MAT 280: Assignment #3

Due on Monday, May 16, 2016

Prof. Thomas Strohmer MF 13:30 - 15:00

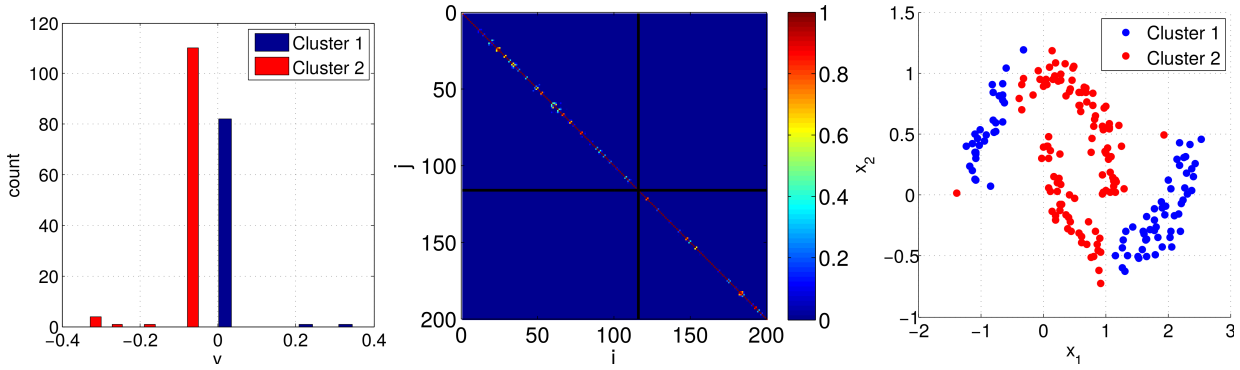
Wenhao Wu

Contents

Problem 1

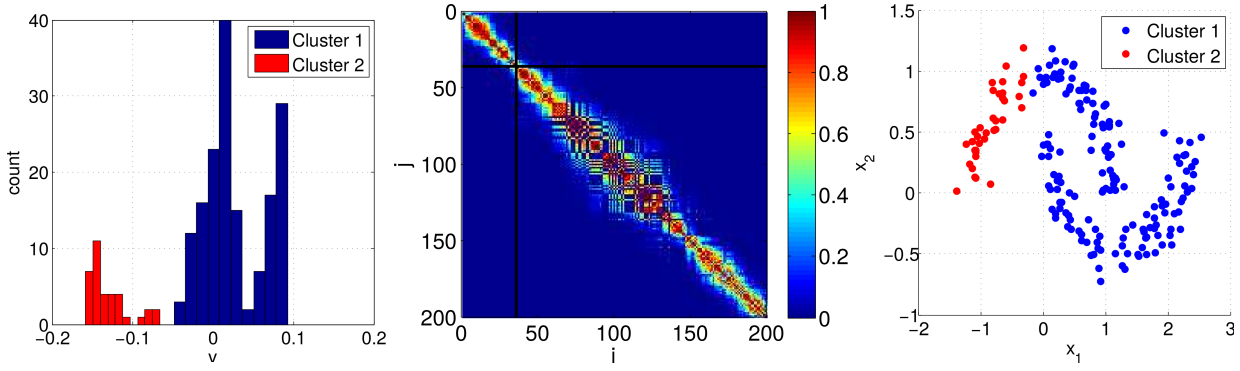
Download the dataset `crescents.mat` from the Class website and load it into Matlab. It contains two-hundred points in two dimensions. If you plot it, you see that the data form two half-moon-like clusters. Clearly, k-means directly applied to this dataset will fail to cluster the data according to these two shapes. Use the graph Laplacian or diffusion maps (followed by k-means) to try to cluster the data as good as possible according to the half-moon shapes. You can use Matlabs k-means function to do the actual clustering once you transformed the data.

