Clustering: K-means

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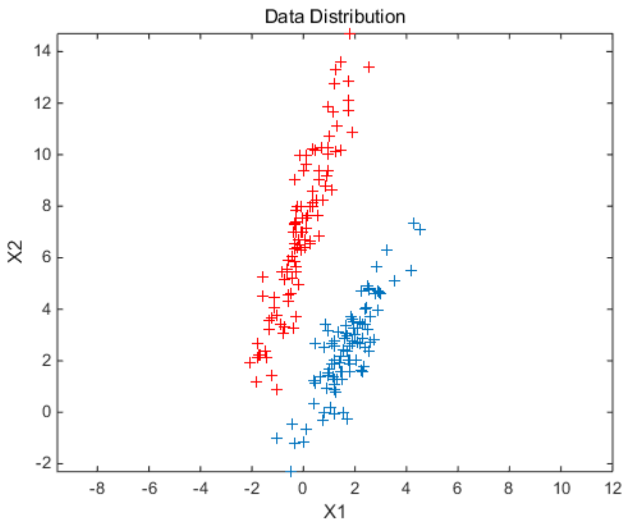
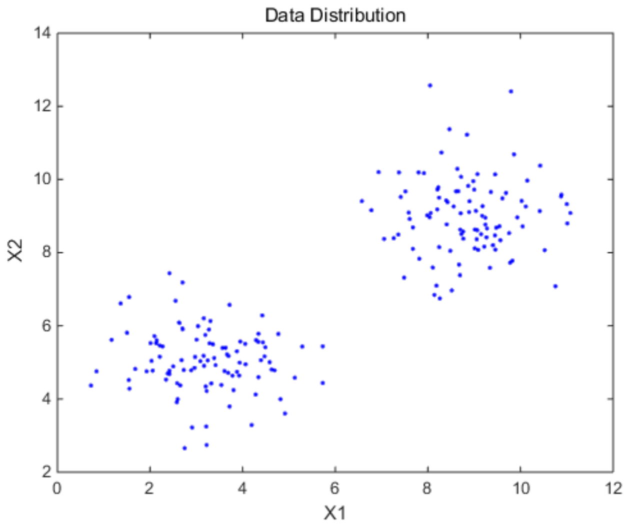
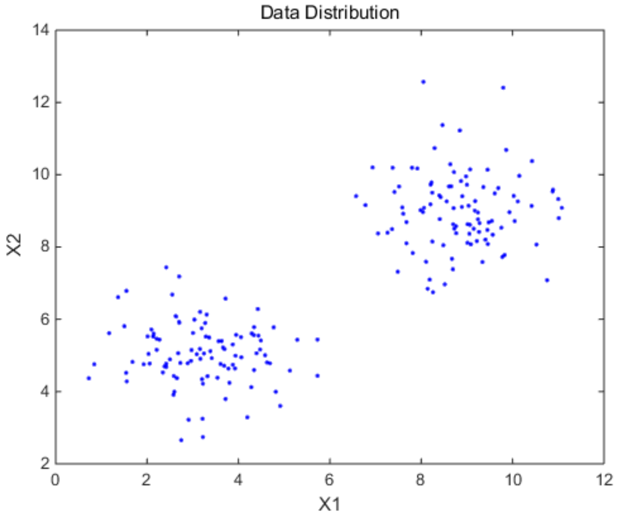
Supervised vs. Unsupervised Learning

<table>
<tr><th>Supervised Learning</th><th>Unsupervised Learning</th></tr>
<tr><td>Building a model from labeled data</td><td>Clustering from unlabeled data</td></tr>
<tr><td>
</td><td>
</td></tr>
<tr><td>$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$
$\{y^{(1)}, y^{(2)}, \cdots, y^{(m)}\}$ $\Rightarrow$ Classification</td><td>$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$ $\Rightarrow$ Clustering</td></tr>
</table>

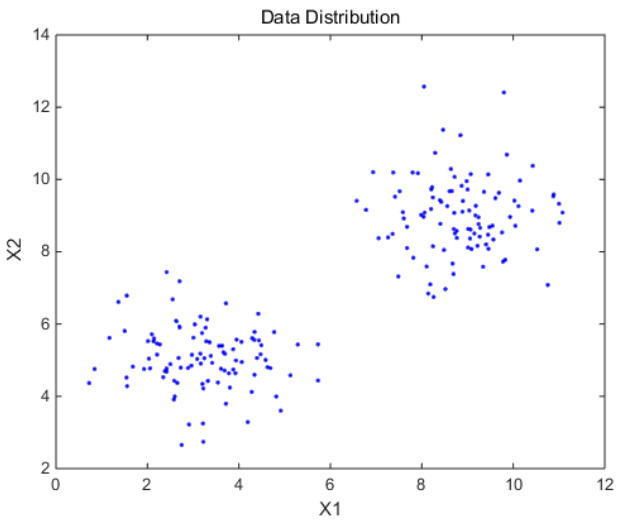
Data Clustering

- Data clustering is an unsupervised learning problem
- Given:
  - m unlabeled examples $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$
  - the number of partitions k
- Goal: group the examples into k partitions



$$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\} \quad \Rightarrow \quad \text{Clustering}$$

Data Clustering: Similarity



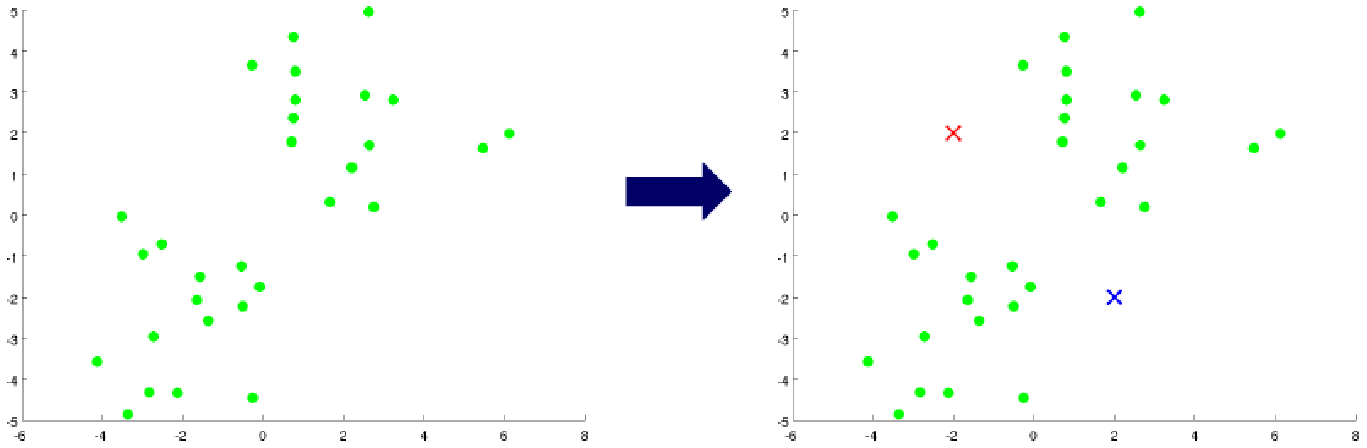
$$\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\} \quad \Rightarrow \quad \text{Clustering}$$

- The only information clustering uses is the mutual similarity between samples
- A good clustering is one that achieves:
  - high within-cluster similarity
  - low inter-cluster similarity

K-means: (Iterative) Algorithm

1) Initialization

- Input
  - k: the number of clusters
  - Training set $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$
- Randomly initialize cluster centers anywhere in $\mathbb{R}^n$

