IE 529 Fall 2016 Computational Assignment 2

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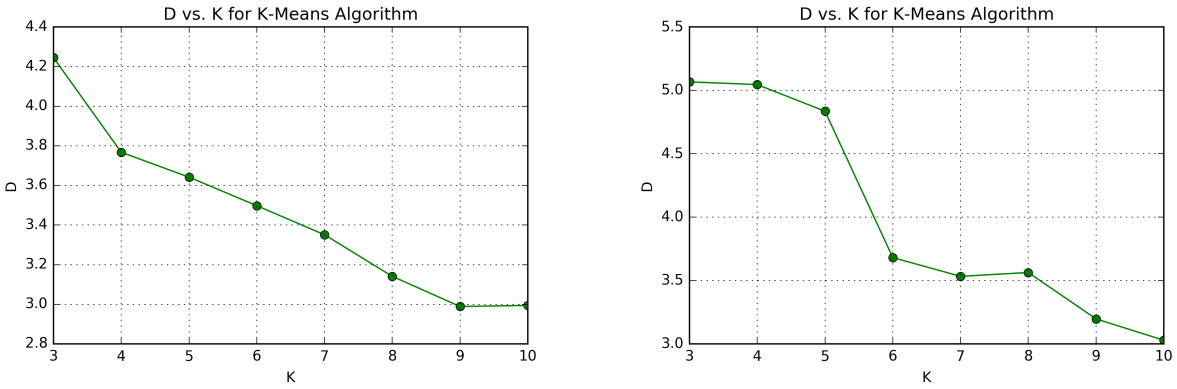
I. Lloyd's (K-means)Algorithm

1. In this part, the polynomial regression is conducted on the given dataset. The derivation is relatively simple, here we only give one simple version.



(a) clustering.txt (b) bigClusteringData.txt

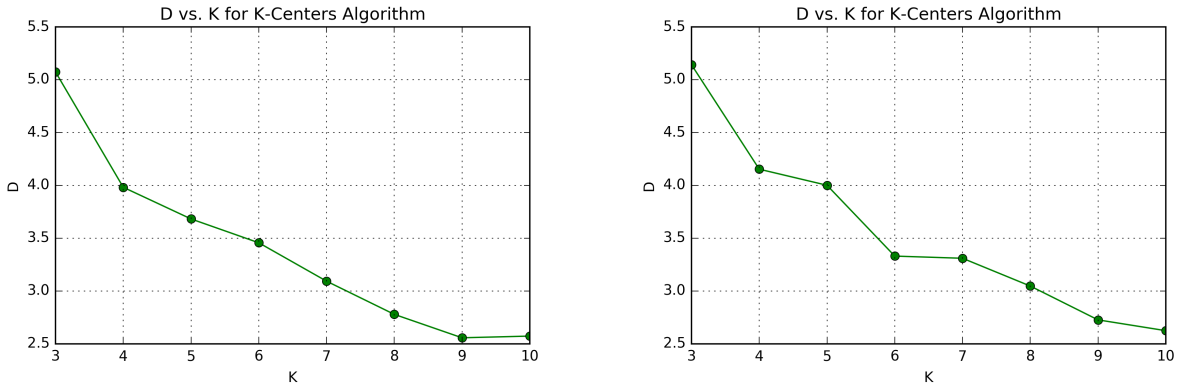
Figure 3: Change of Distoration versus Cluster Number K for K-Means Algorithm

```python
import numpy as np
import time

def kMeans(X, K, tol=0.00001, random_state=None, verbose=True):
    """ function to implement the Lloyd's algorithm for k-means problem """
    np.random.seed(random_state)
    t0 = time.time()

    N, d = X.shape  # number of observations and dimensions
    index = np.random.choice(range(N), size=K, replace=False)
    Y = X[index, :]  # initial k centers
    C = np.zeros(N)
    D = 100
    count = 0
    diff = 100  # difference between D1 and D0

    while diff >= tol:
        D0 = D
        for i in range(N):
            # assign centers to ith data
            C[i] = np.argmin(np.sum((Y - X[i, :]) ** 2, axis=1))

        D = 0
        # re-compute the new centers
```

```
        for j in range(K):
            Y[j, :] = np.mean(X[C == j, :], axis=0)

        # compute the loss
        loss = np.zeros((N, K))
        for i in range(K):
            loss[:, i] = np.sqrt(np.sum((X - Y[i, :])**2, axis=1))
        D = np.max(np.min(loss, axis=1))
        diff = abs(D - D0)
        count += 1

    if verbose is True:
        t = np.round(time.time() - t0, 4)
        print('K-Means finished in ' + str(t) + 's, ' + str(count) + ' iters')

    return Y, C, D
```

Listing 1: K-Means Algorithm Python Code

II. Greedy K-centers Algorithm



(a) clustering.txt

(b) bigClusteringData.txt

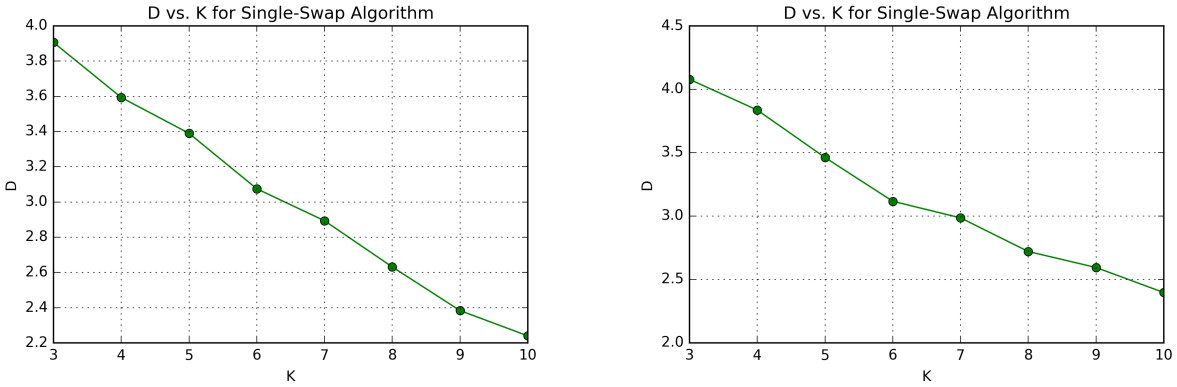
Figure 6: Change of Distoration versus Cluster Number K for K-Center Algorithm

```
import numpy as np
import time

def kCenters(X, K, random_state=None, verbose=True):
    """ function to implement the greedy k-centers algorithm """
    np.random.seed(random_state)
    t0 = time.time()

    N, d = X.shape
    # find the initial center
    index = np.random.choice(range(N), size=1)
    Q = np.zeros((K, d))
    Q[0, :] = X[index, :]
    idx = [index]

    i = 1
```

```
    while i < K:
        distance = np.zeros((N, i))
        for j in range(i):
            distance[:, j] = np.sum((X - Q[j, :])**2, axis=1)
        min_distance = np.min(distance, axis=1)
        new_index = np.argmax(min_distance)
        idx.append(new_index)
        Q[i, :] = X[new_index, :]
        i += 1

    loss = np.zeros((N, K))
    for i in range(K):
        loss[:, i] = np.sqrt(np.sum((X - Q[i, :])**2, axis=1))
    D = np.max(np.min(loss, axis=1))
    C = np.argmin(loss, axis=1)

    if verbose is True:
        t = np.round(time.time() - t0, 4)
        print('K-Centers is finished in ' + str(t) + 's')

    return Q, C, D, idx
```

