Assignment 3

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Question 1:

a) K Means Clustering

In [1]:
```
import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.cluster import SpectralClustering
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
```

In [2]:
```
def k_means_clustering(X, k, y):
    initial_centroids = X[np.random.choice(X.shape[0],k,replace = False)]
    centroids = initial_centroids.copy()
    distance_matrix = np.zeros((centroids.shape[0],X.shape[0]))
    minimum_dist_matrix = np.zeros((centroids.shape[0],X.shape[0]))
    prev_minimum_dist_matrix = np.ones((centroids.shape[0],X.shape[0]))
    iterations = 0
    while(np.array_equal(minimum_dist_matrix, prev_minimum_dist_matrix) == F
alse):
        iterations += 1
        prev_minimum_dist_matrix = np.copy(minimum_dist_matrix)
        minimum_dist_matrix = np.zeros((centroids.shape[0],X.shape[0]))
        distance_matrix = np.zeros((centroids.shape[0],X.shape[0]))
        for i,centroid in enumerate(centroids):
            distance_matrix[i] = np.sqrt(np.sum((X-centroid)**2,axis=1))

        for i,j in enumerate(np.argmin(distance_matrix,axis=0)):
            minimum_dist_matrix[j][i] = 1

        for i in range(k):
            data_points = X[np.where(minimum_dist_matrix[i] == 1)]
            if data_points.size:
                centroids[i] = np.mean(data_points,axis = 0)

    print("Total Iterataions: ",iterations)
    return initial_centroids, centroids, np.array([X[minimum_dist_matrix[i]
== 1] for i in range(k)]),\
            np.array([y[minimum_dist_matrix[i] == 1] for i in range(k)])
```

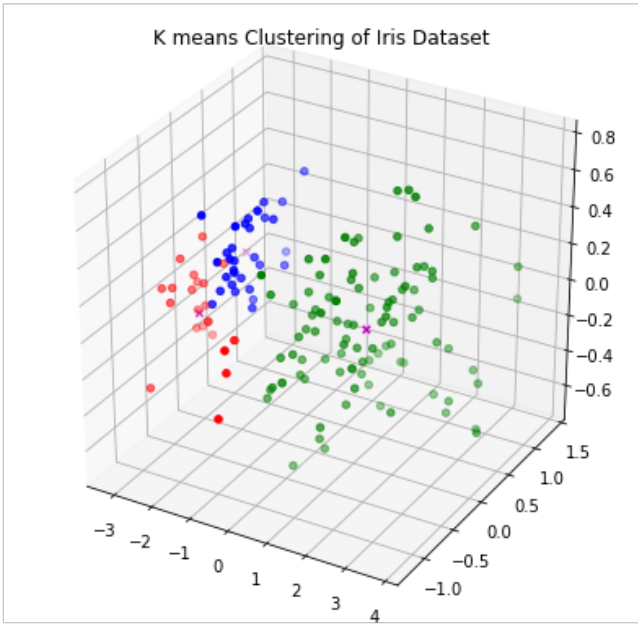
In [3]:
```
def plot_clusters(clusters, centroids_new,title):
    fig = plt.figure(figsize=(7,7))
    ax = fig.add_subplot(111, projection='3d')
    ax.scatter(clusters[0][:, 0], clusters[0][:, 1], clusters[0][:, 2], c="r
")
    ax.scatter(clusters[1][:, 0], clusters[1][:, 1], clusters[1][:, 2], c="g
")
    if clusters.shape[0] == 3:
        ax.scatter(clusters[2][:, 0], clusters[2][:, 1], clusters[2][:, 2],
c="b")
    ax.scatter(centroids_new[:, 0], centroids_new[:, 1], centroids_new[:, 2]
, c="m", marker="x")
    plt.title(title)
    plt.show()
```