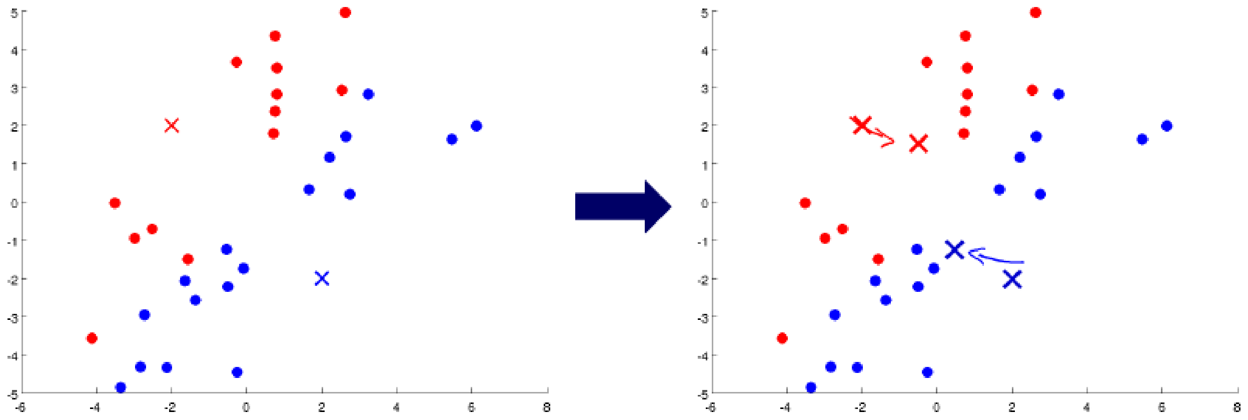


Training set data

Place centroids at random locations (K=2)

K-means: (Iterative) Algorithm

2) Iteration



Cluster Assignment

- For each point $x^{(i)}$
- Find nearest centroid μ_k
- Assign the point $x^{(i)}$ to cluster k

Move centroids

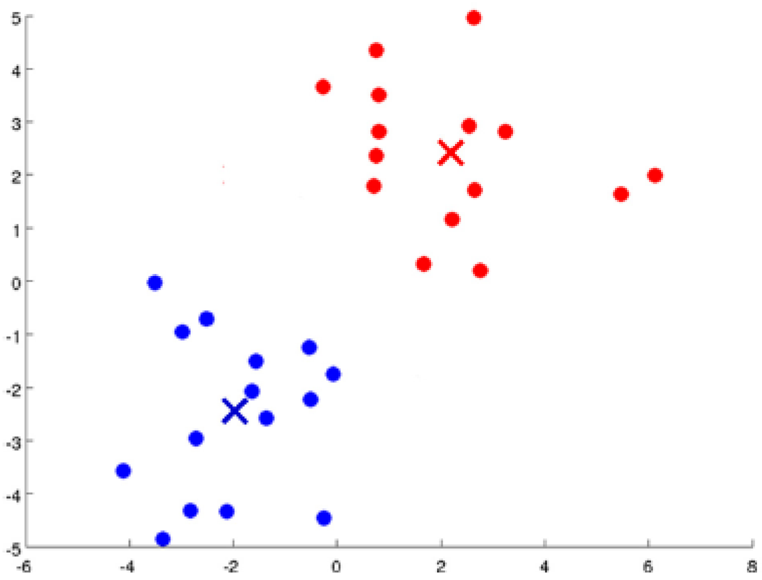
- Move centroids to mean of all points assigned to cluster k

- Repeat until convergence
  - A possible convergence criteria: cluster centers do not change anymore

