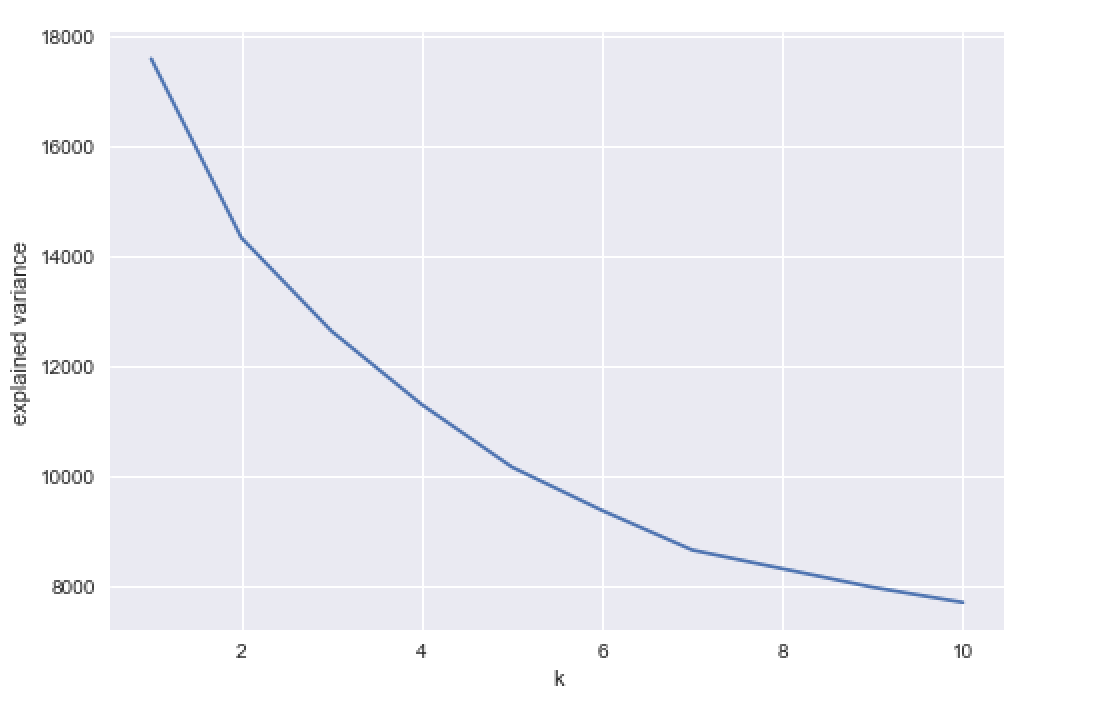
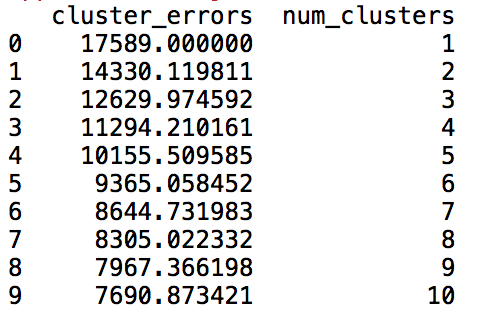
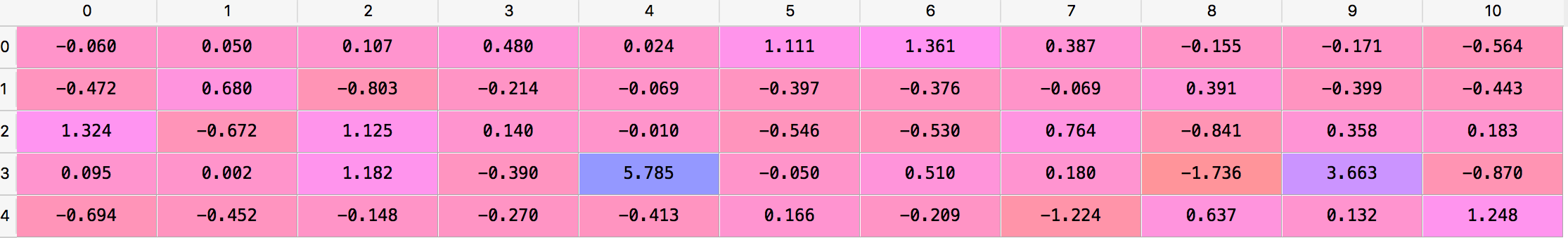
* K-means clustering: Given a set of n observations xi, which is d-dimensional real vector, K-means clustering n observations into k partitions as to minimize the within-cluster sum of squares.
* Preprocessing: since we have high-dimensional feature spaces and various ranges of values involved, we normalize the data first.
* Choosing optimal number of clusters
* Elbow’s method: it uses the percentage of variance that is explained as a function of the number of clusters. (explained variance) – explained variance measures the proportion to which model with k accounts for the variance of a given dataset. The first clusters will add much information that would explain a lot of variance but at some point the marginal gain of information will decrease and this point is the optimal k we choose.
* We choose the optimal K from the point where the marginal gain in explained variance drops.



