Multivariate Analysis (slides 9)

- Today we consider k-means clustering.
- We will address the question of selecting the appropriate number of clusters.
- Properties and limitations of the algorithm will be explored.

k-means clustering

- The aim is to divide the data into k distinct groups so that observations within a group are similar, whilst observations between groups are different.
- *k-means clustering* is an iterative, rather than a hierarchical, clustering algorithm.
- This means that at each stage of the algorithm data points will be assigned to a fixed number of clusters (contrast with hierarchical clustering where the number of clusters ranges from the number of data points down to a single cluster).
- We will discuss ways of selecting an appropriate k from a statistical viewpoint, but there may be expert knowledge as to the appropriate number of clusters.
- Alternatively, there may be previous results from preliminary data exploration, *i.e.*, we could start the k-means algorithm at the result of a hierarchical clustering.

k-means clustering

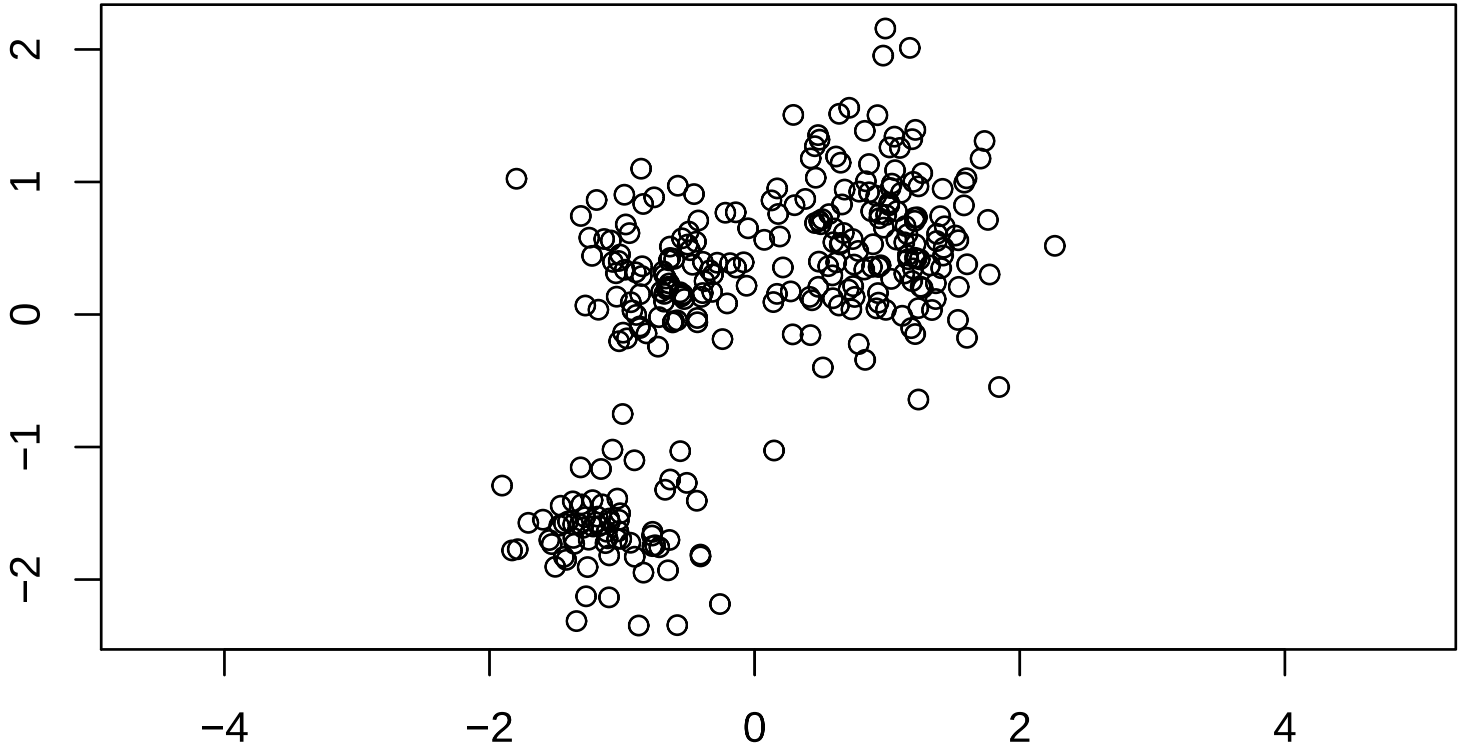
- It is simple and computationally efficient, but can sometimes be sensitive to the selection of starting points.
- Running the k-means algorithm several times for different starting values can help check whether results are robust.
- We will see an example of the problems this can cause.

Pseudo code

1. Choose the number of clusters k and designate cluster centers.
2. Assign each data point to the cluster whose center is closest.
3. For cluster i, calculate its centroid $C_i^T = (C(i)_1, C(i)_2, \ldots, C(i)_m)$, where m denotes the number of variables in an observation (these are found by averaging variables scores for data points within the cluster).
4. Calculate the **sum of squared distances of each object to its cluster centroid**:
$$\text{SS} = \sum_{i=1}^{n} \sum_{j=1}^{m} (x_{ij} - C(i)_j)^2$$
Here we assume a total of n observations. We want the SS value to be as small as possible.
5. Re-assign each observation to the cluster whose centroid is closest.
6. Repeat (3)-(5) until convergence.

Simulated Data

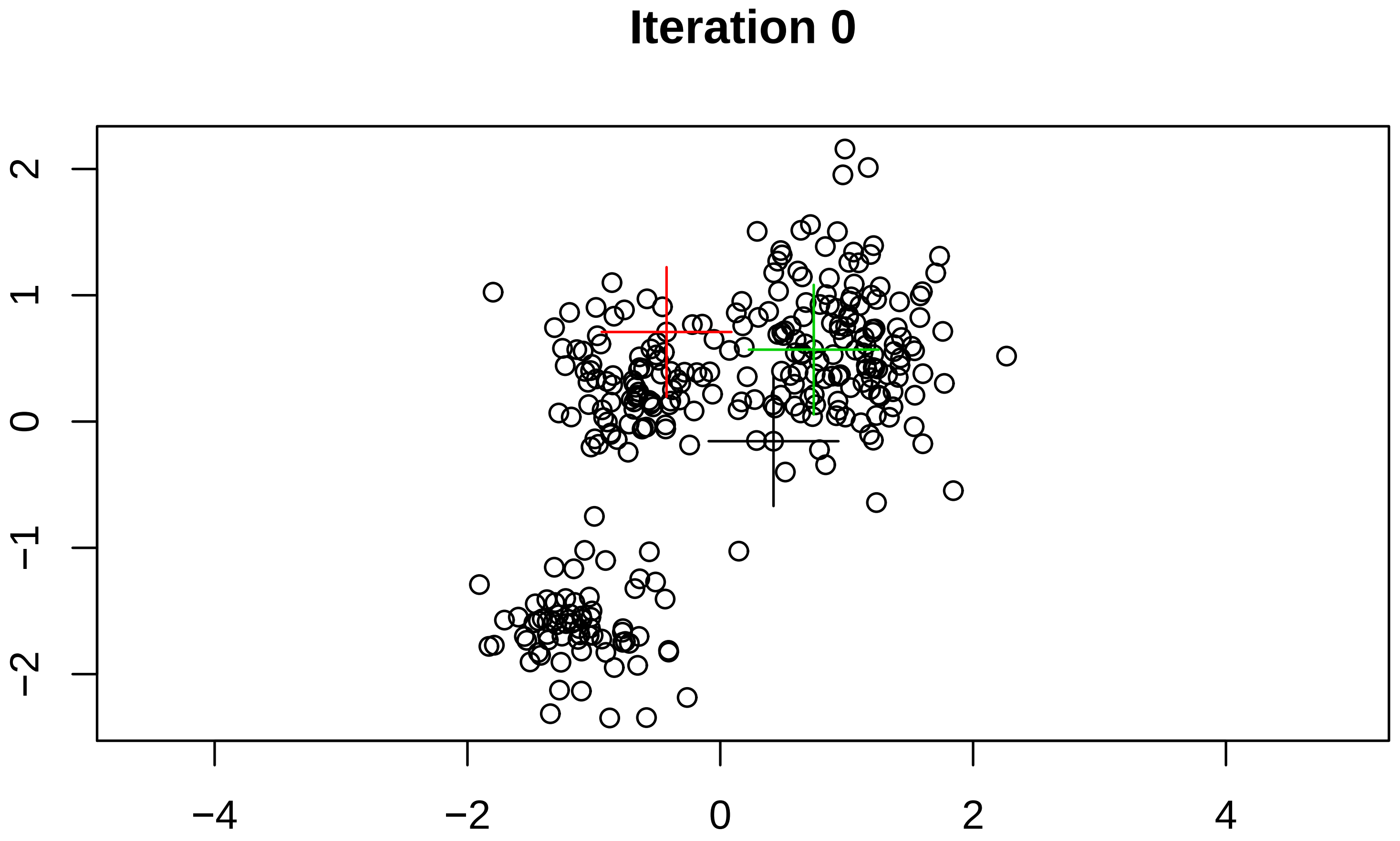
- Consider the following simulated data.



