Clustering

Introduction to Data Science
University of Colorado Boulder
SLIDES ADAPTED FROM LAUREN HANNAH

Clustering Lab

- Review of k-means
- Work through k-means example
- Connection to GMM

k-means

procedure KMeans(X, M)
  $s \leftarrow \infty$
  $Z \leftarrow \text{AssignToClosestCluster}(X, M)$
  while $s > \text{Score}(X, Z, M)$ **do** ▷ Iterate until score stops changing
    $s \leftarrow \text{Score}(X, Z, M)$ ▷ Compute score for old configuration
    $Z \leftarrow \text{AssignToClosestCluster}(X, M)$
    for $k \in \{1, \dots, K\}$ **do** ▷ For each cluster mean
      $v \leftarrow 0, \mu_k \leftarrow \vec{0}$
      for $i \in \{1, \dots, N\}$ **do** ▷ For each observation
        if $z_i = k$ **then** ▷ If the observation is assigned to cluster k
          $\mu_k \leftarrow \mu_k + x_i$ ▷ Add observation to sum
          $v \leftarrow v + 1$ ▷ Count points in cluster k
      $\mu_k \leftarrow \frac{\mu_k}{v}$ ▷ Divide by number of observations
  return Z

Score

procedure Score(X, Z, M) ▷ Current objective function

  $s \leftarrow 0$

  for $i \in \{1, \ldots, N\}$ **do** ▷ For each observation

    $s \leftarrow s + ||x_i - \mu_{z_i}||$ ▷ Accumulate how far it is from its mean

Find closest

procedure AssignToClosestCluster(X, M)