Listing 2: K-Centers Algorithm Python Code

III. Single-Swap Algorithm



(a) clustering.txt

(b) bigClusteringData.txt

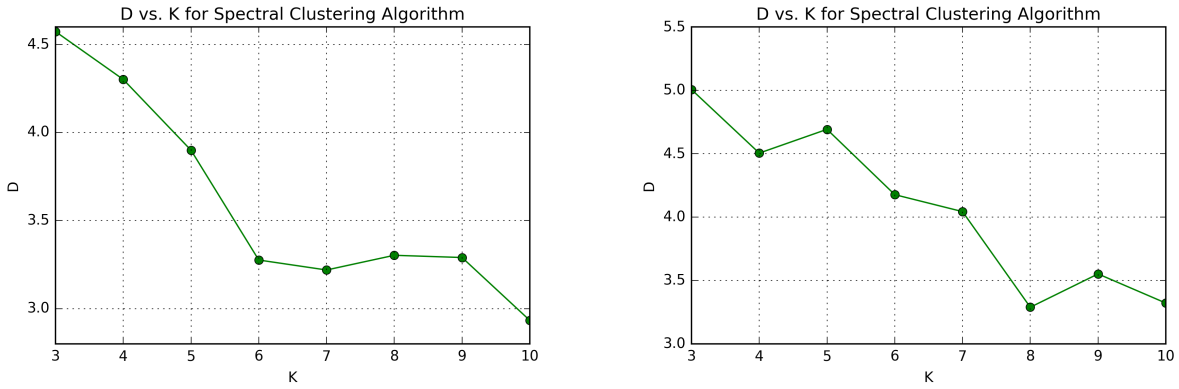
Figure 9: Change of Distoration versus Cluster Number K for Single-Swap Algorithm

```
import numpy as np
import time
from k_centers import kCenters

def singleSwap(X, K, tau=0.05, random_state=None, verbose=True):
    """ function to implement the single-swap for k-centers algorithm """
    t0 = time.time()

    # calculate the initial centers
    Q, _, pre_cost, _ = kCenters(X, K, random_state=random_state,
                                 verbose=False)
    N, d = X.shape
```

```
    # compute the distance based on current centers
    distance = np.zeros((N, K))
    for idx in range(K):
        distance[:, idx] = np.sqrt(np.sum((X - Q[idx, :])**2, axis=1))
    cost = np.max(np.min(distance, axis=1))  # calculate cost

    i = 0
    while i < K:
        if i == 0:
            min_dist = np.min(distance[:, 0:], axis=1)
        elif i == (K - 1):
            min_dist = np.min(distance[:, :-1], axis=1)
        else:
            min_dist = np.minimum(np.min(distance[:, :i], axis=1),
                                  np.min(distance[:, (i + 1):], axis=1))
        swap = False  # keep recording whether or not swaped
        for j in range(N):
            tmp_dist = np.sqrt(np.sum((X - X[j, :])**2, axis=1))
            new_cost = np.max(np.minimum(min_dist, tmp_dist))
            if new_cost / cost < (1 - tau):
                Q[i, :] = X[j, :]
                distance[:, i] = tmp_dist
                swap = True
                cost = new_cost
        i += 1

        if swap is False:
            if i == K - 1:
                break
            else:
                i += 1
        elif (swap is True) and (i == K):
            i = 0

    C = np.argmin(distance, axis=1)

    if verbose is True:
        t = np.round(time.time() - t0, 4)
        print('Single-Swap is finished in ' + str(t) + 's')

    return Q, C, cost
```

Listing 3: Single-Swap Algorithm Python Code

IV. Spectral Clustering Algorithm



(a) clustering.txt

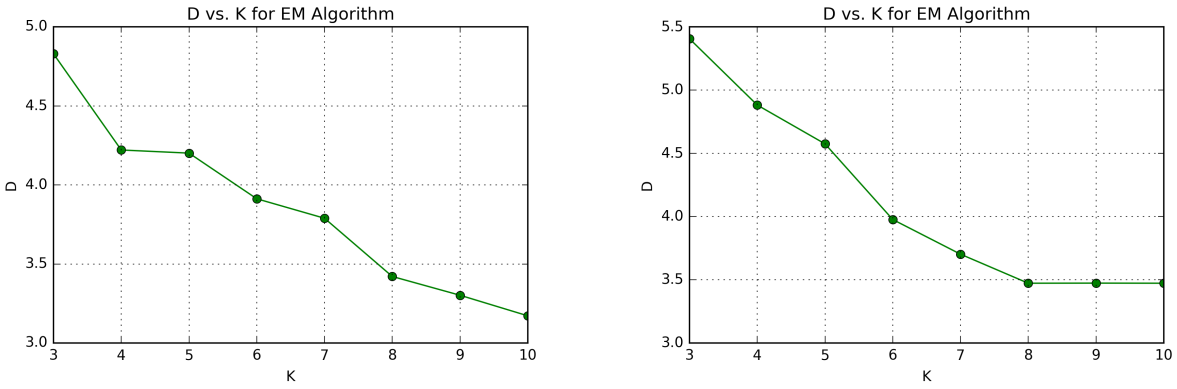
(b) bigClusteringData.txt

Figure 12: Change of Distoration versus Cluster Number K for Spectral Clustering

```python
import numpy as np
import time
from k_centers import kCenters

def spectralClustering(X, K, random_state=None, verbose=True):
    """ function to implement the spectral clustering algorithm """
    t0 = time.time()

    N, d = X.shape
    W = np.zeros((N, N))  # adjacency matrix W
    for i in range(N):
        distance = np.sqrt(np.sum((X - X[i, :])**2, axis=1))
        W[:, i] = distance

    diag = np.sum(W, axis=1)
    D = np.diag(diag)  # diagnoal matrix D
    L = D - W # Laplacian matrix L
    L = np.identity(N) - np.dot(np.linalg.inv(D), W)
    eigvals, U = np.linalg.eigh(L)
    U = U[:, -K:]  # first K eigenvectors

    # call k-means for clustering
    _, C, _, idx = kCenters(U, K, random_state=random_state, verbose=False)

    Q = X[idx, :]
    loss = np.zeros((N, K))
    for i in range(K):
        loss[:, i] = np.sqrt(np.sum((X - Q[i, :])**2, axis=1))
    D = np.max(np.min(loss, axis=1))

    if verbose is True:
        t = np.round(time.time() - t0, 4)
        print('Spectral Clustering finished in ' + str(t) + 's')

    return W, U, Q, C, D
```