- We want to cluster the data into, say, three groups.

k-Means Clustering: Iteration 0a

- We start by randomly generating three centers (prototypes).



k-Means Clustering: Iteration 0a

The initial partition can be constructed in several ways, *e.g.*,

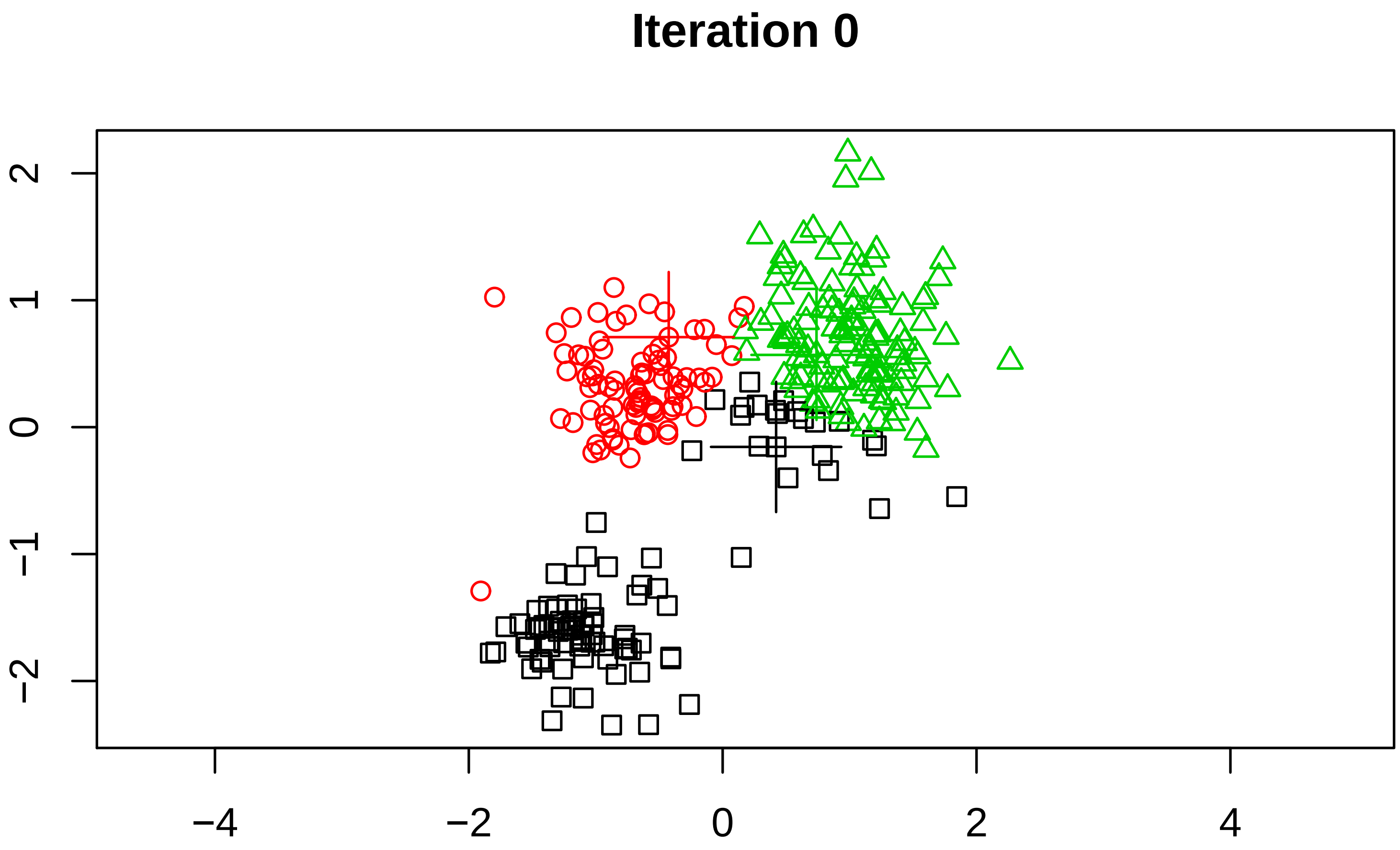
1. A random selection of k observations.

2. Specify selection based on prior knowledge.

3. By using results from an exploratory hierarchical clustering algorithm.

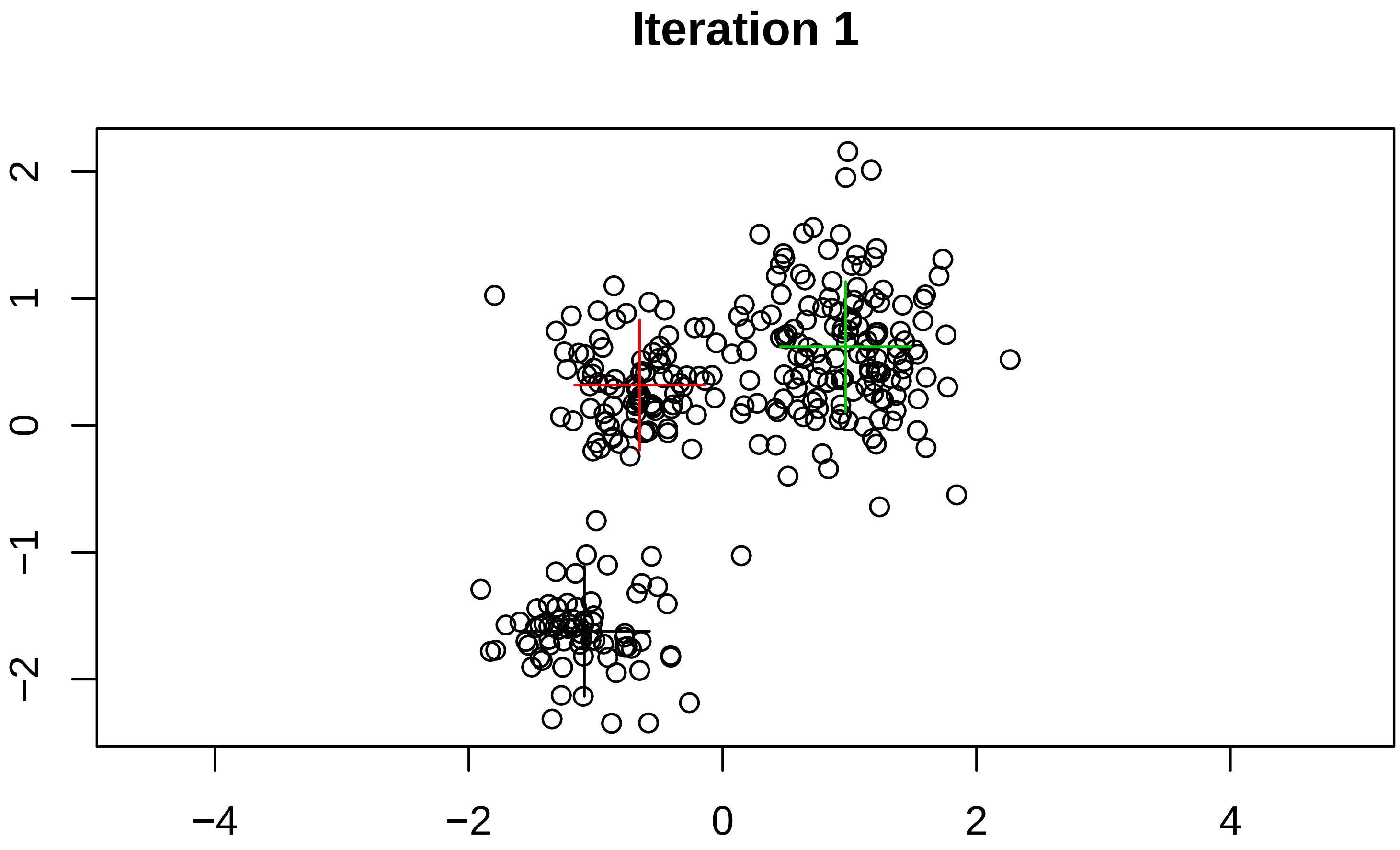
k-Means Clustering: Iteration 0b

- Label points according to which center is closest.



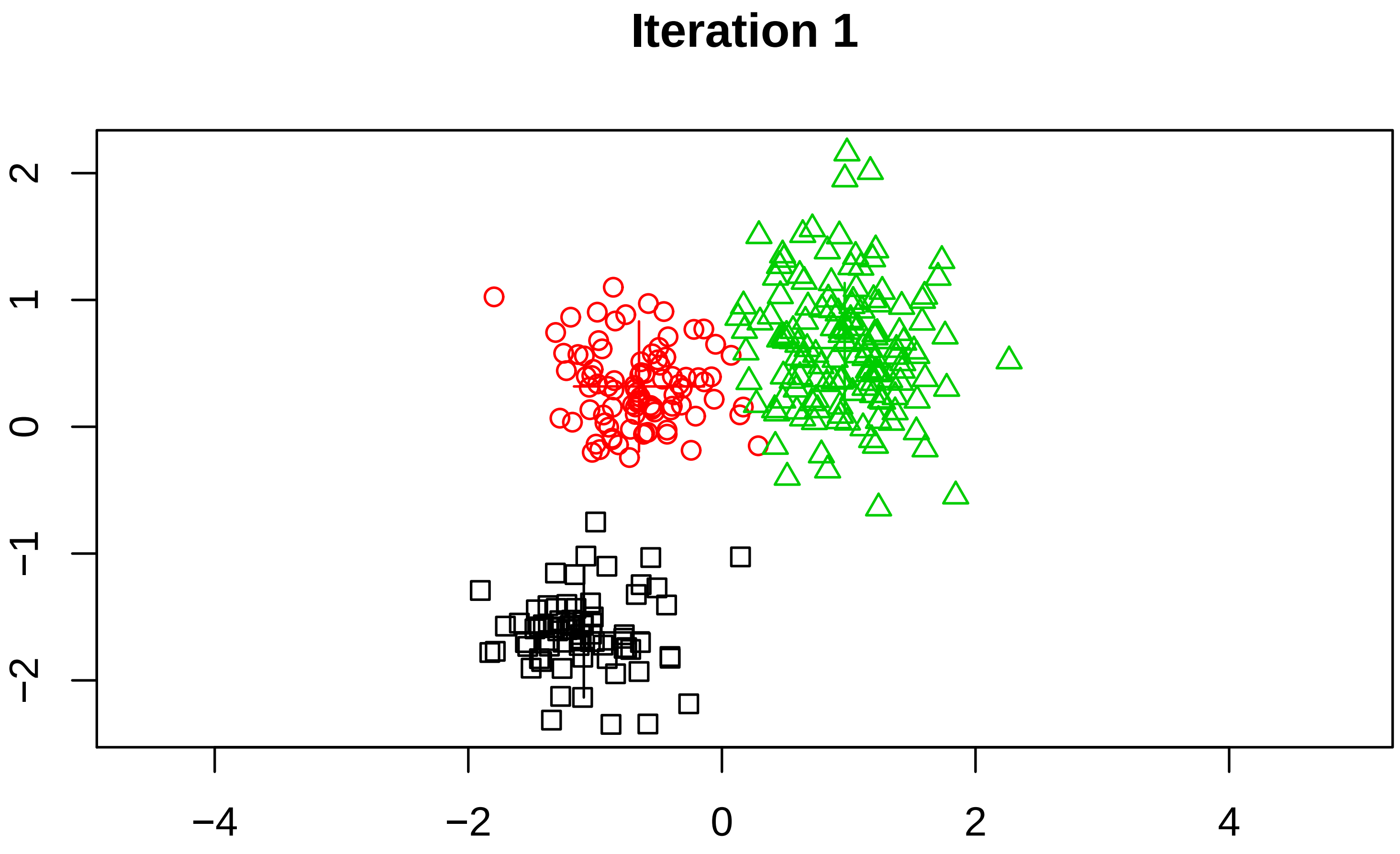
k-Means Clustering: Iteration 1a

- Update the values for the three centers (prototypes).