  $Z \leftarrow$ Vector(N) ▷ Initialize assignments Z as a N-vector

  for $i \in \{1, \ldots, N\}$ **do** ▷ For each observation

    $d \leftarrow -\infty$

    for $k \in \{1, \ldots, K\}$ **do**

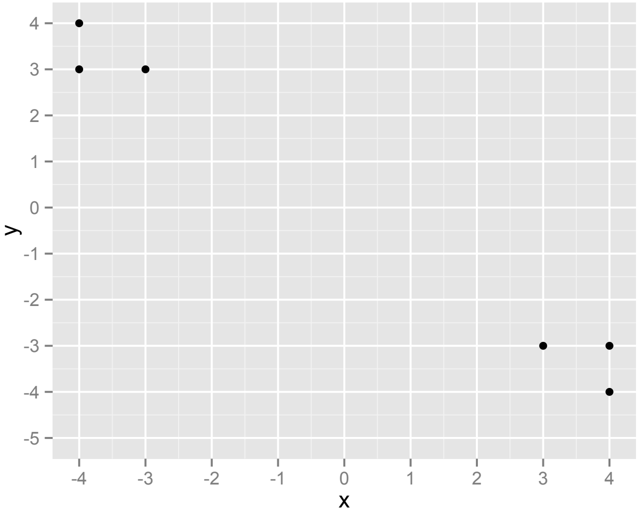
      if $||x_i - \mu_k|| < d$ **then**

        $z_i \leftarrow k$

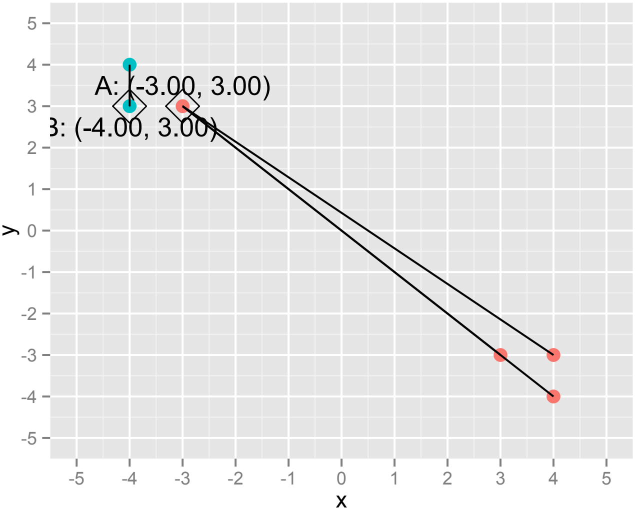
        $d < -||x_i - \mu_k||$

  return Z

Two Points



Two Points



Two Points

$$\mu_A = \frac{1}{4}\left((-3,3)+(3,-3)+(4,-3)+(4,-4)\right)$$

$$=$$

$$\mu_B = \frac{(-4,3)+(-4,4)}{2}$$

$$=$$

Two Points

$$\mu_A = \frac{1}{4}\left((-3,3)+(3,-3)+(4,-3)+(4,-4)\right)$$

$$= (2,-1.75)$$

$$\mu_B = \frac{(-4,3)+(-4,4)}{2}$$

$$=$$

Two Points

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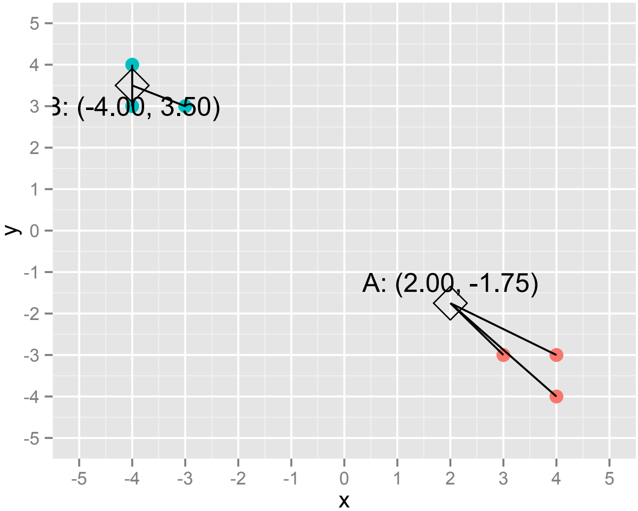
$$= (2,-1.75)$$

$$\mu_B = \frac{(-4,3)+(-4,4)}{2}$$

$$= (-4,3.5)$$

Two Points



Two Points

$$\mu_A = \frac{(3,-3)+(4,-3)+(4,-4)}{3}$$

$$=$$

$$\mu_B = \frac{(-4,3)+(-4,4)+(-3,3)}{3}$$

$$=$$

Two Points

$$\mu_A = \frac{(3,-3)+(4,-3)+(4,-4)}{3}$$

$$= (3.67,-3.33)$$

$$\mu_B = \frac{(-4,3)+(-4,4)+(-3,3)}{3}$$

$$=$$

Two Points

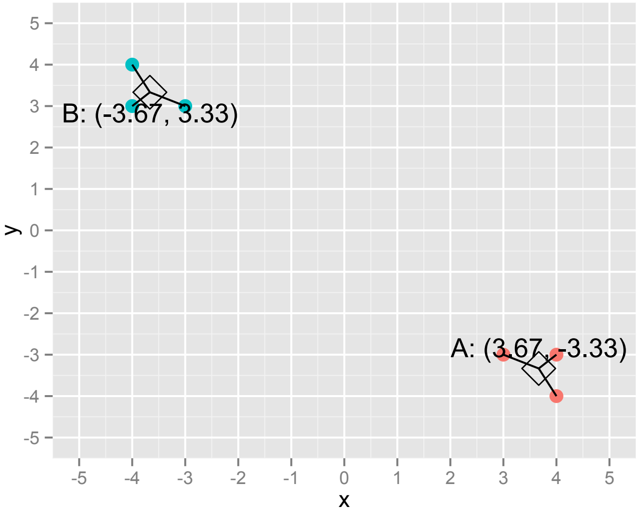
$$\mu_A = \frac{(3,-3)+(4,-3)+(4,-4)}{3}$$

