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[1]:
```
import random
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
import warnings
warnings.filterwarnings("ignore")
import seaborn as sns
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
from sklearn.manifold import TSNE
from sklearn.cluster import KMeans
from sklearn.metrics import calinski_harabaz_score
from sklearn import metrics
from scipy.spatial.distance import cdist
from sklearn.metrics import silhouette_score
from gap_statistic import optimalK
from yellowbrick.cluster.elbow import kelbow_visualizer
```

1 k-Means Clustering "By Hand"

1.1 1

[2]:
```
x_1 = [5,8,7,8,3,4,2,3,4,5]
x_2 = [8,6,5,4,3,2,2,8,9,8]
def get_data(x_1,x_2, k):
    random.seed(20)
    X = list(map(lambda x, y:(x,y), x_1, x_2))
    data = {'x_1': x_1, 'x_2': x_2, 'X': X}
    data = pd.DataFrame(data)
    centers = random.sample(X, k)
    data['label'] = 'undecided'
    for i in range(len(x_1)):
        if data['X'][i] in centers:
            data['label'][i] = data['X'][i]
        else:
            data['label'][i] = random.choice(centers)
    data['distance_dict'] = [0]*len(x_1)
```

```
    return data
labeled_data = get_data(x_1, x_2, k=3)
labeled_data
```

[2]:

	x_1	x_2	X	label	distance_dict
0	5	8	(5, 8)	(3, 3)	0
1	8	6	(8, 6)	(8, 6)	0
2	7	5	(7, 5)	(7, 5)	0
3	8	4	(8, 4)	(8, 6)	0
4	3	3	(3, 3)	(3, 3)	0
5	4	2	(4, 2)	(7, 5)	0
6	2	2	(2, 2)	(7, 5)	0
7	3	8	(3, 8)	(3, 3)	0
8	4	9	(4, 9)	(3, 3)	0
9	5	8	(5, 8)	(7, 5)	0

We can see the initialized labels of each obeservation in the column named label.

1.2 2

[3]:
```
def dis(x, y):
    return ((x[0]-y[0])**2 + (x[1]-y[1])**2)**0.5
def dis_dict(x, centers):
    dic = {}
    for center in centers:
        dic[(center)] = dis(x, center)
    return dic

def update_label(data):
    centers = set(data['label'].unique())
    data['distance_dict'] = data.apply(lambda x:
                                       dis_dict(x['X'], centers), axis = 1)
    data['label'] = data.apply(lambda x:min(x['distance_dict'],
                                            key=x['distance_dict'].get),
                                        axis = 1)
    print(set(data['label'].unique()))
    df = data.groupby('label')[['x_1','x_2']].mean()
    df['new_label'] = df.apply(lambda x:(x['x_1'], x['x_2']), axis = 1)
    df = df.reset_index()
    for i in range(len(data)):
        for j in range(len(df)):
            if data['label'][i] == df['label'][j]:
                data['label'][i] = df['new_label'][j]
    centers = set(data.label.unique())
    data['distance_dict'] = data.apply(lambda x:
                                       dis_dict(x['label'], centers), axis = 1)
    data['label'] = data.apply(lambda x:min(x['distance_dict'],
```

```
                                                    key=x['distance_dict'].get),
                                      axis = 1)
    return data
def finish_kmean(data):
    while True:
        labels = set(data['label'].unique())
        new_data = update_label(data)
        new_labels = set(data['label'].unique())
        if labels == new_labels:
            break
        else:
            data = new_data
    return data
k3_data = get_data(x_1,x_2,3)
k3_data = finish_kmean(get_data(x_1,x_2,3))
```

```
{(8, 6), (7, 5), (3, 3)}
{(3.0, 2.3333333333333335), (5.5, 7.75), (6.0, 5.666666666666667)}
{(3.0, 2.3333333333333335), (7.666666666666667, 5.0), (4.25, 8.25)}
```

Here we see the cluster centroids in different iteration rounds. The last line represents the final (converged) cluster centroids.

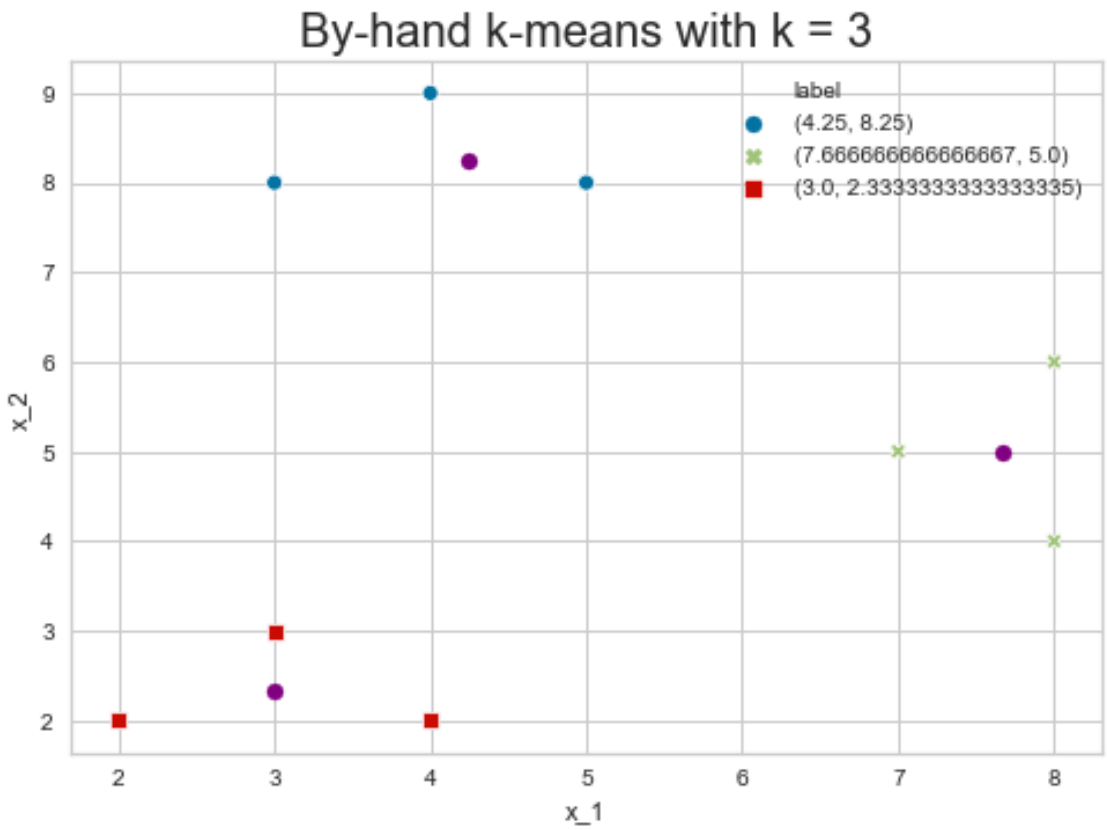
[4]:
```
X = list(map(lambda x, y:(x,y), x_1, x_2))
k3_kmeans = KMeans(n_clusters=3, random_state=0).fit(X)
k3_kmeans.cluster_centers_
```

[4]:
```
array([[7.66666667, 5.        ],
       [4.25      , 8.25      ],
       [3.        , 2.33333333]])
```

Now we used the package in sklearn to check our answers. We can see that the answers from the sklearn package match our results, which justifies our calculation.

