Topic No. 8

1. K-means
2. GMM
3. EM
4. DASH publishing in Linux
5. Preparing Proposal Presentation

Partitioning Algorithms: Basic Concept

- Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

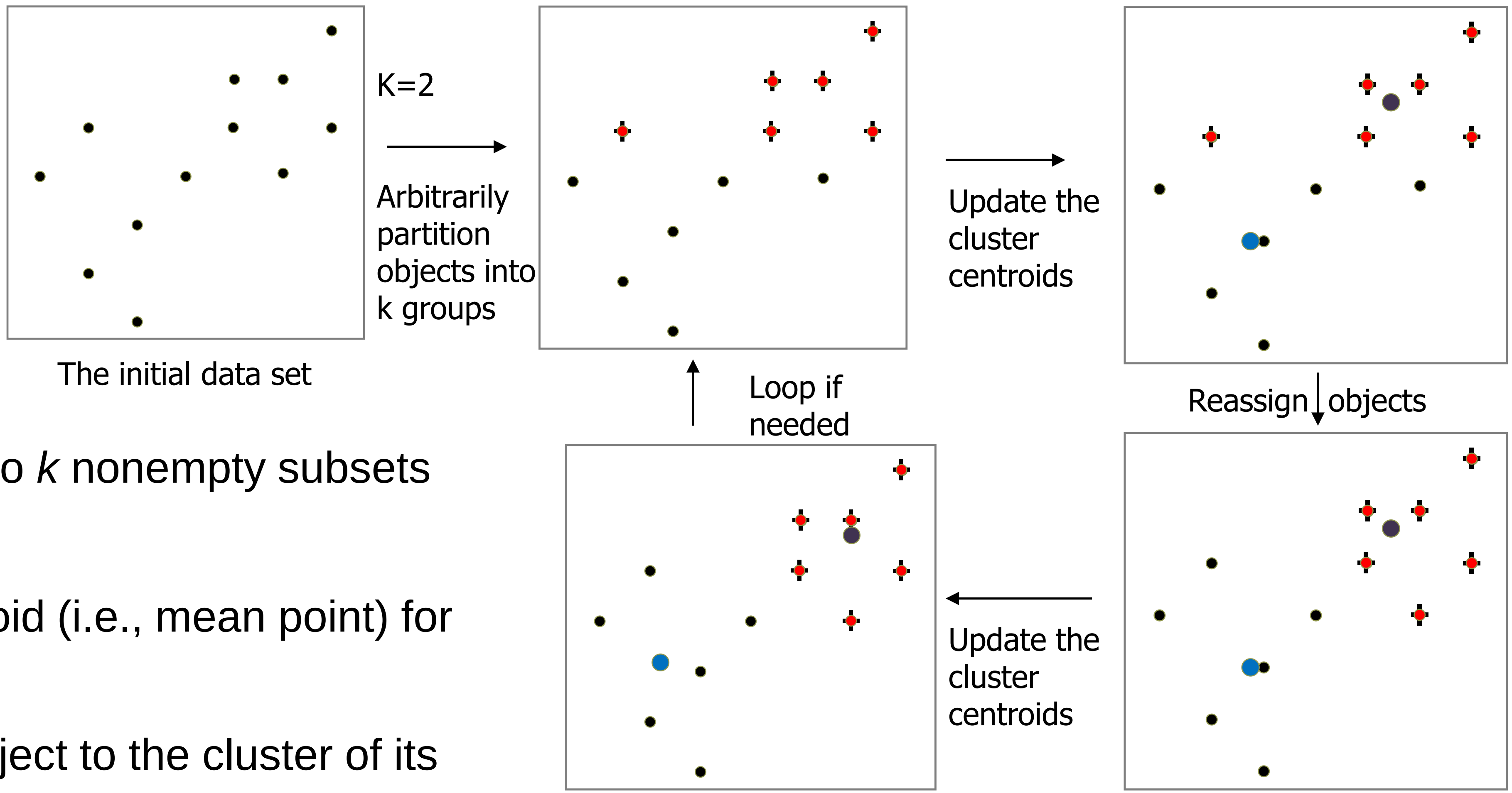
$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (p - c_i)^2$$

- Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion
  - Global optimal: exhaustively enumerate all partitions
  - Heuristic methods: *k-means* and *k-medoids* algorithms
  - *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
  - *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

The *K-Means* Clustering Method

- Given *k*, the *k-means* algorithm is implemented in four steps:
  - Partition objects into *k* nonempty subsets
  - Compute seed points as the centroids of the clusters of the current partitioning (the centroid is the center, i.e., *mean point*, of the cluster)
  - Assign each object to the cluster with the nearest seed point
  - Go back to Step 2, stop when the assignment does not change