Answer: We tried to cluster the data using graph Laplacian where the weighted adjacency matrix $\mathbf{W}$ is evaluated with $\epsilon = 0.001$, 0.01 and 0.1, respectively. When $\epsilon = 0.001$ (Fig. 1), spectral clustering fails as the entries of the second eigenvector of $\mathbf{L}$ concentrates around 0. This is because ϵ is so small that almost no two points are considered to be close to each other. On the other hand, when $\epsilon = 0.1$ (Fig. 2), the spectral clustering fails again since for large ϵ the points that are rather far apart are still considered as neighbors. When $\epsilon = 0.01$ (Fig. 3), we can see that the points within each "arc" are close to one another while the points from the two different "arcs" are far apart. As a result, $\mathbf{v}_2$ concentrates into two spikes and the two "arcs" are clearly separated by k-means algorithm.



(a) Histogram of $\mathbf{v}_2$. (b) $\mathbf{W}$ ordered and clustered. (c) Clustering.

Figure 1: Clustering result for $\epsilon = 0.001$.

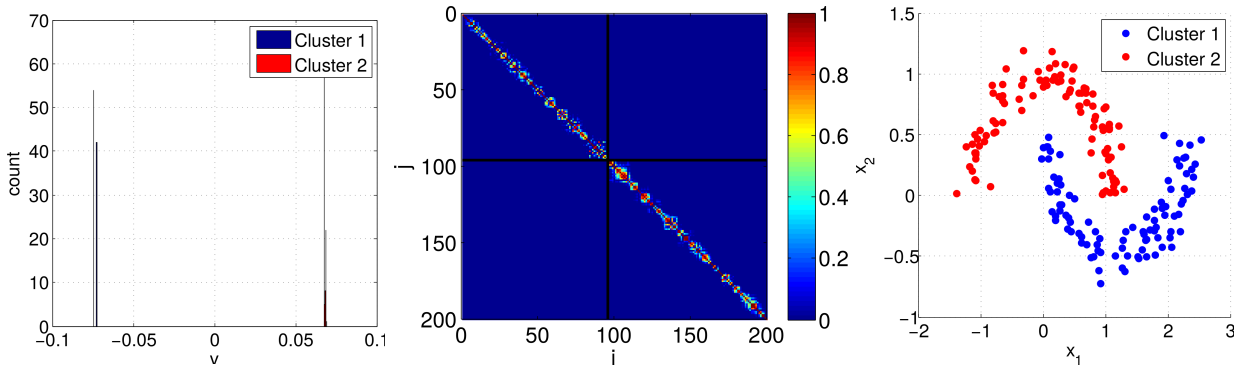


(a) Histogram of $\mathbf{v}_2$. (b) $\mathbf{W}$ ordered and clustered. (c) Clustering.

Figure 2: Clustering result for $\epsilon = 0.1$.

Source code:

Problem 1 continued on next page...



(a) Histogram of $\mathbf{v}_2$. (b) $\mathbf{W}$ ordered and clustered. (c) Clustering.