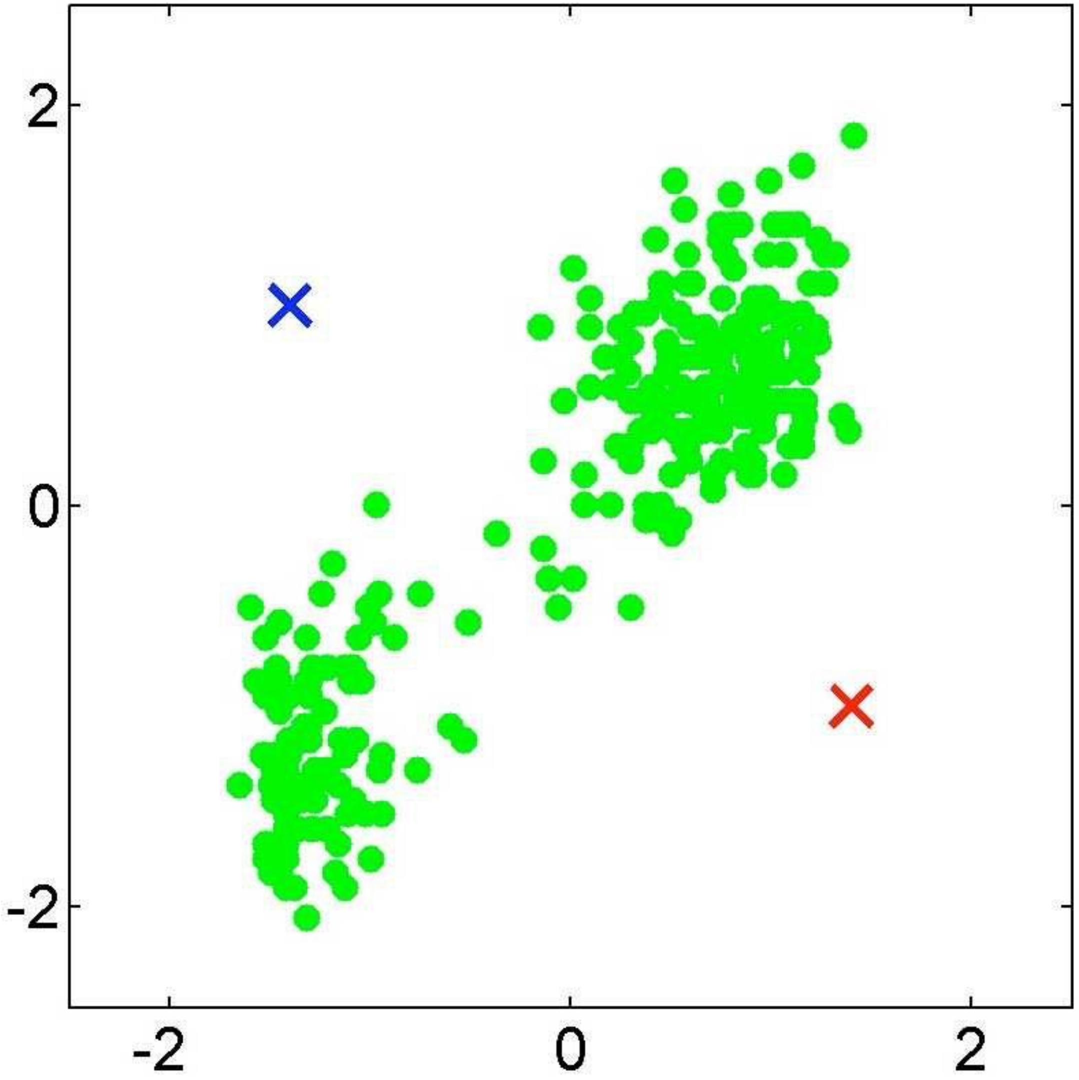
K-means: (Iterative) Algorithm

3) Output

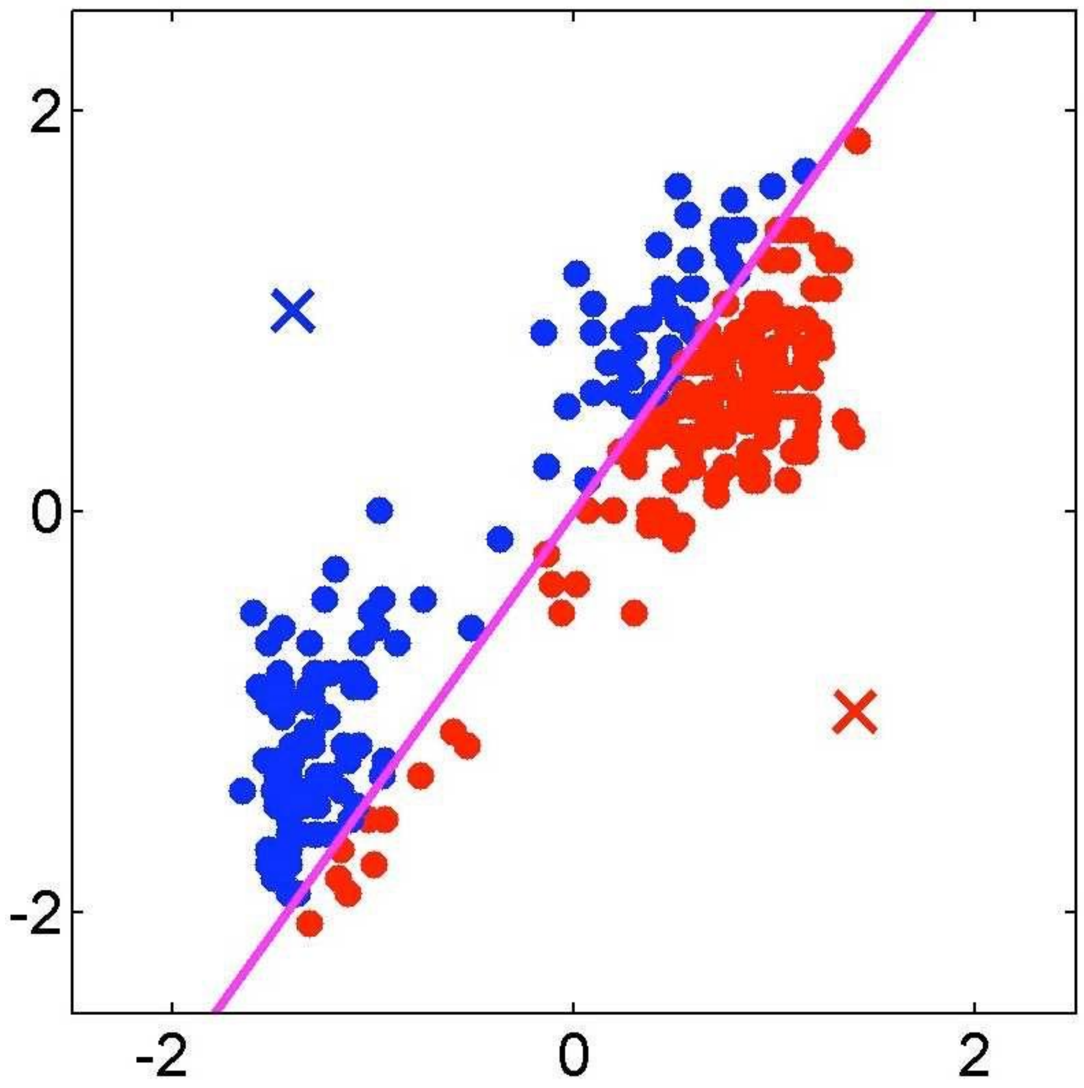
- c (label) : index (1 to k) of cluster centroid (centers)
- μ: averages (mean) of points assigned to cluster $\{\mu_1, \mu_2, \cdots, \mu_k\}$



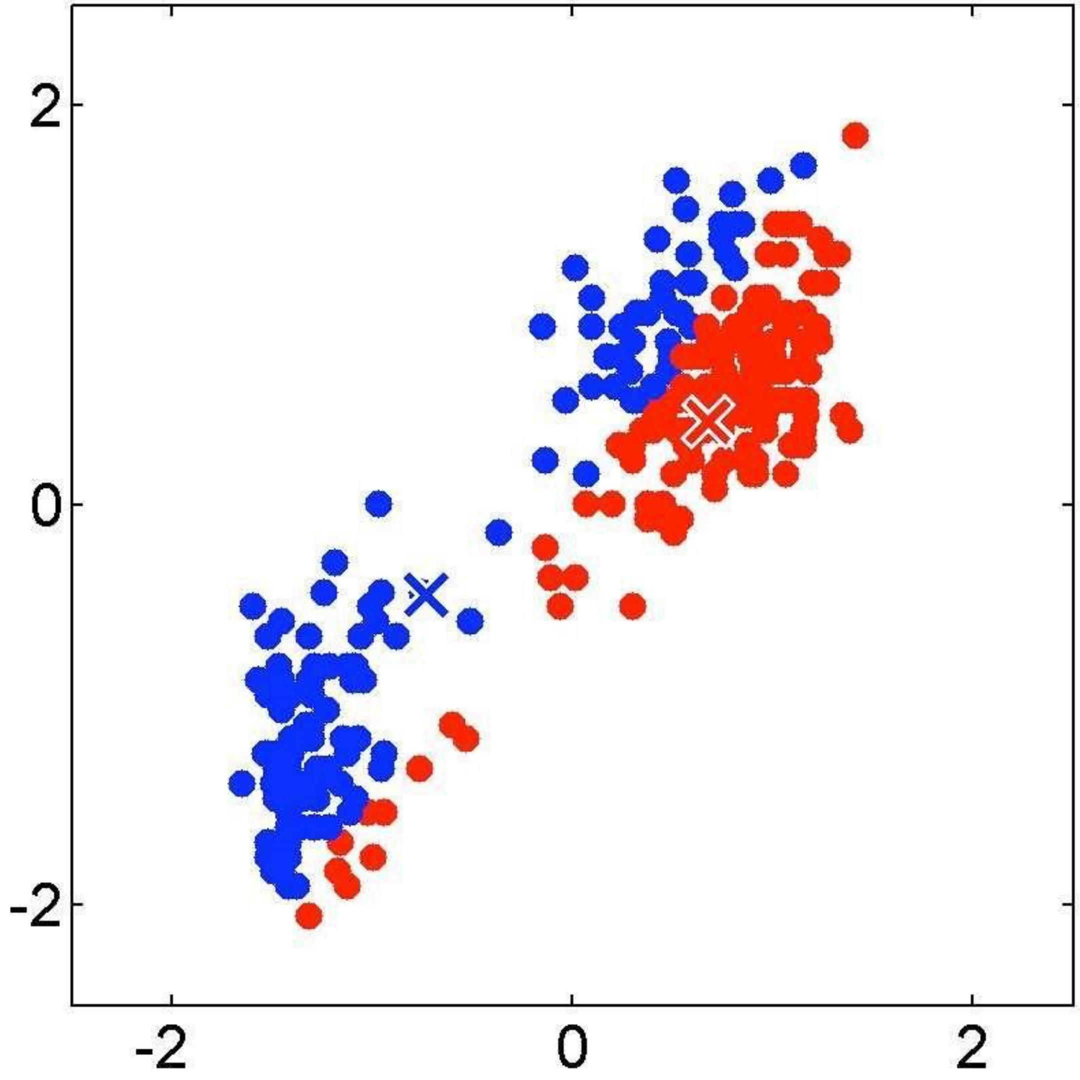
Initialization ($k = 2$)



