SciComp with Py

Data Clustering with K Means

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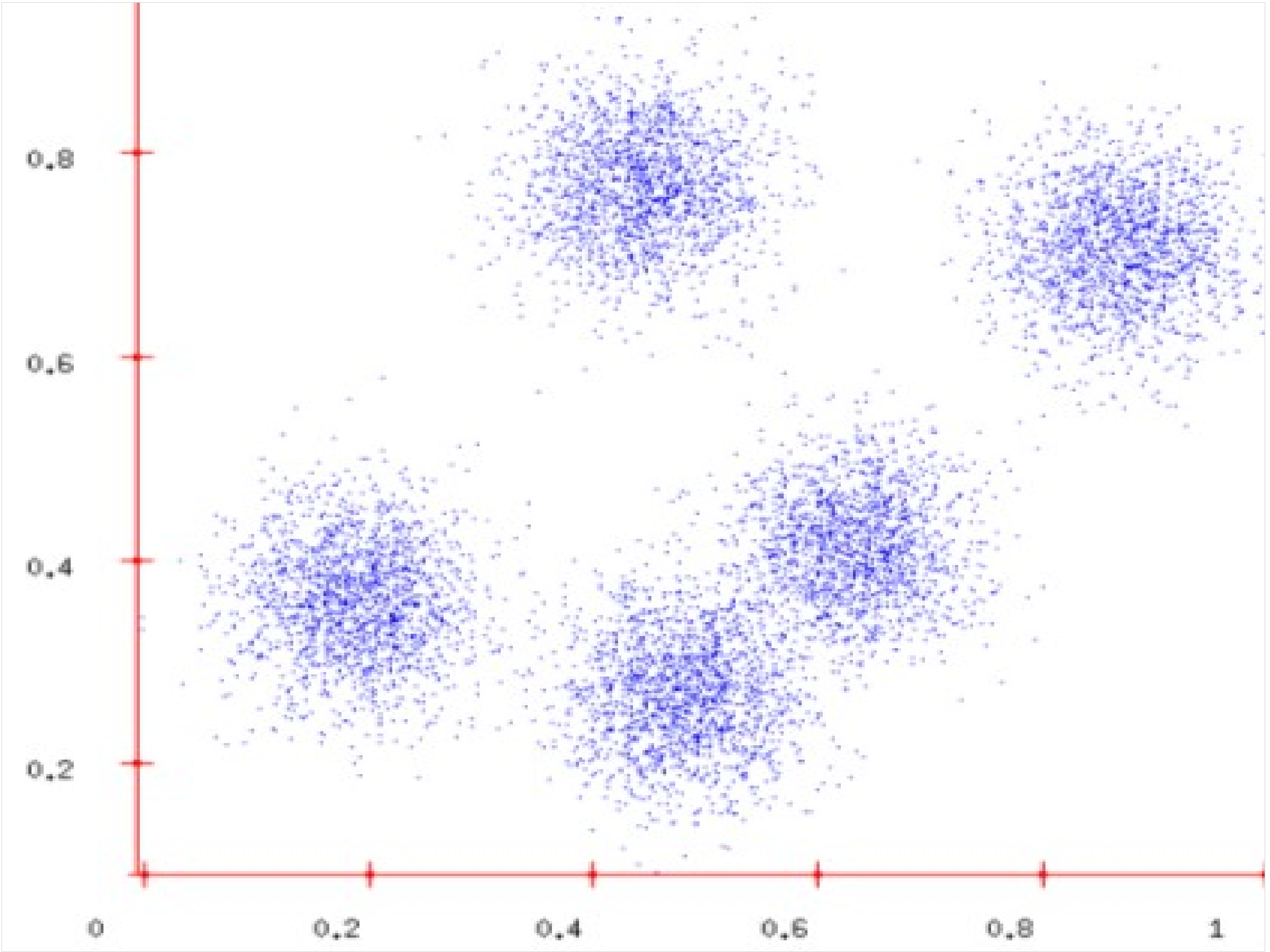
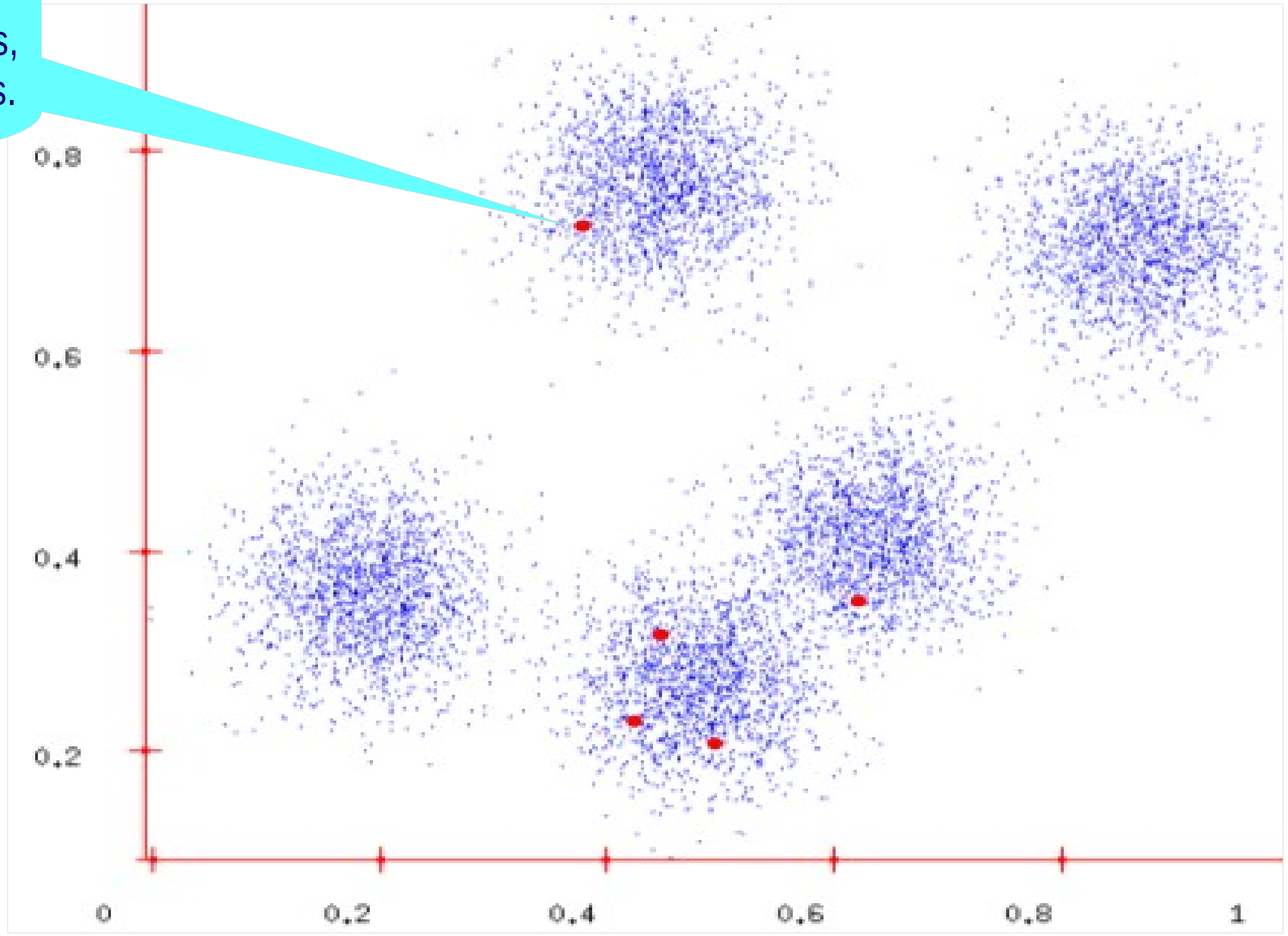
K-Means Illustrated: Step 1: Get Data