An Example of *K-Means* Clustering

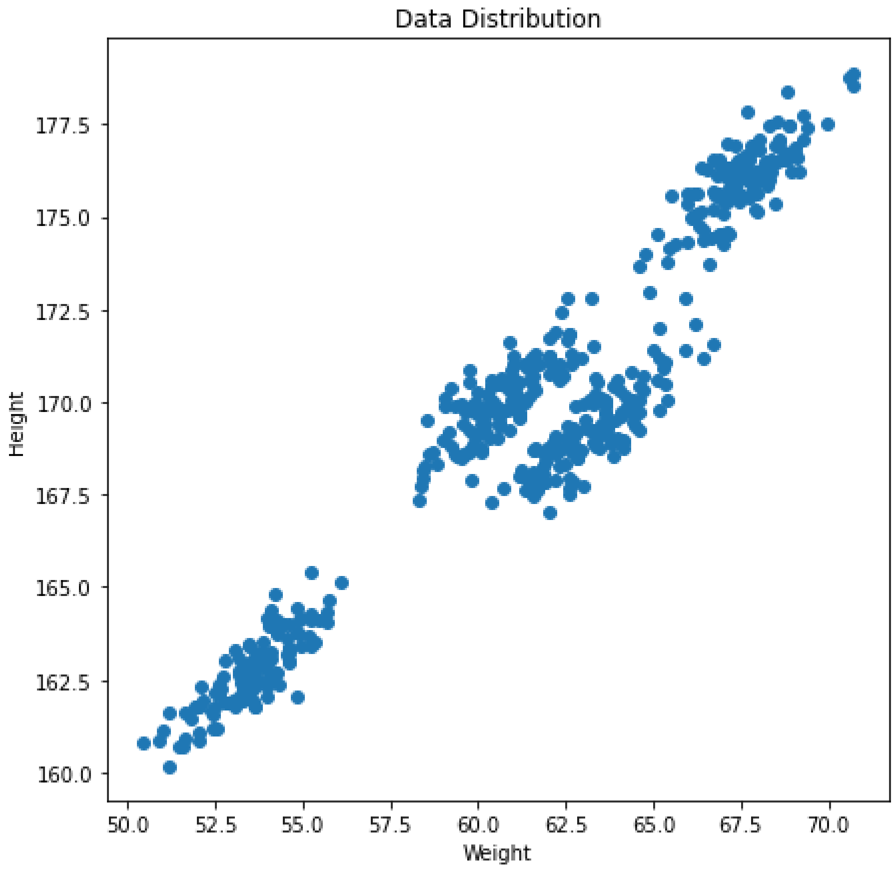


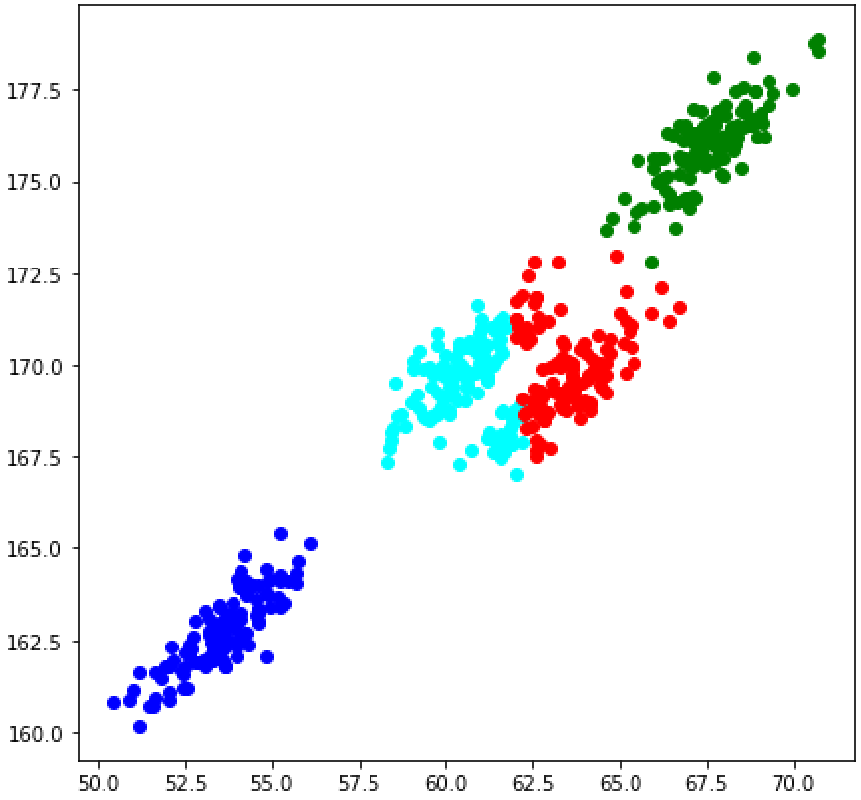
- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

What Is the Problem of the K-Means Method?

- The k-means algorithm is sensitive to outliers !
  - Since an object with an extremely large value may substantially distort the distribution of the data
- All the clusters created have a circular shape
  - Will not work when the distribution of points is ***not*** in a circular form

K-means


Data Distribution
177.5
175.0
172.5
170.0
167.5
165.0
162.5
160.0
Height
50.0
52.5
55.0
57.5
60.0
62.5
65.0
67.5
70.0
Weight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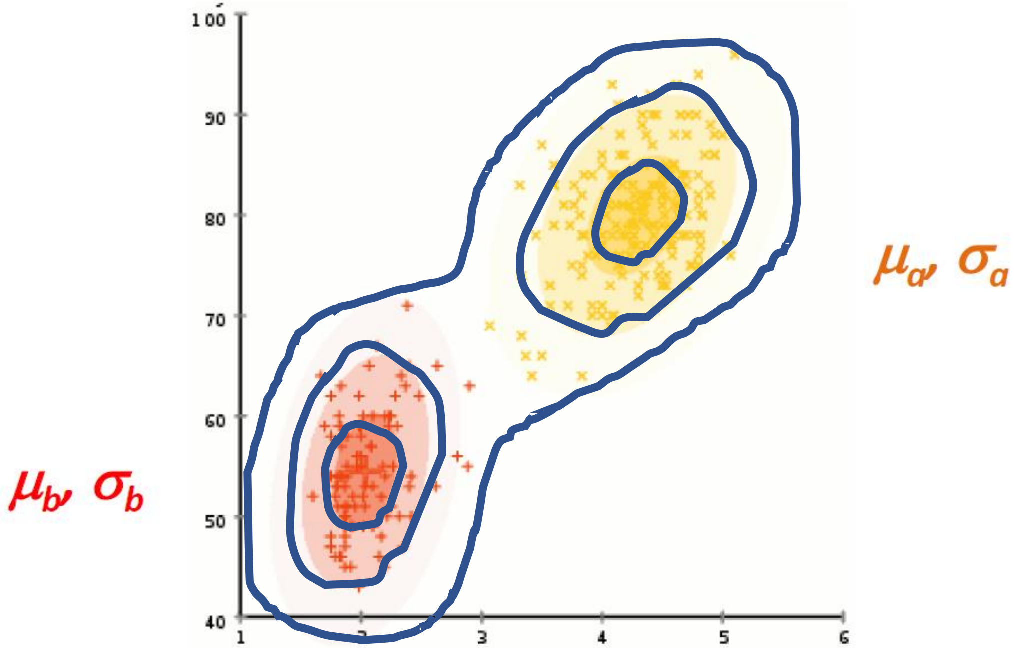
Gaussian Mixture Model

- Assume data points are from several Gaussian distributions

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \qquad \sum_{k=1}^{K} \pi_k = 1 \qquad 0 \leqslant \pi_k \leqslant 1$$

- Not necessarily the same Gaussian
- For each data point, estimate the corresponding Gaussian
- How?



Gaussian Mixture Model

- likelihood

$$p(\mathbf{X}|\pi,\mu,\Sigma) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- Log likelihood

$$\ln p(\mathbf{X}|\pi,\mu,\Sigma) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

Summation inside of log → makes it difficult to solve

EM — Expectation Maximization

1. EM
   - A popular iterative refinement algorithm
   - Assign each object to a cluster according to **a weight (prob. distribution).**
   - New means are computed based on weighted measures.
2. General idea
   - Starts with an initial estimate (“guess”) of **the parameter vector.**
   - Iteratively rescores the patterns against the mixture density produced by the parameter vector.
   - The rescored objects are used to update the parameter estimates.
   - Objects belong to the same cluster, if they are placed by their scores in a particular component distribution.