Assigning Points



Recomputing the Cluster Centers



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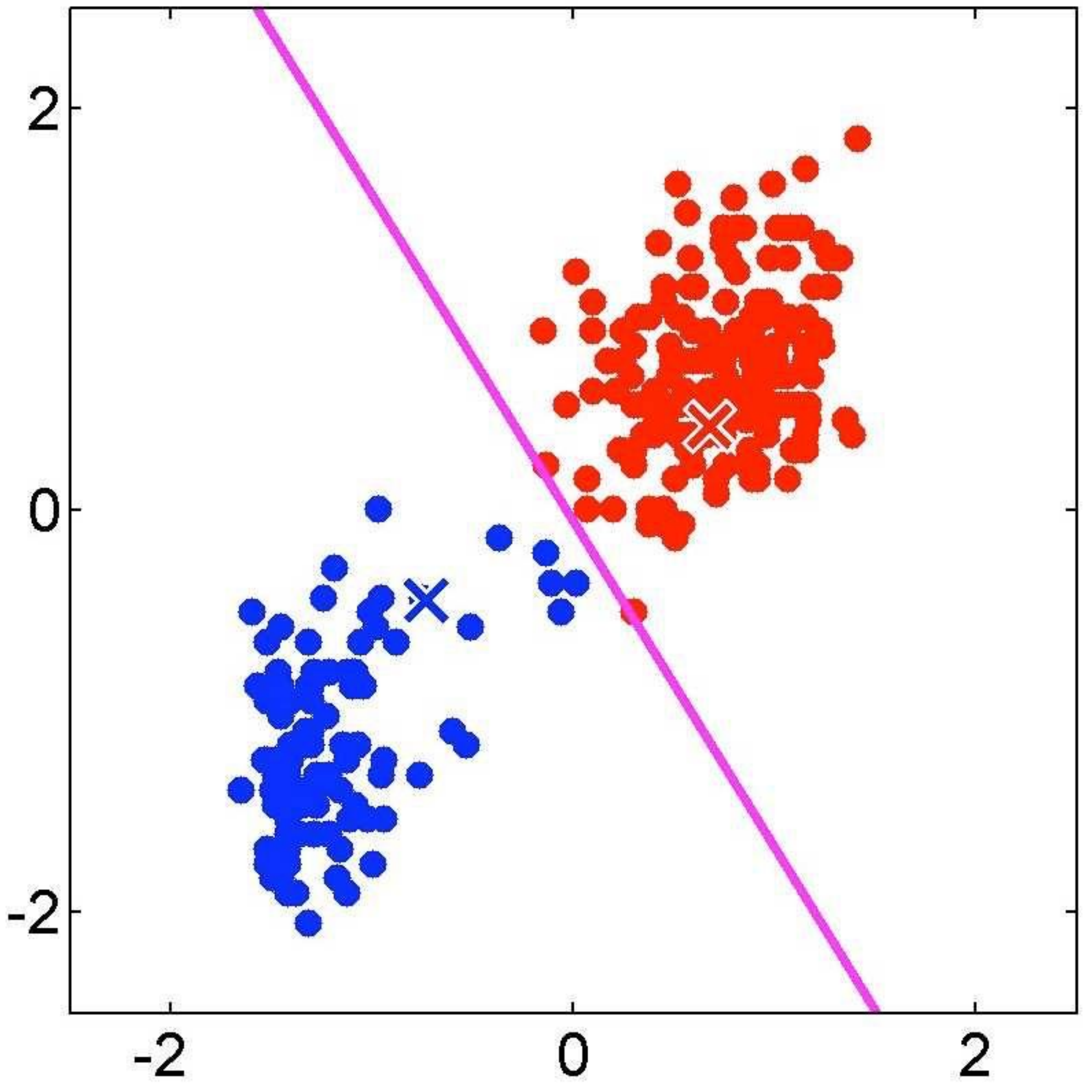

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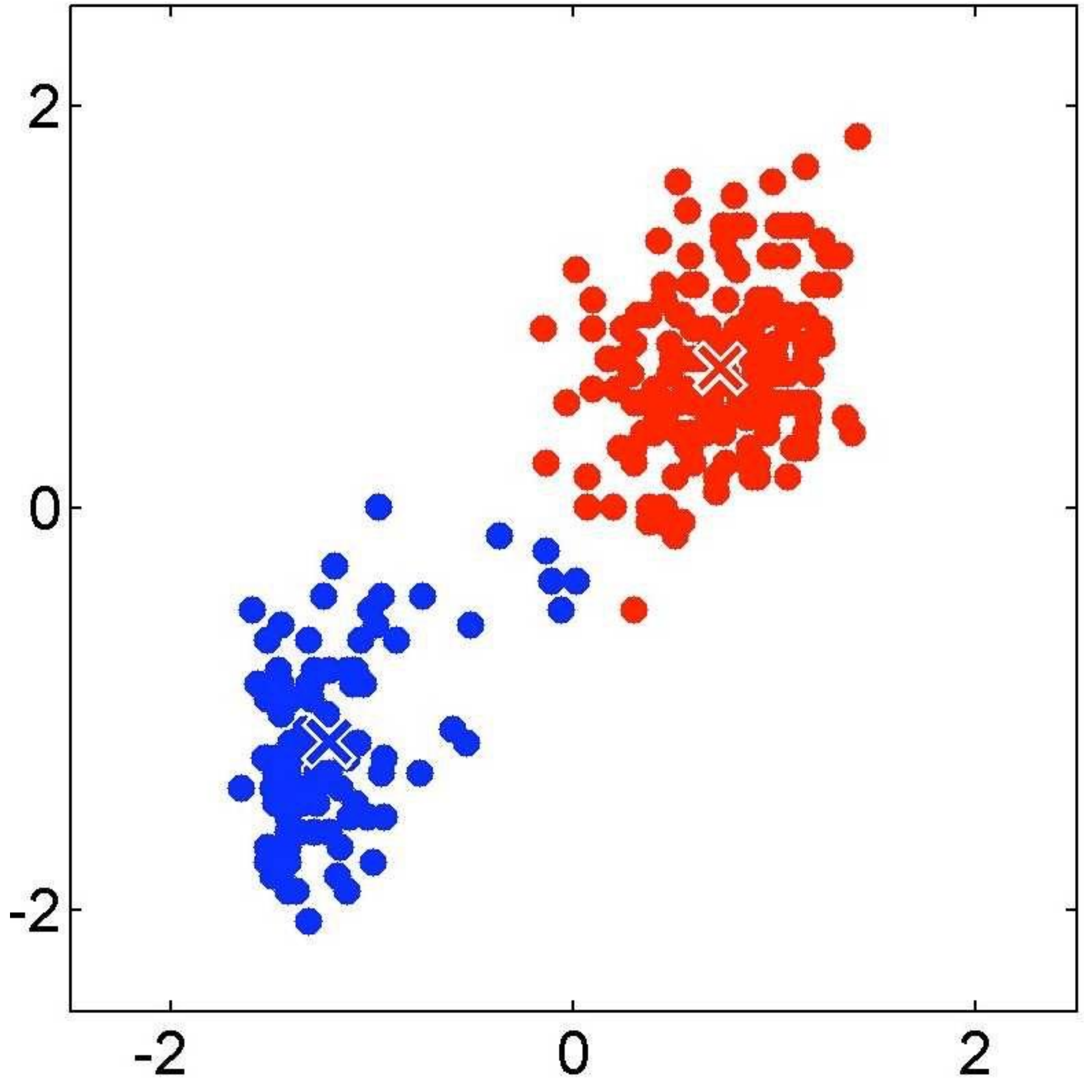

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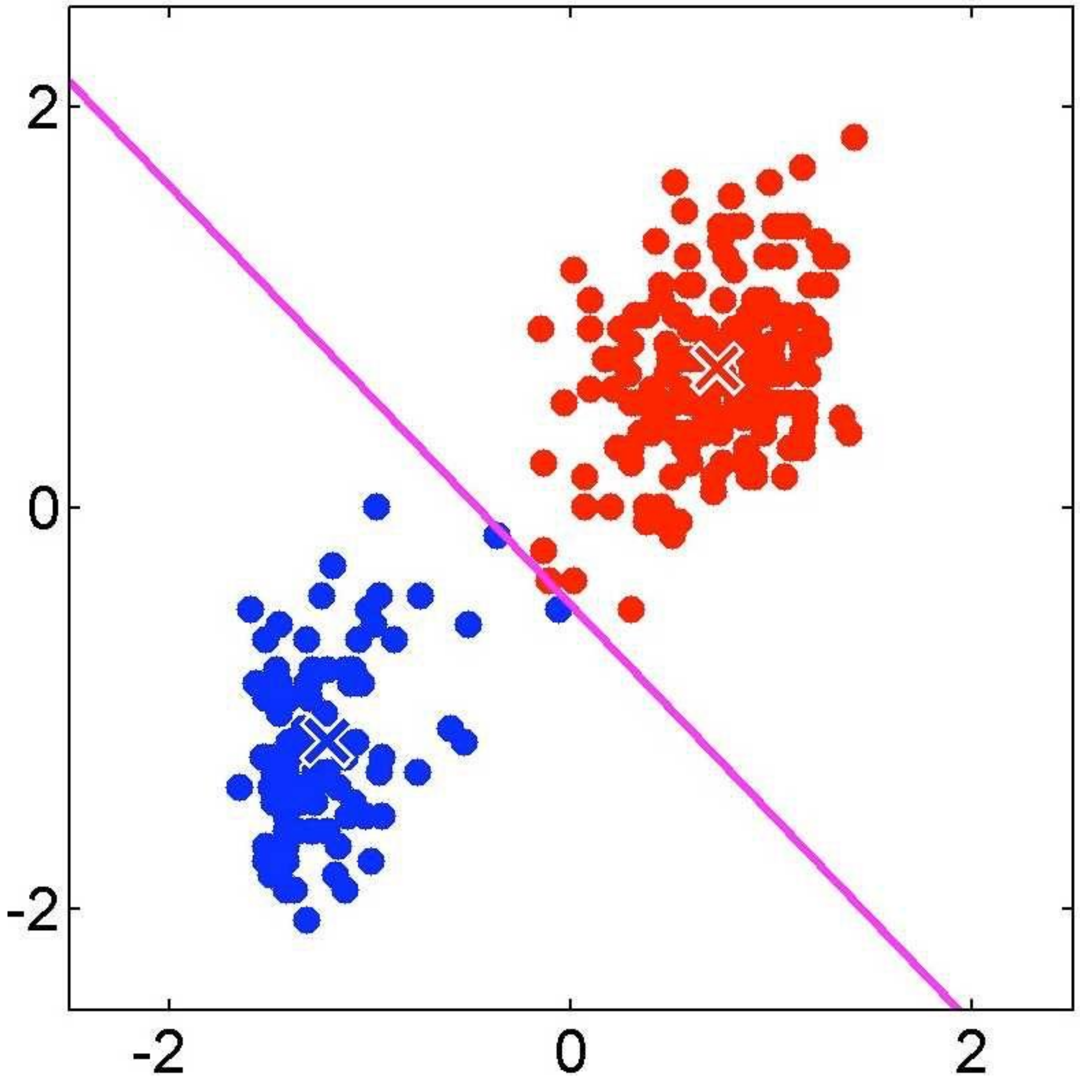