We have some 2D data to cluster

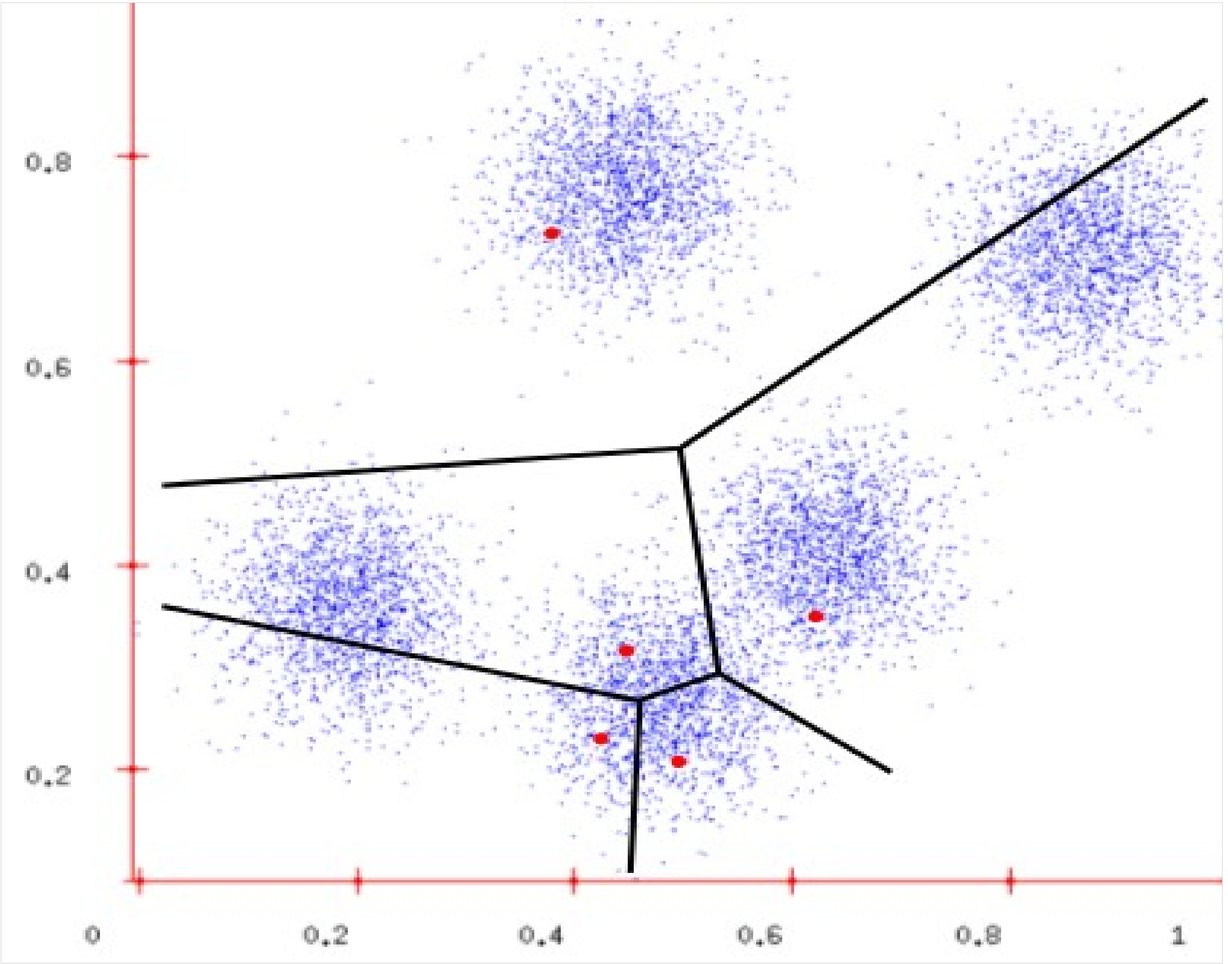
K-Means Illustrated: Step 2: Choose Centroids

Red dots are 2D centroids,
i.e. feature vectors. In n-dim spaces,
centroids are n-dimensional vectors.