* The optimal k can be picked at 5, in which marginal gain in explained variance has remarkably decreased.
* Showing explained variance in chart

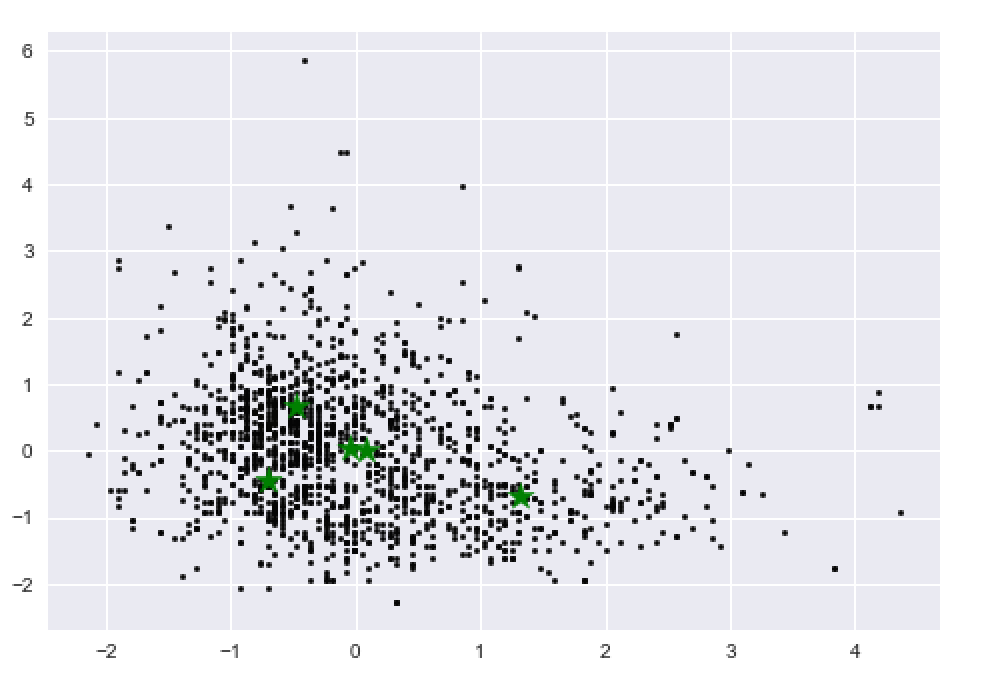