Figure 3: Clustering result for $\epsilon = 0.01$.

```
clear all;
close all;
clc;

load('crescents.mat');
[p, n] = size(x);
% figure;
% scatter(x(1,:), x(2, :))

epsilon = 0.01;
W = exp(-pdist2(x', x') .^ 2 / epsilon);

L = diag(sum(W)) - W;
[V, D] = eig(L);
v = real(V(:, 2));
idx = kmeans(v, 2);

figure;
scatter(x(1, idx == 1), x(2, idx == 1), [], 'MarkerEdgeColor', 'b', '
    ↪ MarkerFaceColor', 'b'), hold on;
scatter(x(1, idx == 2), x(2, idx == 2), [], 'MarkerEdgeColor', 'r', '
    ↪ MarkerFaceColor', 'r');
xlabel('x_1', 'fontsize', 16), ylabel('x_2', 'fontsize', 16);
legend('Cluster␣1', 'Cluster␣2')
set(gca, 'fontsize', 16);
grid on;

figure;
[n1,v1] = hist(v(idx == 1));
[n2,v2] = hist(v(idx == 2));
bar(v1, n1, 'hist')
hold on;
h = bar(v2, n2, 'hist'); hold off
set(h,'facecolor','r');
```

```
legend('Cluster 1', 'Cluster 2');
xlabel('v', 'fontsize', 16), ylabel('count', 'fontsize', 16);
set(gca, 'fontsize', 16);
grid on;

[~, idx_sort] = sort(v);
figure;
imagesc(W(idx_sort, idx_sort)), hold on;
if idx(idx_sort(1)) == 1
    n_cluster1 = sum(idx == 1);
else
    n_cluster1 = sum(idx == 2);
end

plot(n_cluster1 * ones(1, n), 1 : n, 'k', 'linewidth', 2);
plot(1 : n, n_cluster1 * ones(1, n), 'k', 'linewidth', 2);
colorbar;
axis equal
set(gca, 'fontsize', 16);
xlim([0, 200]), ylim([0, 200]);
xlabel('i', 'fontsize', 16), ylabel('j', 'fontsize', 16);
```

Problem 2

Download the dataset `genomedata.mat` from the Class website; it contains Single Nucleid Polymorphisms data from the Human Genome Diversity Project. The data consists of an array consisting of 5000 rows, each row has 1043 different strings. The 5000 rows are Single Nucleid Polymorphisms, the columns correspond to 1043 different individuals. The entries are not numerical values (quite annoyingly), but contain the characters 'AA', 'CC', 'GG', 'TT', 'AG', 'AC', 'TC', 'TG', and (even more annoyingly) also '–', the latter represents missing measurements. Your goal is to cluster the data into a small set of clusters. After loading the file into Matlab, you need to convert the characters into numerical values. It is up to you which conversion you use (you can use the file `gen2vec.m` to do the actual conversion, once you have chosen a conversion rule). Since the data are high-dimensional you first need to reduce the dimension before clustering. You should attempt the dimension reduction via PCA as well as via diffusion maps. In both cases you need to decide how many dimensions you want to use. Also, in both cases you may want to use Matlabs k-means function to do the actual clustering after dimension reduction.
Note: Your results may differ from mine, because you will likely choose a different conversion rule. I did not get a meaningful clustering via PCA, but did achieve reasonable clustering via diffusion maps.

Answer: To cast the 9 possible character pairs into numerical values, we design the mapping on to the complex plane as shown in Fig. 4, which has the following desirable (heuristically) properties:

- The "hybrid" character pairs are close to their parental "pure" character pairs.
- The mappings are highly symmetric.
- '–' is not biased towards any non-empty character pair.

To determine the number of clusters for k-means algorithm, the number of clusters k is determined with Gap statistic [1, 2], which selects $\hat{k}$ as the smallest k producing a gap within one standard deviation of the gap at $k+1$.

Problem 2 continued on next page...

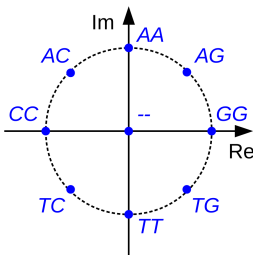


Figure 4: Mapping the characters into numerical values (complex-valued).

The dimension reduction and clustering results given by PCA are shown in Fig. 5. As we can see, although the dimension of the data is high, there are only few large singular values (a). We select the first two principle components (complex-valued) and try to cluster them into 2 groups. The distributions of the real and imaginery parts for the 2 clusters are shown in (c) which is not ideal. In (b) we can see that none of the $k \in [1, 10]$ satisfies the Gap statistic criterion, suggesting that PCA fails to provide a meaningful input to k-means.

For diffusion maps we set the time scale $t = 20$ and ϵ to be 1/10 of the median of $\|\mathbf{x}_i - \mathbf{x}_j\|_2^2$. We reduce the dimension of the original data down to 3 so that a visualization is possible. As shown in Fig. 6, based on the Gap statistic, the data should be clustered into 2 groups. And from the 3-D visualization and the scatter plot, the clustering is rather clear based solely on the first dimension.