b) Iris Dataset

In [4]:
```
iris_dataset = np.genfromtxt("data/iris.csv",delimiter=",")
iris_dataset = iris_dataset[:,:4]
c1, c2, c3 = [0] * 50, [1] * 50, [2] * 50
y = np.array(c1 + c2 + c3)
pca = PCA(n_components=3)
pca.fit(iris_dataset)
iris_dataset = pca.transform(iris_dataset)
centroids_iris, centroids_new_iris, clusters_iris, y_iris = k_means_clusteri
ng(iris_dataset, 3, y)
print("Old Centroids: ",centroids_iris, sep="\n")
print("New Centroids: ",centroids_new_iris, sep="\n")
```

```
Total Iterataions:  4
Old Centroids:
[[-2.469056    0.13788731  0.10126308]
 [ 2.31967279 -0.24554817 -0.34992218]
 [-2.68420713  0.32660731 -0.02151184]]
New Centroids:
[[-2.4107173  -0.39626231 -0.04877788]
 [ 1.40541808 -0.05731672 -0.00301217]
 [-2.56366574  0.47149799  0.04551806]]
```

In [5]:
```
plot_clusters(clusters_iris, centroids_new_iris,"K means Clustering of Iris
Dataset")
```

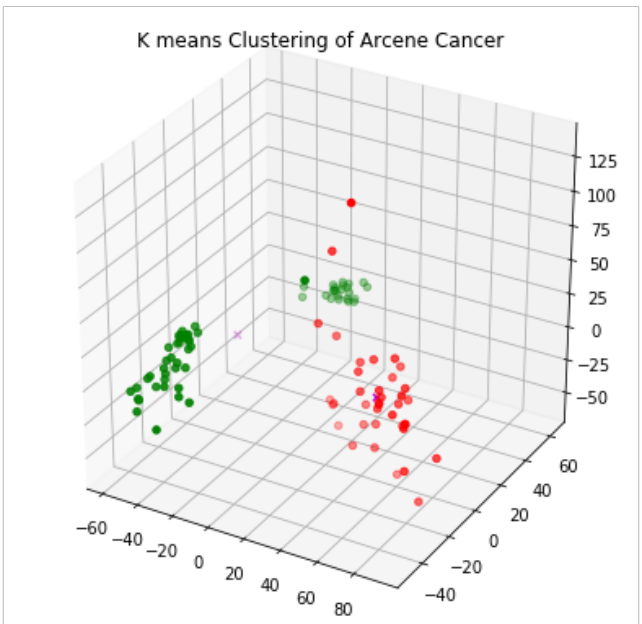


c) 1. Cancer Dataset

In [6]:
```
file = open('data/arcene_train.data')
X = np.array([list(map(int, file.readline().strip().split(' '))) for _ in ra
nge(100)])

file = open('data/arcene_train.labels')
y = np.array([int(file.readline().strip()) for _ in range(100)])

y[y == -1] = 0
scaler = StandardScaler()
X_std = scaler.fit_transform(X)
pca = PCA(n_components=3)
pca.fit(X_std)
X_cancer= pca.transform(X_std)
centroids_cancer, centroids_new_cancer, clusters_cancer,y_cancer = k_means_c
lustering(X_cancer, 2, y)
print("Old Centroids: ",centroids_cancer, sep="\n")
print("New Centroids: ",centroids_new_cancer, sep="\n")
```

```
Total Iterataions:  5
Old Centroids:
[[-48.19983782 -23.29887297   2.42939306]
 [-48.80106952 -10.8254401    8.69807006]]
New Centroids:
[[ 55.98040236  -9.92193407   1.57410511]
 [-34.31056919   6.0811854   -0.9647741 ]]

/home/user/anaconda3/lib/python3.6/site-packages/sklearn/utils/validation.py:
475: DataConversionWarning: Data with input dtype int64 was converted to floa
t64 by StandardScaler.
  warnings.warn(msg, DataConversionWarning)
```

In [7]:
```
plot_clusters(clusters_cancer, centroids_new_cancer,"K means Clustering of A
rcene Cancer")
```