Listing 4: Spectral Clustering Algorithm Python Code

V. Expectation Maximization (EM) Algorithm



(a) clustering.txt

(b) bigClusteringData.txt

Figure 15: Change of Distoration versus Cluster Number K for EM Algorithm

```
import numpy as np
import time

class EM(object):
    """ self-defined calss for EM algorithm """

    def __init__(self, m, threshold=0.01, random_state=None, maxIter=500):
        """ initialize the EM algorithm """
        self.m = m
        self.threshold = threshold
        self.random_state = random_state
        self.maxIter = maxIter
        self.w = None
        self.gamma = None
        self.mu = None
        self.sigma = None
        self.gaussianProb = None
        self.logLikelihood = None
        self.distance = None
        self.D = None

    def train(self, x, verbose=False):
        """ function to perform EM algorithm on X """
        t0 = time.time()
        np.random.seed(self.random_state)

        # initialize the mean and covariance matrix
        self.initialize(x)

        # iterate through E and M steps
        for i in range(1, self.maxIter + 1):
            self.estep(x)
            self.mstep(x)
            if abs(self.logLikelihood[-1] - self.logLikelihood[-2]) \
               / abs(self.logLikelihood[-2]) < self.threshold:
                for i in range(self.m):
```

```
                    self.distance[:, i] = np.sqrt(np.sum((x - self.mu[i])**2,
                                                         axis=1))
                self.D = np.max(np.min(self.distance, axis=1))
                if verbose is True:
                    t = np.round(time.time() - t0, 4)
                    print('Reach threshold at', i,
                          'th iters in ' + str(t) + 's')
                return

        for i in range(self.m):
            self.distance[:, i] = np.sqrt(np.sum((x - self.mu[i])**2, axis=1))
        self.D = np.max(np.min(self.distance, axis=1))
        if verbose is True:
            t = np.round(time.time() - t0, 4)
            print('Stopped, reach the maximum iteration ' + str(t) + 's')

    def initialize(self, x):
        """ function to initialize the parameters """
        n, dim = x.shape  # find the dimensions
        self.distance = np.zeros((n, self.m))
        self.w = np.ones(self.m) * (1 / self.m)
        self.gamma = np.zeros((n, self.m))
        self.gaussianProb = np.zeros((n, self.m))
        self.mu = [None] * self.m
        self.sigma = [None] * self.m
        self.logLikelihood = []

        cov = np.cov(x.T)
        mean = np.mean(x, axis=0)
        for k in range(self.m):
            self.mu[k] = mean + np.random.uniform(-0.5, 0.5, dim)
            self.sigma[k] = cov

        # update gamma
        self.gamma = self.gammaprob(x, self.w, self.mu, self.sigma)

        # calculate the expectation of log-likelihood
        self.logLikelihood.append(self.likelihood())

    def estep(self, x):
        """ function to conduct E-Step for EM algorithm """
        self.gamma = self.gammaprob(x, self.w, self.mu, self.sigma)

    def mstep(self, x):
        """ function to conduct M-Step for EM algorithm """
        n, dim = x.shape
        sumGamma = np.sum(self.gamma, axis=0)
        self.w = sumGamma / n

        for k in range(self.m):
            self.mu[k] = np.sum(x.T * self.gamma[:, k], axis=1) / sumGamma[k]
            diff = x - self.mu[k]
            weightedDiff = diff.T * self.gamma[:, k]
            self.sigma[k] = np.dot(weightedDiff, diff) / sumGamma[k]
            if np.linalg.matrix_rank(self.sigma[k]) != 3:
                randv = np.random.random(dim) / 10000
                self.sigma[k] = self.sigma[k] + np.diag(randv)

        # calculate the expectation of log-likelihood
```

```
96          self.logLikelihood.append(self.likelihood())
97
98      def gammaprob(self, x, w, mu, sigma):
99          """ function to calculate the gamma probability """
100         for k in range(self.m):
101             self.gaussianProb[:, k] = self.gaussian(x, mu[k], sigma[k])
102
103         weightedSum = np.sum(w * self.gaussianProb, axis=1)
104         gamma = ((w * self.gaussianProb).T / weightedSum).T
105
106         return gamma
107
108     def gaussian(self, x, mu, sigma):
109         """ function to calculate the multivariate gaussian probability """
110         inversion = np.linalg.inv(sigma)
111         part1 = (-0.5 * np.sum(np.dot(x - mu, inversion) * (x - mu), axis=1))
112         part2 = 1 / ((2 * np.pi) ** (len(mu) / 2) *
113                      (np.linalg.det(sigma) ** 0.5))
114
115         pdf = part2 * np.exp(part1)
116
117         return pdf
118
119     def likelihood(self):
120         """ function to calculate the log likelihood """
121         log = np.log(np.sum(self.w * self.gaussianProb, axis=1))
122         logLikelihood = np.sum(log)
123
124         return logLikelihood
125
126     def get_label(self):
127         """ function to predict the classes using calculated parameters """
128         label = np.argmax(self.w * self.gaussianProb, axis=1)
129
130         return label
```