We also tried to cluster this data set with spectral clustering (unnormalized), which is closely related to diffusion maps. The results are shown in Fig. 7. The Gap statistic suggest that $k = 5$, though most data concentrates on two "spikes" as in the diffusion map approach.

Source code:

```
import math
import cmath
import numpy as np
import pandas as pd
from numpy.linalg import svd
from numpy.random import uniform
from scipy import io
from scipy.linalg import eigh
from scipy.spatial.distance import pdist, squareform
from sklearn.cluster import KMeans

import matplotlib as mpl
import matplotlib.pyplot as plt
from mpl_toolkits.axes_grid1.inset_locator import inset_axes
from mpl_toolkits.axes_grid1.inset_locator import mark_inset
from mpl_toolkits.mplot3d import Axes3D
import seaborn as sns

%matplotlib qt
sns.set()
axis_font = {'size':'16'}
mpl.rcParams['xtick.labelsize'] = 16
mpl.rcParams['ytick.labelsize'] = 16
```

```
data = io.loadmat('genomedata.mat')
map_gen = {'AA': complex(0.0, 1.0),
           'CC': complex(-1.0, 0.0),
           'GG': complex(1.0, 0.0),
           'TT': complex(0.0, -1.0),
           'AG': complex(1.0 / math.sqrt(2), 1.0 / math.sqrt(2)),
           'AC': complex(-1.0 / math.sqrt(2), 1.0 / math.sqrt(2)),
           'TC': complex(-1.0 / math.sqrt(2), -1.0 / math.sqrt(2)),
           'TG': complex(1.0 / math.sqrt(2), -1.0 / math.sqrt(2)),
           '--': complex(0.0, 0.0)}

X_raw = [[string.strip() for string in row[0][0].strip().split('\t')] for
    ↪ row in data['X']]
X = np.array([[map_gen[string] for string in row] for row in X_raw])
n, p = X.shape
X = X - np.mean(X, axis=0) * np.ones(p)

random_state = 8 # The random state used by the KMeans

# The function to evaluate the gap statistic for k-means with different
    ↪ number of clusters
def get_gapstat(X, k_range=np.arange(1, 9), n_sample=20, random_state=8):
    n, p = X.shape

    X_ref = np.empty((n, p, n_sample), dtype='float64')
    for col in range(p):
        X_ref[:, col, :] = uniform(low=X[:, col].min(), high=X[:, col].max
            ↪ (), size=(n, n_sample))

    gapstat = np.empty((n_sample, len(k_range)), dtype='float64')
    for i_k, k in enumerate(k_range):
        km = KMeans(n_clusters=k, random_state=random_state)

        # The inertia of the actual data
        km.fit(X)
        w = km.inertia_

        # The inertia of the reference data
        w_ref = np.empty(n_sample, dtype='float64')
        for i_sample in range(n_sample):
            km.fit(X_ref[:, :, i_sample])
            w_ref[i_sample] = km.inertia_

        gapstat[:, i_k] = np.log(w_ref) - np.log(w)

    return gapstat

k_range = np.arange(1, 9)
n_sample = 20
```