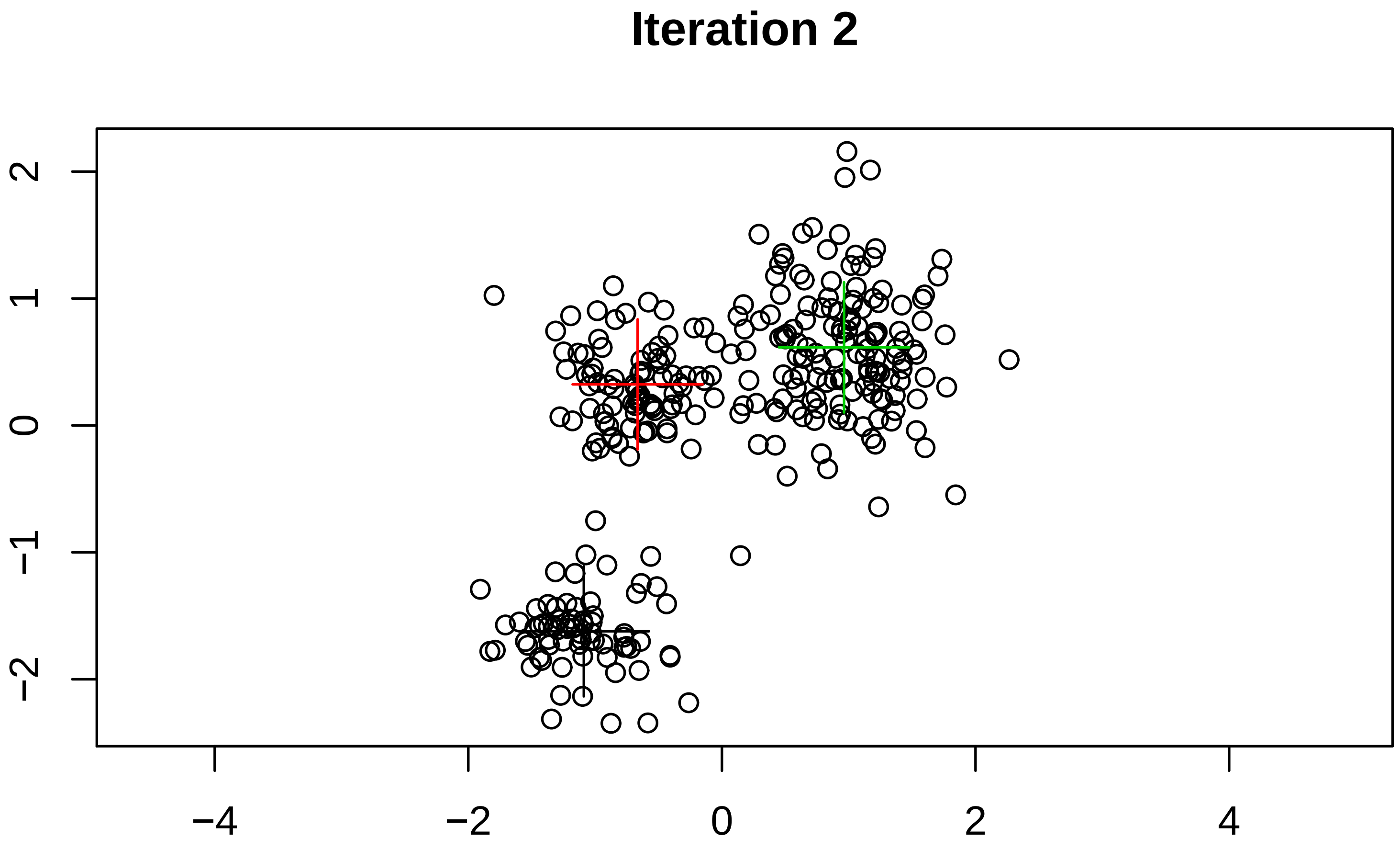
k-Means Clustering: Iteration 1b

- Label points according to which center is closest.



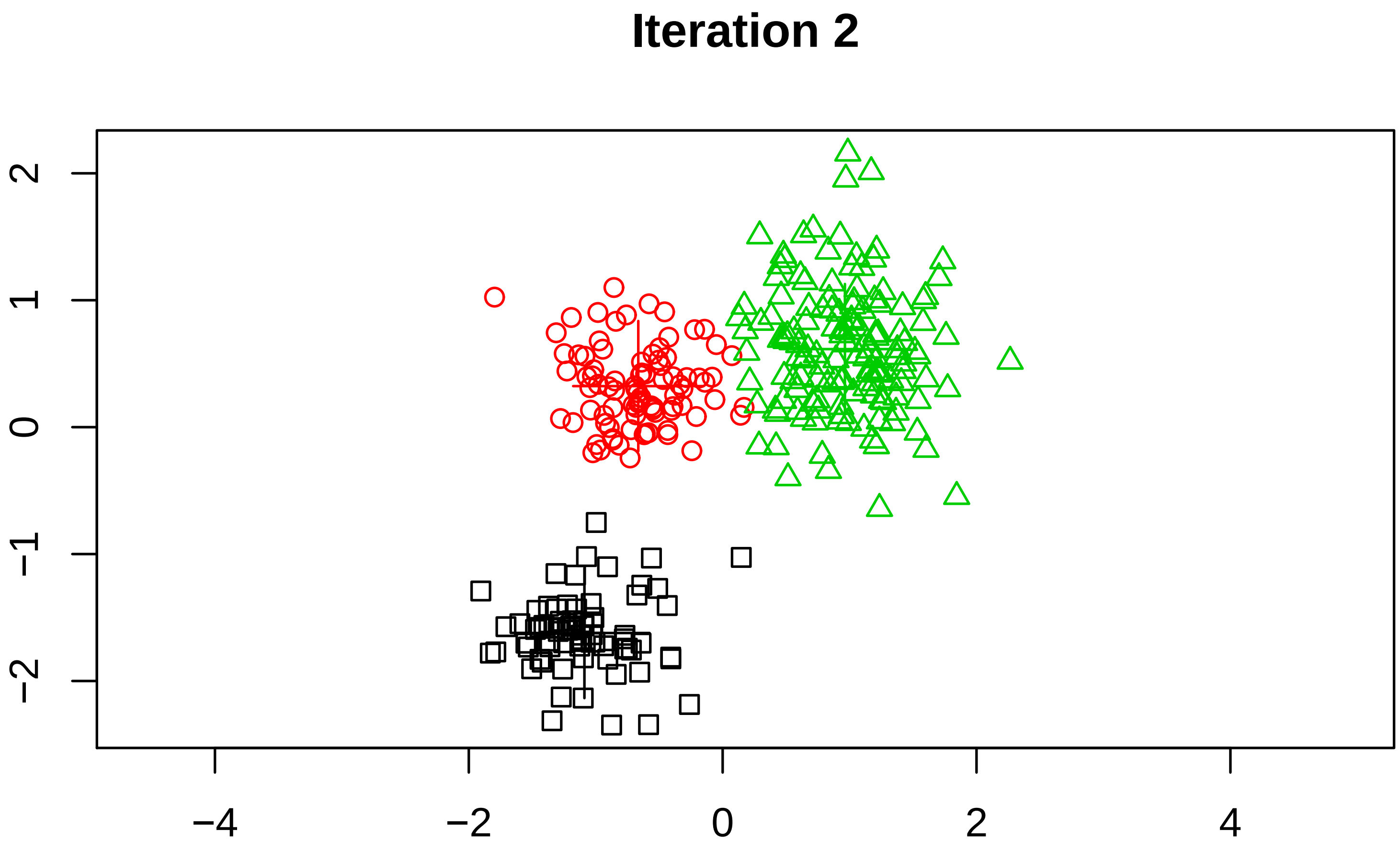
k-Means Clustering: Iteration 2a

- Update the values for the three centers (prototypes).



k-Means Clustering: Iteration 2b

- We label points according to which center is closest.

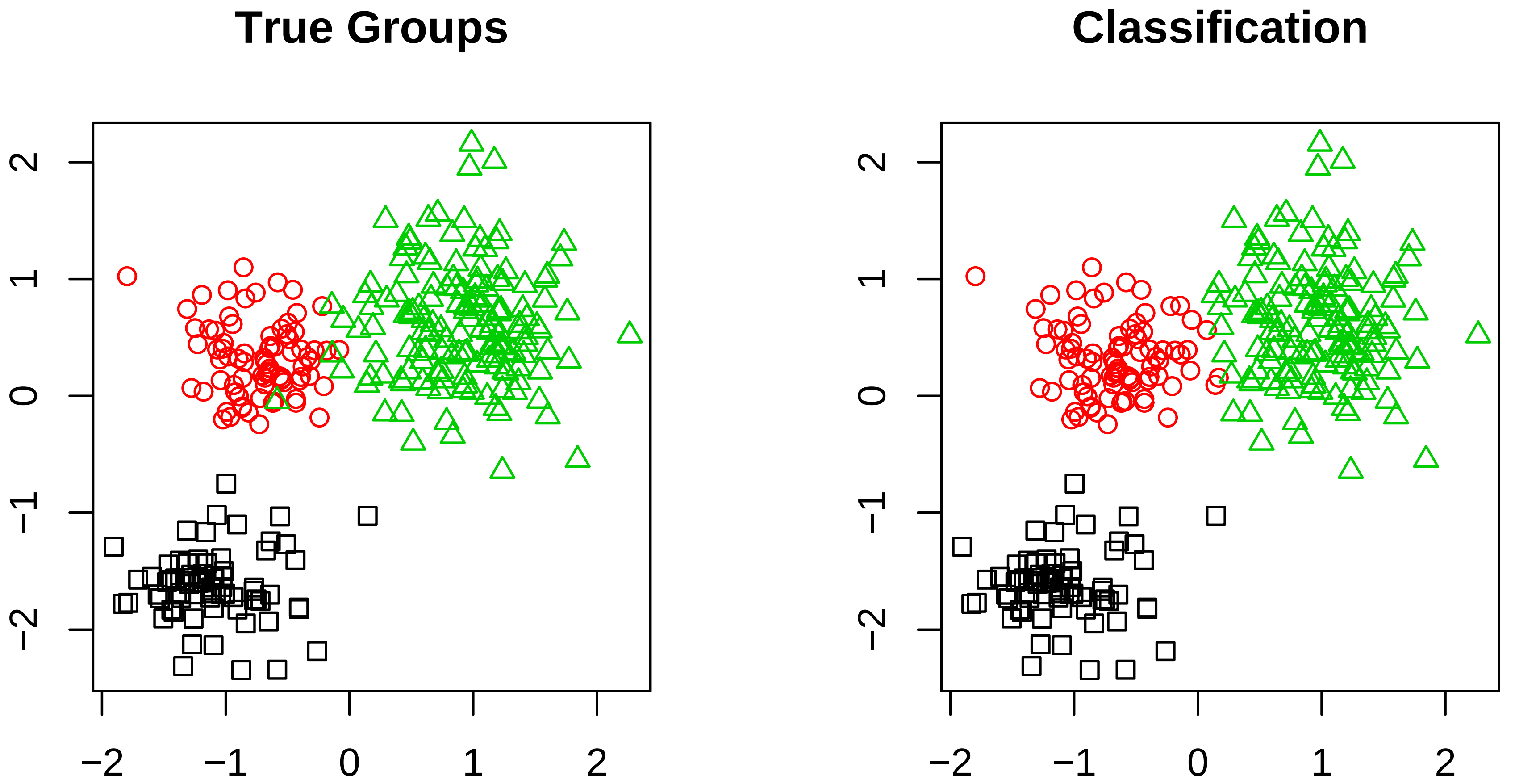


Convergence

- The k-Means algorithm has converged when no points are moved between groups on an iteration.
- Once this happens, the estimates of the centers will no longer change, nor will the allocation of points to groups thereafter.
- This convergence criteria might not be suitable in some cases, *e.g.*, if n is very large, and alternatives are possible, *e.g.*, within cluster sum of squares does not change over 3 iterations *etc.*