Listing 5: EM Algorithm Python Code

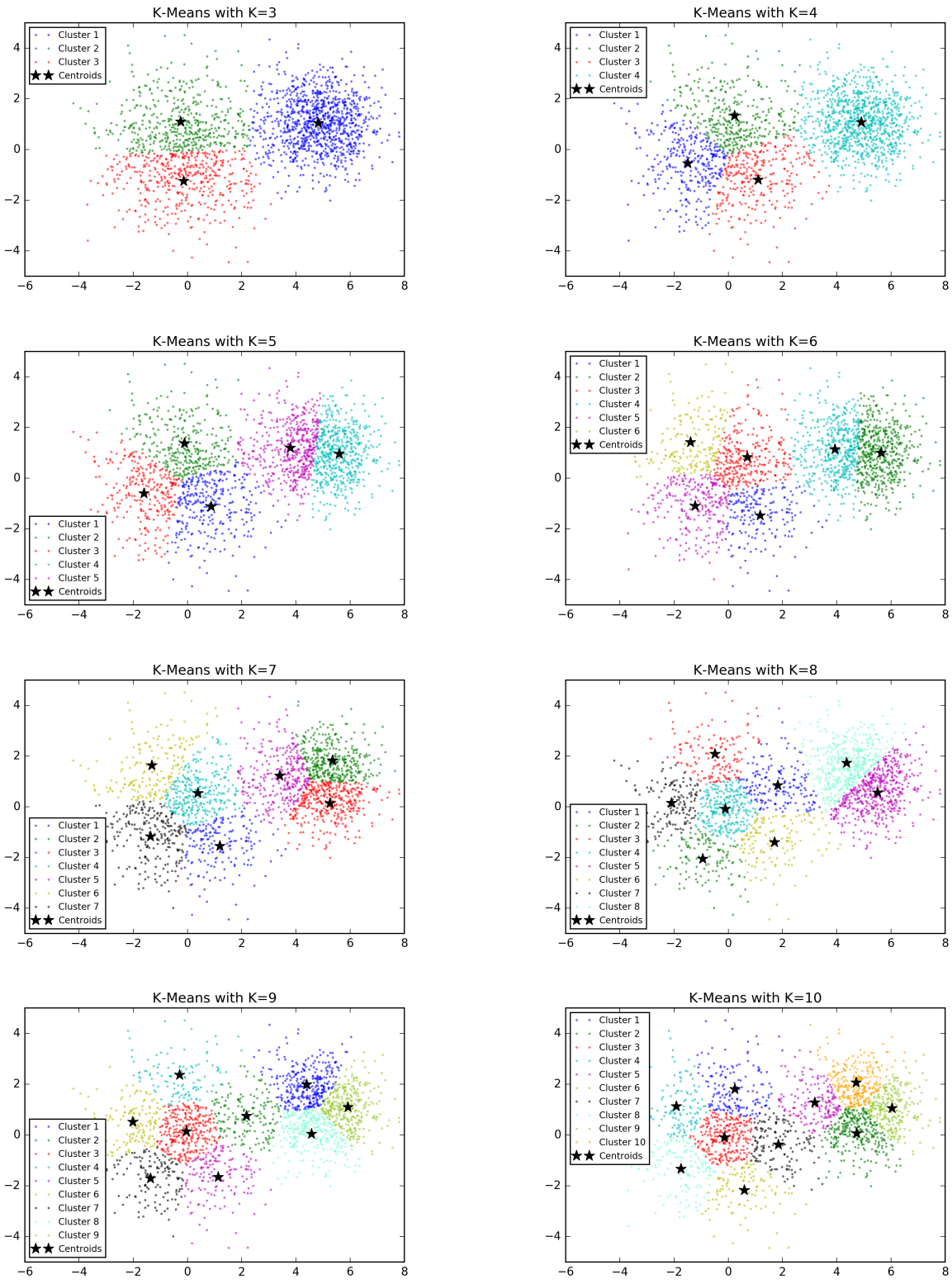


Figure 1: Clustering Result for clustering.txt with K-Means Algorithm

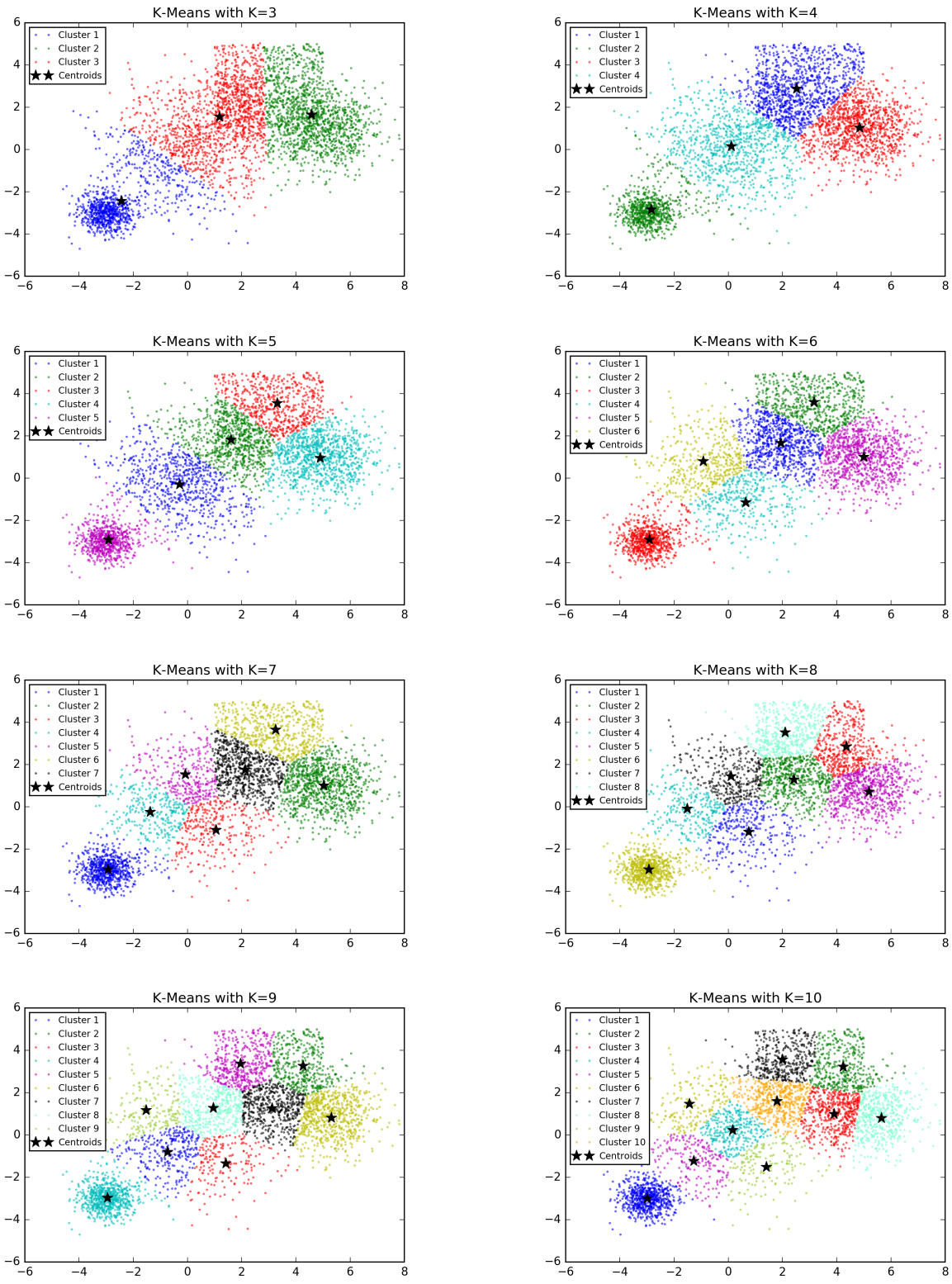


Figure 2: Clustering Result for bigClusteringData.txt with K-Means Algorithm