EM — Expectation Maximization

E-step

Gaussian distribution

Data points

mean

covariance

mixing probability

$$\gamma_j(\mathbf{x}_n) = \frac{\pi_j \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}{\sum_k \pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}$$

ownership weight

each Gaussian model

M-step

$$\boldsymbol{\mu}_j = \frac{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)\mathbf{x}_n}{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)}$$

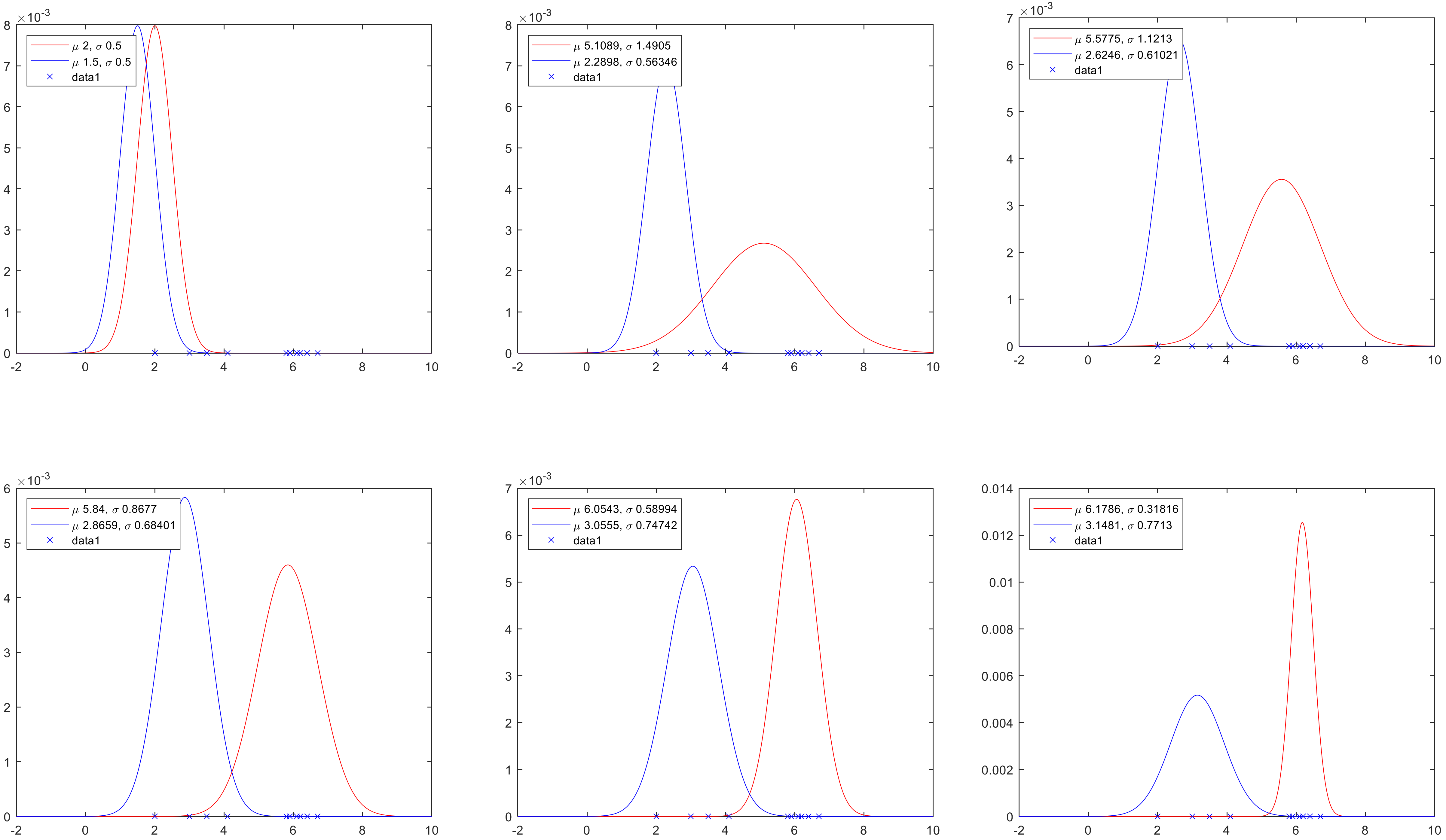
mean

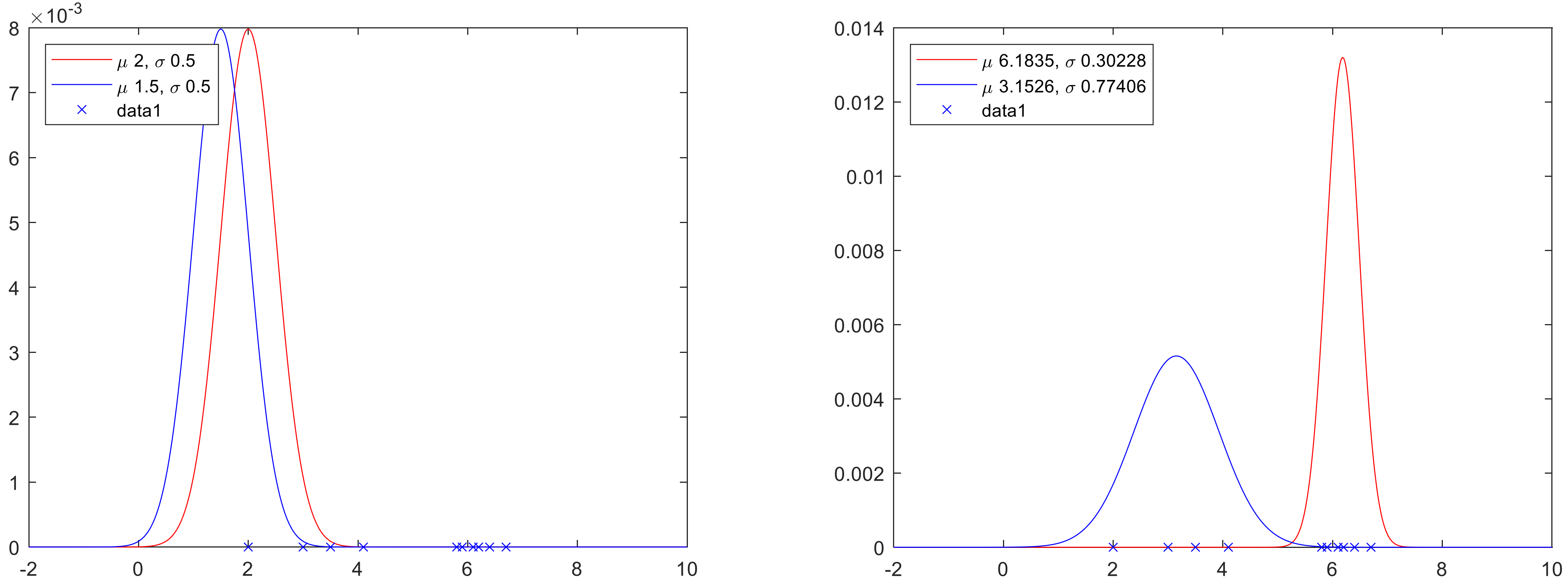
$$\boldsymbol{\Sigma}_j = \frac{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)(\mathbf{x}_n - \boldsymbol{\mu}_j)(\mathbf{x}_n - \boldsymbol{\mu}_j)^{\top}}{\sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)}$$