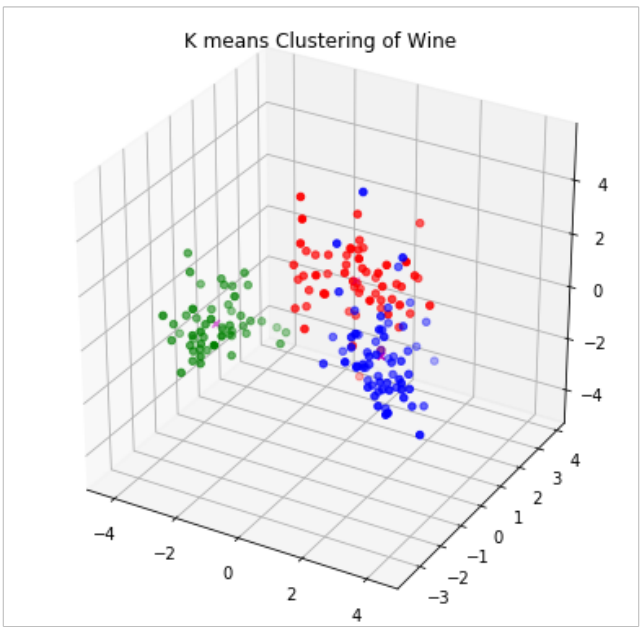


c) 2.Wine Data Set

In [8]:
```
file = open('data/wine.data')
X = np.array([list(map(float, file.readline().strip().split(','))) for _ in
range(178)])
y = X[:,0]
y[y == 1] = 0
y[y == 2] = 1
y[y == 3] = 2

scaler = StandardScaler()
X_std = scaler.fit_transform(X[:,1:])
pca = PCA(n_components=3)
pca.fit(X_std)
X_wine = pca.transform(X_std)
centroids_wine, centroids_new_wine, clusters_wine,y_wine = k_means_clusterin
g(X_wine, 3, y.astype('uint8'))
print("Old Centroids: ",centroids_wine, sep="\n")
print("New Centroids: ",centroids_new_wine, sep="\n")
```

```
Total Iterataions:  10
Old Centroids:
[[ 0.08253578  2.30623459 -0.46357499]
 [ 2.17195527 -2.32730534  0.83172987]
 [ 2.5108743  -0.91807096 -1.77096903]]
New Centroids:
[[-0.23104063  1.82134758  0.24360512]
 [-2.72003575 -1.12565126 -0.23909324]
 [ 2.24048853 -0.73604842 -0.03204334]]
```

In [9]:
```
plot_clusters(clusters_wine, centroids_new_wine,"K means Clustering of Wine"
)
```



Question 2: Internal Measures

RMSSTD:

- The root mean square standard deviation is an evaluation method used to measure the equality of the clustering algorithm. The lower the value of RMSSTD, the better the separation of clusters.
- RMSSTD is a measure of homogeneity within clusters

RMSSTD = $$\sqrt{\frac{\sum\limits_{\substack{j=1..p\\i=1..k}}\sum\limits_{a=1}^{n_{ij}}(x_a-\bar{x_{ij}})^2}{\sum\limits_{\substack{j=1..p\\i=1..k}}(n_{ij}-1)}}$$

where k is the number of clusters,

p is the number of independent variables in dataset,

x_{ij} is the mean of data in variable j and cluster i,

and n_{ij} is the number of data which are in variable p and cluster k.

R- Square:

- RS is used to determine whether there is a significant difference among objects in different groups and that objects in the same group have high similarity.
- The R-squared value is used to determine whether there is a significant difference among objects in different groups and that objects in the same group have high similarity. If RS equals zero, then there is no difference between the groups.
- On the other hand, if RS equals one, then the partitioning of clusters is optimal

$$RS = \frac{SS_t - SS_w}{SS_t}$$

where $SS_t = \sum\limits_{j=1}^{p}\sum\limits_{a=1}^{n_{ij}}(x_a-\bar{x_j})^2$

and $SS_w = \sum\limits_{\substack{j=1..p\\i=1..k}}\sum\limits_{a=1}^{n_{ij}}(x_a-\bar{x_{ij}})^2$

where SS_t is the summation of the distance squared among all variables,

SS_w is the summation of the distance squared among all data in the same cluster,

k is the number of clusters,

p is the number of independent variables in the dataset,

x_j is the mean of data in variable j,

x_{ij} is the mean of the data in variable j and cluster i and

n_{ij} is the number of data which are invariable p and cluster k.