Problem 2 continued on next page...

```
d_pca = 2 # For PCA we reduce the dimension of X down to 3
k_pca = 2 # The expected number of clusters for PCA

_, s_pca, V_pca = svd(X) # svd of X. Note that this is different from
    ↪ matlab in that X = U diag(s) V.
V_pca = np.conjugate(V_pca.T)

X_pca_complex = np.dot(X, V_pca[:, 0 : d_pca]) # Reduce the dimension of X
    ↪  by linear projection, a complex matrix

# Since KMeans does not seem to support complex value, expand the space to
    ↪  2*d_pca dim
X_pca = np.empty((n, 2 * d_pca), dtype="float64")
X_pca[:, 0::2] = X_pca_complex.real
X_pca[:, 1::2] = X_pca_complex.imag

label_pca = KMeans(n_clusters=2, random_state=random_state).fit_predict(
    ↪ X_pca)
gap_pca = get_gapstat(X_pca, k_range=k_range, n_sample=n_sample)

# Distribution of the sinular values
fig, ax = plt.subplots(figsize=(7, 6))
axins = inset_axes(ax, 2, 3, loc=1) # zoom-factor: 2.5, location: upper-
    ↪ left

ax.semilogy(np.arange(p), s_pca, linewidth=2)
ax.grid(True)
ax.set_xlabel('dimension', **axis_font)
ax.set_ylabel('singular value', **axis_font)

axins.semilogy(np.arange(p), s_pca, linewidth=2)
axins.grid(True)
x1, x2, y1, y2 = 0, 20, 50, 2000 # specify the limits
axins.set_xlim(x1, x2) # apply the x-limits
axins.set_ylim(y1, y2) # apply the y-limits
axins.set_xticks(np.arange(0, 20, 5))
mark_inset(ax, axins, loc1=2, loc2=3, fc="none", ec="0.5", lw=2)

fig.savefig('pca_singular.pdf', dpi=10)

# Scatterplot matrix
df_pca = pd.DataFrame({**{'cluster': label_pca}, **{col+1: X_pca[:, col]
    ↪ for col in range(2 * d_pca)}})
sns.pairplot(df_pca, hue='cluster', vars=np.arange(1, 1 + 2 * d_pca))
plt.savefig('pca_scatter.pdf', dpi=10)

# Gap statistics
fig, ax = plt.subplots(figsize=(7, 6))
```

Problem 2 continued on next page...