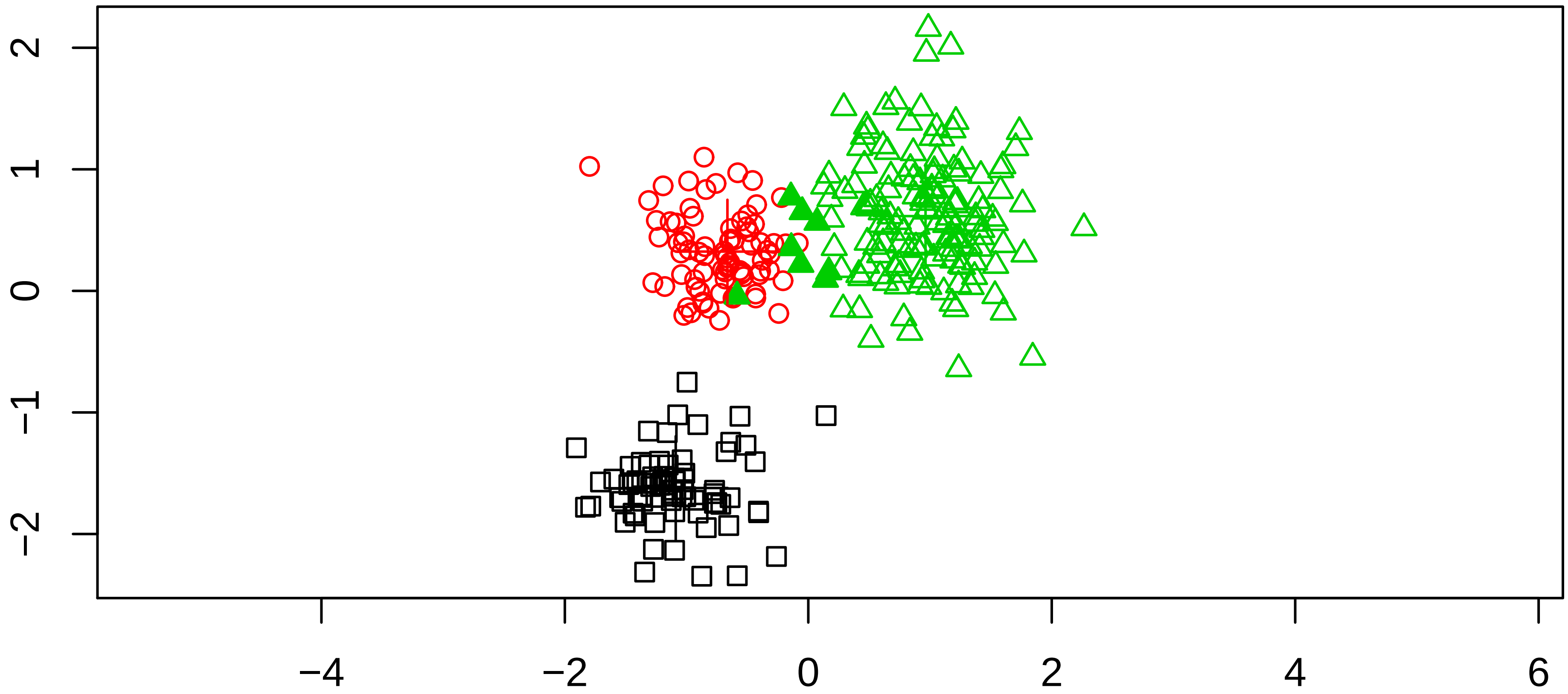
How Did It Do?

- The data from the last example had been simulated, so that there were actually three groups in the data.
- How well did k-means perform at finding these groups?



Any errors?

- The coloured in points were misclassified.
- Only 8/300 were misclassified.

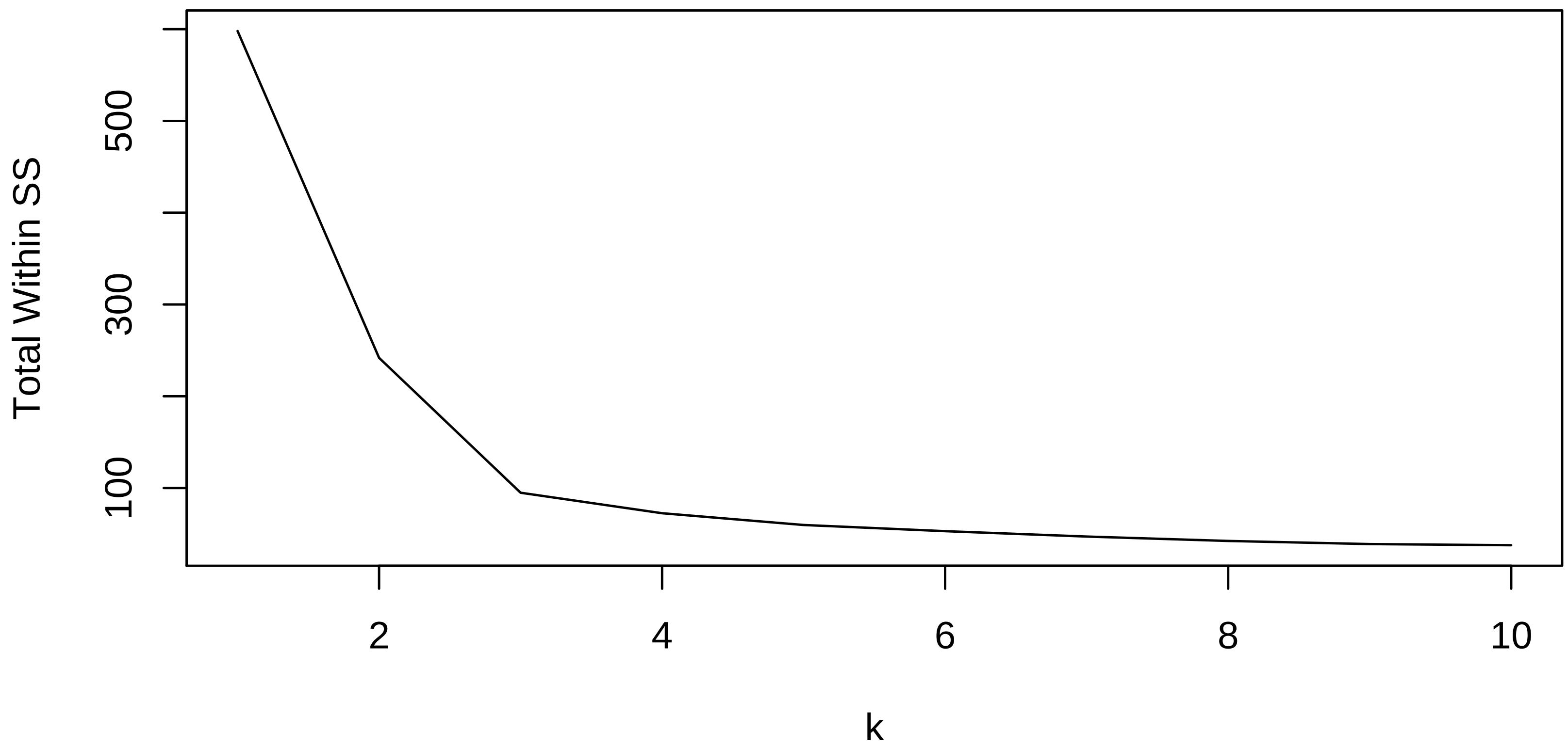


Choosing The Value For k

- This is not an exact science, but there are guidelines.
- Generally we should run the k-means algorithm for a differing number of values for k, *e.g.*, $k = 1, \ldots, 10$.
- When running k-means the aim is to minimize the SS, so why not choose k to minimize the SS?
- However, the more clusters that are fitted the smaller the SS (think of what would happen if we selected $k = n$).
- A general rule is to plot k against SS and look for a 'kink' in the curve. If there is no kink then there is a trade-off between additional complexity by increasing k and better fit by reducing the SS.