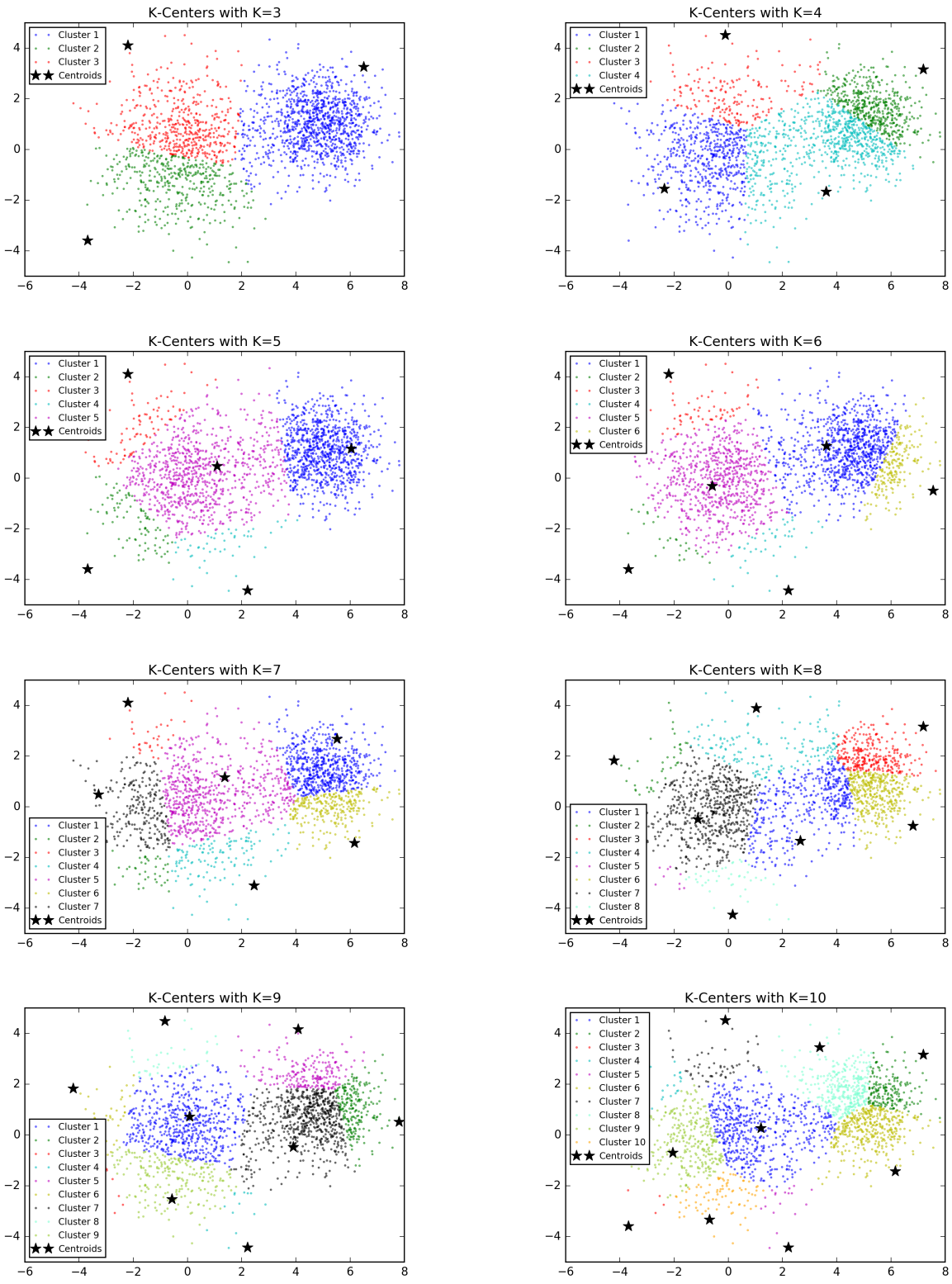


Figure 4: Clustering Result for clustering.txt with K-Center Algorithm

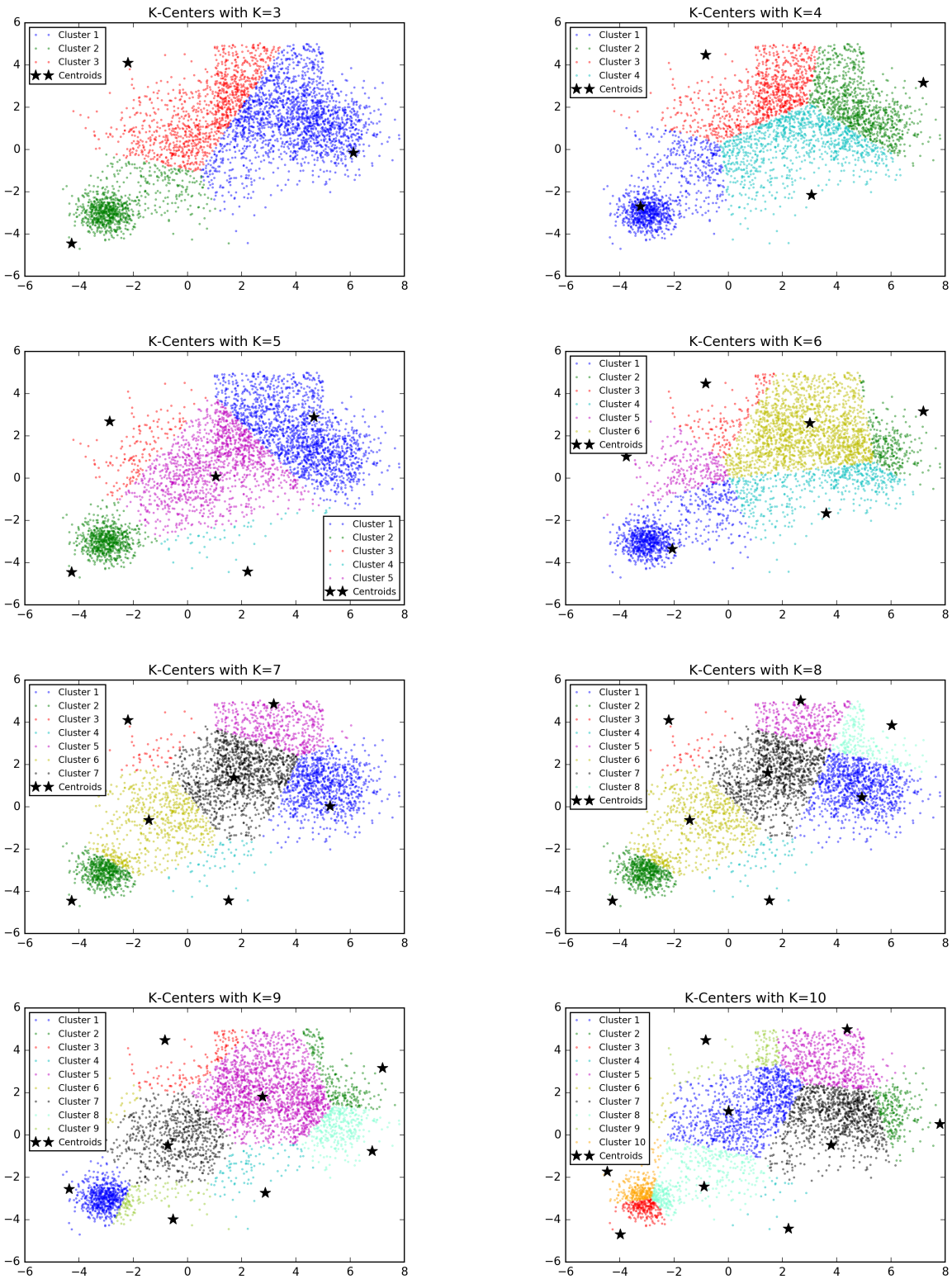


Figure 5: Clustering Result for bigClusteringData.txt with K-Center Algorithm