covariance

$$\pi_j = \frac{1}{N} \sum_{n=1}^{N} \gamma_j(\mathbf{x}_n)$$

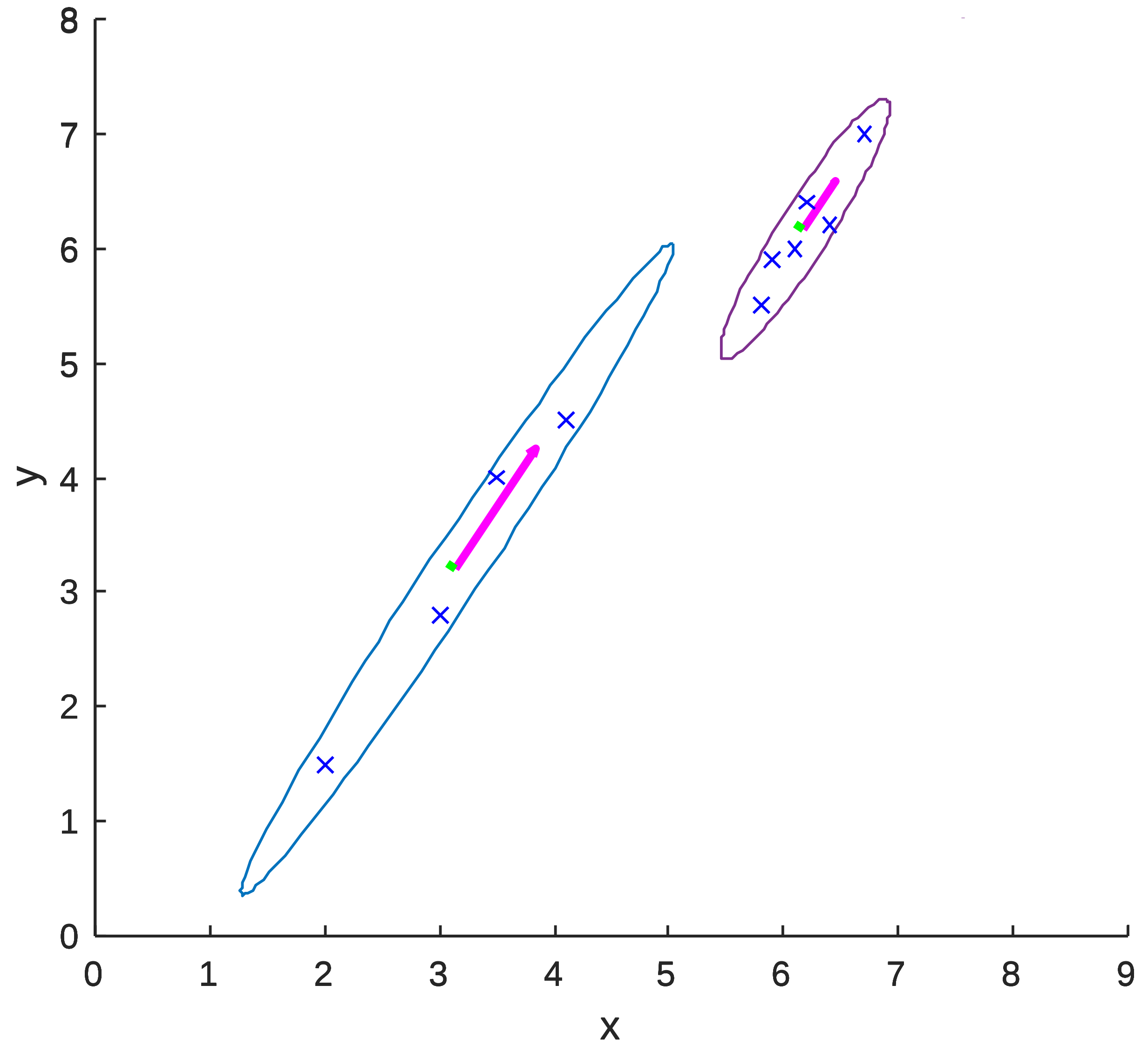
mixing probability


μ 2, σ 0.5
μ 1.5, σ 0.5
data1
μ 5.1089, σ 1.4905
μ 2.2898, σ 0.56346
data1
μ 5.5775, σ 1.1213
μ 2.6246, σ 0.61021
data1
μ 5.84, σ 0.8677
μ 2.8659, σ 0.68401
data1
μ 6.0543, σ 0.58994
μ 3.0555, σ 0.74742
data1
μ 6.1786, σ 0.31816
μ 3.1481, σ 0.7713
data1