Choosing The Value For k

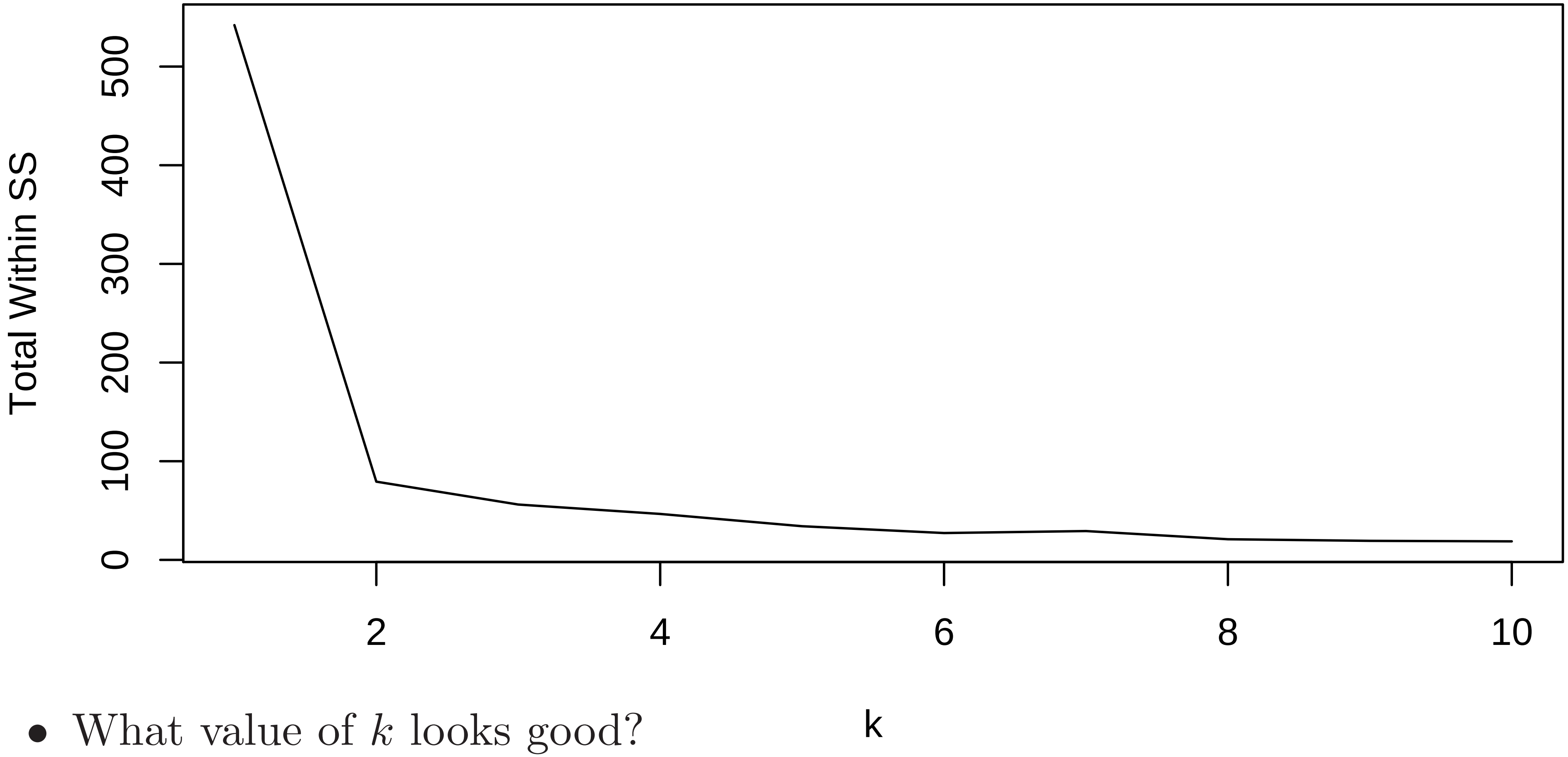
- If we plot the total of the within sum of squares values versus k, then we get the following:



- Notice that the graph flattens very quickly. What k would you use?

Old Faithful Data

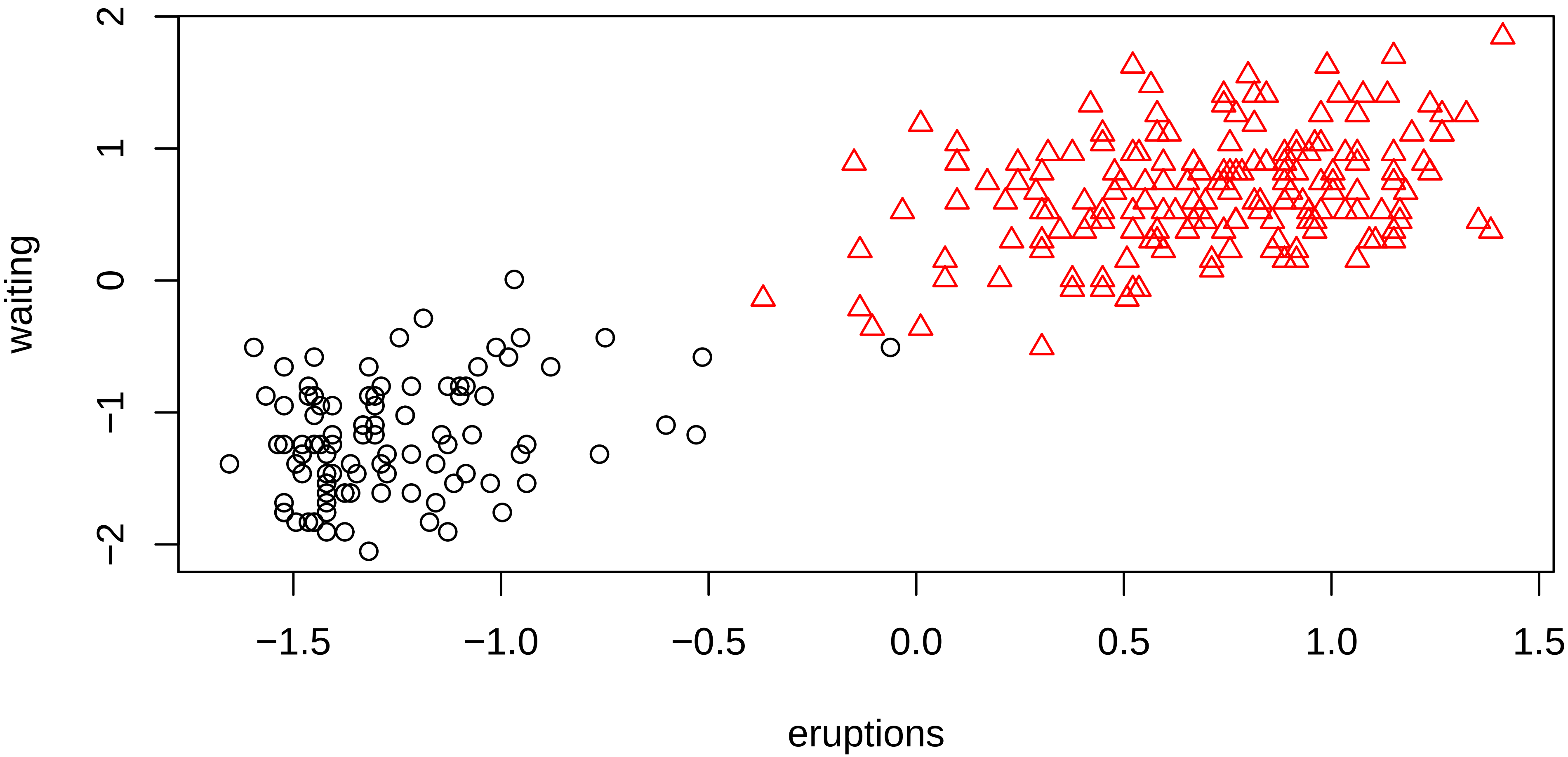
- Running k-means on the standardized Old Faithful data allows a plot of the within sum of squares values versus k:



- What value of k looks good?

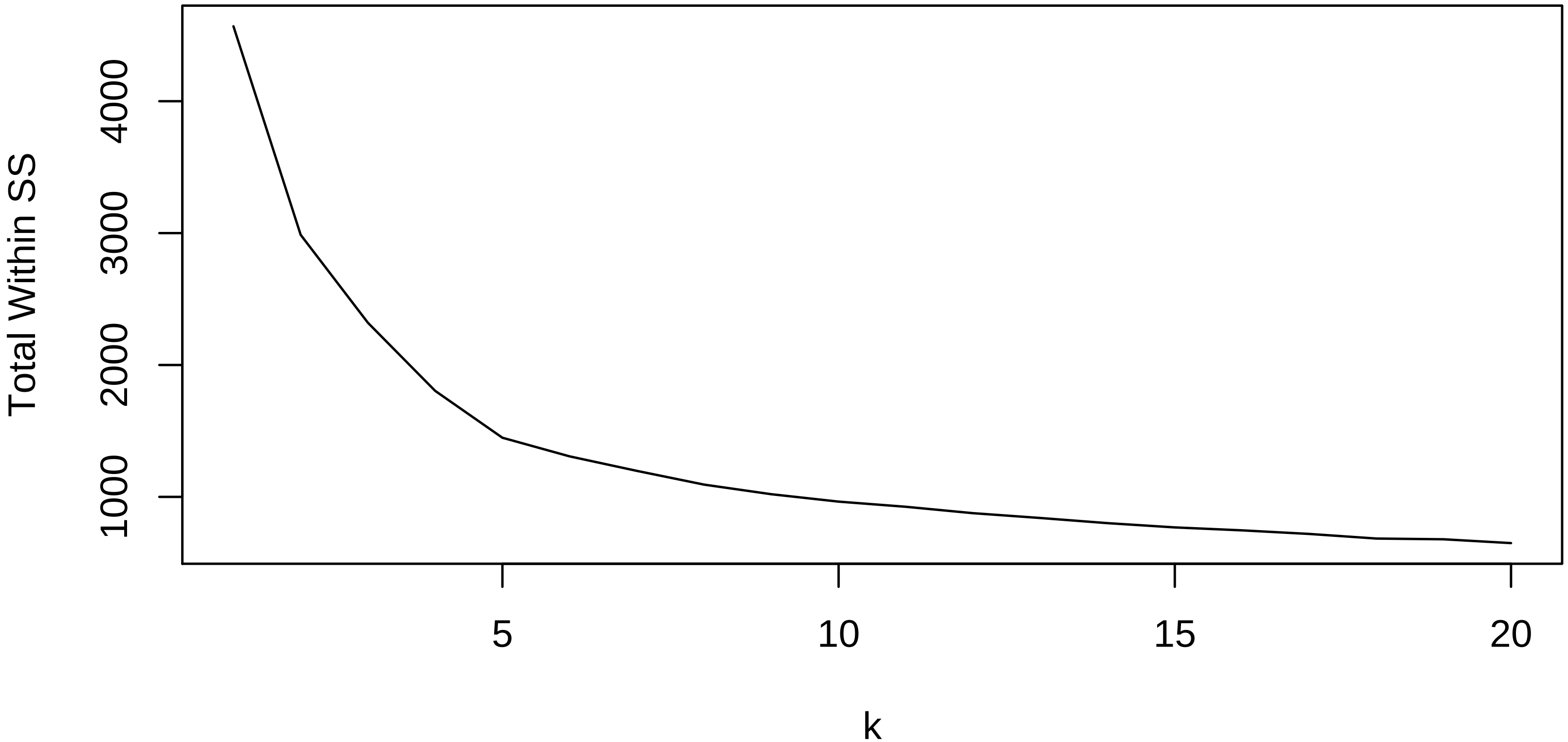
Old Faithful Data

- This provides the following clustering of the data:



Olive Oil Data

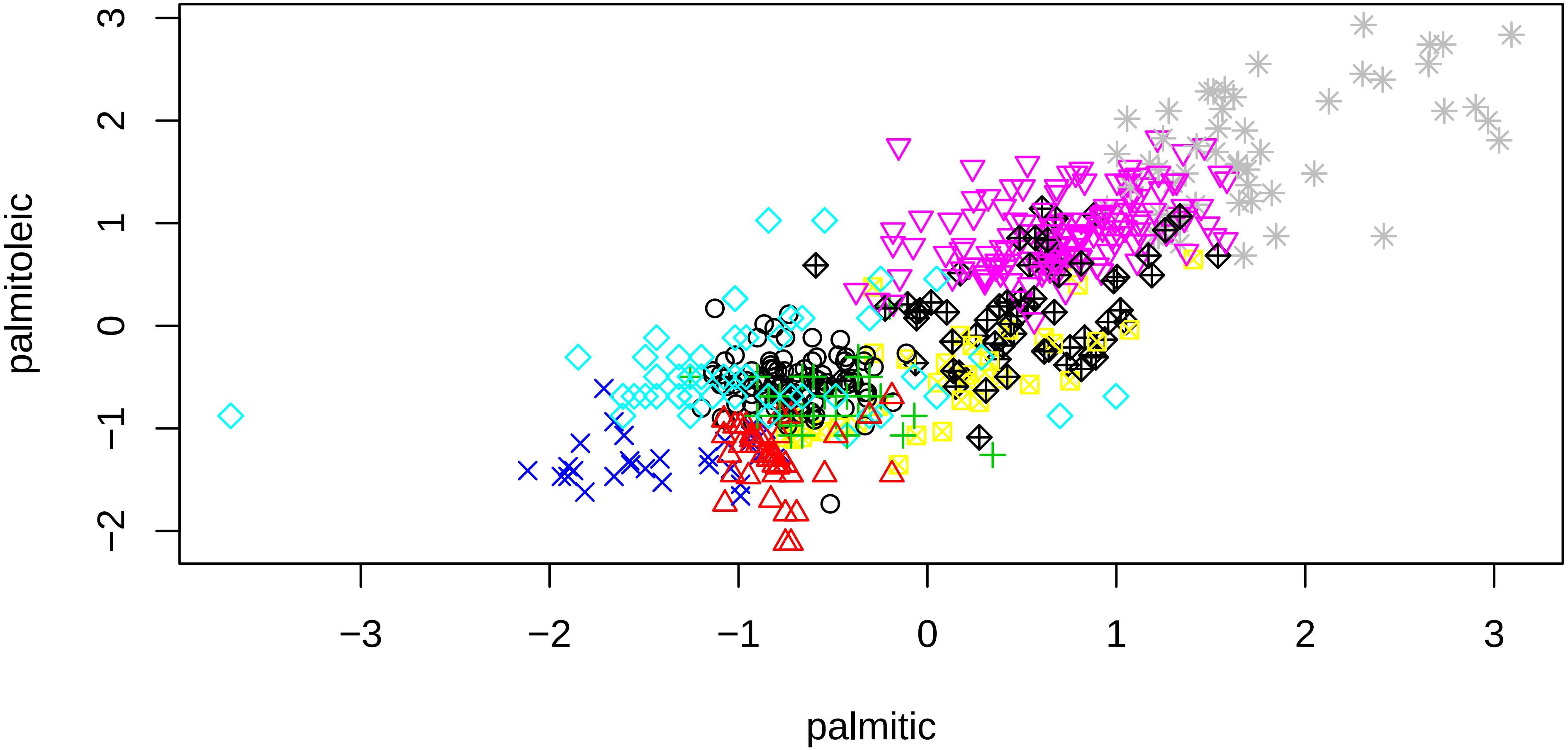
- Running k-means on the standardized olive oil data data allows a plot of the within sum of squares values versus k:



- What value of k looks good? Let's look at $k = 9$.

Olive Oil Data

- This provides the following clustering of the data:



Cross Tabulation

- A cross tabulation of the olive oil regions (rows) and the clusters (columns) shows some agreement:

	4	9	6	7	1	8	3	5	2
1	22	2	0	0	0	0	0	0	1
2	0	32	0	23	0	0	1	0	0
3	0	12	144	1	0	49	0	0	0
4	6	16	0	12	0	2	0	0	0
5	0	0	0	0	65	0	0	0	0
6	0	0	0	0	33	0	0	0	0
7	0	0	0	0	0	0	33	10	7
8	0	0	0	0	0	0	0	50	0
9	0	0	0	0	0	0	1	0	50

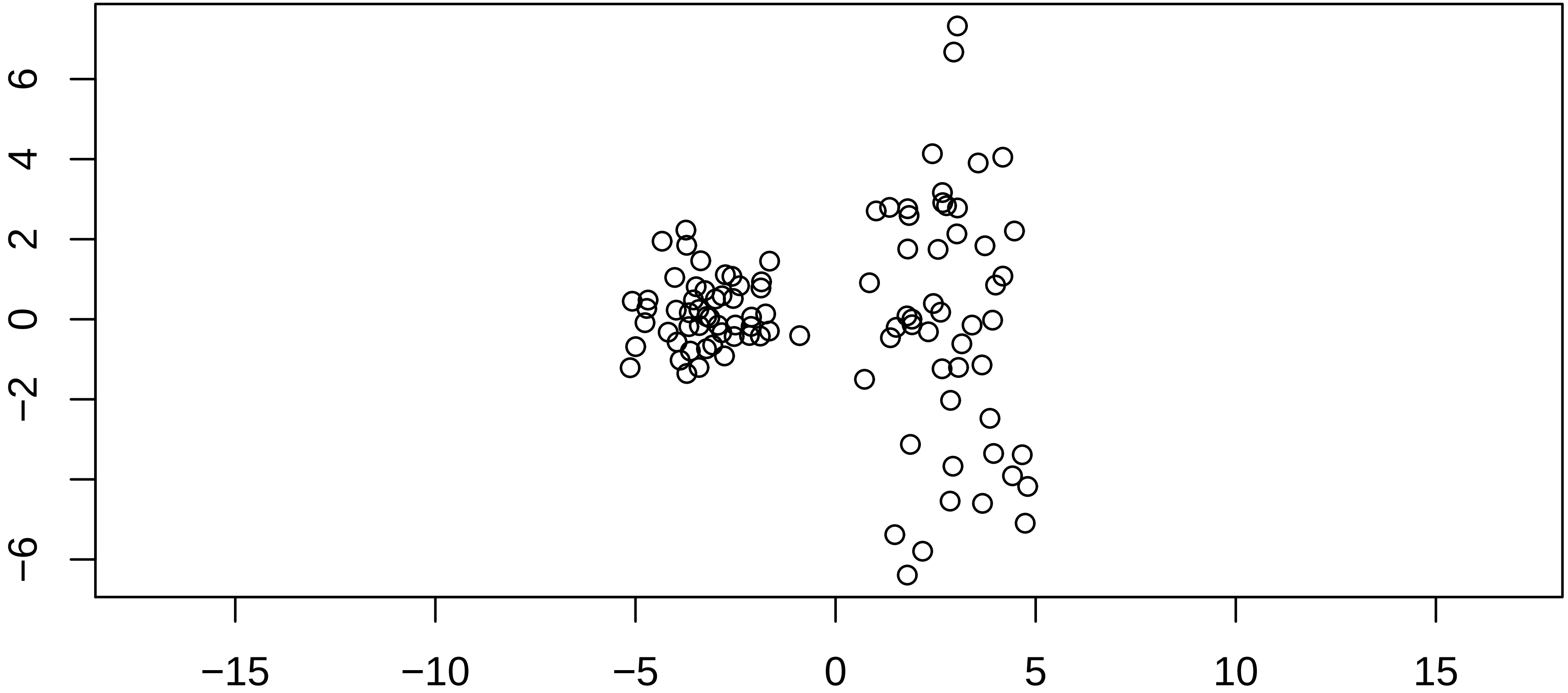
Faithful Data k=2

- Consider the $k = 2$ solution for the Faithful data:

```
Number of clusters: 2

           Number of Obs.   WSS     Avg. Dist. to Centroid
Cluster 1      100         3456.2        4.9
Cluster 2      172         5445.6        4.6
Sum            272         8901.8

Cluster Centroids:

           Cluster 1 Cluster 2 Total Data
eruptions    2.1       4.3         3.5
waiting     54.8      80.3        70.9

Distance Between Cluster Centroids:

           Cluster 1 Cluster 2
Cluster 1   0.0       25.6
Cluster 2  25.6        0.0
```