1.3 3

[5]:
```
k3=sns.scatterplot(data = k3_data, x='x_1',y='x_2', style = 'label',
                   hue = 'label')
labels = k3_data.label.unique()
plot_labels_x = [i[0] for i in labels]
plot_labels_y = [i[1] for i in labels]
plt.scatter(plot_labels_x, plot_labels_y,c = 'purple')
plt.title("By-hand k-means with k = 3", size = 20)
plt.show()
```



1.4 4

[6]:
```
k2_data = get_data(x_1,x_2,2)
k2_data = finish_kmean(k2_data)
```

```
{(7, 5), (3, 3)}
{(5.714285714285714, 6.857142857142857), (3.0, 2.3333333333333335)}
```

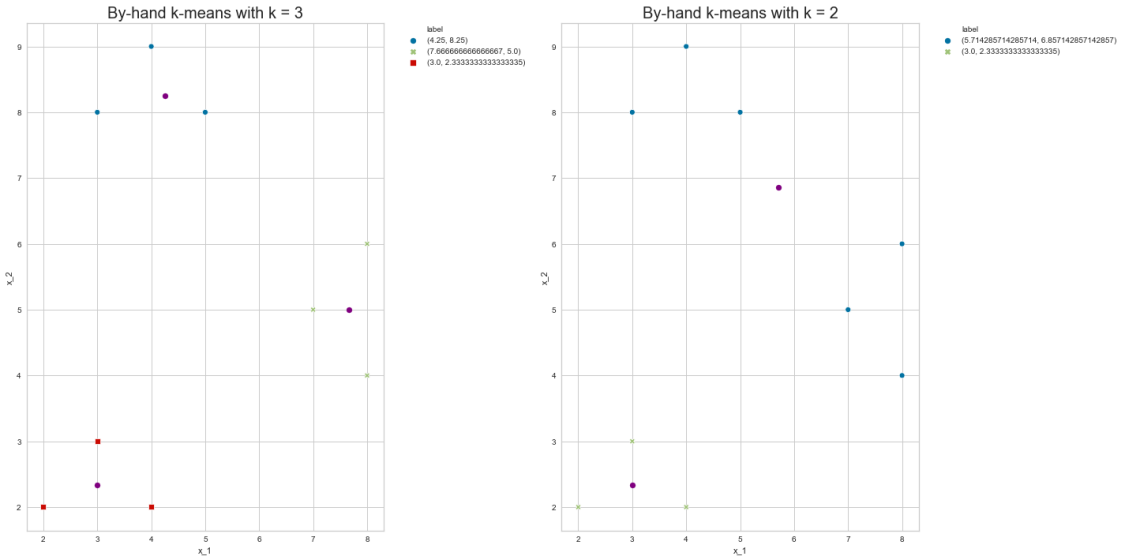
Here we see the cluster centroids in different iteration rounds. The last line represents the final (converged)cluster centroids.

[7]:
```
X = list(map(lambda x, y:(x,y), x_1, x_2))
k2_kmeans = KMeans(n_clusters=2, random_state=0).fit(X)
k2_kmeans.cluster_centers_
```

[7]:
```
array([[3.        , 2.33333333],
       [5.71428571, 6.85714286]])
```

Now we used the package in sklearn to check our answers. We can see that the answers from the sklearn package match our results, which justifies our calculation.

[8]:
```
#visualization
plt.figure(figsize=(20,10))
plt.subplot(1, 2, 1)
k3=sns.scatterplot(data = k3_data, x='x_1',y='x_2', style = 'label',
                   hue = 'label')
labels = k3_data.label.unique()
plot_labels_x = [i[0] for i in labels]
plot_labels_y = [i[1] for i in labels]
plt.scatter(plot_labels_x, plot_labels_y,c = 'purple')
plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0.)
plt.title("By-hand k-means with k = 3", size = 20)

plt.subplot(1, 2, 2)
k2=sns.scatterplot(data = k2_data, x='x_1',y='x_2', style = 'label',
                   hue = 'label')
labels = k2_data.label.unique()
plot_labels_x = [i[0] for i in labels]
plot_labels_y = [i[1] for i in labels]
plt.scatter(plot_labels_x, plot_labels_y,c = 'purple')
plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0.)
plt.title("By-hand k-means with k = 2", size = 20)
plt.tight_layout()
```



1.5 5

[9]:
```
print("k = 2:",k2_kmeans.inertia_)
print("k = 3:",k3_kmeans.inertia_)
```

```
k = 2: 46.952380952380956
```

```
k = 3: 8.833333333333332
```

I think the best value for k is 3. At first, we can clearly observe from the above plots that the data are clustered into 3 groups. It is so clear that we can get the conclusion straightforward. Second, we can use a quantitative method to judge. Here we use the sum of squared distances of samples to their closest cluster center. According to the above results, we can see that when k equals to 3, the the sum of squared distances of samples to their closest cluster center is much smaller. We can try more different k values and the results will be the same.

2 Application

[10]:
```
wiki = pd.read_csv('C:/Users/mac/Desktop/temp/problem-set-7-master/data/wiki.
↪csv')
wiki_std = pd.DataFrame(StandardScaler().fit_transform(wiki))
random.seed(20)
```

2.1 Dimension reduction

2.1.1 6

[11]:
```
pca = PCA(n_components = 2)
pca.fit(wiki_std)
wiki_transformed = pca.fit_transform(wiki_std)
wiki_pca = pd.DataFrame(pca.components_, columns = wiki.columns,
                        index = ['PC_1','PC_2']).T
wiki_pca.iloc[wiki_pca['PC_1'].abs().argsort()[::-1]].head(10)
```

[11]:

	PC_1	PC_2
bi2	0.230924	0.083463
bi1	0.226193	0.056401
use3	0.218809	0.155179
use4	0.214558	0.160887
pu3	0.210863	0.028798
exp1	0.208592	0.070581
use5	0.206539	0.029832
exp2	0.195043	-0.029523
pu1	0.192827	0.008260
pu2	0.190588	0.017671

According to the above dataframe, we can see that bi2, bi1, uses 3 and other 7 variables are the top 10 variables which are highly correlated on the first component. According to the variable explanation, bi2 and bi1 both describes behavioral intention of recommending or using Wikipedia.In addition, variables including use3, use4 and use5 decribe how indiviual uses wikipedia, and the sum of their coeffcients are more than 0.6. According to these facts, we can deduce that people's behavioral intention and how they use wikipedia are strongly related to the first component.

[12]:
```
wiki_pca.iloc[wiki_pca['PC_2'].abs().argsort()[::-1]].head(10)
```

[12]:

	PC_1	PC_2
peu1	0.061228	-0.271727
inc1	0.104667	-0.245469
sa3	0.120376	-0.242287
sa1	0.121658	-0.229924
exp4	0.099873	0.228448
enj2	0.131110	-0.227617
sa2	0.117590	-0.226731
peu2	0.113719	-0.222369
inc3	0.081402	-0.221028
use2	0.147852	0.218648