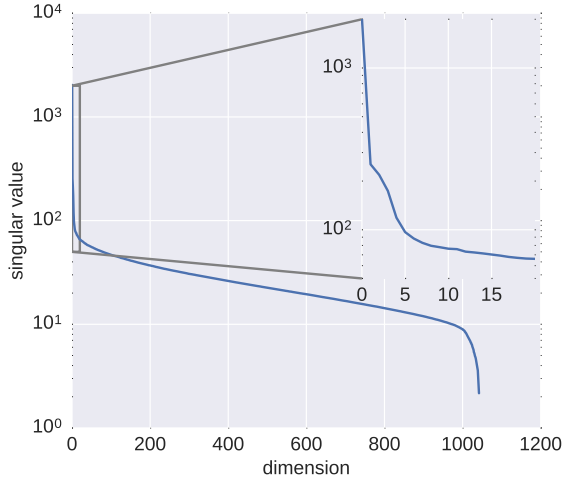
```
ax.errorbar(k_range, np.mean(gap_pca, axis=0), yerr=np.sqrt(1+1/n_sample)*
    ↪ np.std(gap_pca, axis=0))
ax.grid(True)
ax.set_xlabel('$k$', **axis_font)
ax.set_ylabel('Gap', **axis_font)
fig.savefig('pca_gap.pdf', dpi=10)

d_dif = 3 # For PCA we reduce the dimension of X down to 3 for 3-D
    ↪ visualization
k_dif = 2 # The expected number of clusters for diffusion map
t_dif = 20 # The time scale for diffusion map
f = 10 # The factor used to set epsilon according to the median of the
    ↪ square pairwise Euclidean distance

distance = pdist(np.concatenate((X.real, X.imag), axis=1), 'euclidean');
epsilon = np.median(distance ** 2) / f;
W = np.exp(-squareform(distance) ** 2 / epsilon)
D_inv_sqrt = np.diag(1 / np.sqrt(np.sum(W, axis=1)))
MS = np.dot(np.dot(D_inv_sqrt, W), D_inv_sqrt) # The symmetric M matrix

l_dif, V_dif = eigh(MS, eigvals=(n-d_dif-1, n-2)) # Remember to ignore the
    ↪  largest eigen vector
l_dif, V_dif = l_dif[::-1], V_dif[:, ::-1] # The eigen value are now in
    ↪ descending order.

X_dif = np.dot(np.dot(D_inv_sqrt, V_dif), np.diag(l_dif ** t_dif)) # The
    ↪ redued dimension map at time t

label_dif = KMeans(n_clusters=k_dif, random_state=random_state).
    ↪ fit_predict(X_dif)
gap_dif = get_gapstat(X_dif, k_range=k_range, n_sample=n_sample)

df_dif = pd.DataFrame({**{'cluster': label_dif}, **{col+1: 1000*X_dif[:,
    ↪ col] for col in range(d_dif)}})
plot_scatterplot = sns.pairplot(df_dif, hue='cluster', vars=np.arange(1, 1
    ↪  + d_dif))
plt.savefig('dif_scatter.pdf', dpi=10)

fig = plt.figure(1, figsize=(7, 6))
plt.clf()
ax = Axes3D(fig, rect=[0, 0, .95, 1], elev=48, azim=134)
plt.cla()

y = np.choose(label_dif, ['b', 'g'])
ax.scatter(1000*X_dif[:, 0], 1000*X_dif[:, 1], 1000*X_dif[:, 2], c=y)
ax.set_xlabel('1', **axis_font)
ax.set_ylabel('2', **axis_font)
ax.set_zlabel('3', **axis_font)
fig.savefig('dif_3d.pdf', dpi=10)
```

```
# Gap statistics
fig, ax = plt.subplots(figsize=(7, 6))
ax.errorbar(k_range, np.mean(gap_dif, axis=0), yerr=np.sqrt(1+1/n_sample)*
    ↪ np.std(gap_dif, axis=0))
ax.grid(True)
ax.set_xlabel('$k$', **axis_font)
ax.set_ylabel('Gap', **axis_font)

fig.savefig('dif_gap.pdf', dpi=10)

k_spec = 5 # The expected number of clusters for spectral clustering

L = np.diag(sum(W)) - W
_, V_spec = eigh(L)
X_spec = V_spec[:, 1:2] # The reduced dimension data, simply the second
    ↪ smallest eigen vector of L
label_spec = KMeans(n_clusters=k_spec, random_state=random_state).
    ↪ fit_predict(X_spec)
gap_spec = get_gapstat(X_spec, k_range=k_range, n_sample=n_sample)

fig, ax = plt.subplots(figsize=(7, 6))

c = ['b', 'g', 'r', 'purple', 'orange']
for k in range(k_spec):
    ax.hist(X_spec[label_spec==k, 0], 20, facecolor=c[k], alpha=0.75,
        ↪ label='cluster␣{0}'.format(k))
ax.legend(loc=1, fontsize=16)
ax.set_xlabel('$v$', **axis_font)
ax.set_ylabel('count', **axis_font)
fig.savefig('spec_hist.pdf', dpi=10)

# Gap statistics
fig, ax = plt.subplots(figsize=(7, 6))
ax.errorbar(k_range, np.mean(gap_spec, axis=0), yerr=np.sqrt(1+1/n_sample)
    ↪  * np.std(gap_spec, axis=0))
ax.grid(True)
ax.set_xlabel('$k$', **axis_font)
ax.set_ylabel('Gap', **axis_font)
fig.savefig('spec_gap.pdf', dpi=10)
```

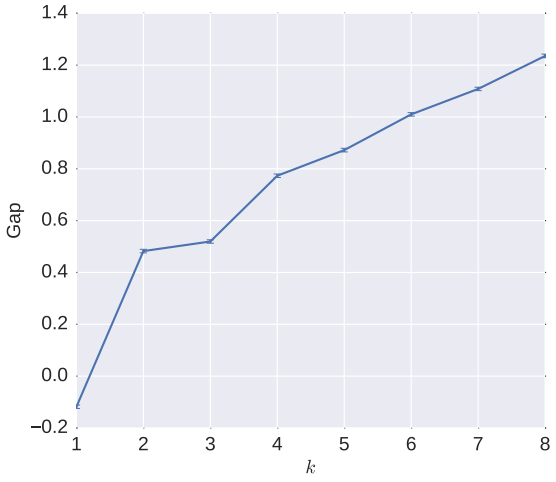
References

[1] Robert Tibshirani, Guenther Walther, and Trevor Hastie. Estimating the number of clusters in a data set via the gap statistic. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63(2):411–423, 2001.