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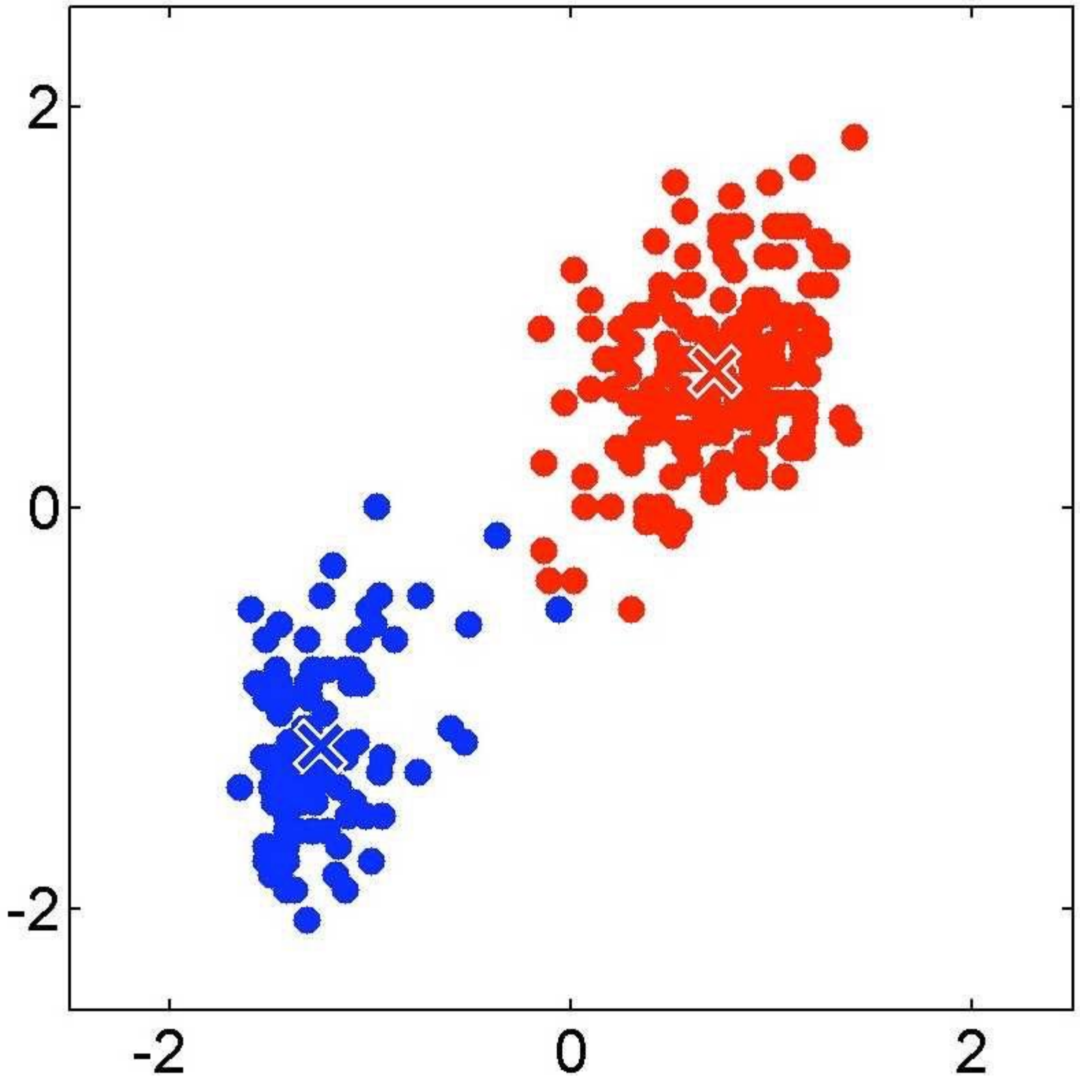