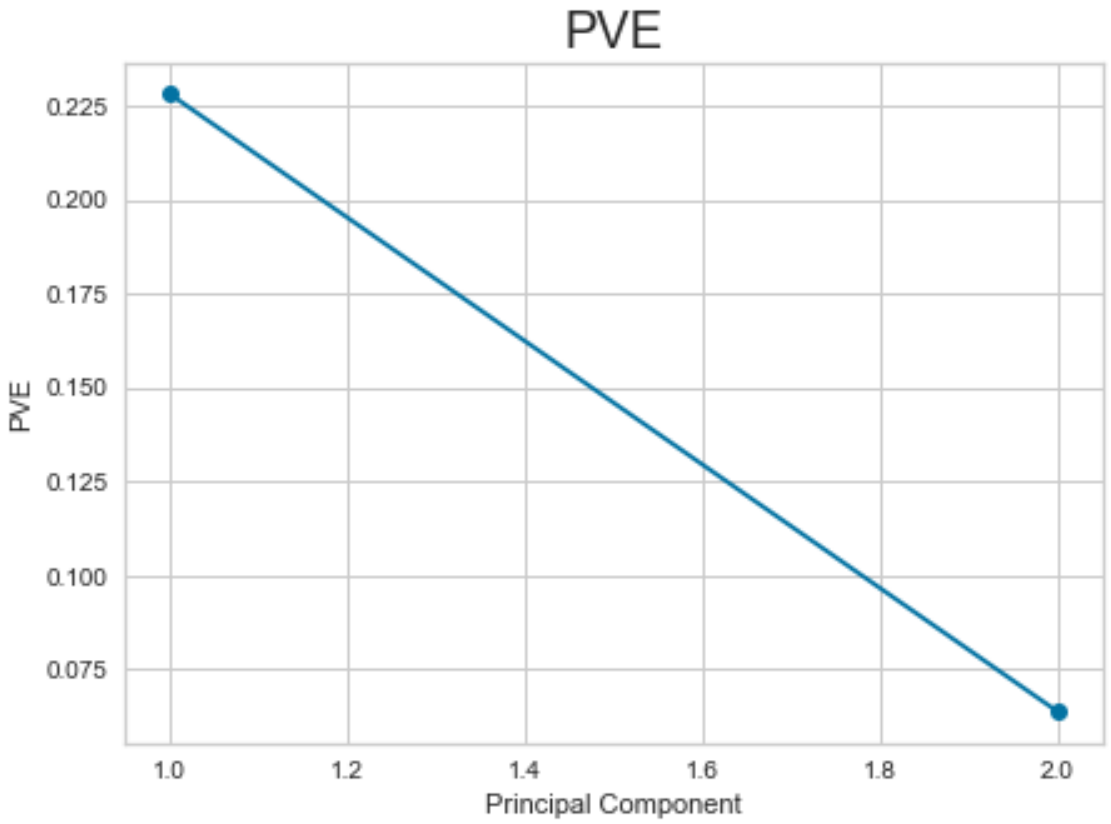
According to the above dataframe, we can see that peu1, inc1, sa 3 and other 7 variables are the top 10 variables which are highly correlated on the second component. Variables including sa1, sa2 and sa3 all decribe the social image of wikipedia, and the absolute value of the sum of coefficients of these three variables are nearly 0.7. We can deduce that the social image of wikipedia is strongly related to the second component.

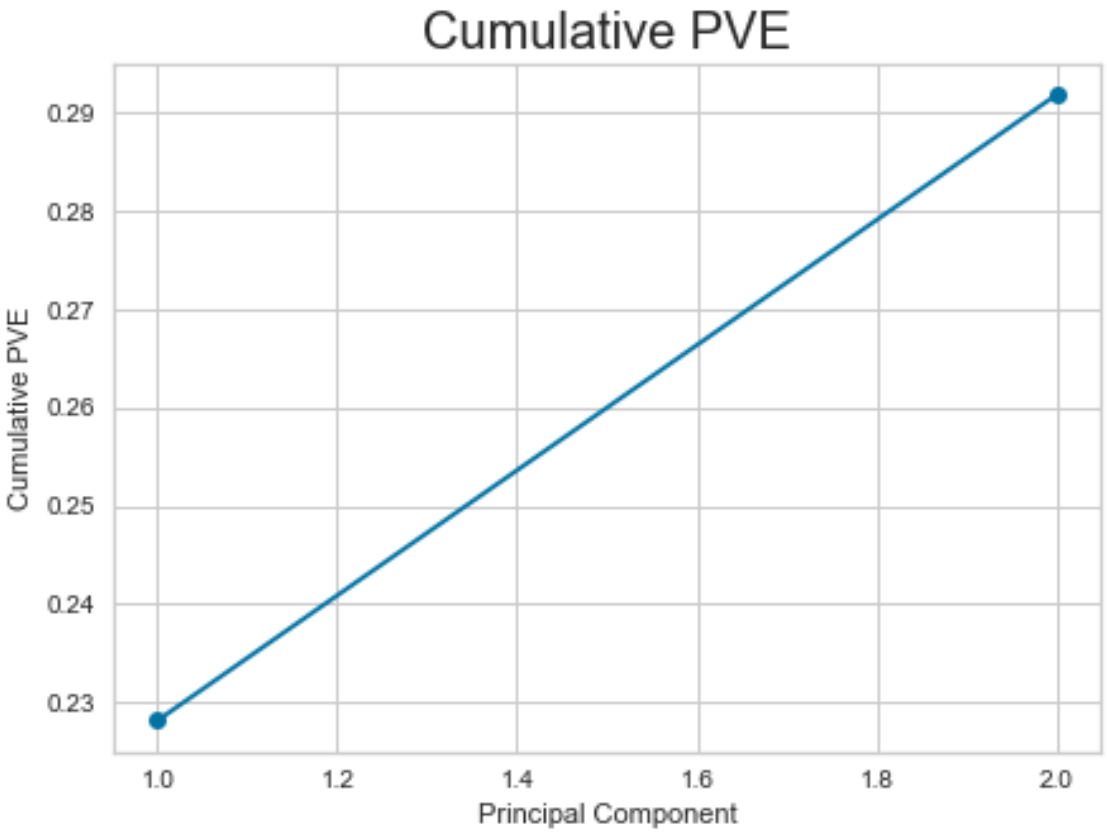
In addition, we can see that in the variables which are more correlated on the first component, the coefficients are all positive. in the variables which are more correlated on the second component, the coefficients are almost negative. Therefore, we may deduce that the two components describe the data in two opposite directions.

2.1.2 7

[13]:
```
plt.figure(figsize=[7,5])
plt.plot([1,2],pca.explained_variance_ratio_,'-o')
plt.ylabel('PVE')
plt.xlabel('Principal Component')
plt.title('PVE', size = 20)

plt.figure(figsize=[7,5])
plt.plot([1,2],np.cumsum(pca.explained_variance_ratio_),'-o')
plt.ylabel('Cumulative PVE')
plt.xlabel('Principal Component')
plt.title('Cumulative PVE', size = 20)
```

[13]:
```
Text(0.5, 1.0, 'Cumulative PVE')
```


PVE
0.225
0.200
0.175
0.150
0.125
0.100
0.075
PVE
1.0
1.2
1.4
1.6
1.8
2.0
Principal Component