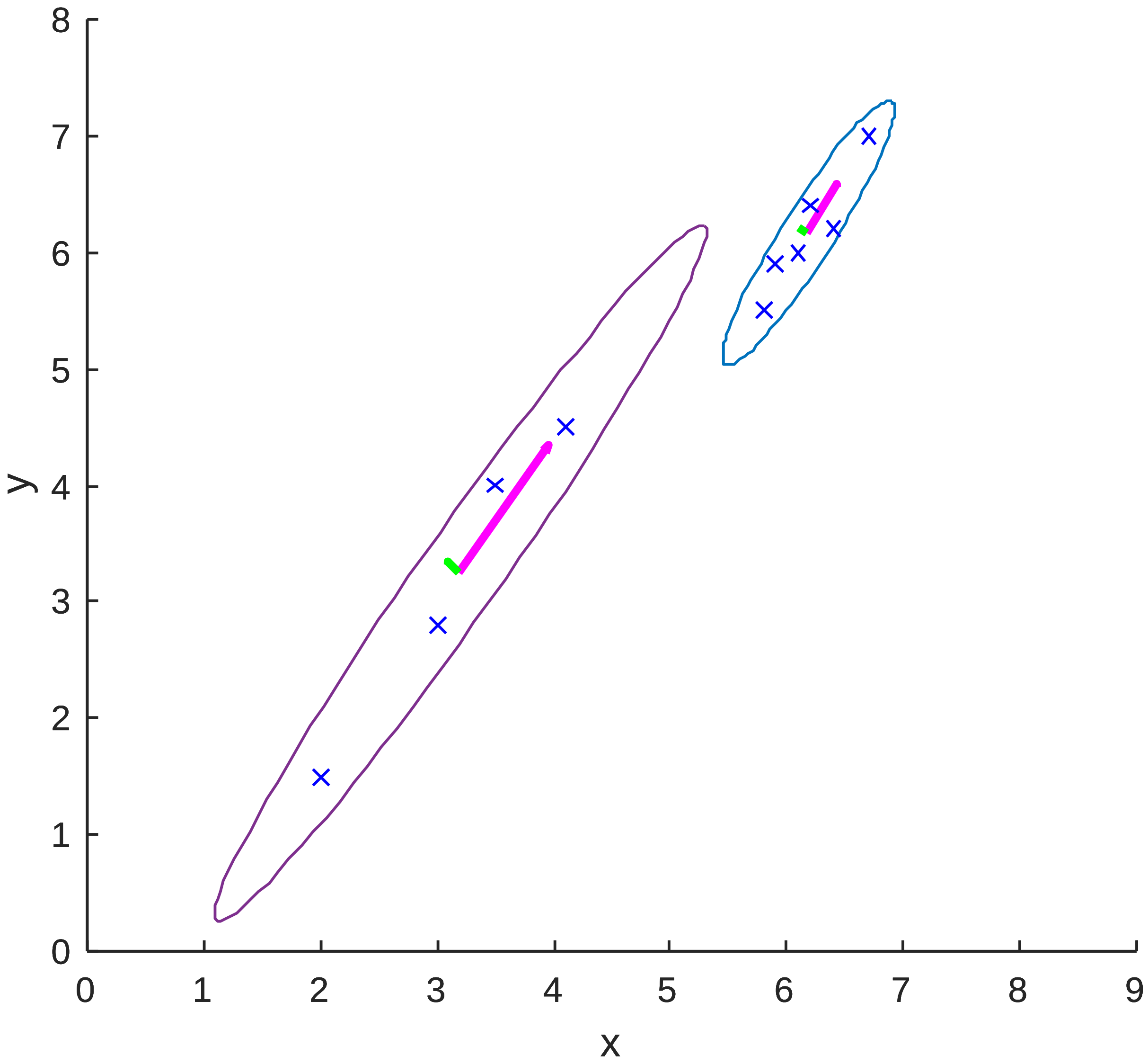


$\times 10^{-3}$
8
7
6
5
4
3
2
1
0
-2
0
2
4
6
8
10
μ 2, σ 0.5
μ 1.5, σ 0.5
data1
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
μ 6.1835, σ 0.30228
μ 3.1526, σ 0.77406
data1

Example of 2D Gaussian Mixture using EM



Example of 2D Gaussian Mixture using EM



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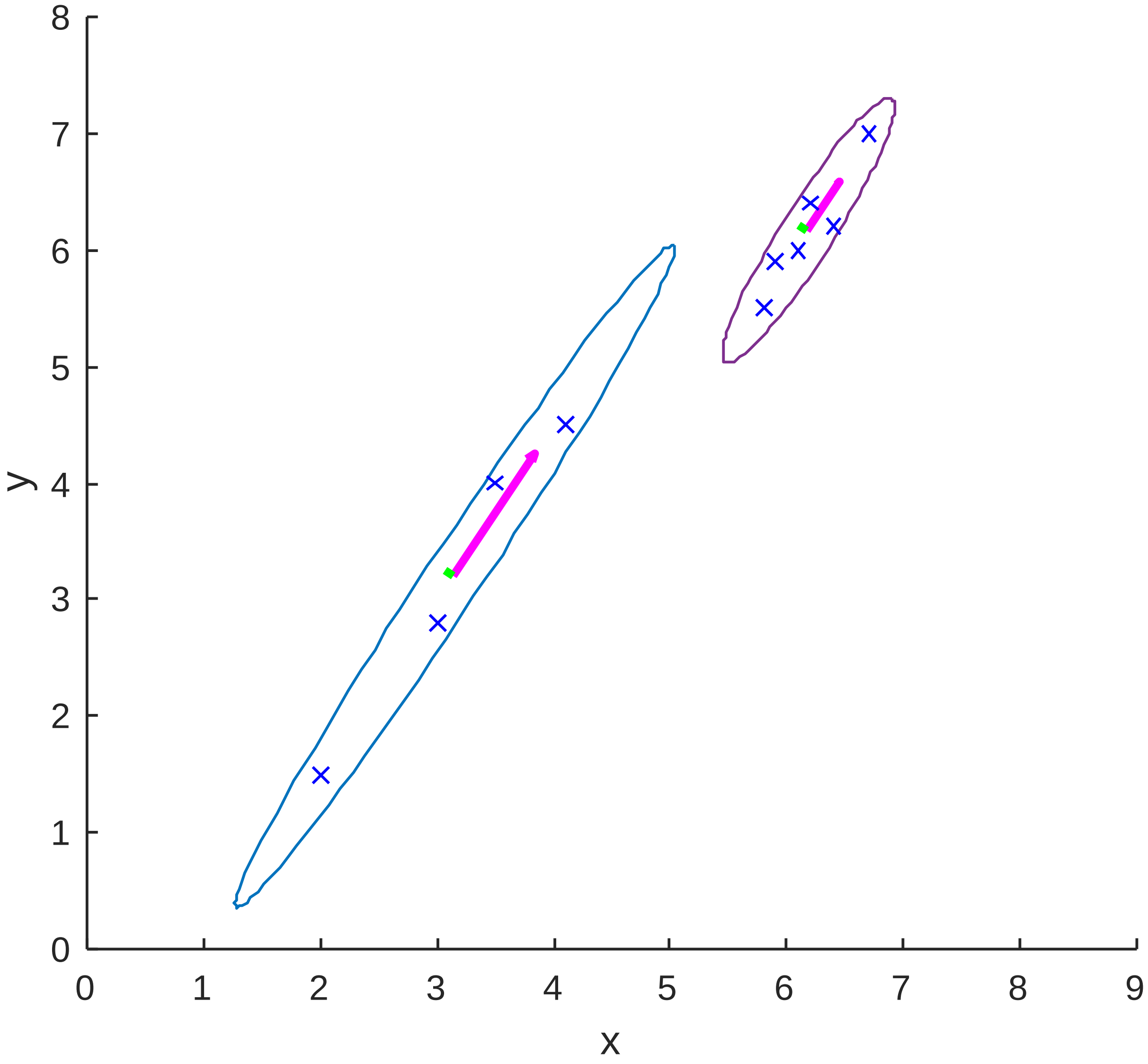