$$= (3.67,-3.33)$$

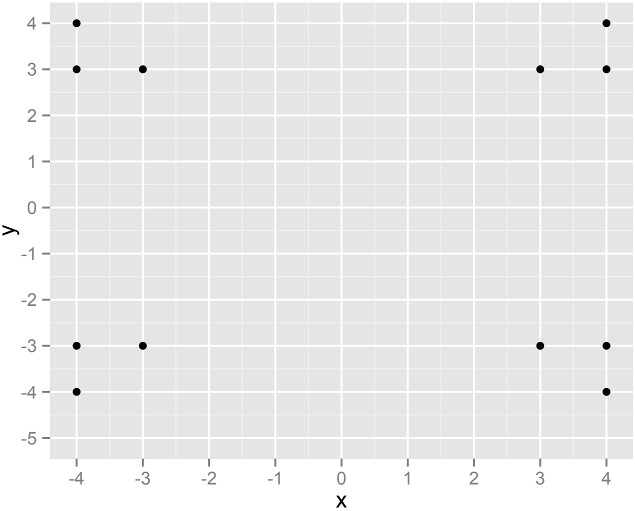
$$\mu_B = \frac{(-4,3)+(-4,4)+(-3,3)}{3}$$

$$= (-3.67,3.33)$$

Two Points



Four Points



Four Points

The observation at $(3,3)$ is the same distance from μ_A and μ_C. If you look at Line 10 in the algorithm, the **first** mean with the smallest distance gets the assignment. So $(3,3)$ gets assigned to cluster A.

$$\mu_A =$$

$$\mu_B =$$

$$\mu_C =$$

$$\mu_D =$$

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$$\mu_A = (-1,1)$$
$$\mu_B =$$
$$\mu_C =$$
$$\mu_D =$$

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$$\mu_B = (-4,0)$$
$$\mu_C =$$
$$\mu_D =$$

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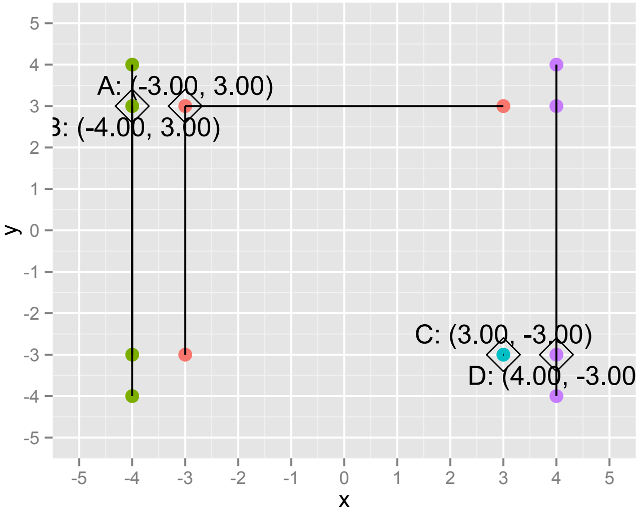
$$\mu_A = (-1, 1)$$
$$\mu_B = (-4, 0)$$
$$\mu_C = (3, -3)$$
$$\mu_D =$$

Four Points

The observation at $(3,3)$ is the same distance from μ_A and μ_C. If you look at Line 10 in the algorithm, the **first** mean with the smallest distance gets the assignment. So $(3,3)$ gets assigned to cluster A.

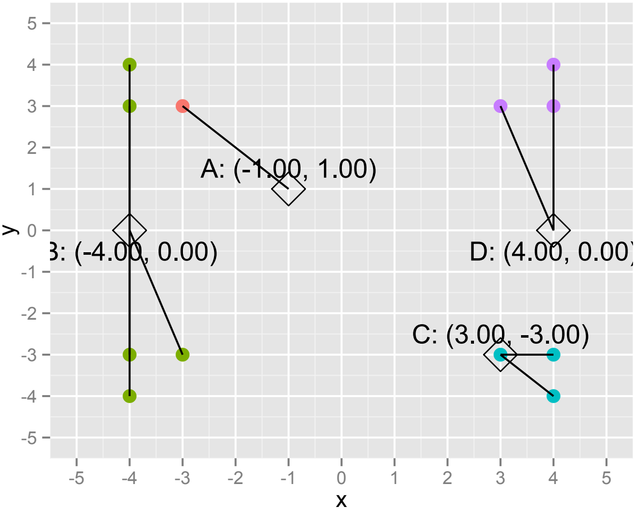
$$\mu_A = (-1,1)$$
$$\mu_B = (-4,0)$$
$$\mu_C = (3,-3)$$
$$\mu_D = (4,0)$$