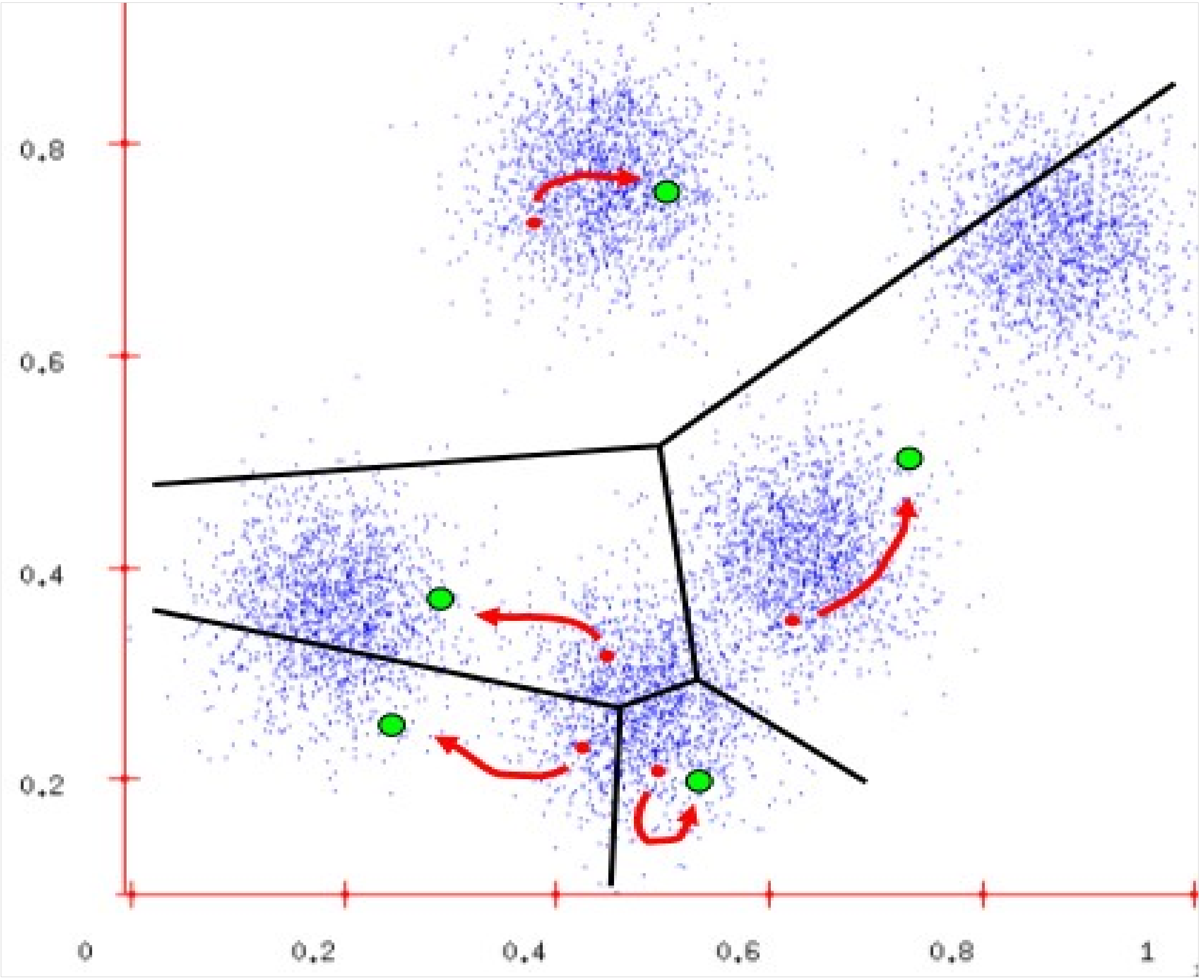
Pick a number of clusters you want and guess a centroid for each cluster; *guessing* typically refers to *random selection*

K-Means Illustrated: Step 3: Cluster Assignment



Each data item (i.e., feature vector) is assigned to a cluster on the basis of its closeness (e.g., euclidean distance) to a centroid; these centroids are referred to as *means* (this explains the means part of K-Means)

K-Means: Step 4: Adjust Centroids



Each centroid is adjusted by moving it to the center (mean) of its cluster; if centroid adjustment is small, stop; else recurse to step 3

K-Means in Pseudocode

1) Choose number of clusters you want to have (K)
2) Randomly choose K centroids (i.e., K feature vectors)
3) Assign all data items to one of the K clusters on the basis of their closeness to the randomly selected centroids
4) Adjust each centroid by moving it to the center of its cluster by setting the value of each feature to the mean of the values of that feature in all data items in the cluster
5) Note the amount of adjustment, i.e., the distance each centroid moves (this is called *inertia*)
6) If the amount of adjustment is greater than a threshold, go to step 3; this means the clusters are still unstable
7) If the amount of adjustment is smaller than a threshold, return