In [10]:
```
def rmsstd(clusters):
    k = clusters.shape[0]
    ssd = np.zeros(clusters.shape)
    for i in range(k):
        mean = np.mean(clusters[i][0],axis=0)
        ssd[i] = np.sum((clusters[i][0] - mean)**2)
    numerator = np.sum(ssd)
    denominator = 0
    for i in range(k):
        for j in range(clusters[i][0].shape[1]):
            denominator += clusters[i][0].shape[0] - 1
    rmsstd_val = np.sqrt(numerator/denominator)
    return rmsstd_val

def rs(clusters):
    k = clusters.shape[0]
    ssd = np.zeros(clusters.shape)
    total_ssd = np.zeros(clusters.shape)

    means = []
    for i in range(k):
        mean = np.mean(clusters[i][0],axis=0)
        ssd[i] = np.sum((clusters[i][0] - mean)**2)
        means.append(list(mean))
    ss_w = np.sum(ssd)
    total_mean = np.mean(means, axis = 0)
    for i in range(k):
        total_ssd[i] = np.sum((clusters[i][0] - total_mean)**2)
    ss_t = np.sum(total_ssd)

    rs_val = (ss_t - ss_w) / ss_t
    return rs_val
```

In [11]:
```
print("Iris Dataset - RMSSTD: ", rmsstd(clusters_iris.reshape(clusters_iris.
shape[0],1)))
print("Iris Dataset - RS: ", rs(clusters_iris.reshape(clusters_iris.shape[0]
,1)))
```

```
Iris Dataset - RMSSTD:  0.5620830706277432
Iris Dataset - RS:  0.8433797163492809
```

In [12]:
```
print("Cancer Dataset - RMSSTD: ", rmsstd(clusters_cancer.reshape(clusters_c
ancer.shape[0],1)))
print("Cancer Dataset - RS: ", rs(clusters_cancer.reshape(clusters_cancer.sh
ape[0],1)))
```

```
Cancer Dataset - RMSSTD:  25.29265829394243
Cancer Dataset - RS:  0.5279806006610025
```

In [13]:
```
print("Wine Dataset - RMSSTD: ", rmsstd(clusters_wine.reshape(clusters_wine.
shape[0],1)))
print("Wine Dataset - RS: ", rs(clusters_wine.reshape(clusters_wine.shape[0]
,1)))
```

```
Wine Dataset - RMSSTD:  0.9894786178727465
Wine Dataset - RS:  0.6682811640878119
```

Observations:

- The RMSSTD value is less for Iris Dataset which means that the clustering for that dataset is pretty good.
- Whereas the RMSSTD value for Cancer is very high which indicates that it is very bad clustering. This is because the 10,000 variables is reduced to 3 variables.
- On the other hand, the RMSSTD value for Wine dataset is very much better compared to Cancer dataset.
- If RS = 1 then it indiates optimal clustering. Here it is observed that for Iris Dataset it is high and for Cancer Dataset it is low.

Question 2: External Measures

Purity is a simple and transparent evaluation measure. Normalized mutual information can be information-theoretically interpreted. The Rand index penalizes both false positive and false negative decisions during clustering. The F measure in addition supports differential weighting of these two types of errors.

Purity:

To compute purity , each cluster is assigned to the class which is most frequent in the cluster, and then the accuracy of this assignment is measured by counting the number of correctly assigned documents and dividing by N. Formally:

$$\text{purity}(\Omega, \mathbb{C}) = \frac{1}{N} \sum_k \max_j |\omega_k \cap c_j|$$

F-measure

F1 score (also F-score or F-measure) is a measure of a test's accuracy. It considers both the precision p and the recall r of the test to compute the score: p is the number of correct positive results divided by the number of all positive results returned by the classifier, and r is the number of correct positive results divided by the number of all relevant samples (all samples that should have been identified as positive). The F1 score is the harmonic average of the precision and recall, where an F1 score reaches its best value at 1 (perfect precision and recall) and worst at 0.