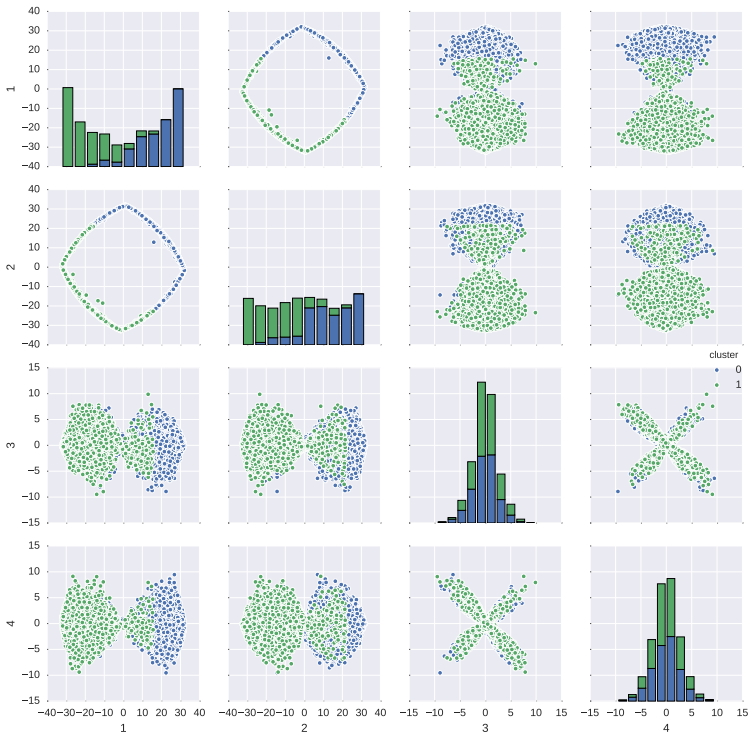
[2] Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. *The elements of statistical learning: data mining, inference and prediction.* Springer, second edition, 2008.



(a) Distribution of λ.

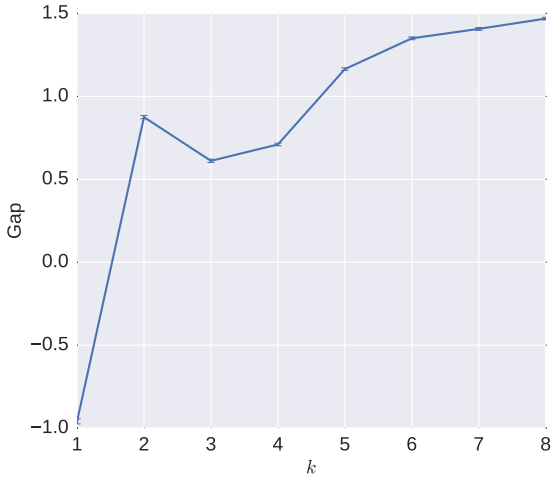


(b) Gap statistic.

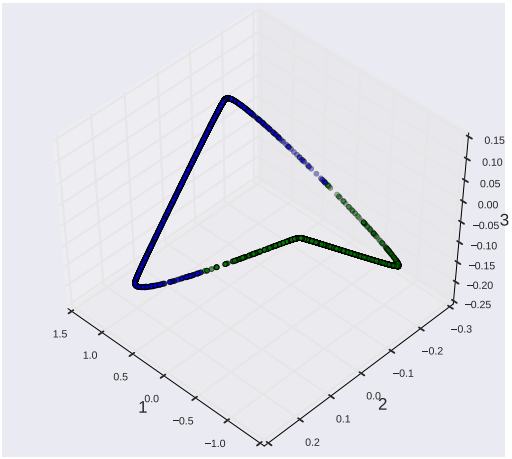


(c) Scatter plot of the real and imaginery part of the first 2 principle components.