Four Points



A: (-3.00, 3.00)
3: (-4.00, 3.00)
C: (3.00, -3.00)
D: (4.00, -3.00
y
x
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2
3
4
5

Four Points



Four Points

$$\mu_A =$$

$$\mu_B =$$

$$\mu_C =$$

$$\mu_D =$$

Four Points

$$\mu_A = (-3, 3)$$
$$\mu_B =$$
$$\mu_C =$$
$$\mu_D =$$

Four Points

$$\mu_A = (-3, 3)$$
$$\mu_B = (-3.8, -0.6)$$
$$\mu_C =$$
$$\mu_D =$$

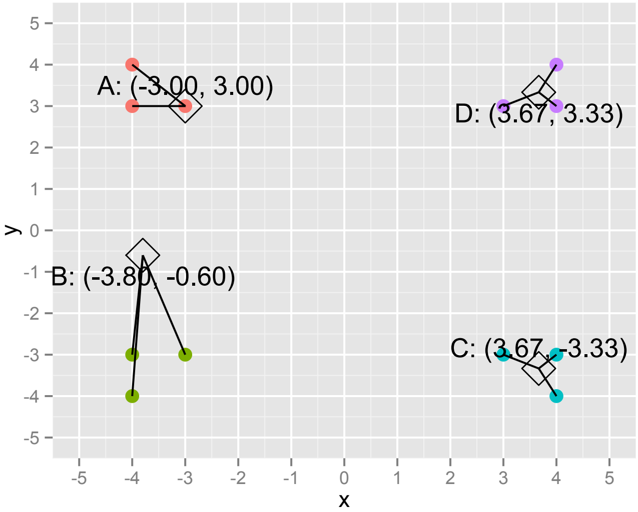
Four Points

$$\mu_A = (-3, 3)$$
$$\mu_B = (-3.8, -0.6)$$
$$\mu_C = (3.67, -3.33)$$
$$\mu_D =$$

Four Points

$$\mu_A = (-3, 3)$$
$$\mu_B = (-3.8, -0.6)$$
$$\mu_C = (3.67, -3.33)$$
$$\mu_D = (3.67, 3.33)$$

Four Points


A: (-3.00, 3.00)
D: (3.67, 3.33)
B: (-3.80, -0.60)
C: (3.67, -3.33)
y
x
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2
3
4
5

Four Points

$$\mu_A =$$
$$\mu_B =$$
$$\mu_C =$$
$$\mu_D =$$

Four Points

$$\mu_A = (-3.67, 3.33)$$
$$\mu_B =$$
$$\mu_C =$$
$$\mu_D =$$

Four Points

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$$\mu_B = (-3.67, -3.33)$$
$$\mu_C =$$
$$\mu_D =$$

Four Points

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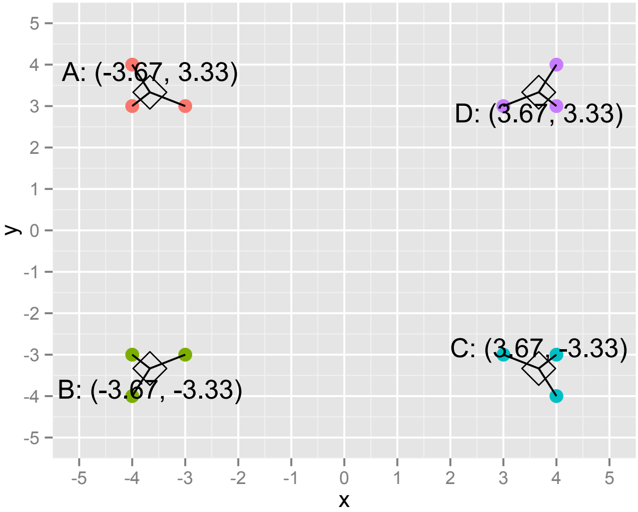
$$\mu_B = (-3.67, -3.33)$$
$$\mu_C = (3.67, -3.33)$$
$$\mu_D =$$