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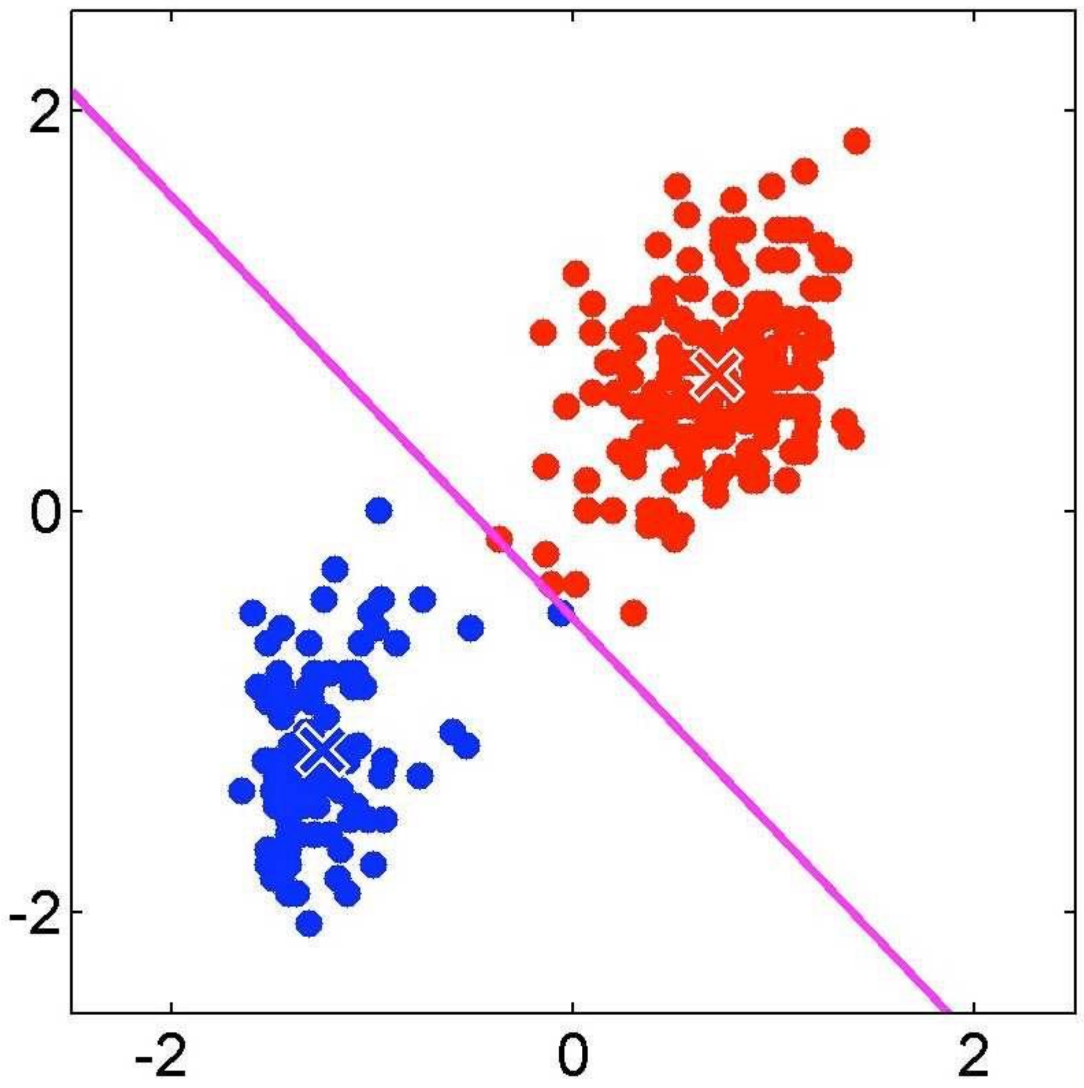
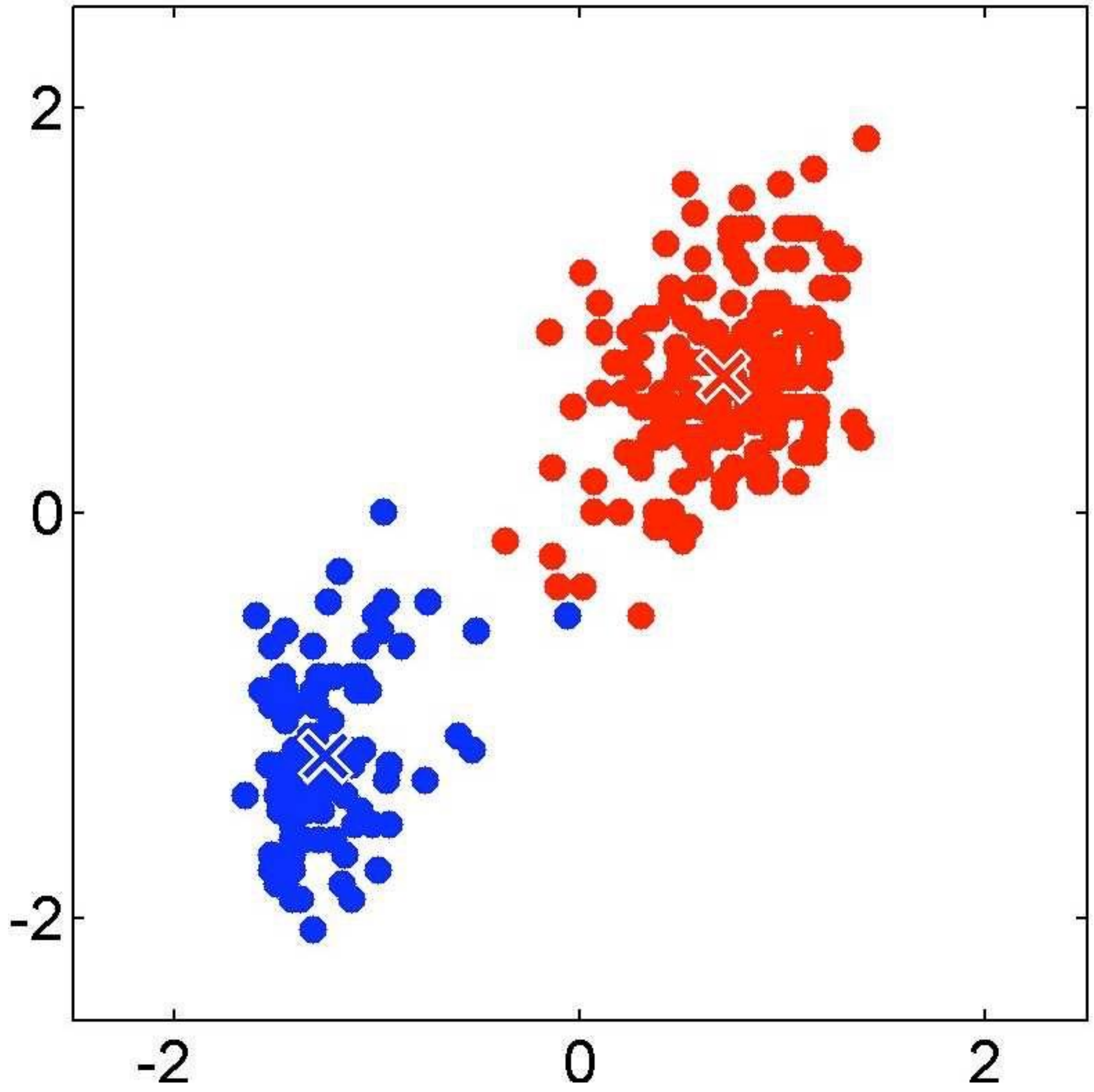


Recomputing the Cluster Centers



Summary: K-means Clustering

- (Iterative) Algorithm

Randomly initialize k cluster centroids $\mu_1, \mu_2, \cdots, \mu_k \in \mathbb{R}^n$

Repeat {

for $i = 1$ to m

$c_i :=$ index (from 1 to k) of cluster centroid closest to $x^{(i)}$

for $k = 1$ to k

$\mu_k :=$ average (mean) of points assigned to cluster k

}

K-means: Optimization Point of View (Optional)

- c_i = index of cluster $(1, 2, \cdots, k)$ to which example $x^{(i)}$ is currently assigned
- μ_k = cluster centroid
- μ_{c_i} = cluster centroid of cluster to which example $x^{(i)}$ has been assigned

- Optimization objective:

$$J(c_1, \cdots, c_m, \mu_1, \cdots, \mu_k) = \frac{1}{m} \sum_{i=1}^{m} \|x^{(i)} - \mu_{c_i}\|^2$$

$$\min_{c_1, \cdots, c_m,\ \mu_1, \cdots, \mu_k} J(c_1, \cdots, c_m, \mu_1, \cdots, \mu_k)$$

Expectation Maximization (EM) Algorithm

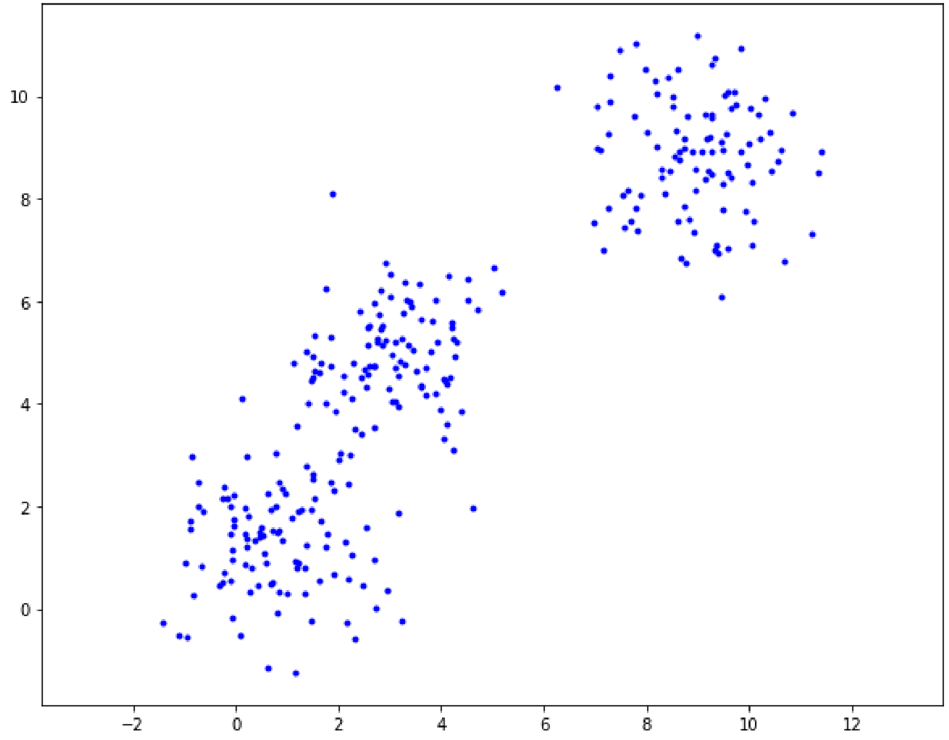
- It is a "chicken and egg" problem (dilemma)
  - Q: if we knew c_is, how would we determine which points to associate with each cluster center?
  - A: for each point $x^{(i)}$, choose closest c_i