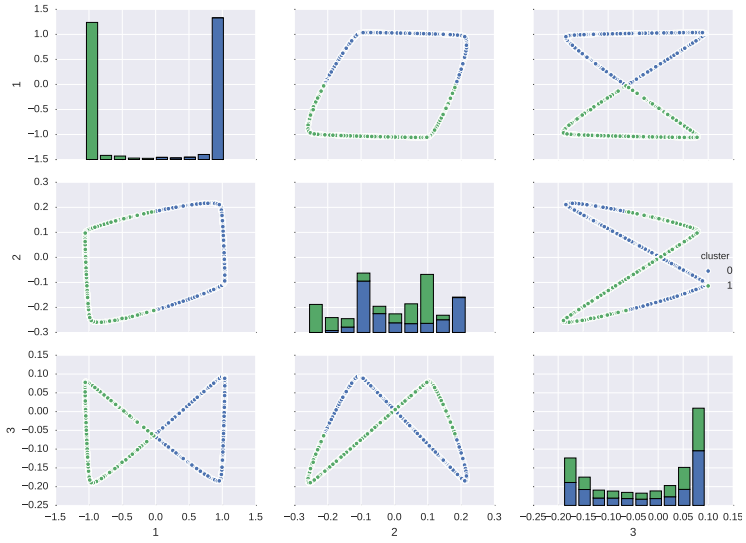
Figure 5: Dimension reduction and clustering by PCA.



(a) Gap statistic.

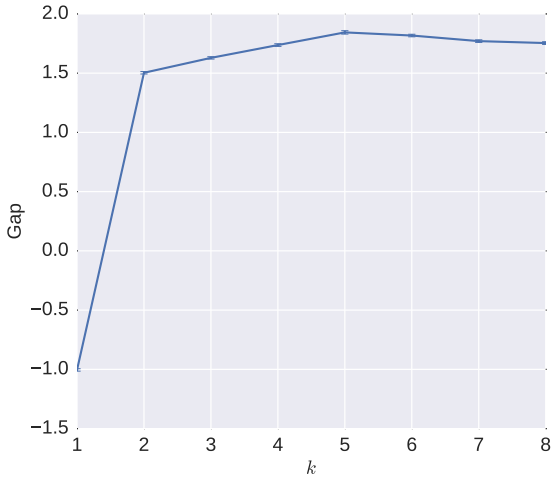


(b) 3-D visualization of the clustering.

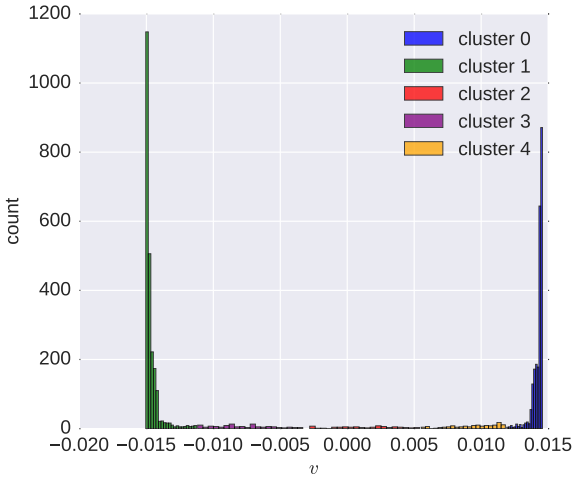


(c) Scatter plot of the reduced dimension data.

Figure 6: Dimension reduction and clustering by diffusion maps.



(a) Gap statistic.



(b) Histogram of the second eigenvector of $\mathbf{L}$.

Figure 7: Dimension reduction and clustering by spectral method.