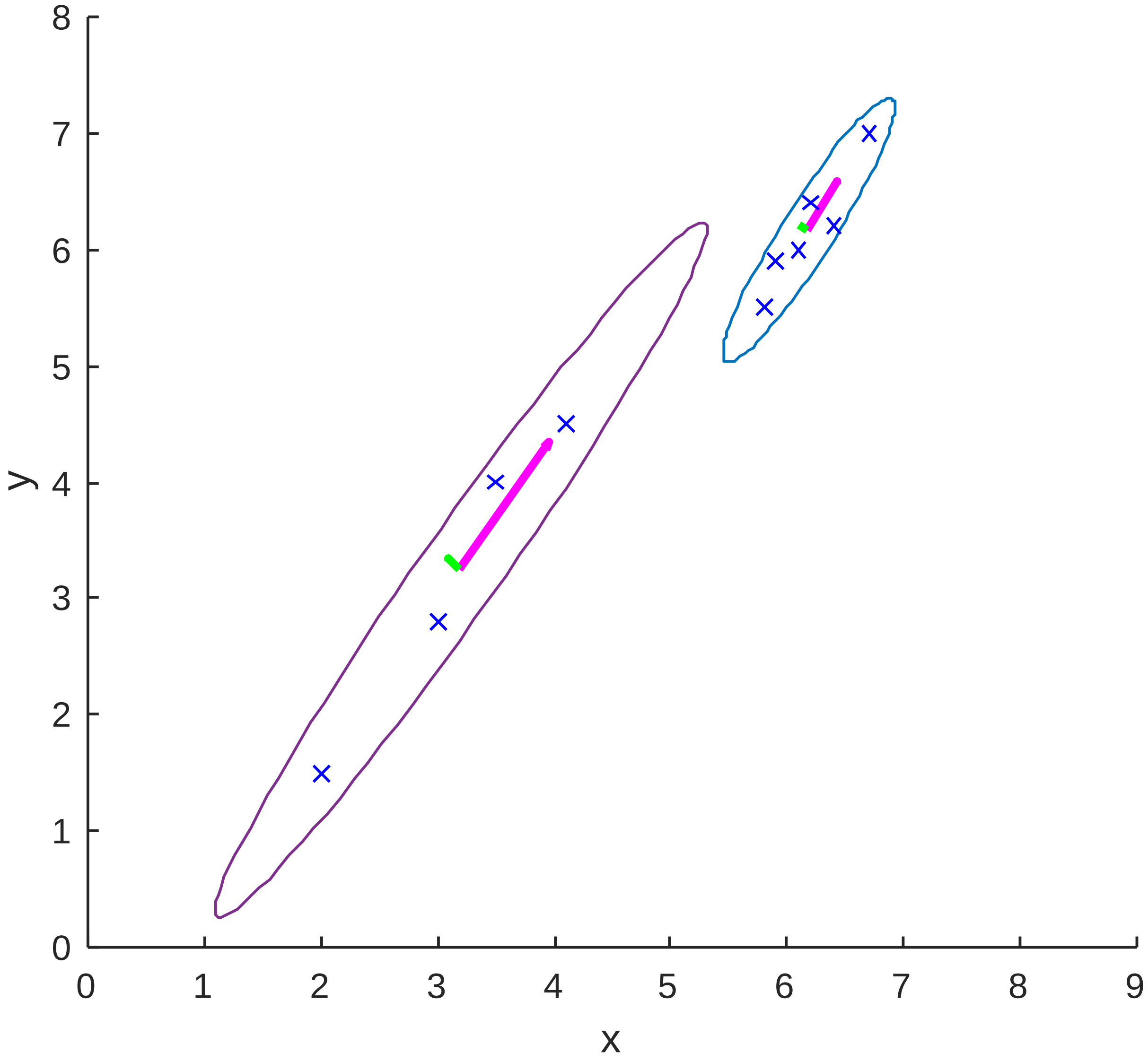

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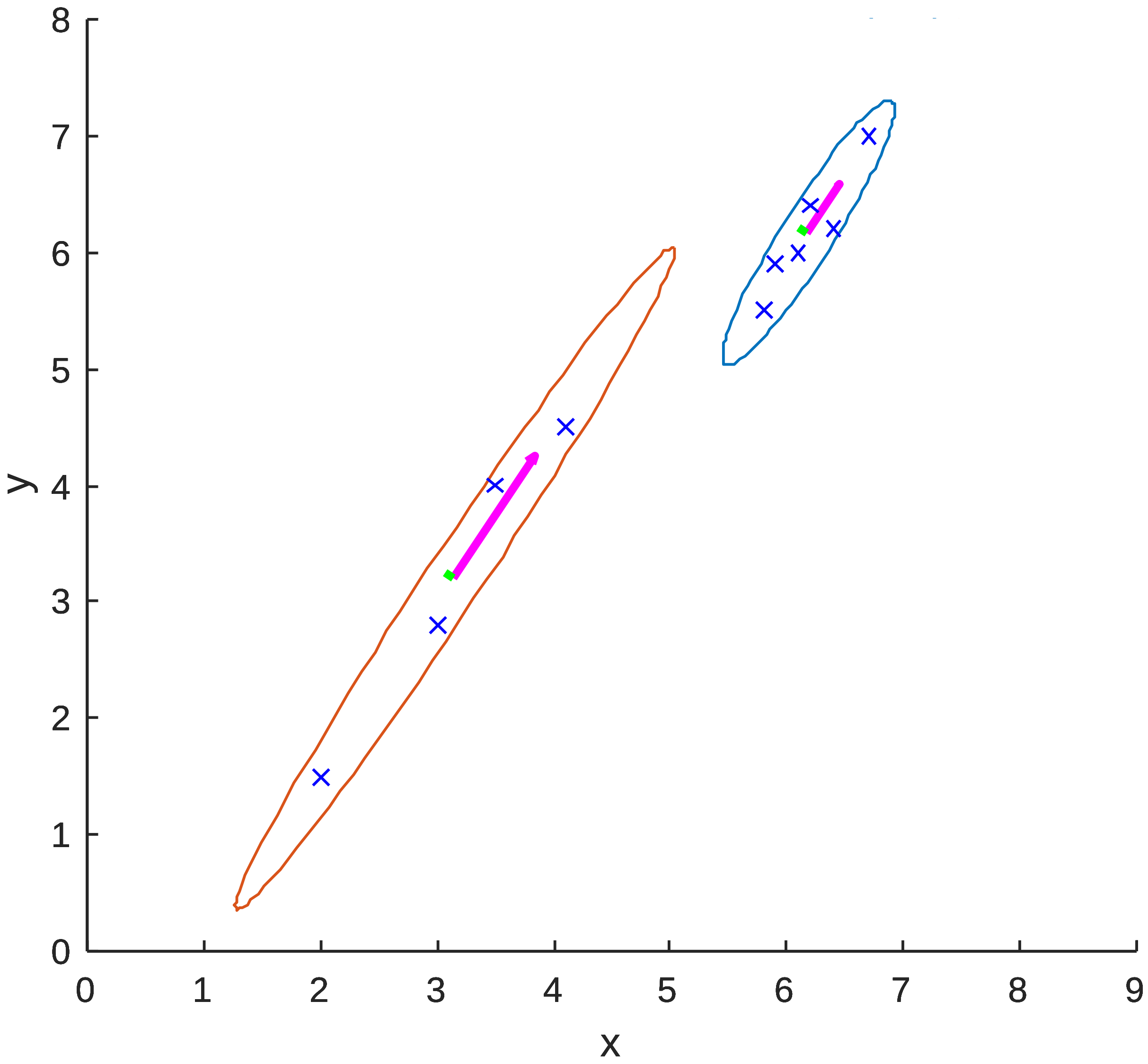