* Cluster centers for k=3

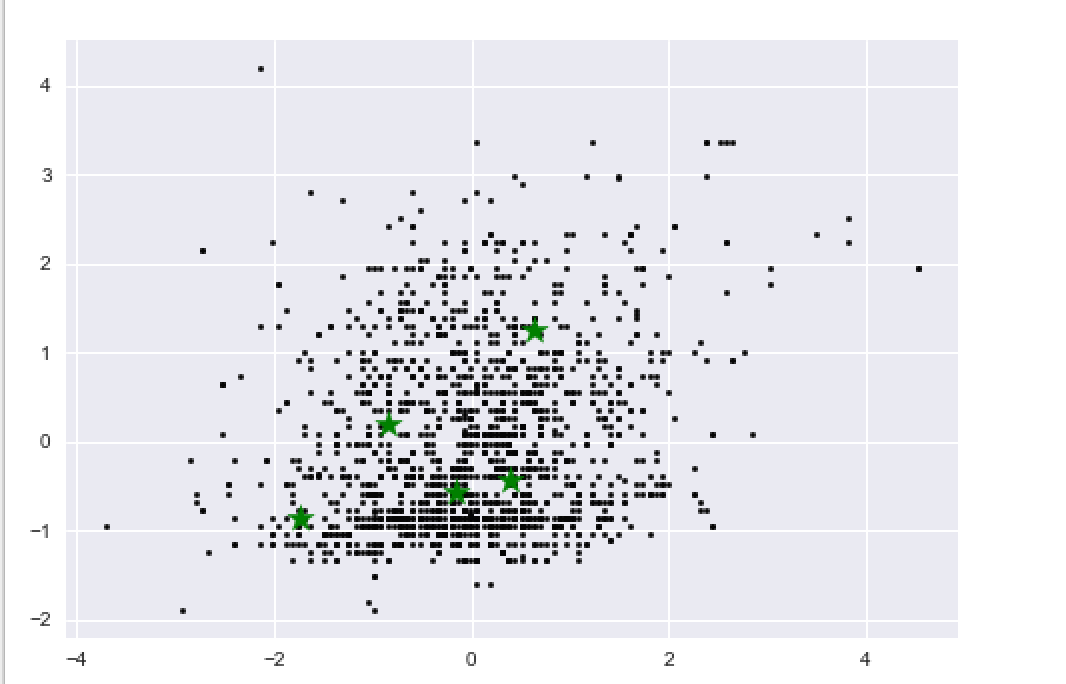


* Several visualization of feature vs. feature graphs as in terms of clusters

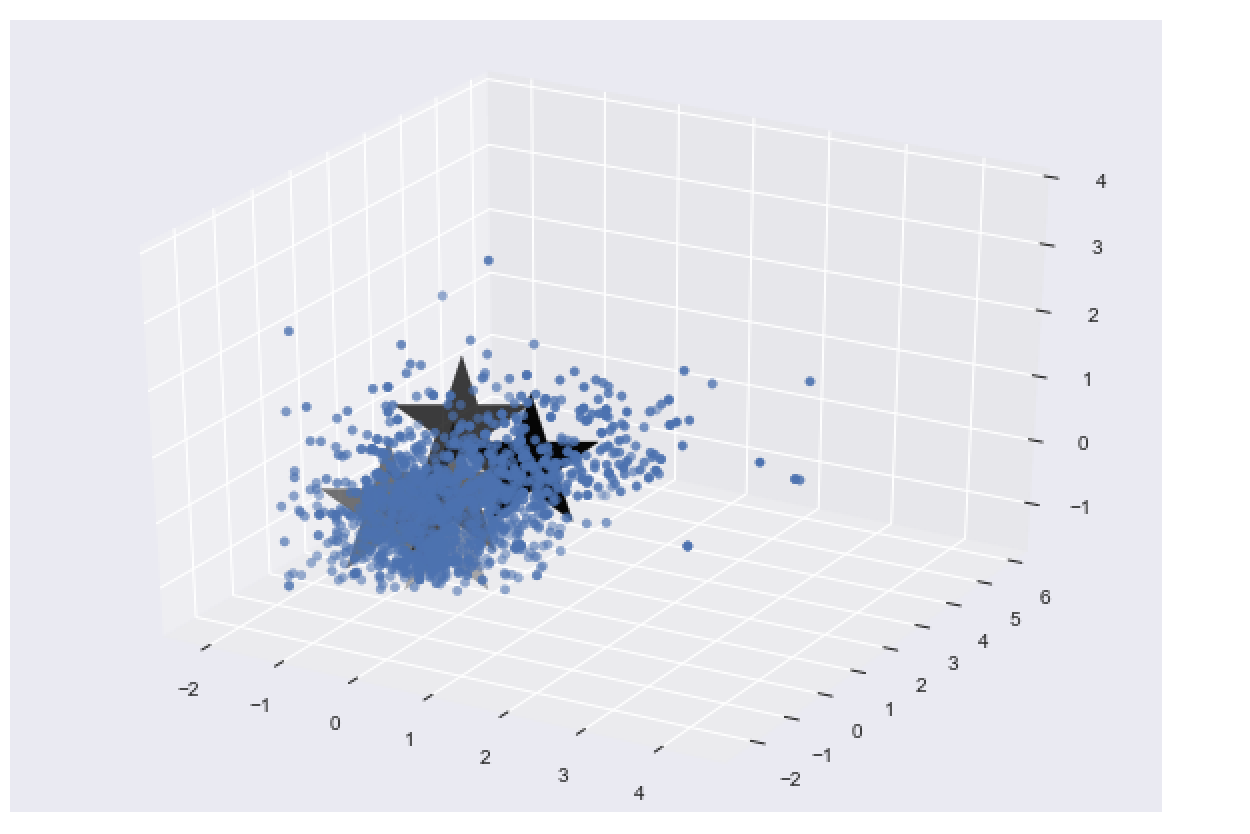
