activeSiteClustering

February 8, 2017

In [1]:
```
import os
os.chdir('/Users/ken/Desktop/repos/activeSiteClustering')
from clustering import cluster, similarity, io, utils
import numpy as np
import sys
from random import seed, random
from math import floor
import matplotlib.pyplot as plt
%matplotlib inline
```

In [2]:
```
# similarity metric:
# 9-dimensional vector of basic chemical and morphological features
# Hand-tuned examples showed it can separate different sizes
#       and charge distributions
# Can easily incorporate more variables in the future
#     (e.g. charge variance)
# Comparison takes Euclidean distance between two vectors

activeSites = io.read_active_sites('data')

seed()
rand1 = int(floor(random()*len(activeSites)))
rand2 = int(floor(random()*len(activeSites)))

#Range
print('\n----------------')
print('This value will be between 0 and 1:')
print('\tSimilarity (random):',
      similarity.compute_similarity(activeSites[rand1],
                                    activeSites[rand2]))

#Reflexive
print('\nThis value will be 1:')
print('\tSimilarity A <-> A:',
      similarity.compute_similarity(activeSites[rand1],
                                    activeSites[rand1]))
```

```
        #Symmetric
        print('\nThese values will be the same:')
        print('\tSimilarity A -> B:',
              similarity.compute_similarity(activeSites[rand1],
                                            activeSites[rand2]))
        print('\tSimilarity B -> A:',
              similarity.compute_similarity(activeSites[rand2],
                                            activeSites[rand1]))
```

```
Read in 136 active sites

----------------
This value will be between 0 and 1:
        Similarity (random): 0.1916944851

This value will be 1:
        Similarity A <-> A: 1.0

These values will be the same:
        Similarity A -> B: 0.1916944851
        Similarity B -> A: 0.1916944851
```

In [3]:
```
        # partitioning algorithm:
        # Implemented K-Means
        # Reason: straightforward, well-documented and known to converge
        # downside: non-deterministic. testing required many runs of func
        #     to catch small bugs.

        # hierarchical algorithm:
        # agglomerative with centroid linkage
        # Reason: similar to above... simple linkage calculation,
        #        intuitive implementation.
        # downside: super slow compared to k-means. but being
        #        deterministic helped with debugging.

        print('clustering by partition')
        p_clust = cluster.cluster_by_partitioning(activeSites,num_clusters=7)
        print('done')
        print('-----------------------')
        print('clustering by hierarchy')
        h_clust = cluster.cluster_hierarchically(activeSites,num_clusters=7)
        print('done')
```

```
clustering by partition
done
-----------------------
clustering by hierarchy
```

```
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
Number of Clusters: 10
done
```

In [4]:
```
# quality metric:
# Used average inter-object distance among clusters in clustering
#    (low=good).
# Slight variation on what was presented in class,
#    averaging pairwise distances *within* clusters
#    before averaging these cluster averages. This prevented
#    skewing by large clusters (common in hierarchical here)
# To compare two clusterings together, I took the log ratio of the two

p_qual = []
h_qual = []
ratio = []

num_clusters = [3,5,7,10,15]

for num in num_clusters:
    print('\n')
    print('---------',num,'-----------')
    print('----------------------')

    print('clustering by partition')
    p_clust = cluster.cluster_by_partitioning(activeSites,
                                              num_clusters=num)
    p_qual.append(cluster.quality(p_clust))

    print('done')
    print('----------------------')
    print('clustering by hierarchy')

    h_clust = cluster.cluster_hierarchically(activeSites,
                                             num_clusters=num)
    h_qual.append(cluster.quality(h_clust))
```

```
            print('done')

            ratio.append(cluster.compare(p_clust,h_clust))
```

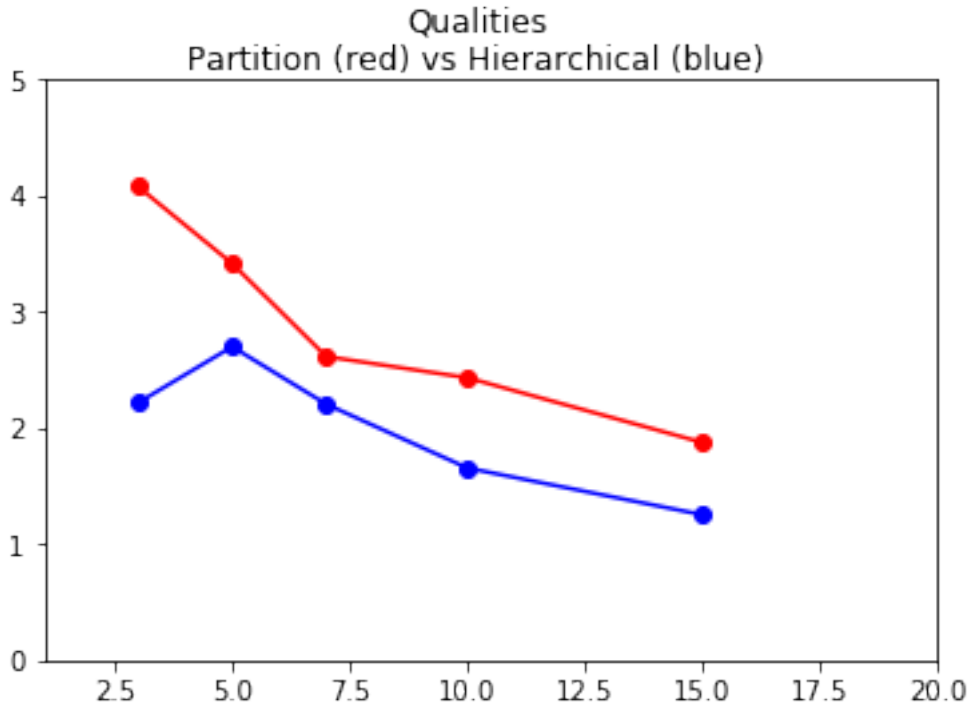
```
--------- 3 -----------
-----------------------
clustering by partition
done
-----------------------
clustering by hierarchy
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
Number of Clusters: 10
done
```