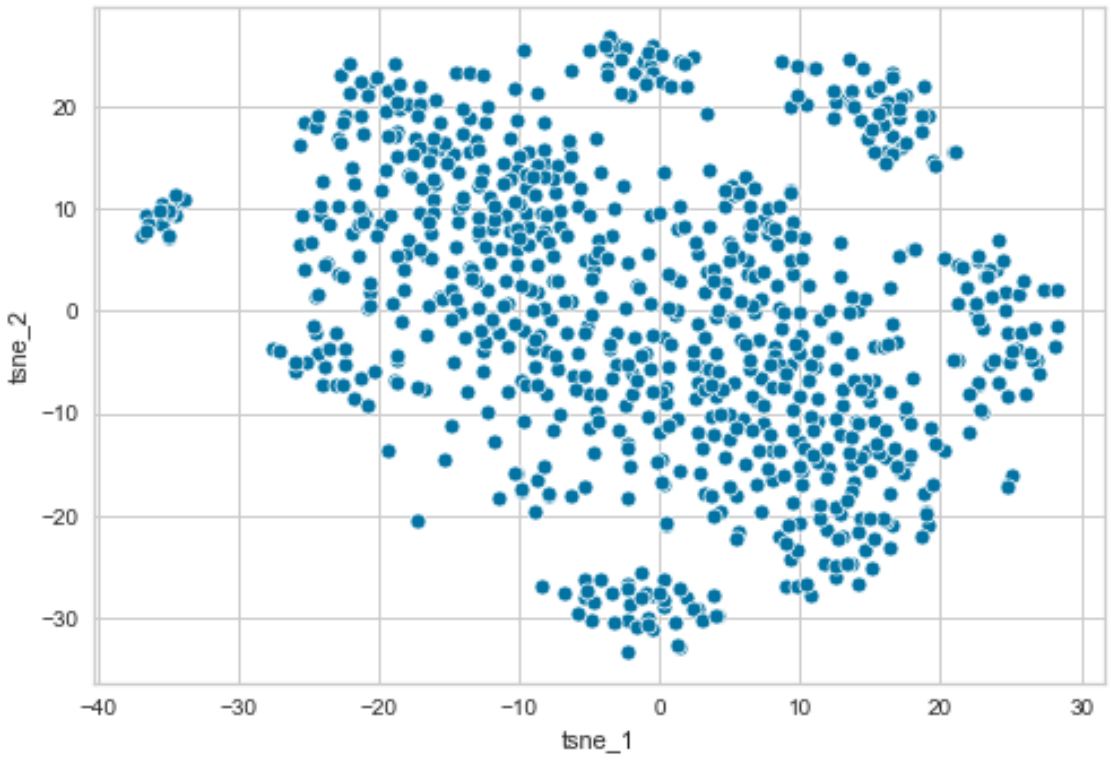
[14]:
```
print('Total variance being explained: ', np.cumsum(pca.
↪explained_variance_ratio_)[-1])
```

```
Total variance being explained:  0.291831013133461
```

2.1.3 8

[15]:
```
tsne = TSNE(n_components=2, random_state = 20)
tsne_results = tsne.fit_transform(wiki_std)
tsne_results = pd.DataFrame(tsne_results)
tsne_results = tsne_results.rename(columns = {0:'tsne_1', 1:'tsne_2'})

sns.scatterplot(x='tsne_1', y='tsne_2', palette=sns.color_palette("hls",␣
↪10),data=tsne_results,legend="full")
```

[15]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x20df2c1ff48>
```



According to the above plot, we can see that the data are mainly composed by a huge group of observations and several scattered much smaller groups (about 5).This phenomenon shows one advantage of t-SNE over PCA: t-SNE are better able to avoid the problem of overlapping. At the same time, since the different groups of data are clearly represented in the above plot, we can find that according to t-SNE as a non-linear algorithm, it can more accurately capture the complex polynomial relationship between features compared to PCA.

2.2 Clustering

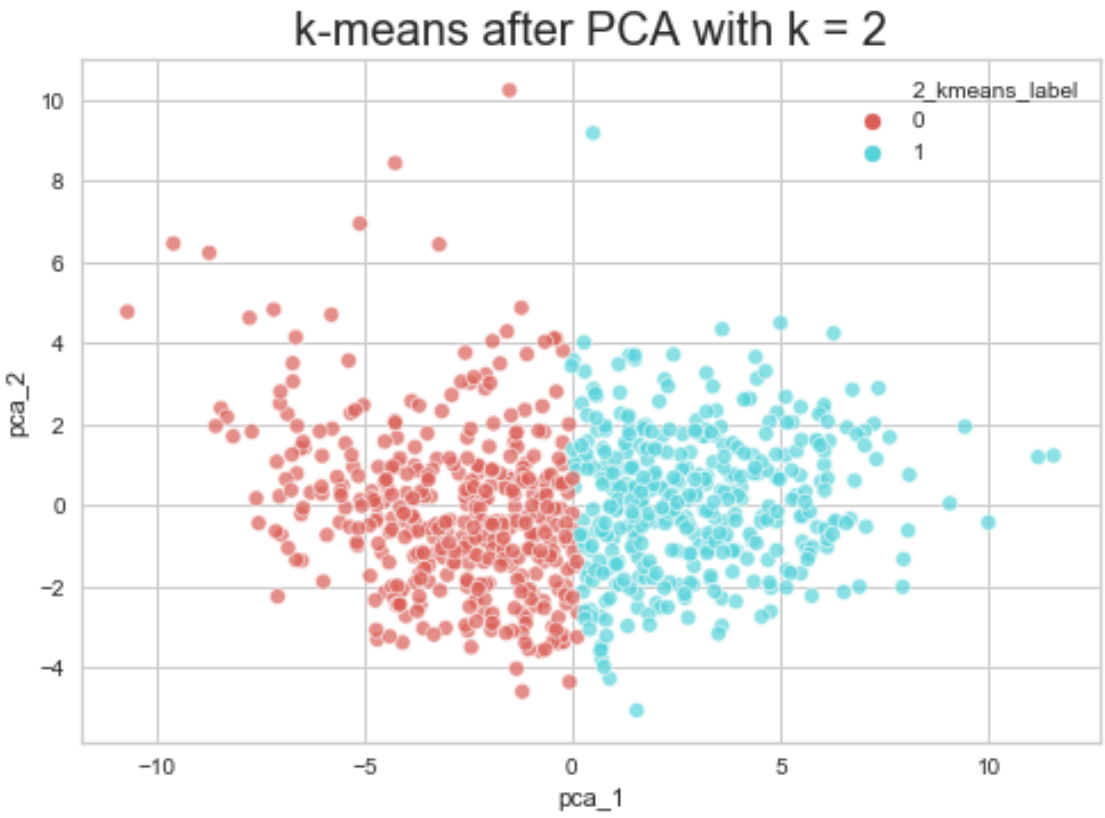
2.2.1 9

[16]:
```
wiki_transformed = pd.DataFrame(wiki_transformed)
wiki_transformed = wiki_transformed.rename(columns = {0:'pca_1', 1:'pca_2'})
k2_wiki = KMeans(n_clusters=2, random_state=20).fit(wiki_transformed)
k2_wiki.cluster_centers_

k3_wiki = KMeans(n_clusters=3, random_state=20).fit(wiki_transformed)
k3_wiki.cluster_centers_

k4_wiki = KMeans(n_clusters=4, random_state=20).fit(wiki_transformed)
k4_wiki.cluster_centers_