1. Volatile acidity vs. citric acid



1. pH vs. alcohol

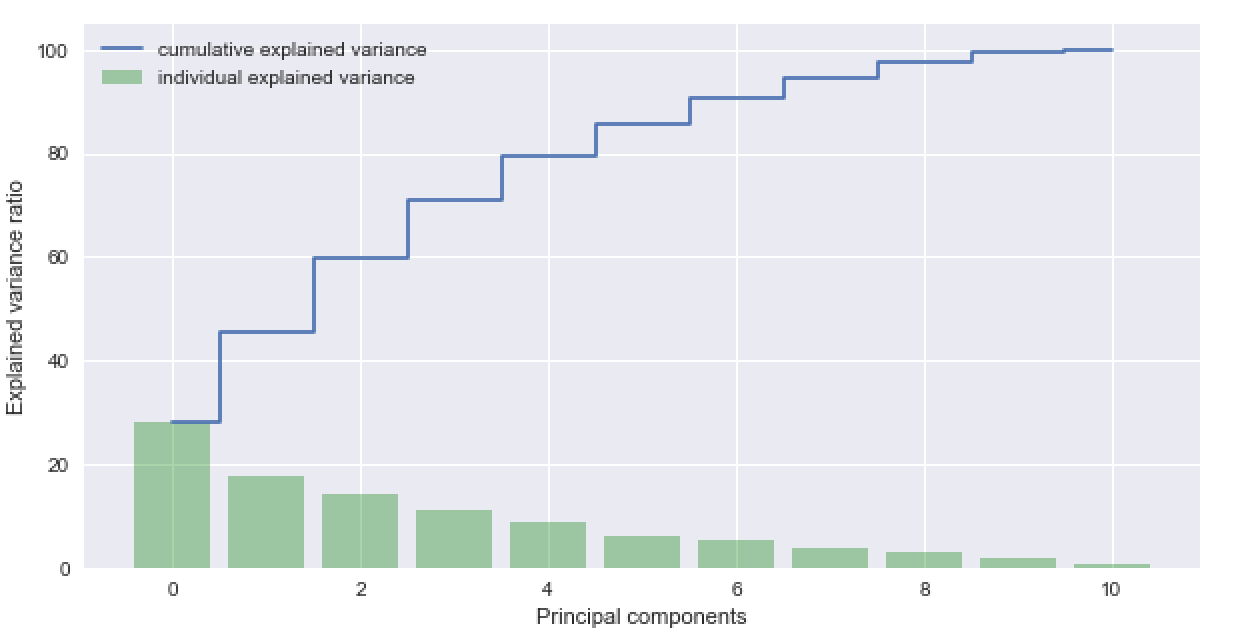


* In 3D visualization with three features: fixed acidity, volatile acidity, and citric acid



