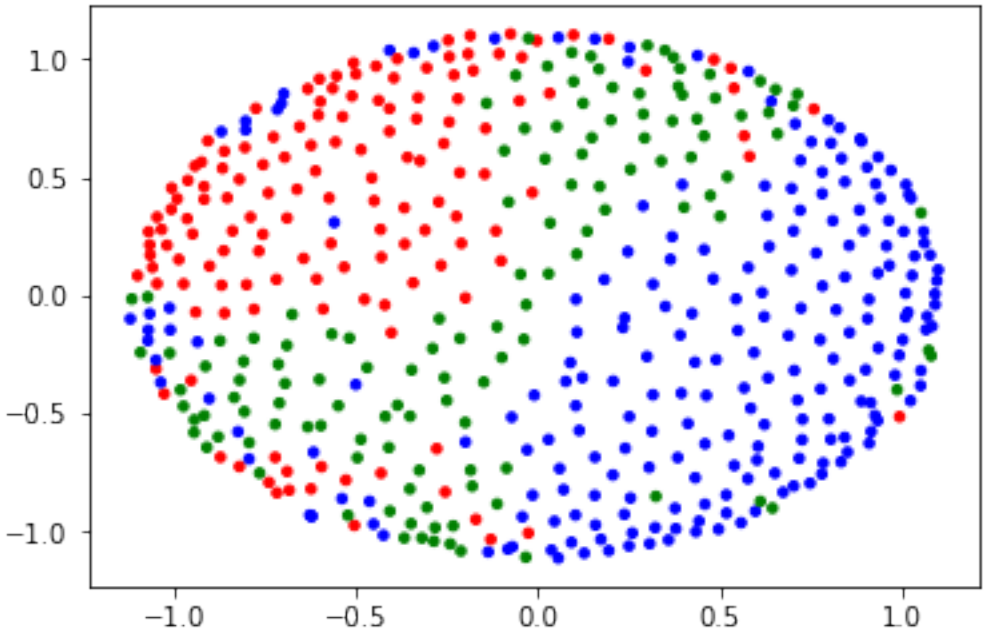
Let's visualize with MDS. Note that MDS is a slow algorithm and we can't do all 1700+ data points quickly, so we will take a random sample.

```
In [92]: import random
         n_items = euclidean_dists.shape[0]
         subset = random.sample(range(n_items),500)

         fit = mds.fit(euclidean_dists[subset][:,subset])
         pos = fit.embedding_

In [93]: cols = [['b', 'g', 'r', 'c', 'm', 'y', 'k'][l] for l in labels[subset]]
         plt.scatter(pos[:, 0], pos[:, 1], s=12, c=cols)

Out[93]: <matplotlib.collections.PathCollection at 0x117014828>
```


1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0