$$F1 = 2.(\frac{precision.recall}{precision+recall})$$

In [14]:
```
 def confusion_matrix(k, labels):
        cm = np.zeros((k, k), int)
        number_of_datapoints = np.sum([labels[i].size for i in range(k)])
        for i in range(k):
            counts = np.bincount(labels[i])
            target = np.argmax(counts)
            for label in labels[i]:
                cm[label, int(target)] += 1
        return cm

def precision(TP, FP):
    return np.around((TP/(TP+FP)),decimals=3)

def recall(TP, FN):
    return np.around((TP/(TP+FN)),decimals=3)


def f_measure(TP, FP, FN):
    precision_val = precision(TP, FP)
    recall_val = recall(TP, FN)
    return 2 * (precision_val * recall_val) / (precision_val + recall_val)

def cm_metrics(cm):
    FP, FN, TN = [], [], []
    for i in range(cm.shape[0]):
        FP.append(sum(cm[:,i]) - cm[i,i])
        FN.append(sum(cm[i,:]) - cm[i,i])
        temp = np.delete(cm, i, 0)   # delete ith row
        temp = np.delete(temp, i, 1)  # delete ith column
        TN.append(sum(sum(temp)))
    return np.diag(cm),FP, FN, TN



def purity(y, k, class_count):
    sum = 0
    for i in range(k):
        counts = np.bincount(y[i])
        label = np.argmax(counts)
        max_occurances = counts[label]
        sum += min(class_count[i], max_occurances)
    return sum / np.sum(class_count)
```

In [15]:
```
cm = confusion_matrix(3, y_iris)
print("Confusion Matrix: ",cm,sep="\n")
tp, fp, fn, tn = cm_metrics(cm)
f_m = f_measure(tp, fp, fn)
print("Purity: ", purity(y_iris, 3, [50,50,50]))
print("F-Measure: ", f_m)
print("Average F-Measure: ", np.mean(f_m))
```

```
Confusion Matrix:
[[50  0  0]
 [ 4  0 46]
 [ 0  0 50]]
Purity:  0.6666666666666666
F-Measure:  [0.9615784         nan 0.68507561]
Average F-Measure:  nan
```

```
/home/user/anaconda3/lib/python3.6/site-packages/ipykernel_launcher.py:12: Ru
ntimeWarning: invalid value encountered in true_divide
  if sys.path[0] == '':
```

In [16]:
```
cm = confusion_matrix(2, y_cancer)
print("Confusion Matrix: ",cm,sep="\n")
tp, fp, fn, tn = cm_metrics(cm)
f_m = f_measure(tp, fp, fn)
print("Purity: ", purity(y_cancer, 2, [44,56]))
print("F-Measure: ", f_m)
print("Average F-Measure: ", np.mean(f_m))
```

```
Confusion Matrix:
[[28 28]
 [10 34]]
Purity:  0.62
F-Measure:  [0.59579628 0.64133838]
Average F-Measure:  0.6185673306704 64
```

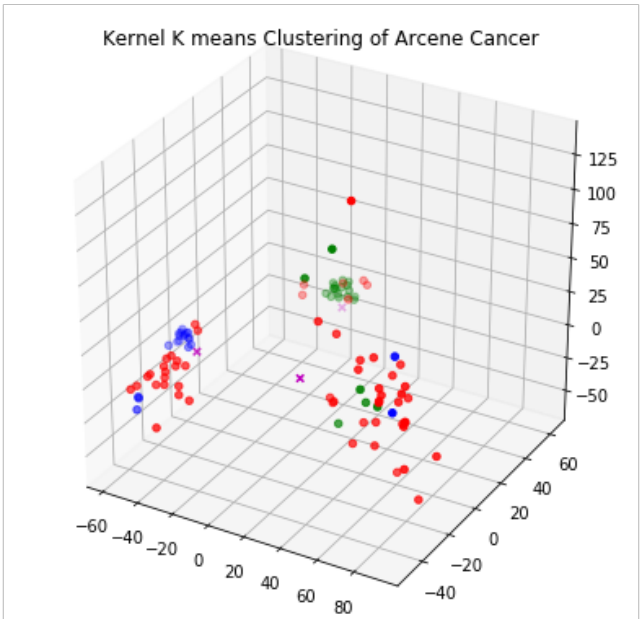
In [17]:
```
cm = confusion_matrix(3, y_wine)
print("Confusion Matrix: ",cm,sep="\n")
tp, fp, fn, tn = cm_metrics(cm)
f_m = f_measure(tp, fp, fn)
print("Purity: ", purity(y_wine, 3, [59,71, 48]))
print("F-Measure: ", f_m)
print("Average F-Measure: ", np.mean(f_m))
```

```
Confusion Matrix:
[[59  0  0]
 [ 9 59  3]
 [ 0  0 48]]
Purity:  0.8707865168539326
F-Measure:  [0.92933619 0.90770071 0.9696033 ]
Average F-Measure:  0.9355467319002727
```