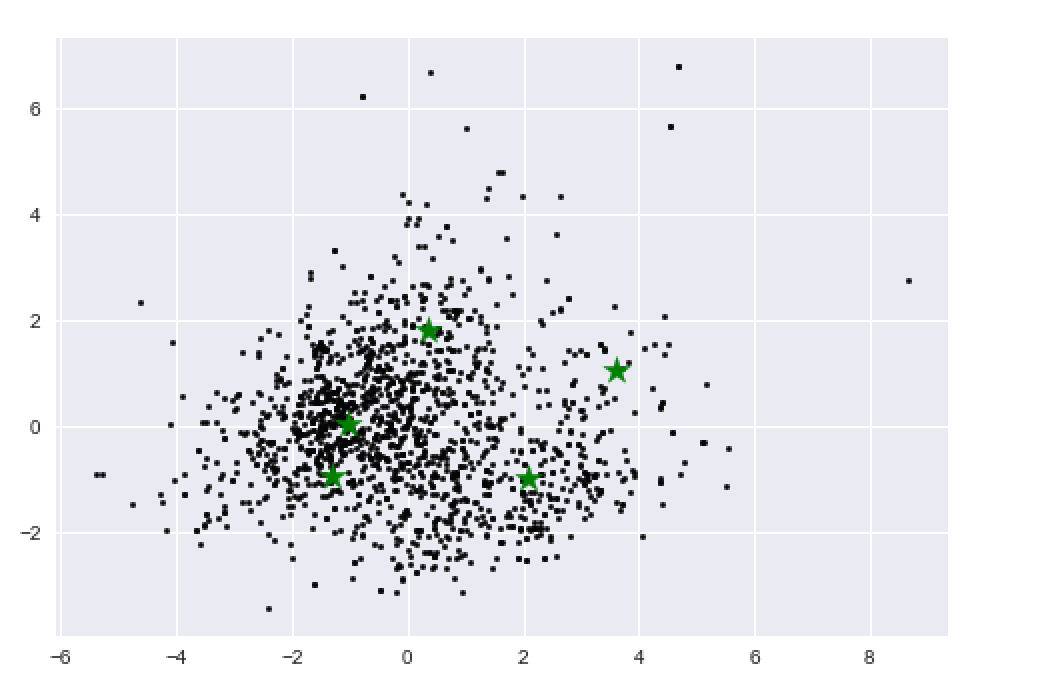
With normalized data for offsetting constraints by different features, we can analyze though visualization that k=5 clustering is precisely classifying the dataset into 5 clusters; however, since the feature space is high-dimensional and with large dataset, 5 means clustering cannot perfectly classify dataset into 5 clusters. We can also see that data points are somewhat concentrated in that it is hard to manipulate the sparse solution with k-means clustering. But, still it is optimal way of clustering for this dataset since with elbow’s method, we attained k=5 and data points are sparsely distributed among these centroids.