pca_analysis = wiki_transformed.copy()
```

```
pca_analysis['2_kmeans_label'] = k2_wiki.labels_
pca_analysis['3_kmeans_label'] = k3_wiki.labels_
pca_analysis['4_kmeans_label'] = k4_wiki.labels_
```

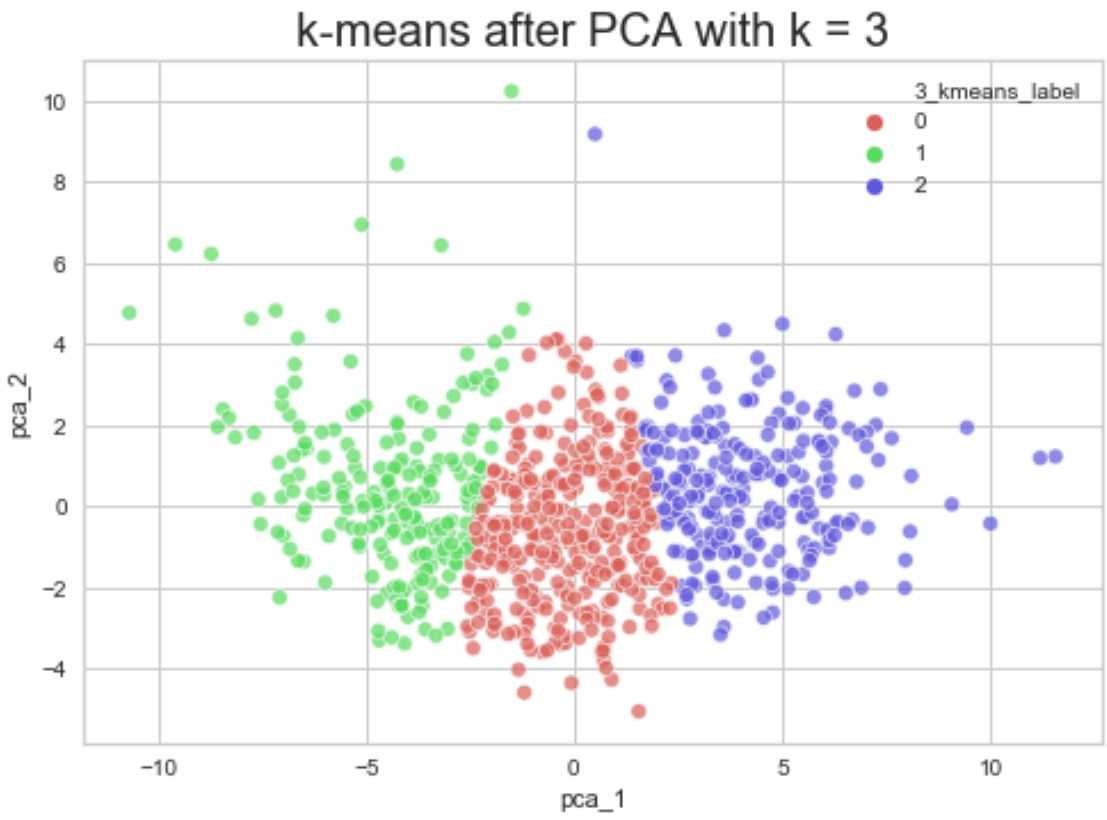
[17]:
```
sns.scatterplot(x='pca_1', y='pca_2', palette=sns.color_palette("hls", 2),data␣
↪= pca_analysis, hue = '2_kmeans_label',
                legend="full",alpha = 0.7)
plt.title('k-means after PCA with k = 2', size = 20)
```

[17]:
```
Text(0.5, 1.0, 'k-means after PCA with k = 2')
```



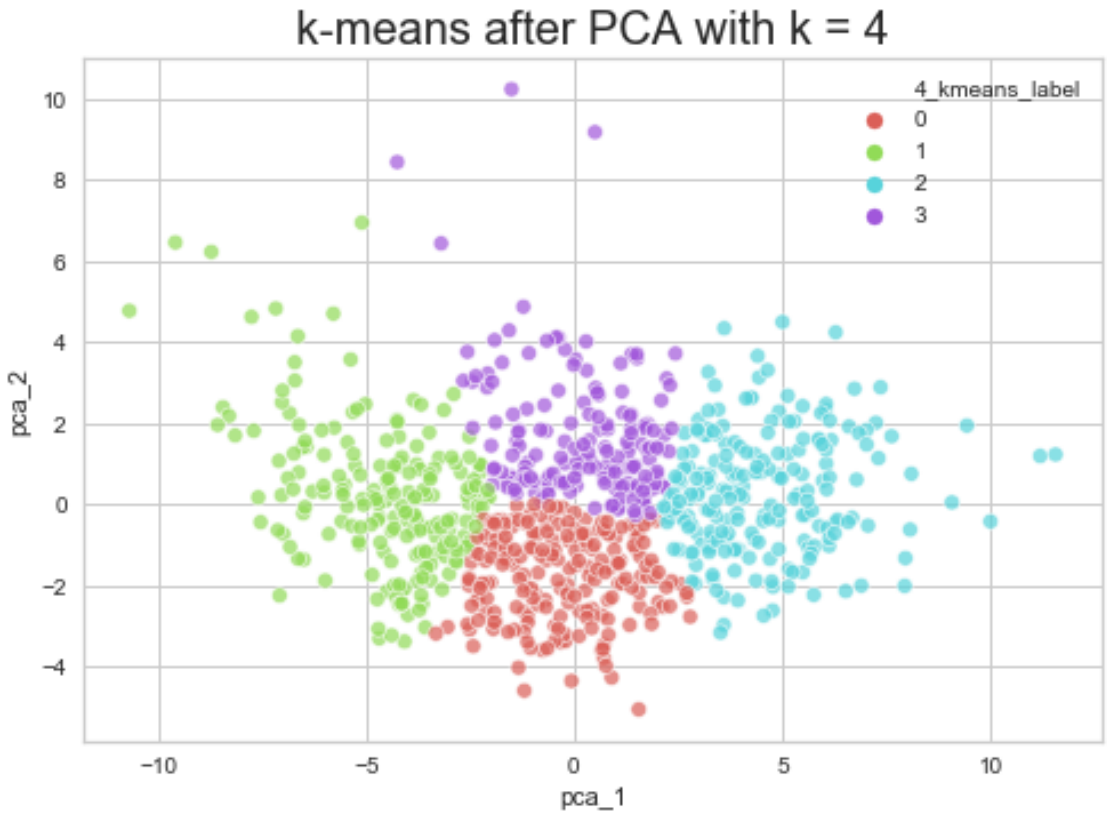
[18]:
```
sns.scatterplot(x='pca_1', y='pca_2', palette=sns.color_palette("hls", 3),data␣
↪= pca_analysis, hue = '3_kmeans_label',
                legend="full",alpha = 0.7)
plt.title('k-means after PCA with k = 3', size = 20)
```

[18]:
```
Text(0.5, 1.0, 'k-means after PCA with k = 3')
```



[19]:
```
sns.scatterplot(x='pca_1', y='pca_2', palette=sns.color_palette("hls", 4),data␣
↪= pca_analysis, hue = '4_kmeans_label',
                legend="full",alpha = 0.7)
plt.title('k-means after PCA with k = 4', size = 20)
```

[19]:
```
Text(0.5, 1.0, 'k-means after PCA with k = 4')
```

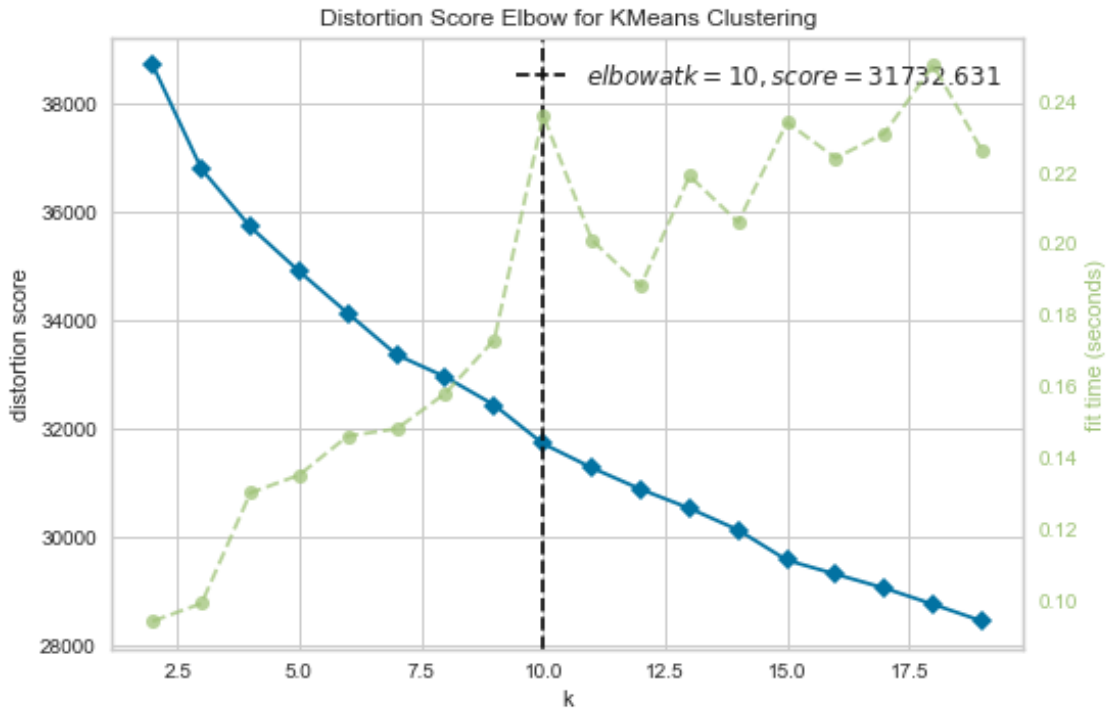