  - Q: if we knew the cluster memberships, how do we get the centers?
  - A: choose c_i to be the mean of all points in the cluster

- Extension of K-means algorithm
  - A special case of Expectation Maximization (EM) algorithm
  - A special case of Gaussian Mixture Model (GMM)
  - Won’t be discussed in this course

Python: Data Generation

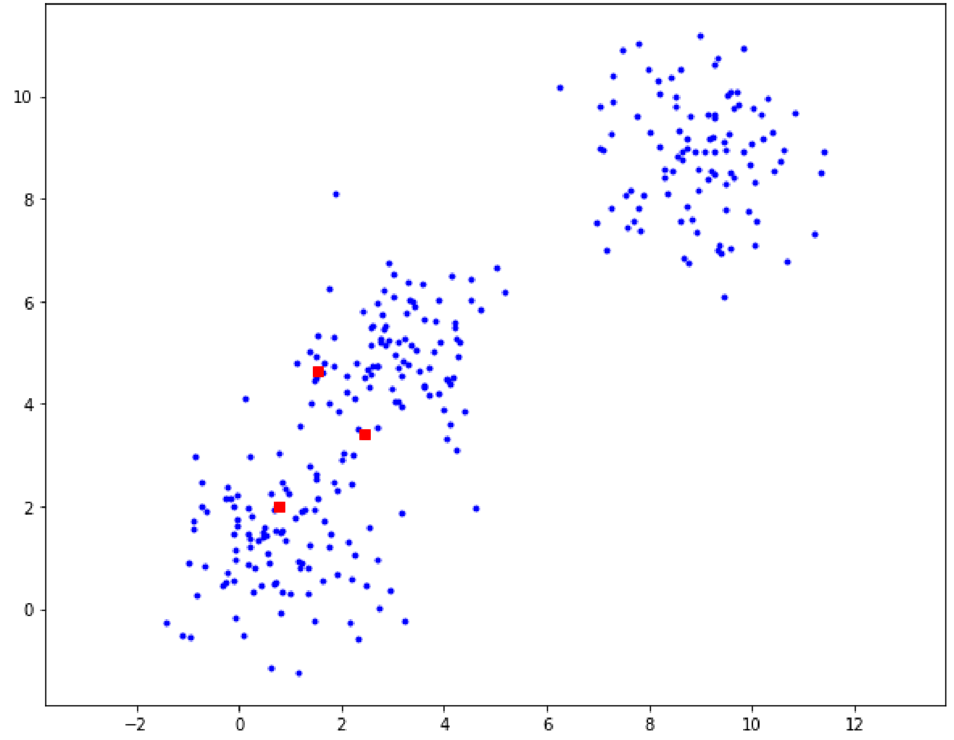
```python
# data generation
G0 = np.random.multivariate_normal([1, 1], np.eye(2), 100)
G1 = np.random.multivariate_normal([3, 5], np.eye(2), 100)
G2 = np.random.multivariate_normal([9, 9], np.eye(2), 100)

X = np.vstack([G0, G1, G2])
```



Python: Data Generation and Random Initialization

```
# data generation
G0 = np.random.multivariate_normal([1, 1], np.eye(2), 100)
G1 = np.random.multivariate_normal([3, 5], np.eye(2), 100)
G2 = np.random.multivariate_normal([9, 9], np.eye(2), 100)

X = np.vstack([G0, G1, G2])
```

```
# The number of clusters and data
k = 3
m = X.shape[0]

# ramdomly initialize mean points
mu = X[np.random.randint(0, m, k), :]
```



Python: K-Means

Randomly initialize k cluster centroids $\mu_1, \mu_2, \cdots, \mu_k \in \mathbb{R}^n$

Repeat {

for $i = 1$ to m

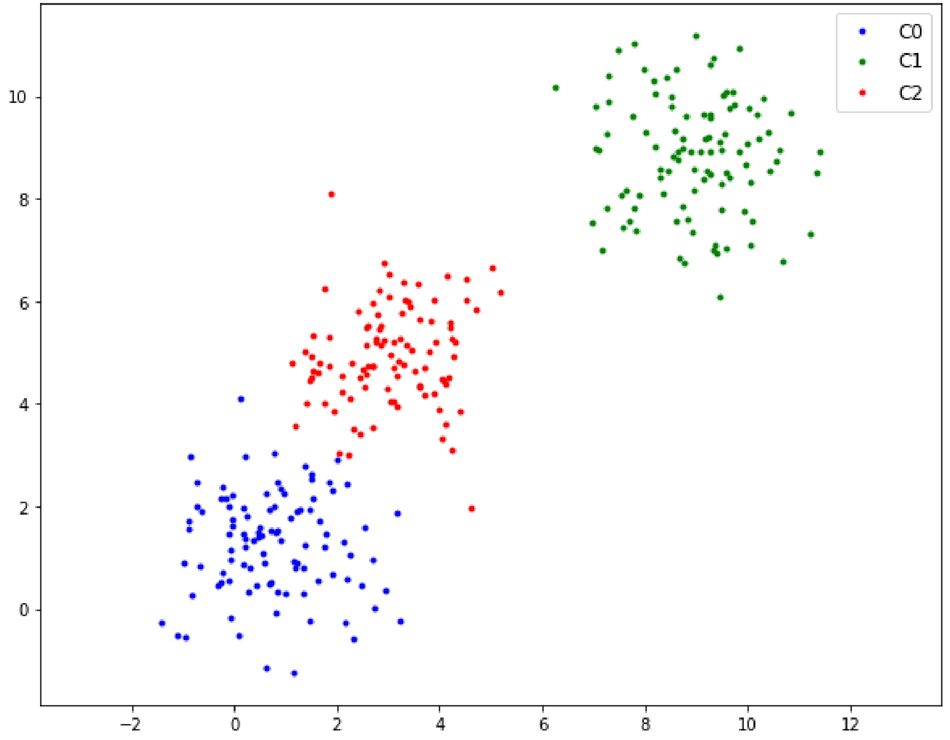
$c_i :=$ index (from 1 to k) of cluster centroid closest to $x^{(i)}$