K Means Advantages and Disadvantages

Advantages: 1) one of the best known clustering algorithm; 2) lots of third-party implementations in the language of your choice; 3) easy to implement if you want to do it from scratch; 4) works really well on static data sets

Disadvantages: 1) the user must specify the number of clusters (k) explicitly; 2) k means can handle only numerical data; 3) k means assumes that data clusters into spherical clusters with each cluster having roughly the same number of samples; 4) doesn't work well with constantly changing data

USENET News Group Posts in SKLEARN

SKLEARN.DATASETS contains posts for 20 USENET newsgroups

These posts are unfiltered so some posts may strike you as offensive

The good news is though that this is real world, raw data

Loading USENET Data

```
>>> import sklearn.datasets
>>> usenet_data = sklearn.datasets.fetch_20newsgroups()
>>> usenet_data.data[10]
u'From: irwin@cmptrc.lonestar.org (Irwin Arnstein)\nSubject: Re: Recommendation on Duc\nSummary: What\'s it worth?\nDistribution: usa\nExpires: Sat, 1 May 1993 05:00:00 GMT\nOrganization: CompuTrac Inc., Richardson TX\nKeywords: Ducati, GTS, How much? \nLines: 13\n\nI have a line on a Ducati 900GTS 1978 model with 17k on the clock.  Runs\nvery well, paint is the bronze/brown/orange faded out, leaks a bit of oil\nand pops out of 1st with hard accel.  The shop will fix trans and oil \nleak.  They sold the bike to the 1 and only owner.  They want $3495, and\nI am thinking more like $3K.  Any opinions out there?  Please email me.\nThanks.  It would be a nice stable mate to the Beemer.  Then I\'ll get\na jap bike and call myself Axis Motors!\n\n-- \n-------------------------------------------------------------------\n"Tuba" (Irwin)      "I honk therefore I am"     CompuTrac-Richardson,Tx\nirwin@cmptrc.lonestar.org              DoD   #0826 (R75/6)\n-------------------------------------------------------------------\n'
```

Getting USENET Data Target Names

```
>>> usenet_data.target_names
['alt.atheism', 'comp.graphics', 'comp.os.ms-windows.misc',
'comp.sys.ibm.pc.hardware', 'comp.sys.mac.hardware', 'comp.windows.x',
'misc.forsale', 'rec.autos', 'rec.motorcycles', 'rec.sport.baseball',
'rec.sport.hockey', 'sci.crypt', 'sci.electronics', 'sci.med', 'sci.space',
'soc.religion.christian', 'talk.politics.guns', 'talk.politics.mideast',
'talk.politics.misc', 'talk.religion.misc']
```

Problem

We know how to find posts related to a user's post by matching the feature vector of the user's post to the feature vectors of all posts in the database. This, of course, does not scale: as the number of posts grows, finding relevant posts becomes more and more time consuming. What we can do is 1) cluster the posts*; 2) find the cluster (or a small number of clusters) closest to the user's post; 3) look for related posts ***only within*** the closest cluster (or clusters).

* Note that I am ignoring, for the sake of simplicity, how and where the clusters are stored. This is a cloud computing problem and, as such, has very little to do with scientific computing.

Getting Posts from Six Newsgroups

```
import sklearn.datasets
## select six neutral groups for training
groups = ['comp.graphics', 'comp.os.ms-windows.misc',
          'comp.sys.ibm.pc.hardware',  'comp.sys.mac.hardware',
          'comp.windows.x', 'sci.space']
## create train data
train_data = sklearn.datasets.fetch_20newsgroups(subset='train',
                                                 categories=groups)
```

source in find_post_with_kmeans.py

Clustering with K-Means

```
## 5) construct a tfidf vectorizer and build feature matrix of train_data
vectorizer = StemmedTfidfVectorizer(min_df=10,
                                    stop_words='english', decode_error='ignore')
train_data_feat_mat = vectorizer.fit_transform(train_data.data)

from sklearn.cluster import Kmeans
## 6) choose number of clusters
num_clusters = 50
## 7) create k-means clustering object
km = KMeans(n_clusters=num_clusters, verbose=1, random_state=3)
## 8) cluster the feature data
clustered_data = km.fit(train_data_feat_mat))
```