According to the above plots, we can see that using the dimension reduction method of PCA, the clustered groups are very closed to one another, and in some regions they overlap.In addition, we can see that many plots also overlap with other plots. This may give us some hints that we may try another non-linear dimension reduction method.

2.2.2 10

The elbow method

[20]:
```
kelbow_visualizer(KMeans(random_state=20), wiki_std, k=(2,20), locate_elbow =␣
↪True)
```



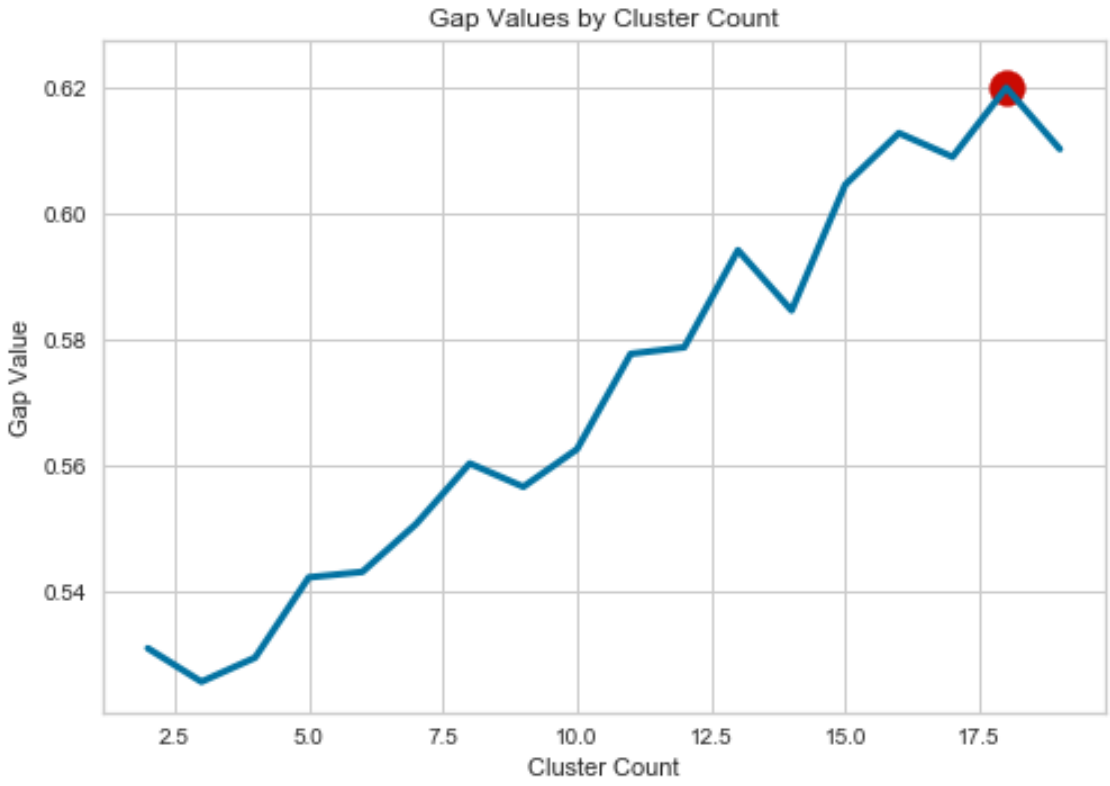
[20]:
```
KElbowVisualizer(ax=<matplotlib.axes._subplots.AxesSubplot object at
0x0000020DF2DB2308>,
                 k=None, locate_elbow=True, metric='distortion', model=None,
                 timings=True)
```

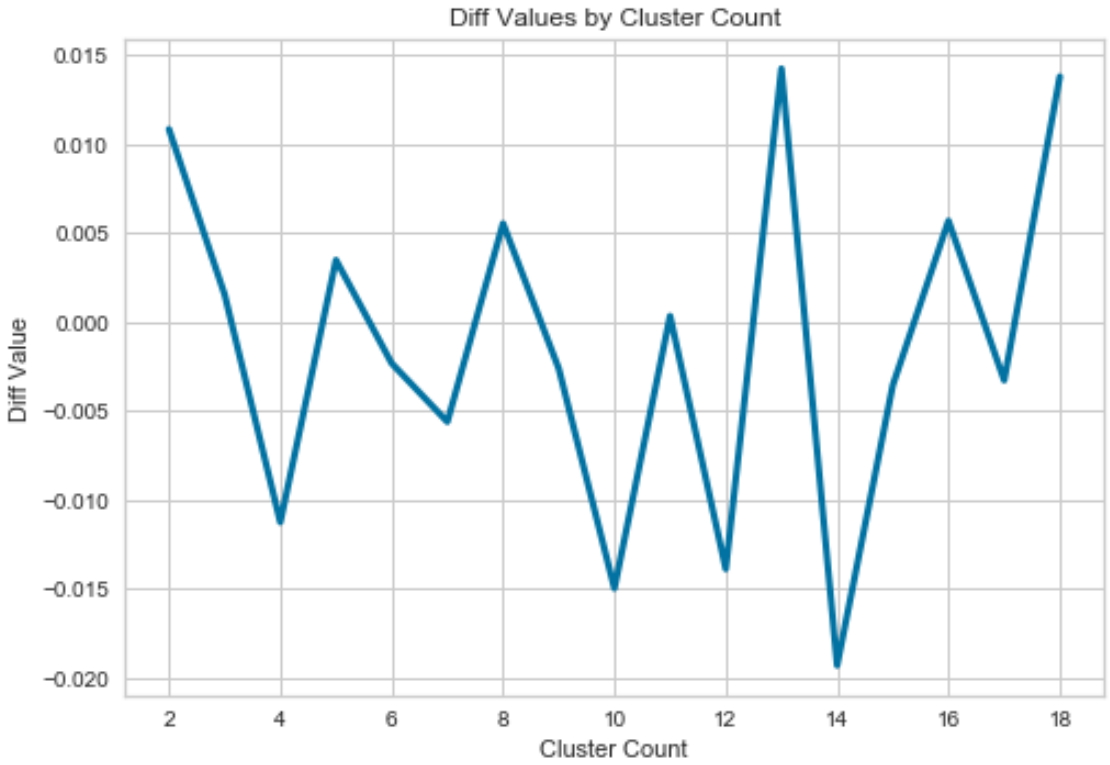
According to the above plot, the optimal k value is 10 if we use the elbow method as the selection standard.

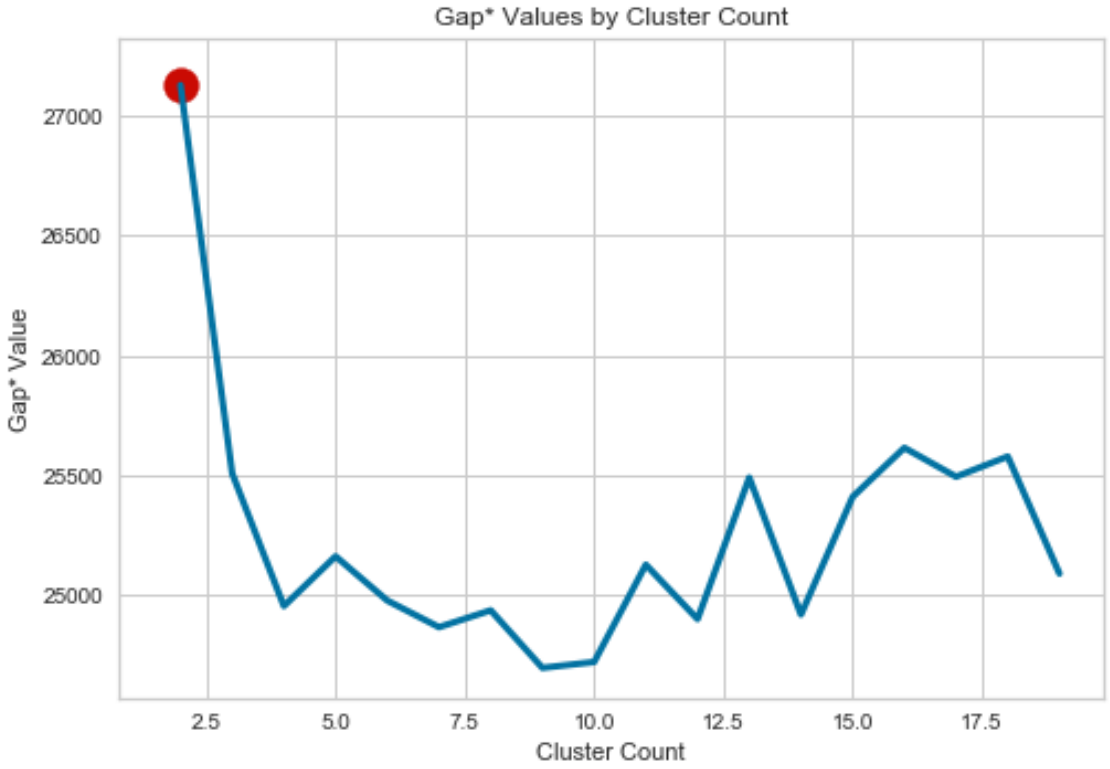
Gap statistic

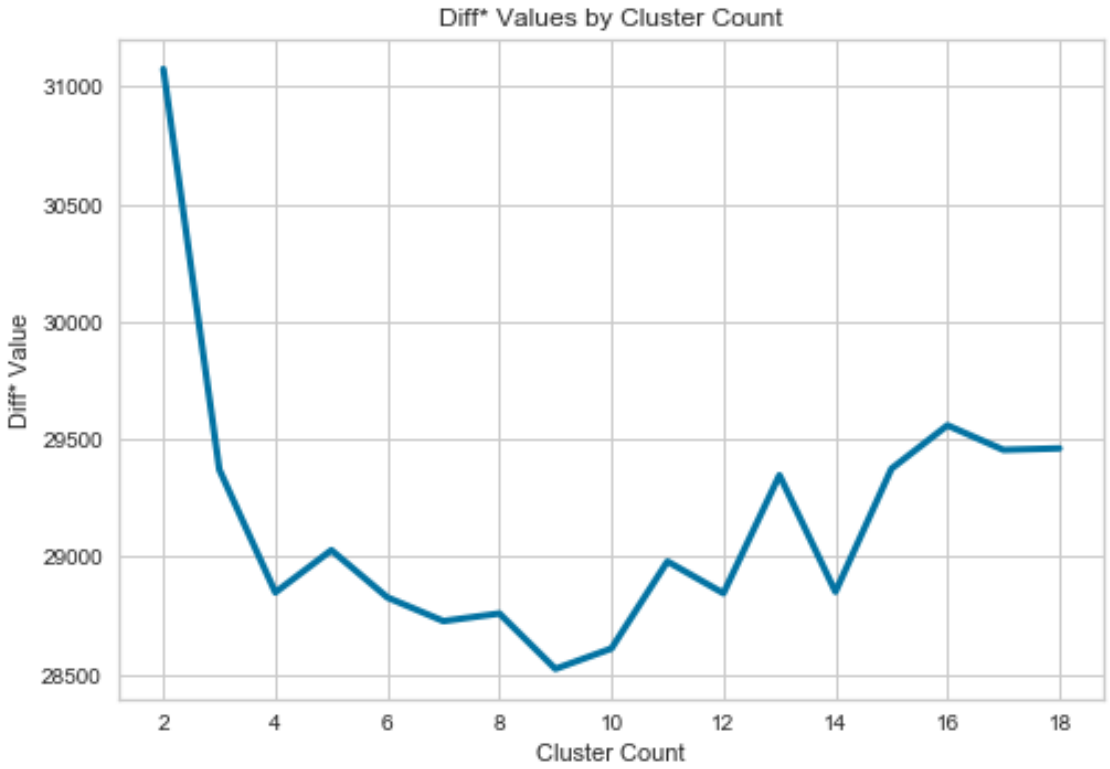
[21]:
```
np.random.seed(124)
opt = optimalK.OptimalK()
k_gap = opt(wiki_std, cluster_array=np.arange(2, 20))
print("According to the above plot, the optimal k value is ", k_gap, " if we␣
 ↪use gap statistic as the selection standard.")
opt.plot_results()
```