for $k = 1$ to k

$\mu_k :=$ average (mean) of points assigned to cluster k

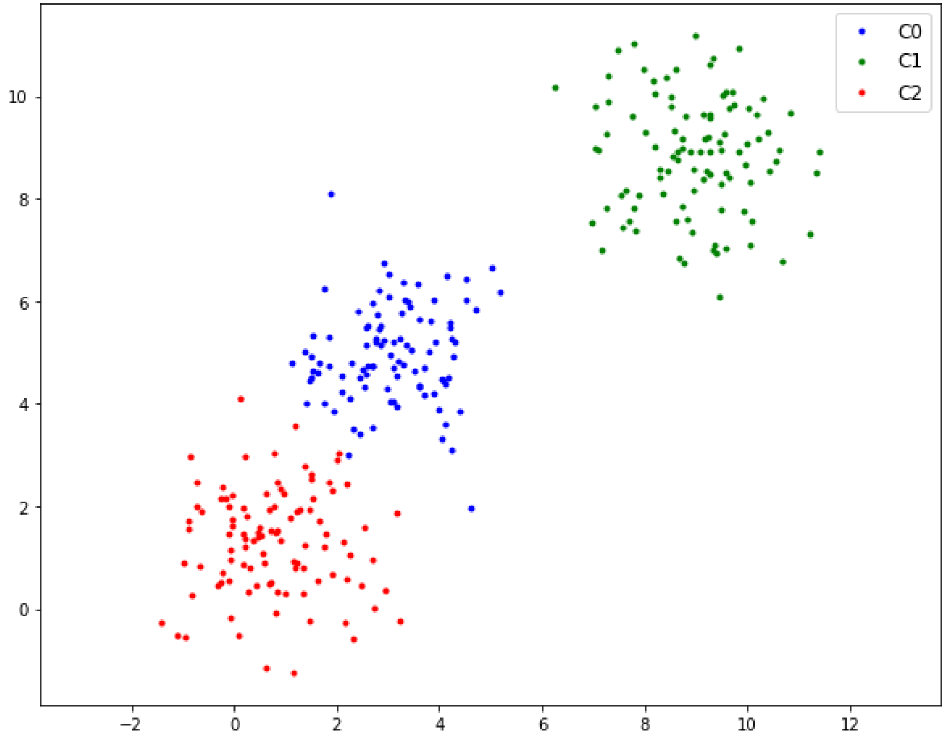
}

```
y = np.empty([m,1])

# Run K-means
for n_iter in range(500):
    for i in range(m):
        d0 = np.linalg.norm(X[i,:] - mu[0,:], 2)
        d1 = np.linalg.norm(X[i,:] - mu[1,:], 2)
        d2 = np.linalg.norm(X[i,:] - mu[2,:], 2)

        y[i] = np.argmin([d0, d1, d2])

    err = 0
    for i in range(k):
        mu[i,:] = np.mean(X[np.where(y == i)[0]], axis = 0)
        err += np.linalg.norm(pre_mu[i,:] - mu[i,:], 2)

    pre_mu = mu.copy()

    if err < 1e-10:
        print("Iteration:", n_iter)
        break
```



Python: K-Means in Scikit-learn

```
# use kmeans from the scikit-learn module

from sklearn.cluster import KMeans

kmeans = KMeans(n_clusters = 3, random_state = 0)
kmeans.fit(X)

plt.figure(figsize = (10,8))
plt.plot(X[kmeans.labels_ == 0, 0],X[kmeans.labels_ == 0, 1], 'b.', label = 'C0')
plt.plot(X[kmeans.labels_ == 1, 0],X[kmeans.labels_ == 1, 1], 'g.', label = 'C1')
plt.plot(X[kmeans.labels_ == 2, 0],X[kmeans.labels_ == 2, 1], 'r.', label = 'C2')
plt.axis('equal')
plt.legend(fontsize = 12)
plt.show()
```



Initialization Issues

- k-means is extremely sensitive to cluster center initialization

- Bad initialization can lead to
  - Poor convergence speed
  - Bad overall clustering

- Safeguarding measures:
  - Choose first center as one of the examples, second which is the farthest from the first, third which is the farthest from both, and so on.
  - Try multiple initialization and choose the best result

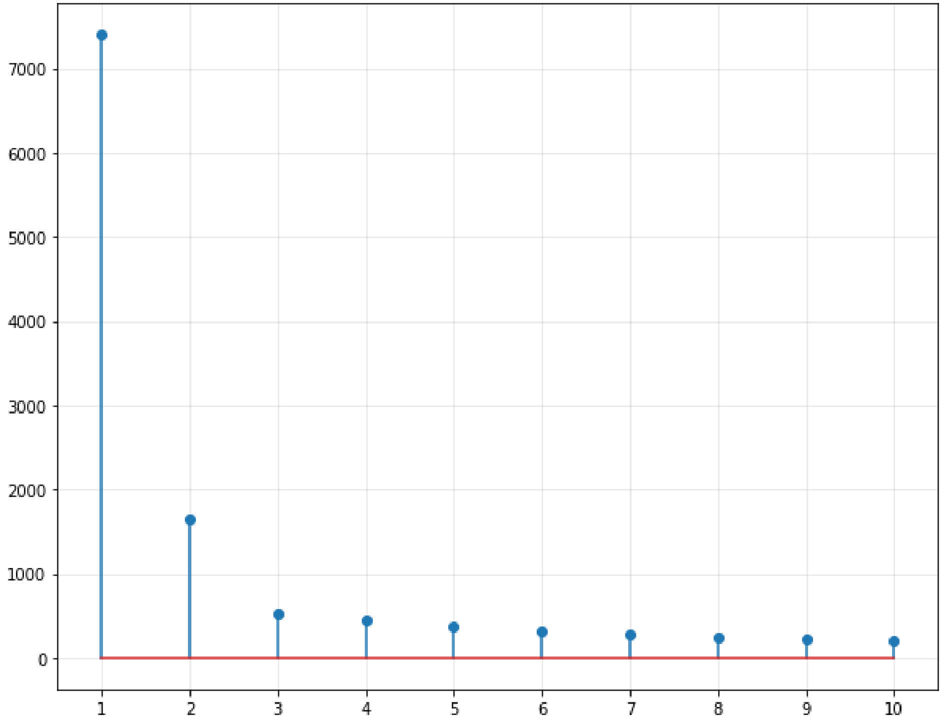
Choosing the Number of Clusters

- Idea: when adding another cluster does not give much better modeling of the data

- One way to select k for the K-means algorithm is to try different values of k, plot the K-means objective versus k, and look at the 'elbow-point' in the plot

Choosing the Number of Clusters

```
cost = []
for i in range(1,11):
    kmeans = KMeans(n_clusters = i, random_state = 0).fit(X)
    cost.append(abs(kmeans.score(X)))
```



K-means: Limitations

- Make hard assignments of points to clusters
  - A point either completely belongs to a cluster or not belongs at all
  - No notion of a soft assignment (*i.e.*, probability of being assigned to each cluster)
  - Gaussian mixture model (we will study later) and Fuzzy K-means allow soft assignments

- Sensitive to outlier examples
  - K-medians algorithm is a more robust alternative for data with outliers

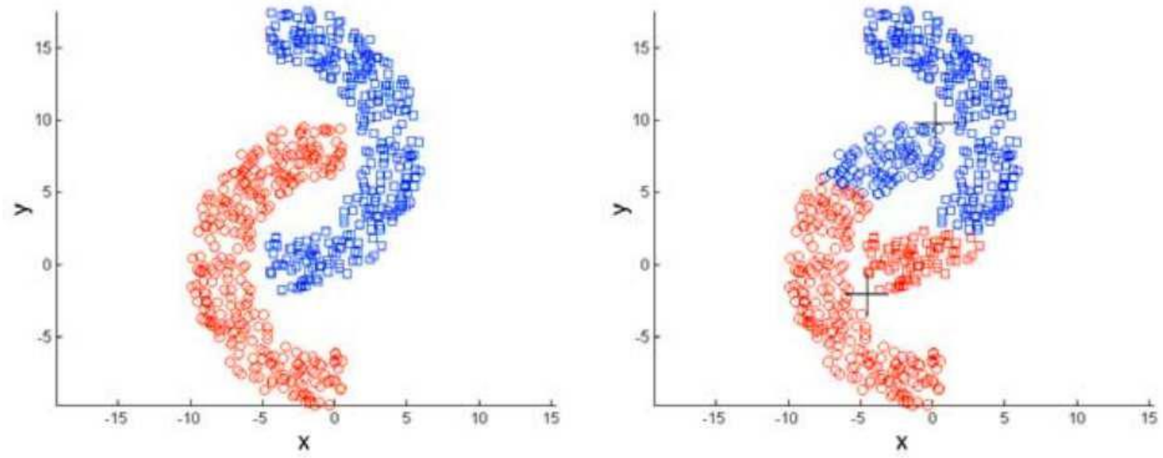
K-means: Limitations

- Works well only for round shaped, and of roughly equal sizes/density cluster

- Does badly if the cluster have non-convex shapes
  - Spectral clustering (we will study later) and Kernelized K-means can be an alternative

K-means: Limitations

- Non-convex/non-round-shaped cluster: standard K-means fails !



- (optional) Connectivity → networks → spectral partitioning

K-means: Limitations

- Clusters with different densities