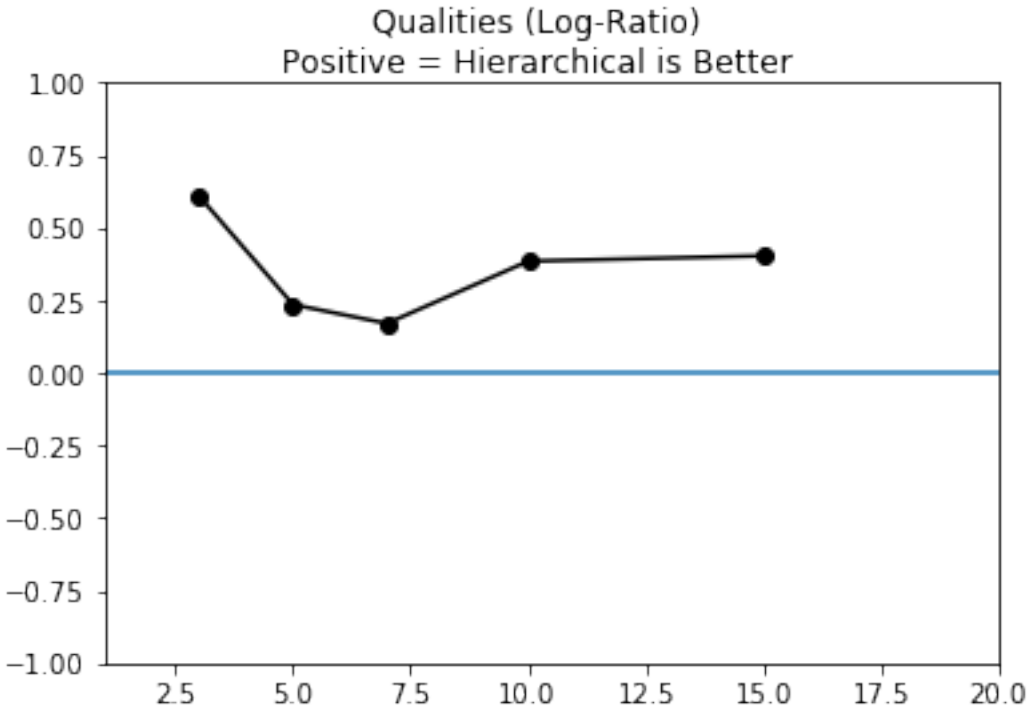
```
--------- 5 -----------
-----------------------
clustering by partition
done
-----------------------
clustering by hierarchy
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
Number of Clusters: 10
done
```

```
--------- 7 -----------
-----------------------
clustering by partition
done
-----------------------
clustering by hierarchy
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
Number of Clusters: 10
done


--------- 10 -----------
-----------------------
clustering by partition
done
-----------------------
clustering by hierarchy
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
Number of Clusters: 10
done


--------- 15 -----------
-----------------------
```

```
clustering by partition
done
-----------------------
clustering by hierarchy
Number of Clusters: 130
Number of Clusters: 120
Number of Clusters: 110
Number of Clusters: 100
Number of Clusters: 90
Number of Clusters: 80
Number of Clusters: 70
Number of Clusters: 60
Number of Clusters: 50
Number of Clusters: 40
Number of Clusters: 30
Number of Clusters: 20
done
```

```
In [5]: fig1 = plt.figure()
        fig1.suptitle('Qualities\nPartition (red) vs Hierarchical (blue)')
        plt.plot(num_clusters,p_qual,color="r",marker='o')
        plt.plot(num_clusters,h_qual,color="b",marker='o')
        plt.axis([1,20,0,5])

        fig2 = plt.figure()
        fig2.suptitle('Qualities (Log-Ratio)\nPositive = Hierarchical is Better')
        plt.plot(num_clusters,ratio,color="k",marker='o')
        plt.plot([0,21],[0,0],marker='_')
        plt.axis([1,20,-1,1])

Out[5]: [1, 20, -1, 1]
```


Qualities
Partition (red) vs Hierarchical (blue)
5
4
3
2
1
0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0


Qualities (Log-Ratio)
Positive = Hierarchical is Better
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0

I'm unsure if my clusters had biological meaning. The fact that the hierarchical clustering consistently had more skewed distributions of cluster sizes whereas the k-means did not makes me skeptical. Of course, this is also compounded by not knowing if the 9 somewhat arbitrary parameters I chose actually translate to functionality (e.g. ligand specificity).

In all, I think the general algorithms employed here could be useful, but would require more detailed input data upon which to cluster the sites.