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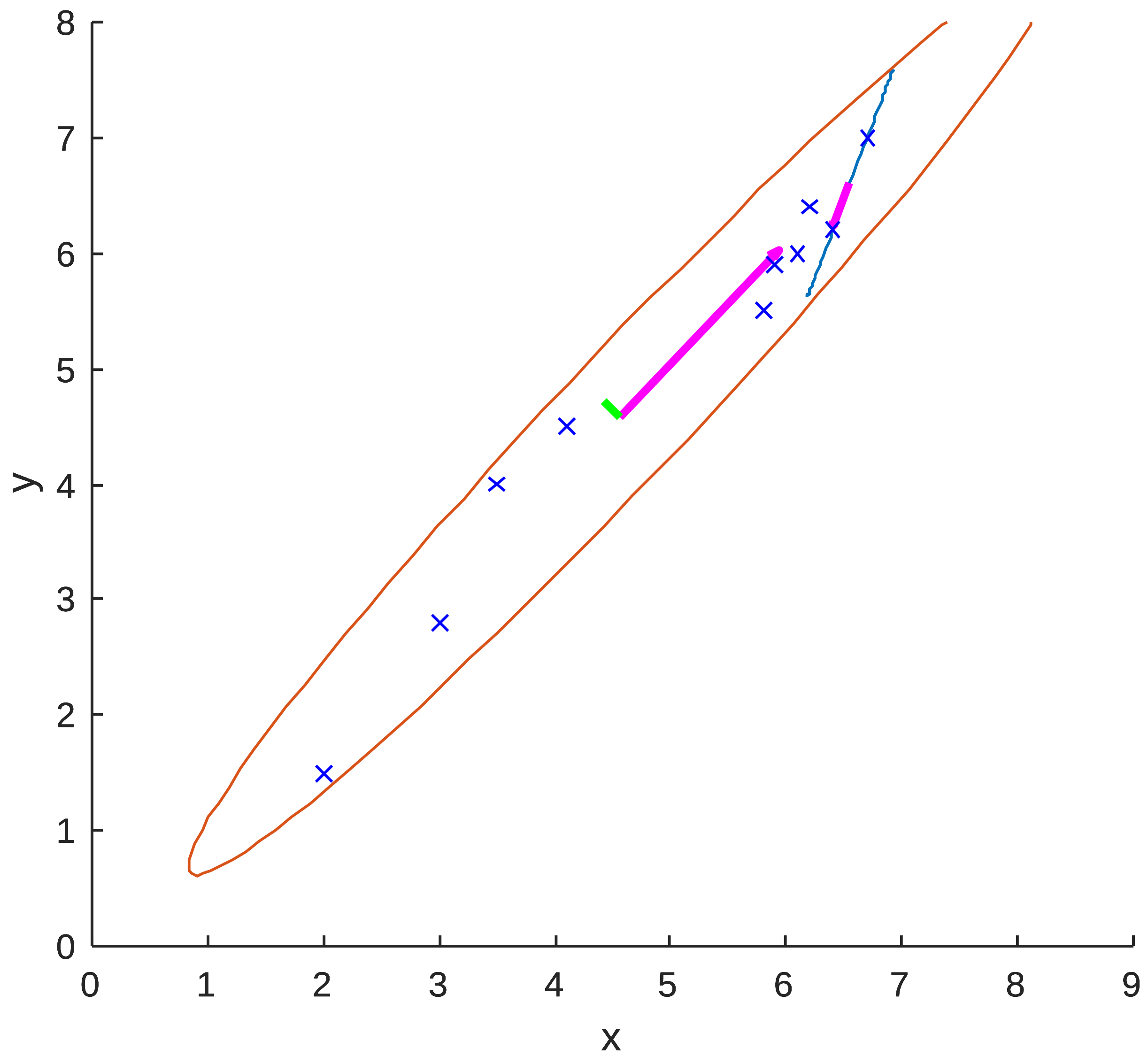