```
According to the above plot, the optimal k value is  18  if we use gap statistic
as the selection standard.
```


Gap Values by Cluster Count
Gap Value
0.62
0.60
0.58
0.56
0.54
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Cluster Count

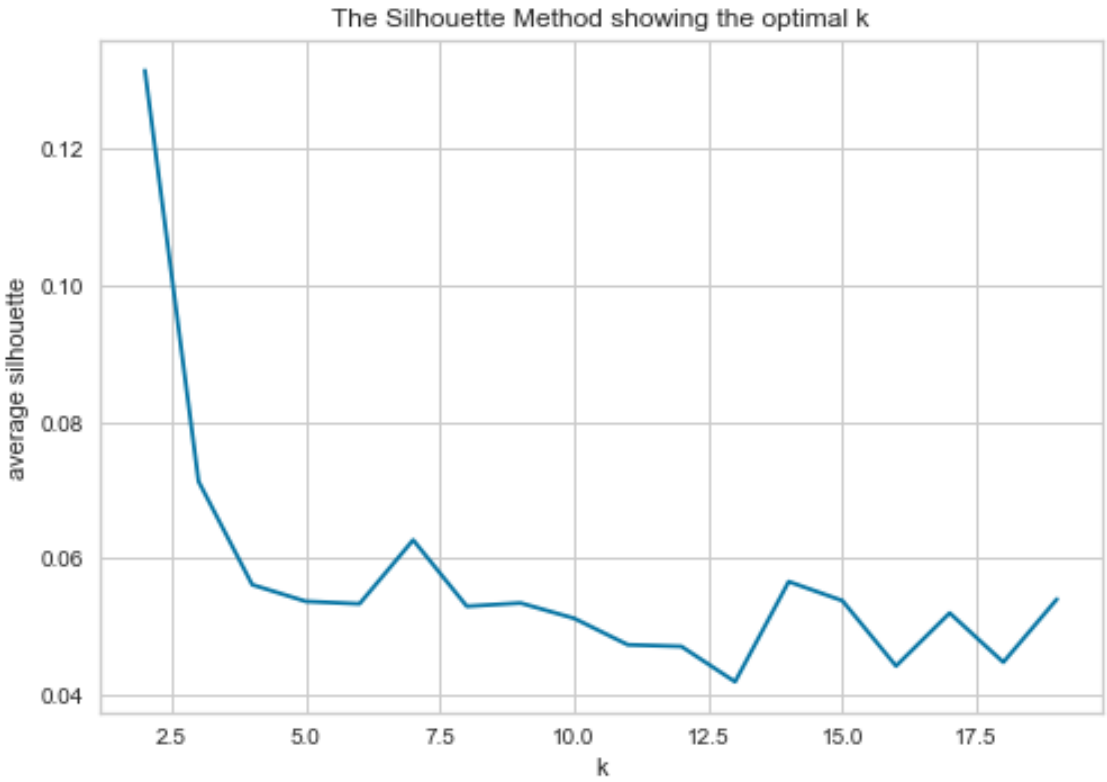

Diff Values by Cluster Count
Diff Value
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
2
4
6
8
10
12
14
16
18
Cluster Count


Gap* Values by Cluster Count
27000
26500
26000
25500
25000
Gap* Value
2.5
5.0
7.5
10.0
12.5
15.0
17.5
Cluster Count



Average silhouette

[22]:
```
avg_sil = {}
K = range(2, 20)
for k in K:
    model = KMeans(n_clusters=k, random_state=20)
    preds = model.fit_predict(wiki_std)
    score = silhouette_score(wiki_std, preds, metric = 'euclidean')
    avg_sil[k] = score
avg_sil_values = list(avg_sil.values())
plt.plot(K, avg_sil_values, 'bx-')
plt.xlabel('k')
plt.ylabel('average silhouette')
plt.title('The Silhouette Method showing the optimal k')
plt.show()
```



Since we get two different optimal k values from the two methods (the elbow method and gap statistic), we use average silhouette to pick one of them. Average silhouette measures the compactness of data after clustering. We want to pick the optimal value with higher average silhouette score. If they have the same scores, we prefer the smaller one.

[23]:
```
if avg_sil[10] >= avg_sil[k_gap]:
    chosen_k = 10
else:
    chosen_k = k_gap
print("According to the above standards, we set the value of optimal k as ",␣
 ↪chosen_k)
```

