Problem 2: Lack of optimality of K-Means

From the hint in the question, let $k=2$ for the dataset, with $\mu_1=2$, $\mu_2=4$

$m=4$

$k=2$

Assume towards a contradiction that these μ will converge towards a globally optimal solution.

K-Means

1. Distance from $x[i]$ to $\mu[k]$, $i \in [1,4]$, $k \in [1,2]$

$x[i]$	$\|x_i-\mu_1\|^2$	$\|x_i-\mu_2\|^2$
$i=1$	1	9
2	0	4
3	1	1
4	4	0

$d = \|x_i - \mu_k\|^2$
$= \left[\sqrt{(x_i-\mu_k)^2}\right]^2$
$= (x_i-\mu_k)^2$

2. Cluster assignment step: $c_i = \min_k \{\|x_i-\mu_k\|^2\}$

	$i=1$	$i=2$	$i=3$	$i=4$
$c[i]$	1	1	1	2

3. Move centroids: μ_k' = avg. of all $x[i]$ assigned to cluster k.

k	avg. value of $x[i]$	μ_k'
1	$\frac{1}{3}(1+2+3)$	2
2	4	4

Since $\mu_1' = \mu_1 = 2$ and $\mu_2' = \mu_2 = 2$, we stop the algorithm.

4. Calculate the distortion J.

$$J(c^{(1)}=1, c^{(2)}=1, c^{(3)}=1, c^{(4)}=2, \mu_1=2, \mu_2=4) = \frac{1}{4}\sum_{i=1}^{4} \|x^{(i)} - \mu_{c^{(i)}}\|^2$$

$$= \frac{1}{4}\left[(1-2)^2 + (2-2)^2 + (3-2)^2 + (4-4)^2\right]$$

$$= \frac{1}{4}(1+0+1+0)$$

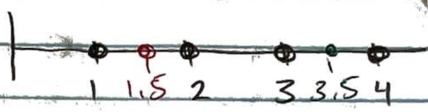
$$J = \frac{1}{2}$$

If $\mu_1=2$ and $\mu_2=4$ were the globally optimal solution, then $J=\frac{1}{2}$ should be the lowest value of the distortion for any other cluster centroids.

But we can achieve a lower distortion if we pick different initializations:

$\mu_1' = 2$

$\mu_2' = 3$



K-Means

1. Distance

i	$\|x_i - \mu_1\|^2$	$\|x_i - \mu_2\|^2$
1	1	4
2	0	1
3	1	0
4	4	1

i	$\|x_i - \mu_1\|^2$	$\|x_i - \mu_2\|^2$
1	0.25	6.25
2	0.25	2.25
3	2.25	0.25
4	6.25	0.25

2. Cluster assignment

	$i=1$	$i=2$	$i=3$	$i=4$
$c[i]$	1	1	2	2

	$i=1$	$i=2$	$i=3$	$i=4$
$c[i]$	1	1	2	2

3. Move centroid

k	avg. value of $x[i]$	μ_k''
1	$\frac{1}{2}(1+2) = 1.5$	1.5
2	$\frac{1}{2}(3+4) = 3.5$	3.5

Since $\mu_k'' \neq \mu_k'$, repeat the algorithm with the new values of μ_k

k	avg. value of $x[i]$	μ_k''
1	$\frac{1}{2}(1+2) = 1.5$	1.5
2	$\frac{1}{2}(3+4) = 3.5$	3.5

Since $\mu_k'' = \mu_k'$, we stop K-means.

4. Calculate the distortion, J'.

$$J'(c^{(1)}=1, c^{(2)}=1, c^{(3)}=2, c^{(4)}=2, \mu_1=1.5, \mu_2=3.5) = \frac{1}{4}\sum_{i=1}^{4} \|x^{(i)} - \mu_{c^{(i)}}\|^2$$

$$= \frac{1}{4}\left[(1-1.5)^2 + (2-1.5)^2 + (3-3.5)^2 + (4-3.5)^2\right]$$

$$= \frac{1}{4}\left[4(0.5)^2\right]$$

$$= 0.25$$

$$J' = \frac{1}{4}.$$

Since $J' = \frac{1}{4} < J = \frac{1}{2}$, the cluster assignment $\mu_1' = 1.5$, $\mu_2' = 3.5$ is more optimal than $\mu_1 = 2$, $\mu_2 = 4$. But k-means converged for $\mu_1 = 2$, $\mu_2 = 4$, implying that this was a global optimum. This is a contradiction $\square$.