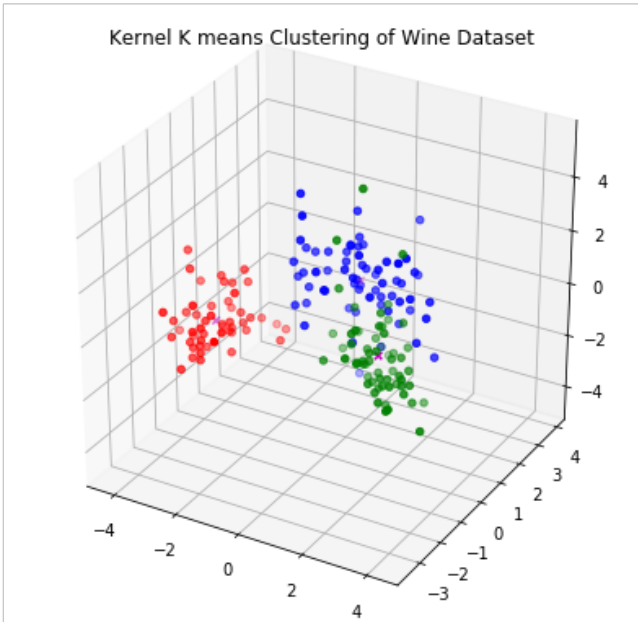
Question 3: Kernel K Means

In [18]:
```
k = 3
clustering = SpectralClustering(n_clusters=k,assign_labels="discretize",rand
om_state=0).fit_predict(X_cancer)
# clustering = SpectralClustering(n_clusters=k,assign_labels="discretize",ra
ndom_state=0).fit_predict(iris_dataset[:100,:])

clusters = np.array([X_cancer[clustering == i] for i in range(k)])
centroids_new = np.array([np.mean(clusters[i],axis=0) for i in range(k)])
plot_clusters(clusters, centroids_new,"Kernel K means Clustering of Arcene C
ancer")
```

```
/home/user/anaconda3/lib/python3.6/site-packages/sklearn/manifold/spectral_em
bedding_.py:234: UserWarning: Graph is not fully connected, spectral embeddin
g may not work as expected.
  warnings.warn("Graph is not fully connected, spectral embedding"
```



In [19]:
```
k = 3
clustering = SpectralClustering(n_clusters=k,assign_labels="discretize",rand
om_state=0).fit_predict(X_wine)
# clustering = SpectralClustering(n_clusters=k,assign_labels="discretize",ra
ndom_state=0).fit_predict(iris_dataset[:100,:])

clusters = np.array([X_wine[clustering == i] for i in range(k)])
centroids_new = np.array([np.mean(clusters[i],axis=0) for i in range(k)])
plot_clusters(clusters, centroids_new,"Kernel K means Clustering of Wine Dat
aset")
```



Observations:

- When compared to the K means on Arcene Cancer dataset the results obtained by Kernel K means is not appealing. It does not create proper clustering. The reson may be the dimensionality reduction from 10,000 to 3 components.
- The clusters formed for Wine dataset using Kernel Kmeans and the normal K means is almost the same.