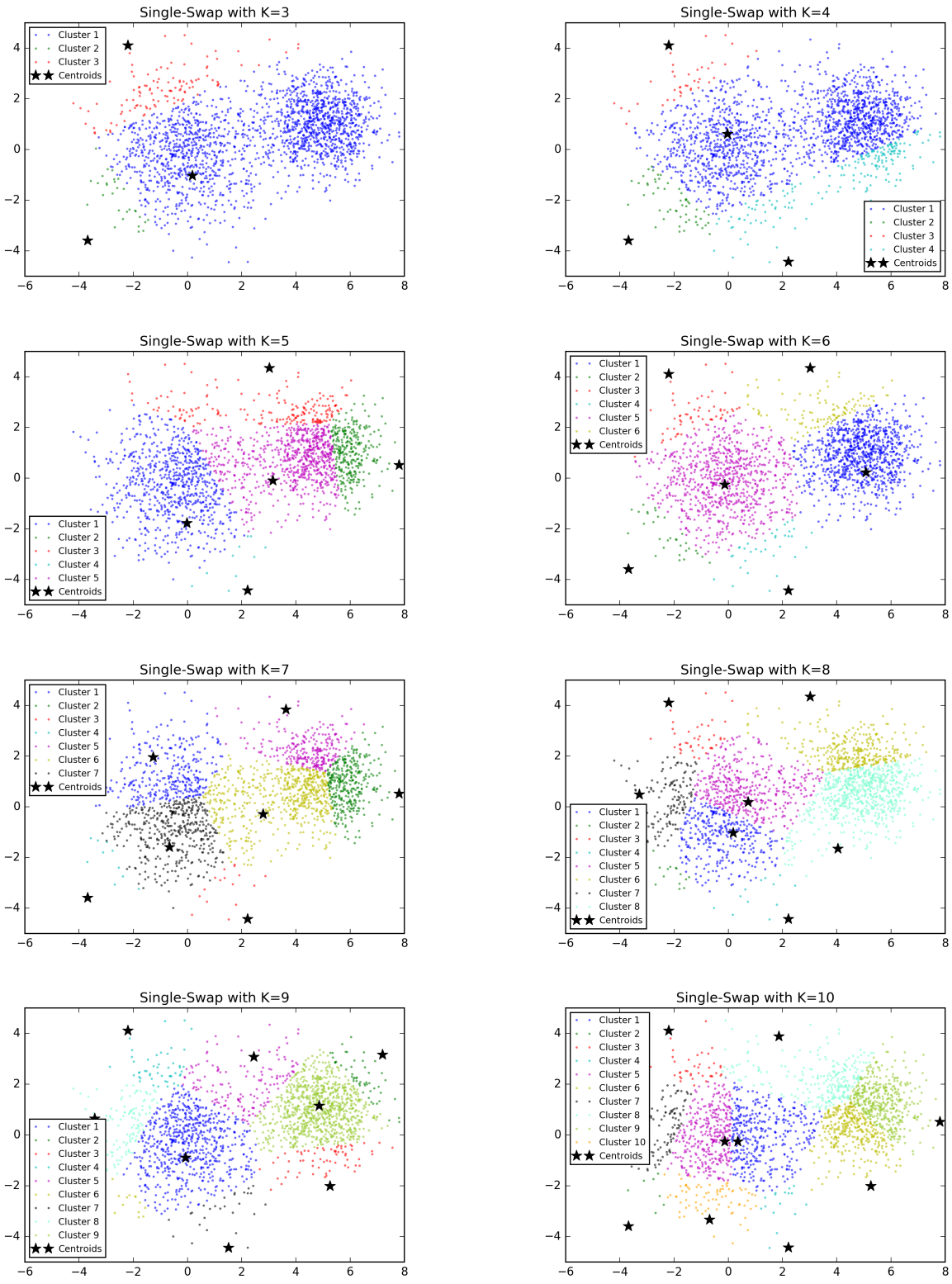


Figure 7: Clustering Result for clustering.txt with Single-Swap Algorithm

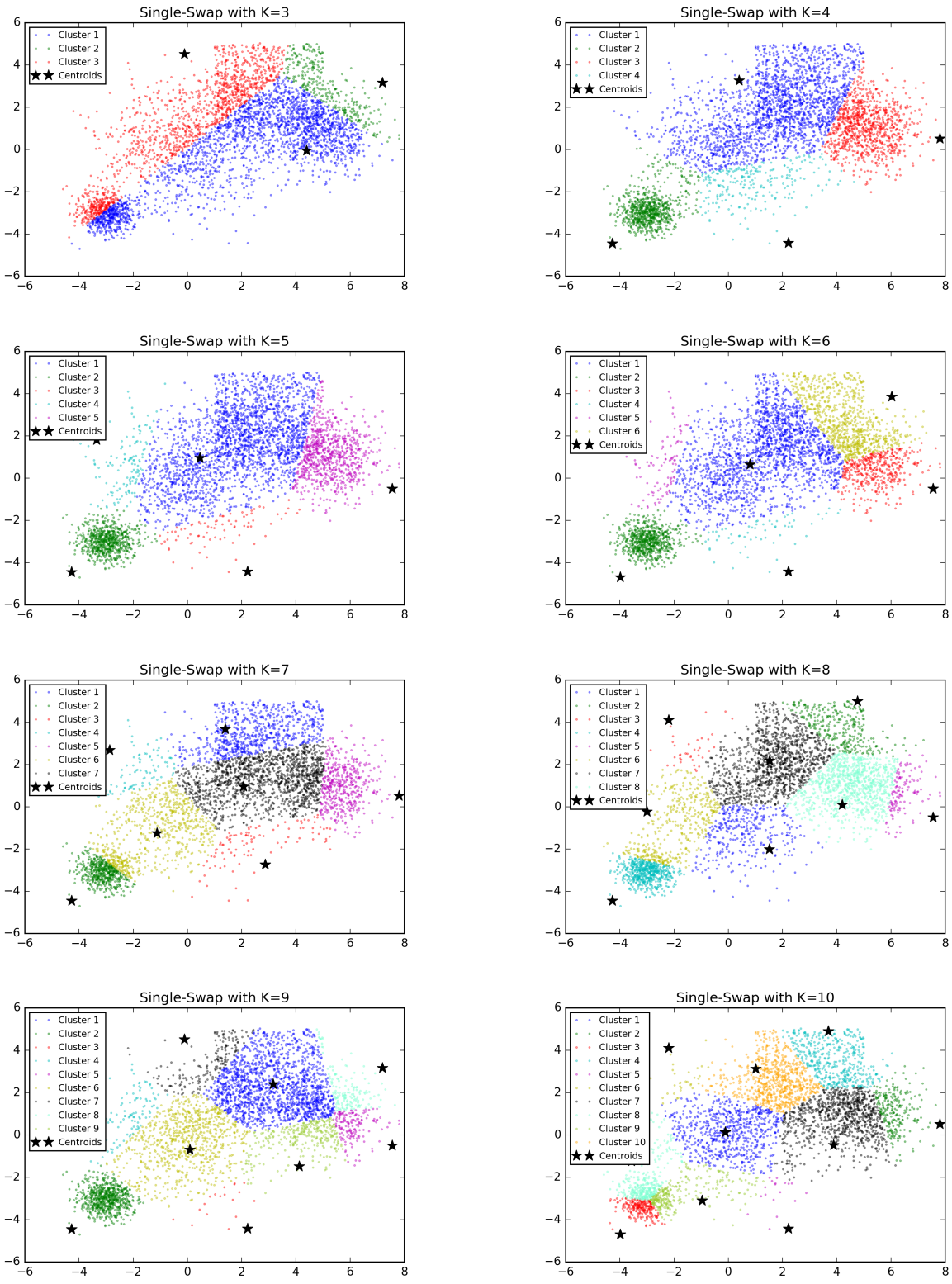


Figure 8: Clustering Result for bigClusteringData.txt with Single-Swap Algorithm