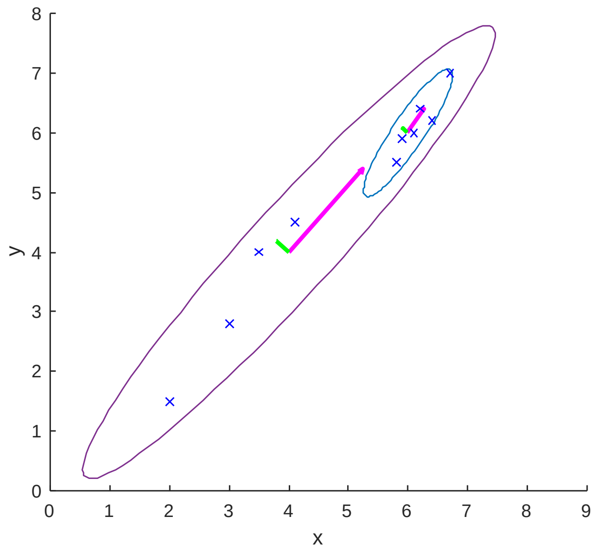

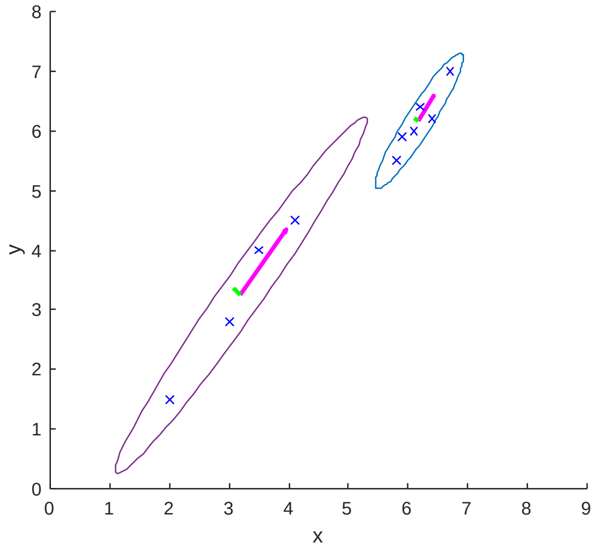

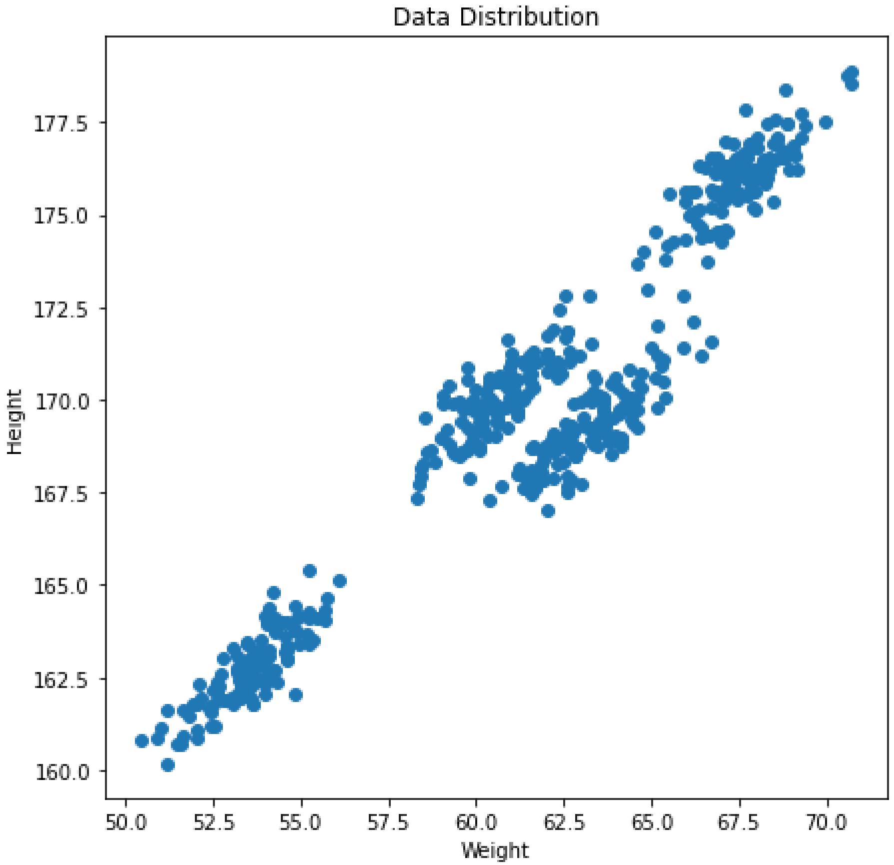

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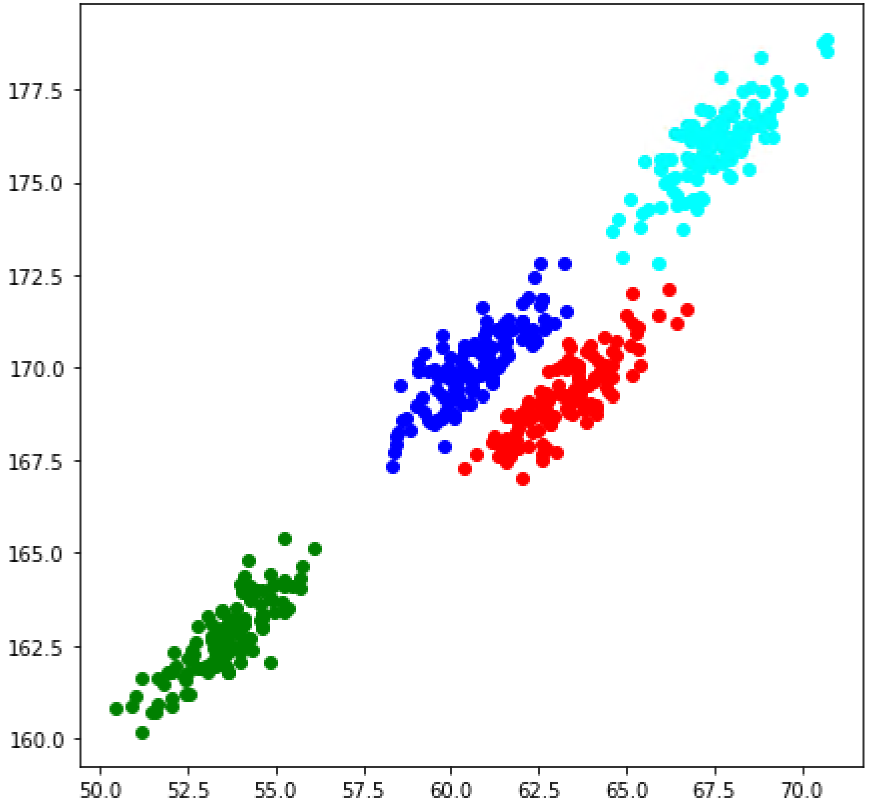

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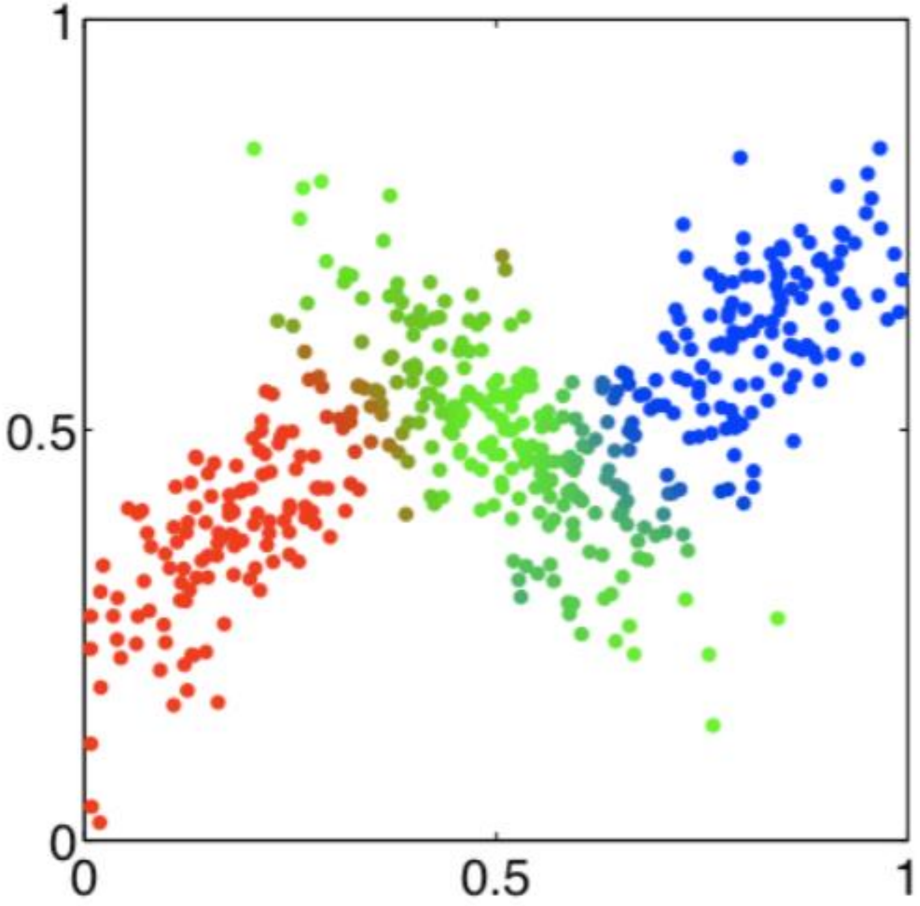
EM estimates weighted contributions of data point to the clusters



http://www.cse.psu.edu/~rtc12/CSE586/lectures/EMLectureFeb3.pdf

EM and *k*-means

k-means clustering is a special case of GMM-EM

1. Constant mixing probability $\pi_j = \frac{1}{k}$
2. Constant covariance matrix $\Sigma = I$
3. Only update mean values

```
from sklearn.mixture import GaussianMixture
import matplotlib.pyplot as plt

data = pd.read_csv('GMM.csv')
gmm = GaussianMixture(n_components=4)
gmm.fit(data)

#predictions from gmm
labels = gmm.predict(data)
frame = pd.DataFrame(data)
frame['cluster'] = labels
frame.columns = ['Weight', 'Height', 'cluster']

plt.figure(figsize=(7,7))
color=['blue', 'green', 'cyan', 'red']
for k in range(0,4):
   data = frame[frame["cluster"]==k]
   plt.scatter(data["Weight"],data["Height"],c=color[k])
plt.show()
```

https://www.analyticsvidhya.com/blog/2019/10/gaussian-mixture-models-clustering/