source in find_post_with_kmeans.py

K-Means: Displaying Clustering Stats

```
# after the clustering is done, each cluster has its own cluster label in [0, 49].
print('km.labels_=%s' % km.labels_)
print('len(km.labels_)=%d' % len(km.labels_))
# there are 3529 samples
# the number of samples is the same as the number of labels
# each label is an integer 0 <= i <= 49. or 0 <= i <= n-1
# where n is the number of clusters.
print('max label = %d' % max(km.labels_))
print('min label = %d' % min(km.labels_))
```

source in find_post_with_kmeans.py

K-Means: Classifying New Post

This is the user post to which we want to find relevant posts

```
new_post = \
    """Disk drive problems. Hi, I have a problem with my hard disk.
After 1 year it is working only sporadically now.
I tried to format it, but now it doesn't boot any more.
Any ideas? Thanks.
"""


new_post_vec = vectorizer.transform([new_post]).getrow(0).toarray()
km_predicted_labels = km.predict(new_post_vec)
print('len(km_predicted_labels)=%d' % len(km_predicted_labels))

## get the top cluster label for the new post
top_new_post_label = km.predict(new_post_vec)[0]

print(top_new_post_label)
```

Predict the labels of the new post vector.

Getting Posts in the Same Post Cluster as the New Post

This is how we can get the numbers of posts in the same cluster as the new post.

```
>>> (km.labels_ == top_new_post_label).nonzero()
(array([  69,   71,  125,  139,  157,  167,  201,  213,  228,  247,  297,
        308,  359,  377,  384,  428,  429,  463,  520,  531,  533,  581,
        650,  676,  727,  773,  779,  806,  807,  808,  905,  935,  939,
        944,  961,  964,  971,  976, 1076, 1114, 1214, 1246, 1266, 1286,
       1311, 1377, 1388, 1427, 1431, 1486, 1495, 1548, 1608, 1716, 1735,
       1752, 1806, 1807, 1809, 1852, 1853, 1864, 1893, 1944, 1985, 1986,
       1990, 1996, 2013, 2015, 2061, 2085, 2151, 2235, 2244, 2257, 2270,
       2339, 2347, 2351, 2414, 2436, 2447, 2463, 2482, 2493, 2494, 2512,
       2516, 2518, 2525, 2565, 2573, 2600, 2619, 2624, 2639, 2667, 2678,
       2705, 2745, 2791, 2800, 2842, 2875, 2907, 2956, 2964, 3018, 3111,
       3145, 3199, 3202, 3225, 3278, 3285, 3296, 3297, 3309, 3310, 3437,
       3458]),)
```

K-Means: Getting Similar Posts

get the posts in the same cluster as the new post

computing distances b/w new post vector and the post feature vectors

```
posts_in_same_cluster = (km.labels_ == top_new_post_label).nonzero()[0]

similar_posts = [ ]
for i in posts_in_same_cluster:
    dist = sp.linalg.norm(new_post_vec - train_data_feat_mat[i])
    similar_posts.append((dist, train_data.data[i]))

similar_posts.sort(key=lambda post: post[0])
```

So, what's the reduction of the search space? Let's find out:

```
>>> len(train_data.filenames)
3529
>>> len(posts_in_same_cluster)
122
```

so, instead of matching aginst 3529 feature vectors, we are matching only against 122, i.e., about 3% of the available feature vectors.

Accessing Similar Posts

similar_posts is a list of 2-tuples of the form (distance, post_text)

accessting distance of top post

```
>>> similar_posts[0][0]
1.0383025802700465
```

printing top post

```
>>> print(similar_posts[0][1])
From: Thomas Dachsel <GERTHD@mvs.sas.com>
Subject: BOOT PROBLEM with IDE controller
Nntp-Posting-Host: sdcmvs.mvs.sas.com
Organization: SAS Institute Inc.
Lines: 25
...
```

Potential Experiments

Experiment with different numbers of clusters and measure recall and precision for each cluster

Experiment with different stemmers and vectorizers in addition to different numbers of clusters

References

W. Richert & L. Coelho. “Building ML Systems with Python”, Ch. 3, Pack, 2013.

A. Moore. “K-Means & Hierarchical Clustering.” CMU, 2001.