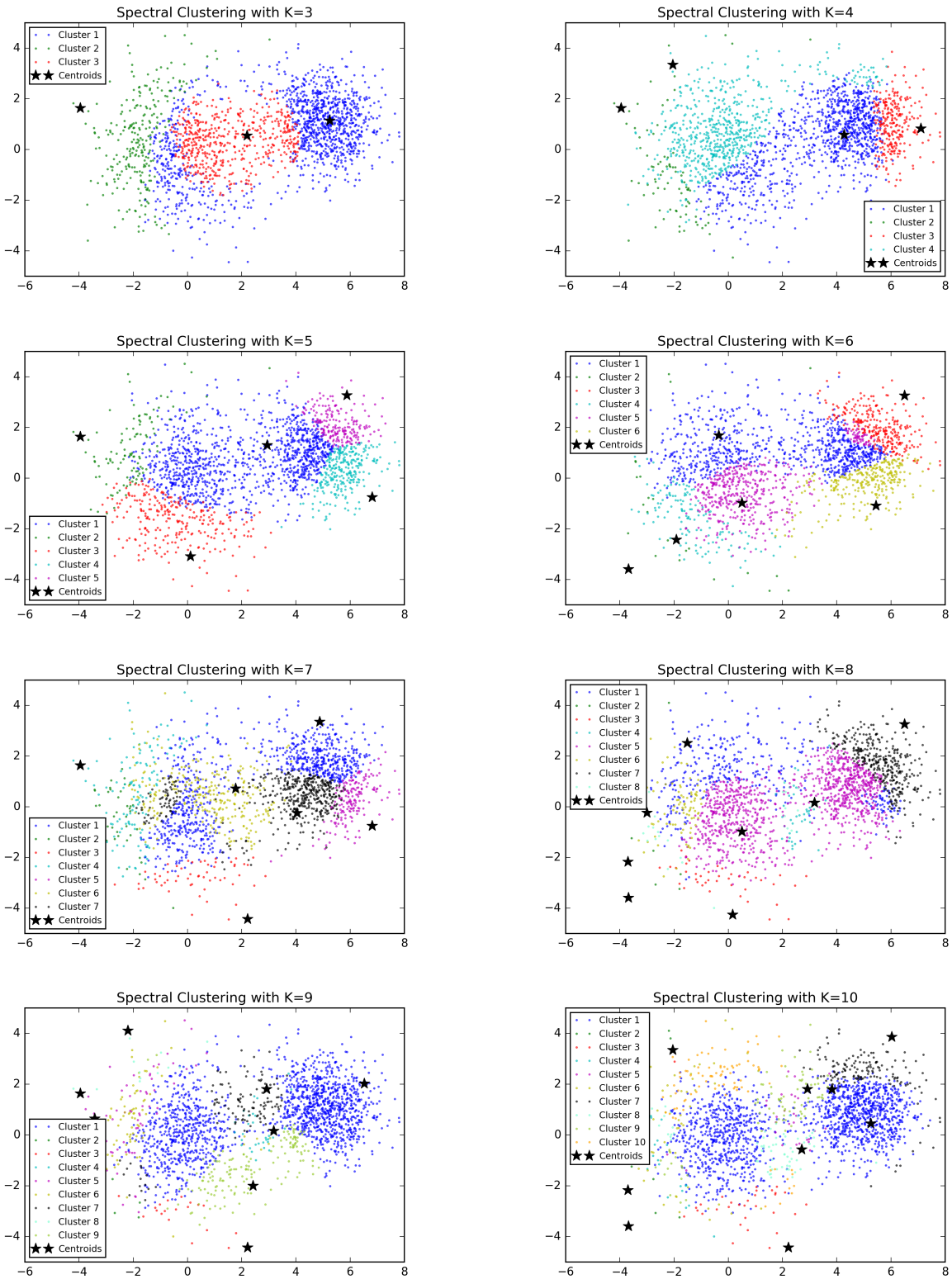


Figure 10: Clustering Result for clustering.txt with Spectral Clustering

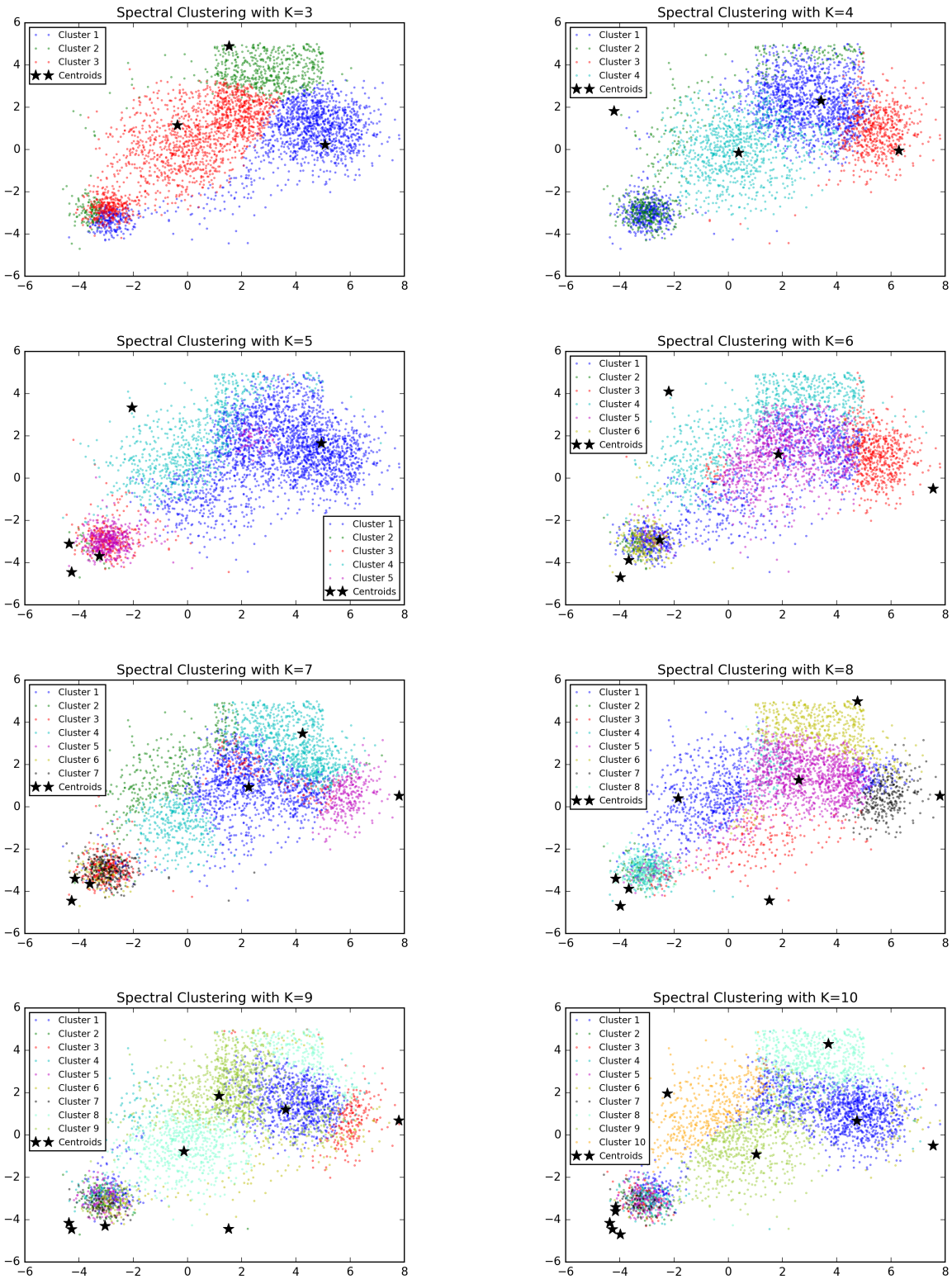


Figure 11: Clustering Result for bigClusteringData.txt with Spectral Clustering