* Evaluation through predicting the labels is not appropriately applied for k-means clustering since the labels are made through the number of clusters and the spherical clusters from clustering helplessly lets clusters to possibly contain multiple overlapped data points. Also, the graphs demonstrate that the normalized data points are roughly concentrated.
* We can still use the labels we attained from 5-means clustering to predict the label and compare with the actual labels: 0.550969355847, but we cannot conclude this accuracy as our precision of K-means clustering as reasoning above.
* PCA(Principal Component Analysis) version of K-means clustering with reduction in feature dimension
* PCA: It is a statistical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated values into a set of values of linearly uncorrelated variables.
  + Choosing the number of principal components

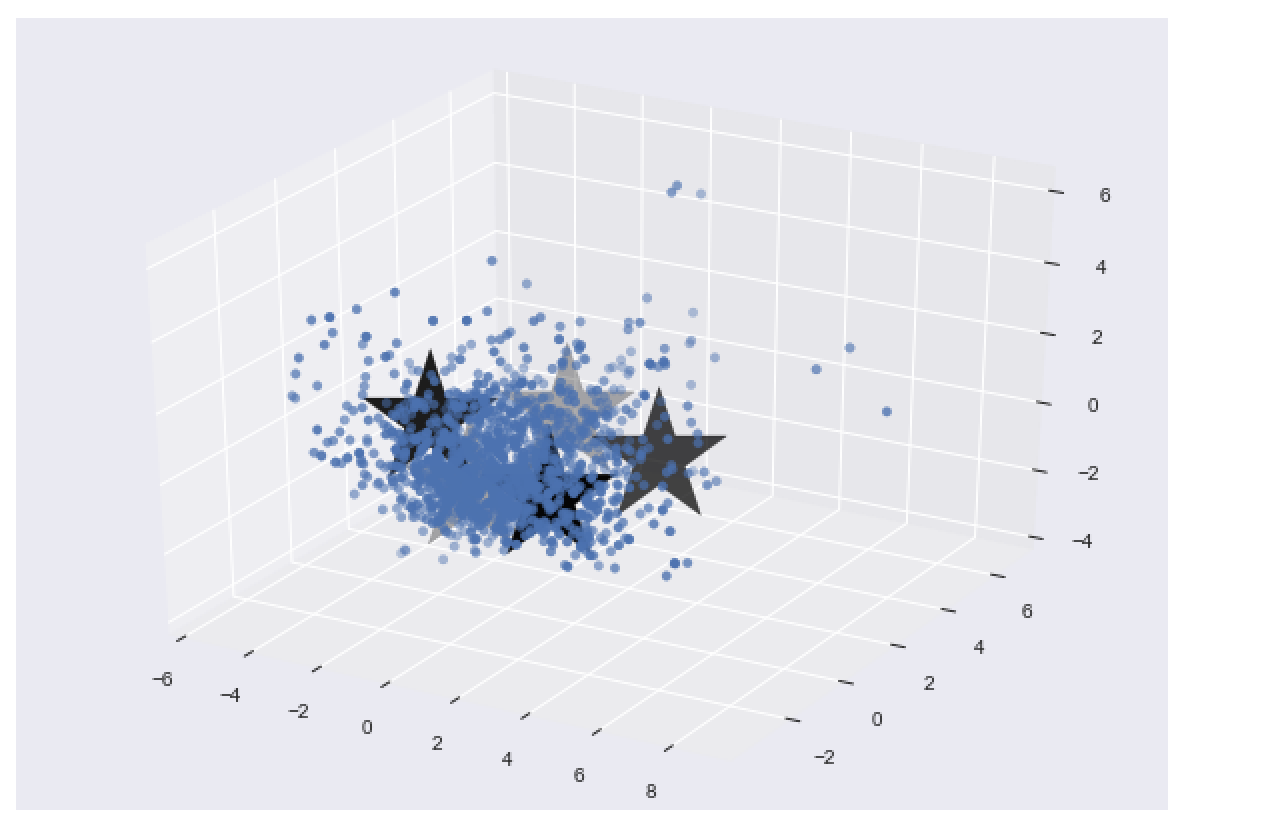


Here, we see 95% and above cumulative explained variance is around 8.

* Now, we know that we can reduce the feature dimension to 8 and use k-means clustering on these reduced dimension.
* The result for first feature and second feature from reduced 8 vectors



* The result in 3D space with first, second and third generated features



* From these two visualizations, we can achieve that K-means have been more spread in the data points and tend to achieve in more sparse way.