Four Points

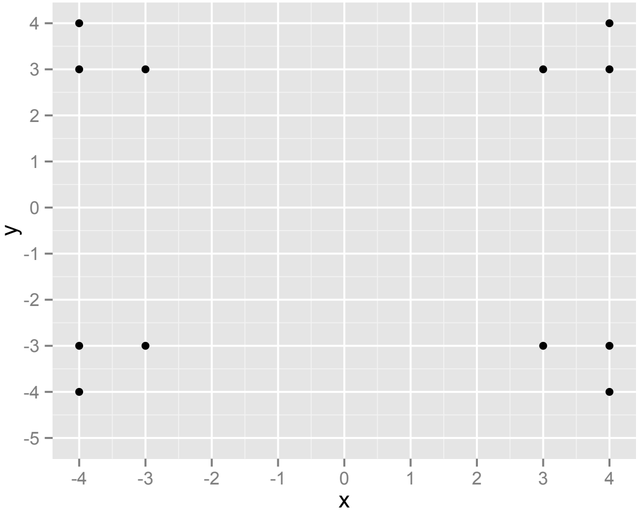
$$\mu_A = (-3.67, 3.33)$$
$$\mu_B = (-3.67, -3.33)$$
$$\mu_C = (3.67, -3.33)$$
$$\mu_D = (3.67, 3.33)$$

Four Points

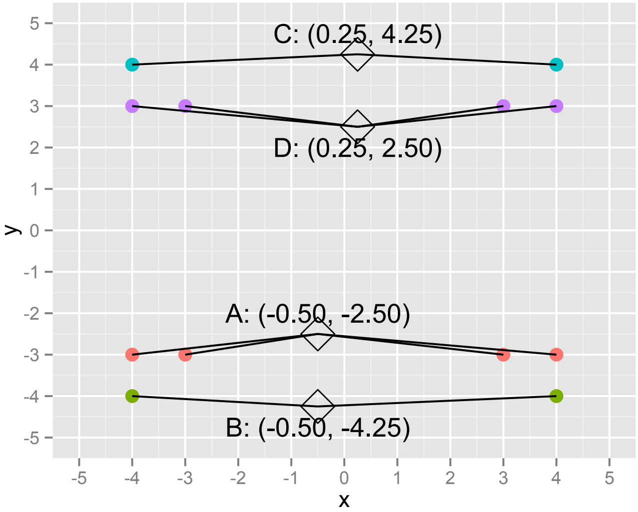


A: (-3.67, 3.33)
D: (3.67, 3.33)
B: (-3.67, -3.33)
C: (3.67, -3.33)
y
x
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
-4
-3
-2
-1
0
1
2
3
4
5

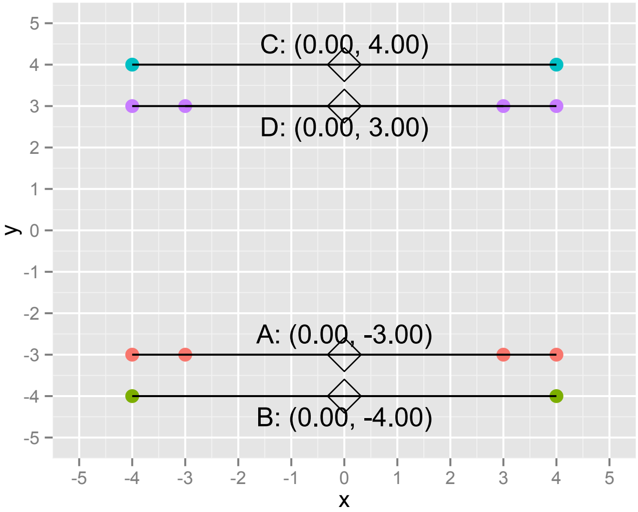
Bad Initialization



Bad Initialization



Bad Initialization



How does it change for GMM?

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Instead of just computing mean, you also compute variance.