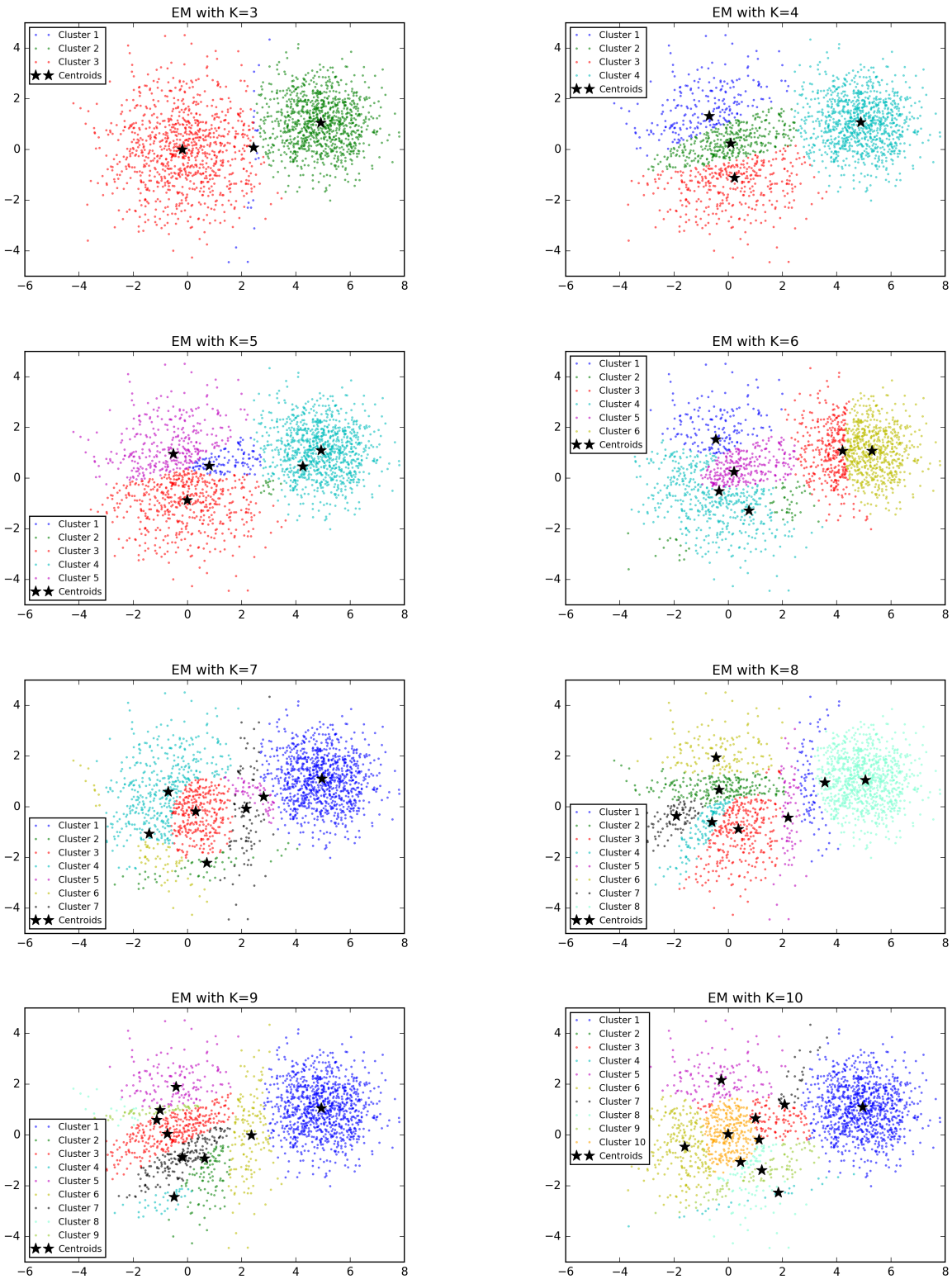


Figure 13: Clustering Result for clustering.txt with EM Algorithm

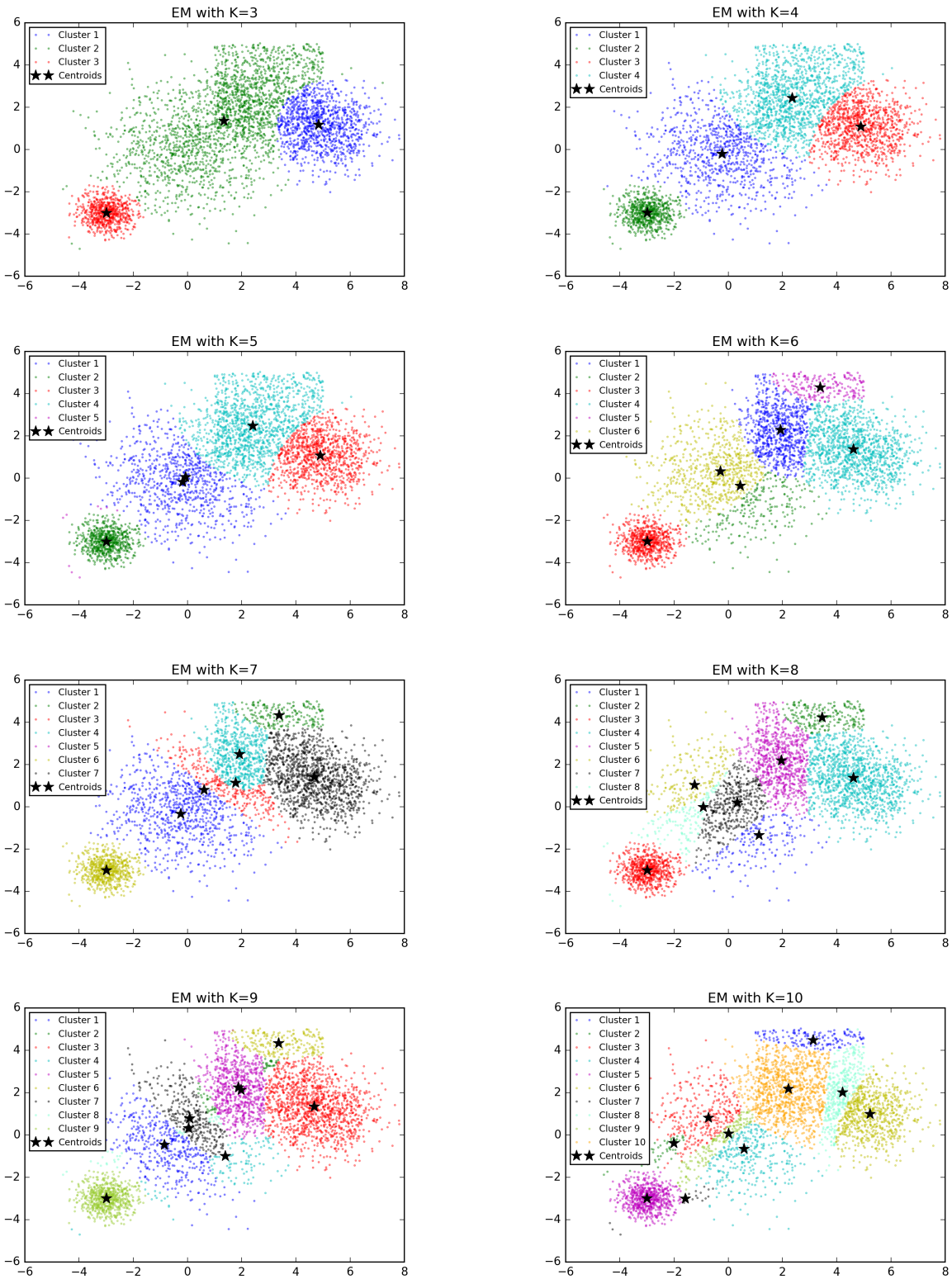


Figure 14: Clustering Result for bigClusteringData.txt with EM Algorithm