Tricky Data

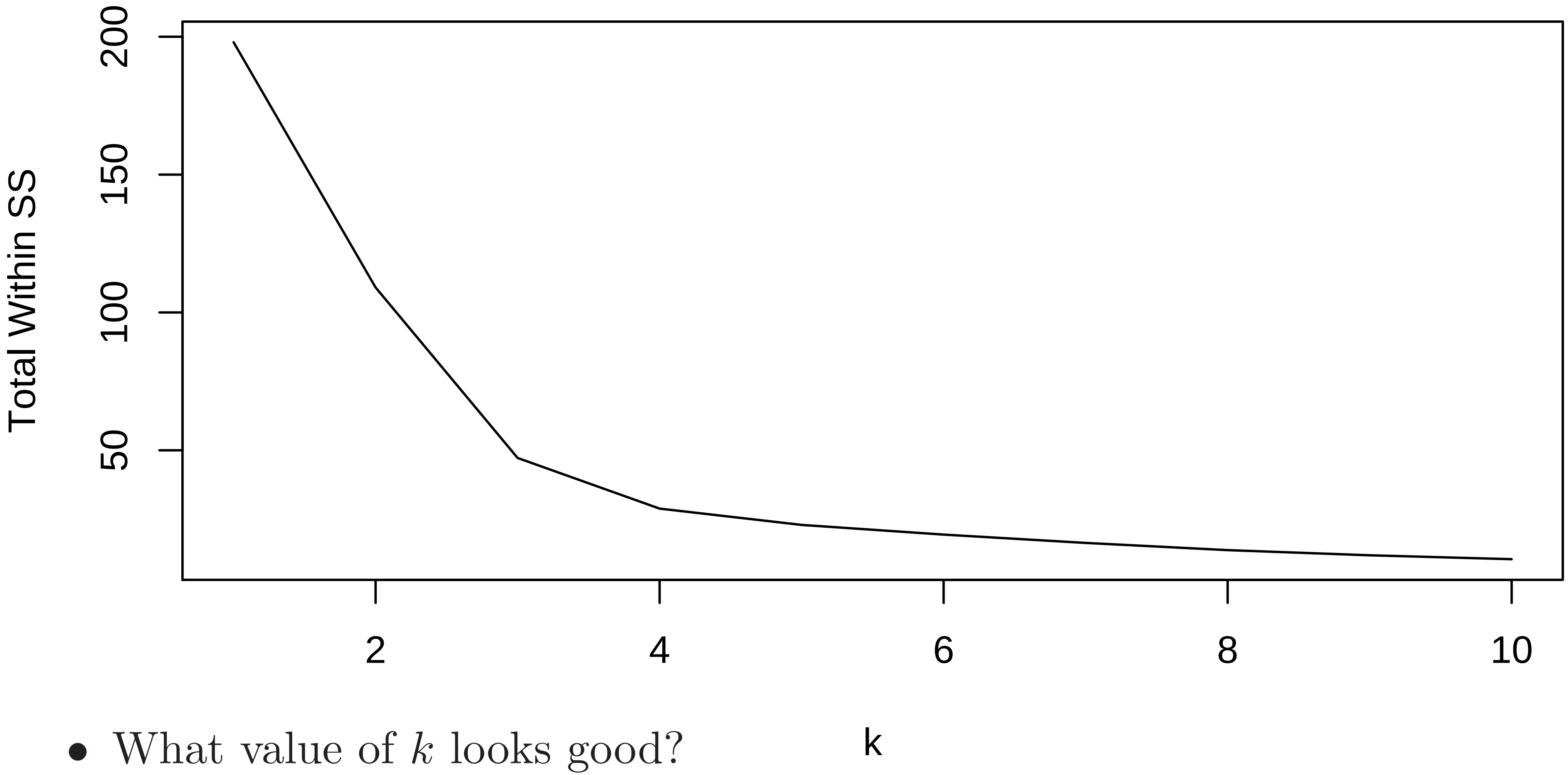
- What if we run k-means on the following, more tricky, standardized data:



- It looks like there should be two groups.

Tricky Data

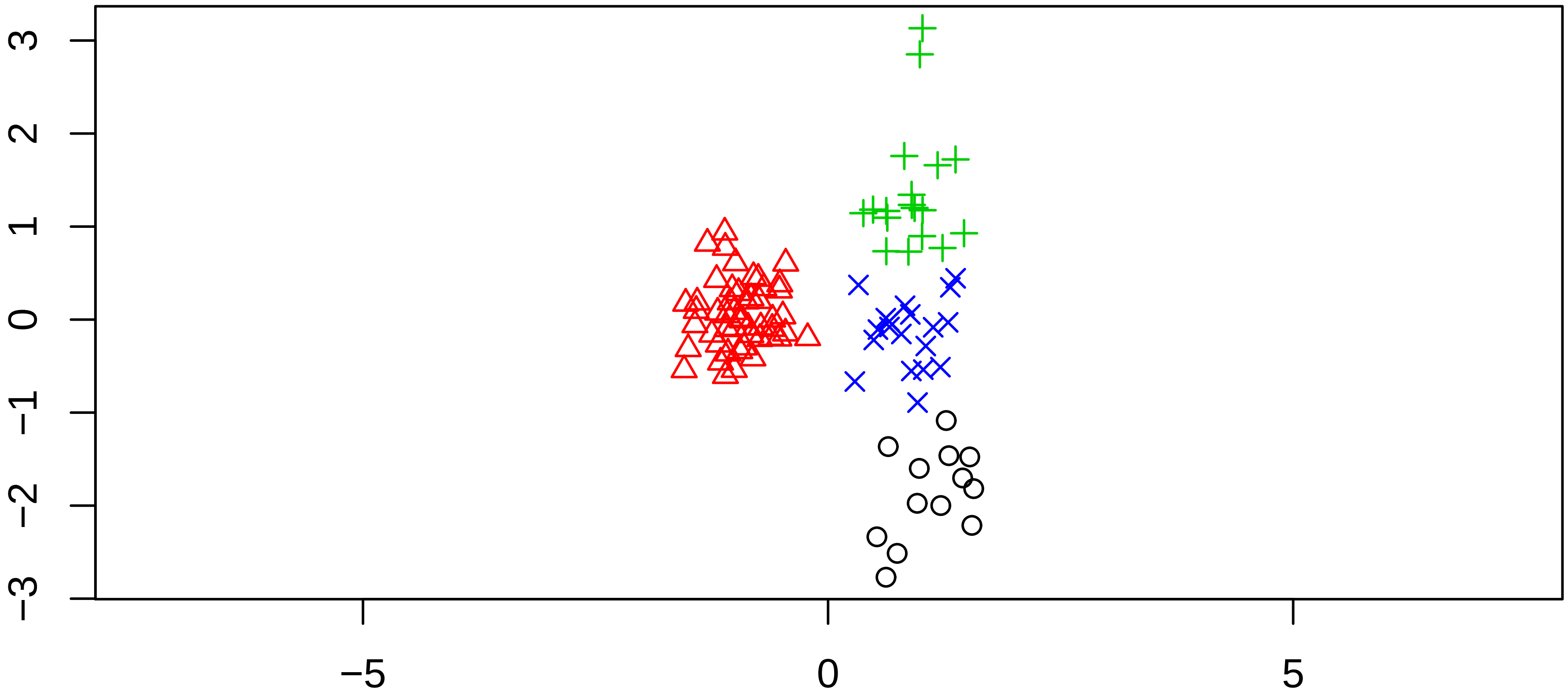
- Plotting the within sum of squares values versus k gives:



- What value of k looks good?

Tricky Data

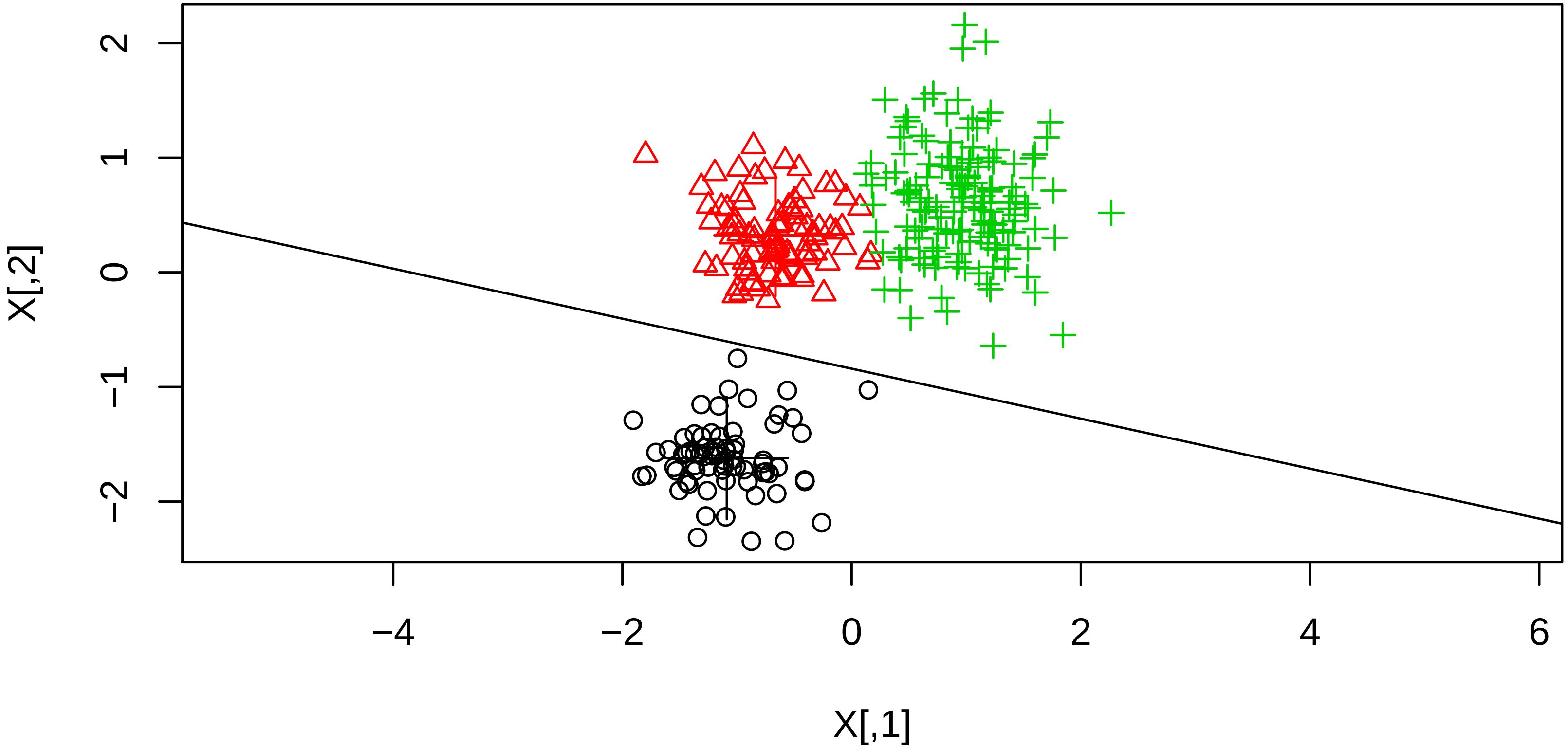
- This provides the following clustering of the data:



- The elliptical group is broken into subgroups. This is because k-means clustering looks for circular clusters.