```
According to the above standards, we set the value of optimal k as  10
```

2.2.3 11

PCA and k-means

[24]:
```
best_wiki = KMeans(n_clusters=chosen_k, random_state=20).fit(wiki_transformed)
best_wiki.cluster_centers_

pca_analysis_best = wiki_transformed.copy()
pca_analysis_best['best_kmeans_label'] = best_wiki.labels_
```

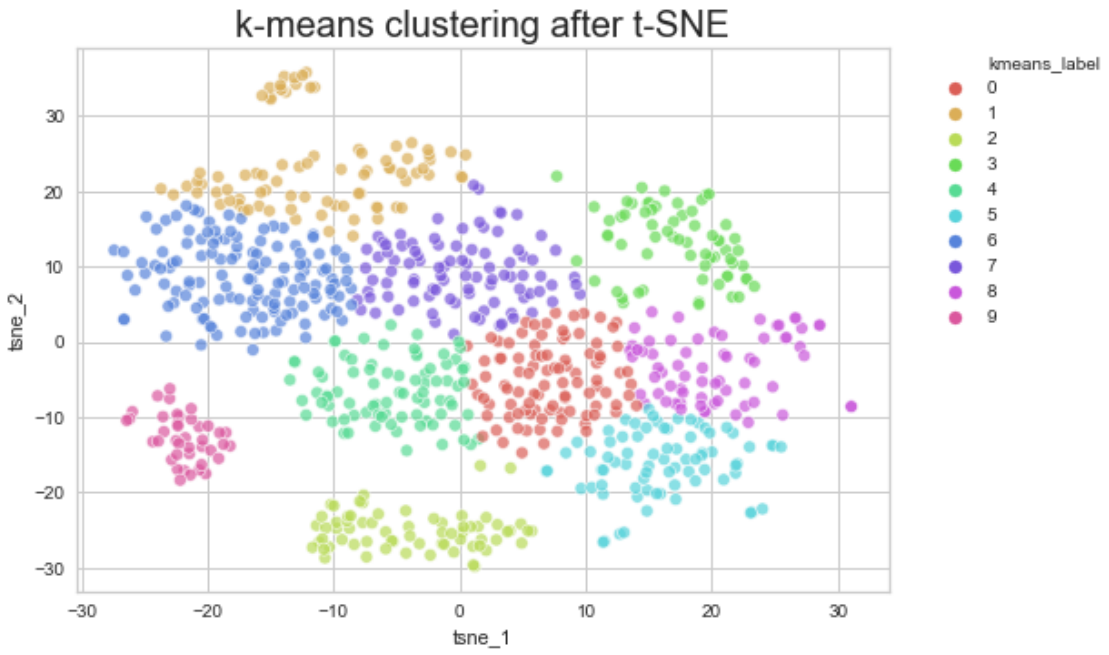
```
sns.scatterplot(x='pca_1', y='pca_2', palette=sns.color_palette("hls",␣
↪chosen_k), data=pca_analysis_best,
                hue = 'best_kmeans_label', legend="full", alpha = 0.7)
plt.title("k-means clustering after PCA", size = 20)
plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0.)
```

[24]: <matplotlib.legend.Legend at 0x20df4e0dd08>

t-SNE and k-means

[25]:
```
best_tsne = TSNE(n_components=2)
tsned_wiki = best_tsne.fit_transform(wiki_std)
tsned_wiki = pd.DataFrame(tsned_wiki)
tsned_wiki = tsned_wiki.rename(columns = {0:'tsne_1', 1:'tsne_2'})
final_wiki = KMeans(n_clusters=chosen_k, random_state=20).fit(tsned_wiki)
final_tsne_ks = tsned_wiki.copy()
final_tsne_ks['kmeans_label'] = final_wiki.labels_

sns.scatterplot(x='tsne_1', y='tsne_2',palette=sns.color_palette("hls",␣
↪chosen_k), data = final_tsne_ks,
                hue = 'kmeans_label', legend="full", alpha = 0.7)
plt.title("k-means clustering after t-SNE", size = 20)
plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0.)
```

[25]: <matplotlib.legend.Legend at 0x20df4e35988>



The good thing is that both the clusterings after PCA and t-SNE do not have much overlapped boundaries. According to the above plots, we can see that the clustering after t-SNE has clearer boundaries. In other words, the groups are more clearly presented in the clustering after t-SNE. However, we can find that t-SNE costs more time than PCA.Besides, in terms of data with high dimensions, PCA will place observations in very near locations, while t-SNE can tackle this problem. t-SNE is more capable of setting observations apart.