Distance From Means

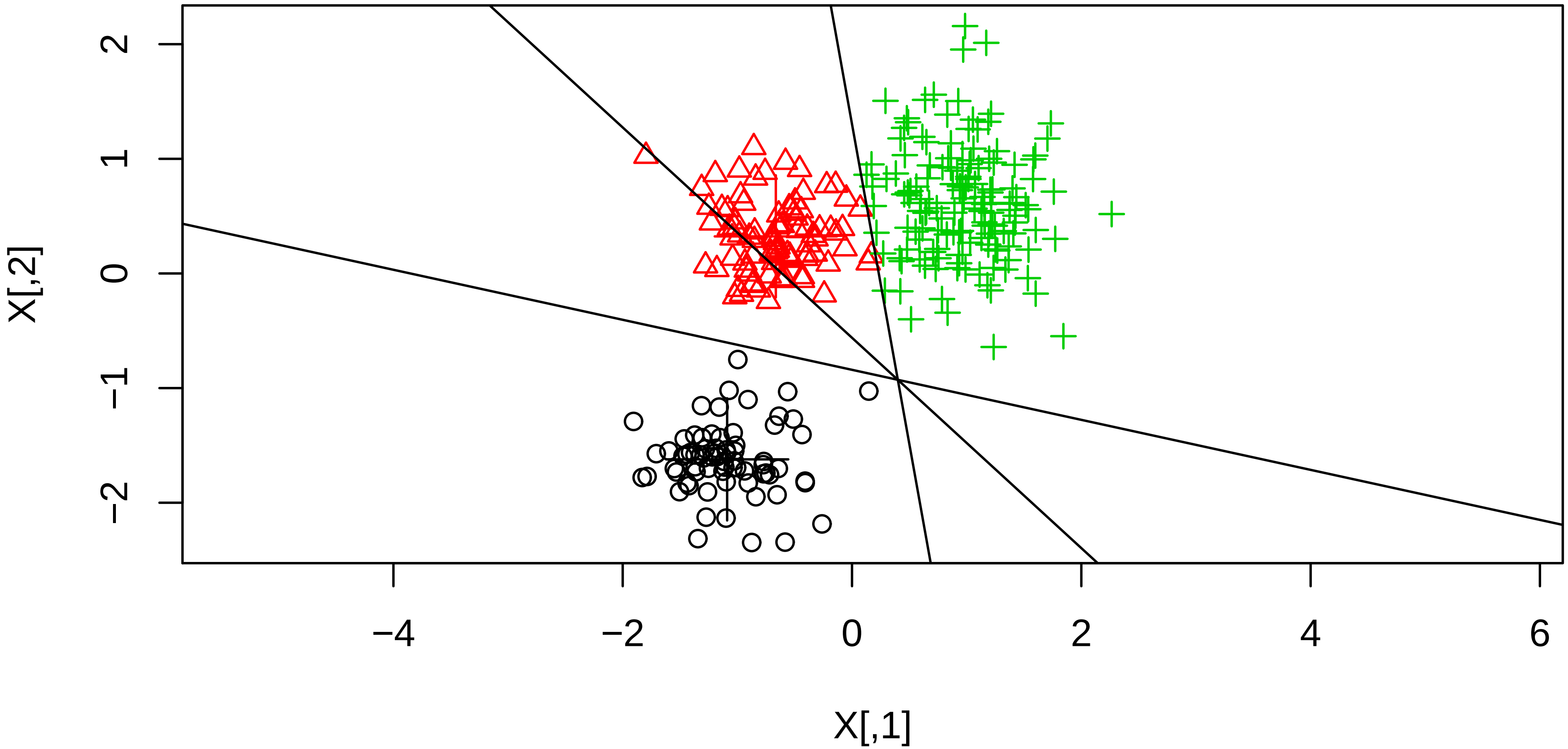
- Return to the first data set.



- Consider the line separating the points that are closest to the mean of the triangles ($\triangle$) and the points closest to the mean of the circles ($\circ$).

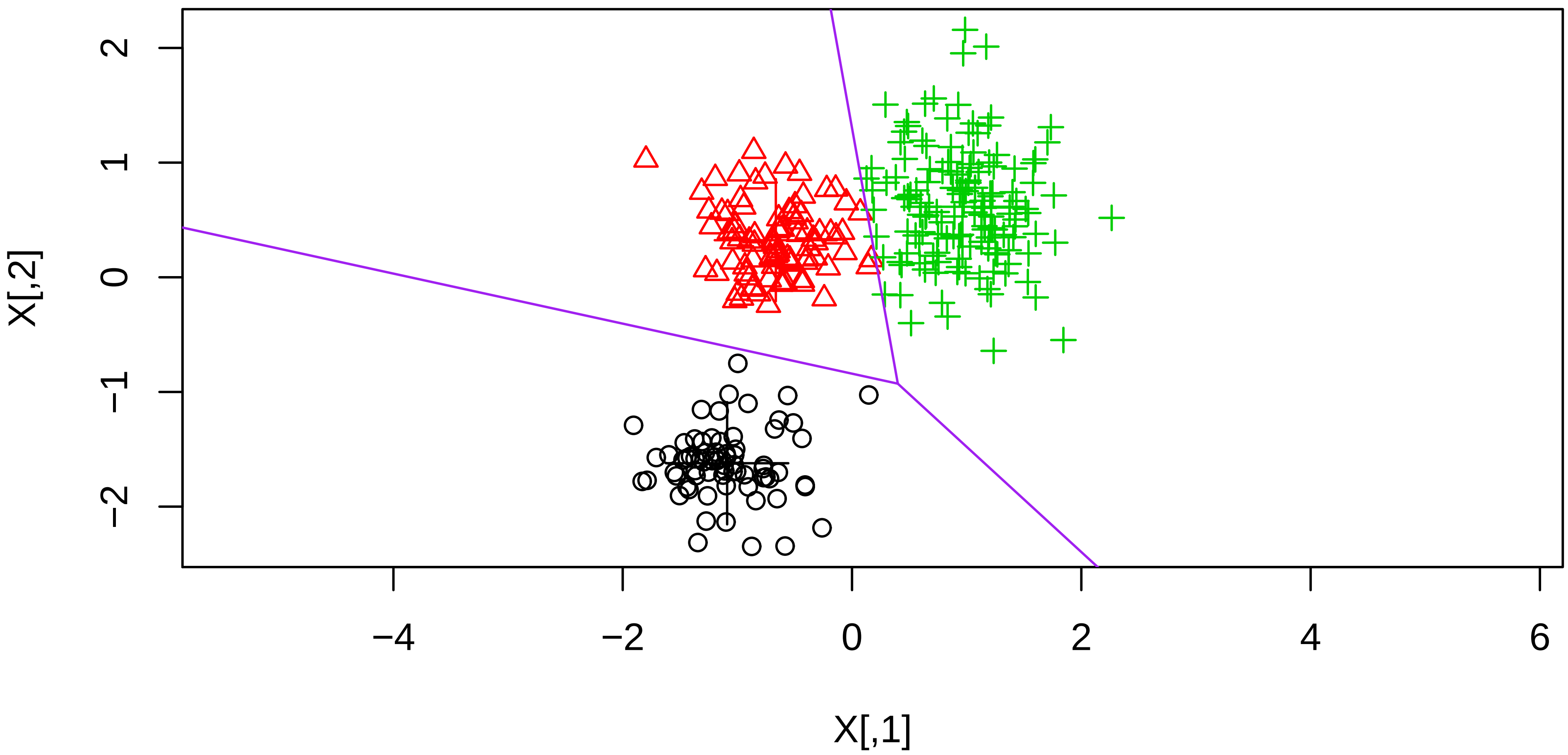
Distance From Means

- Including such lines for each pair of means:



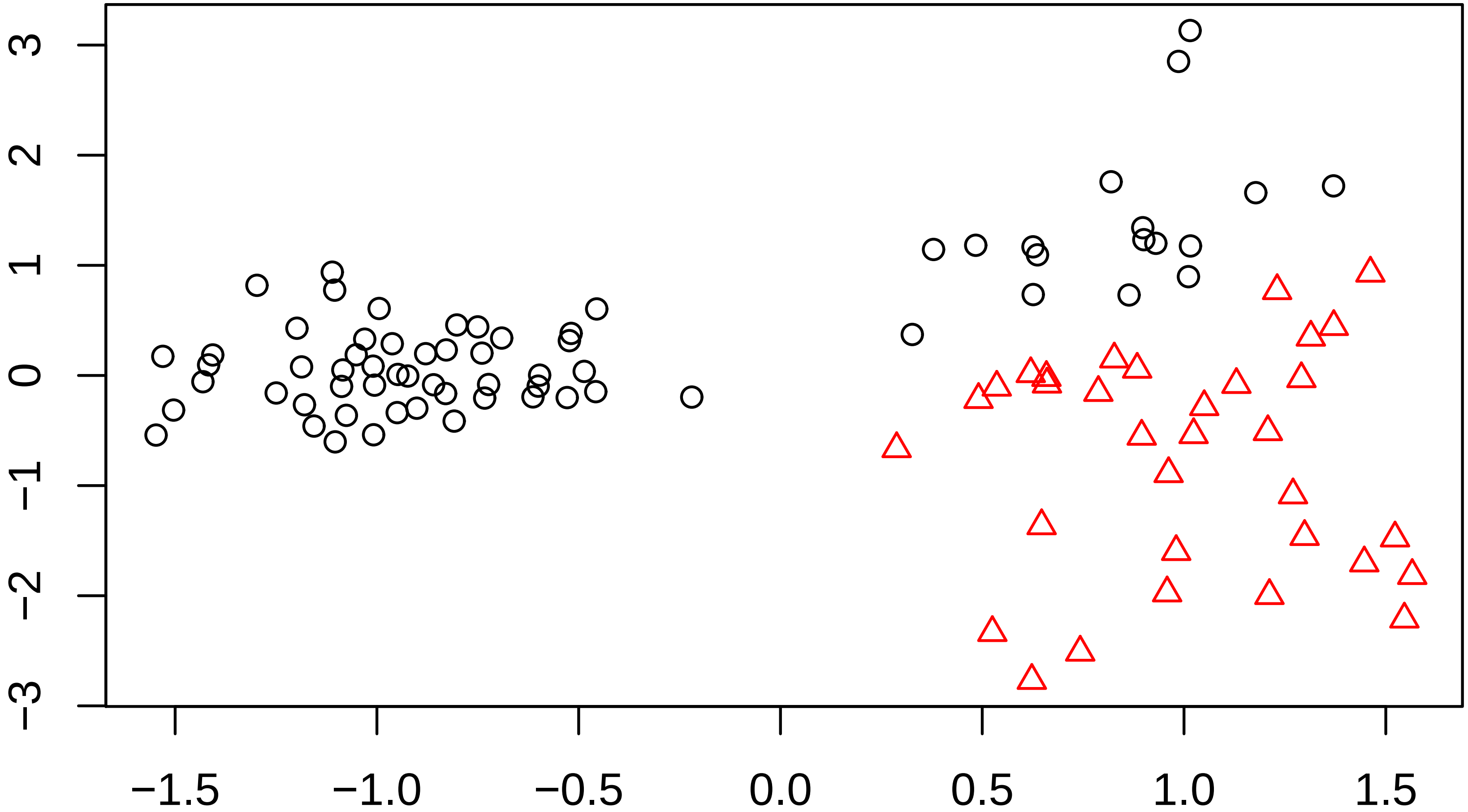
Partitioning Of The Plane

- The plane is partitioned into three polygonal regions depending on which mean is closest.



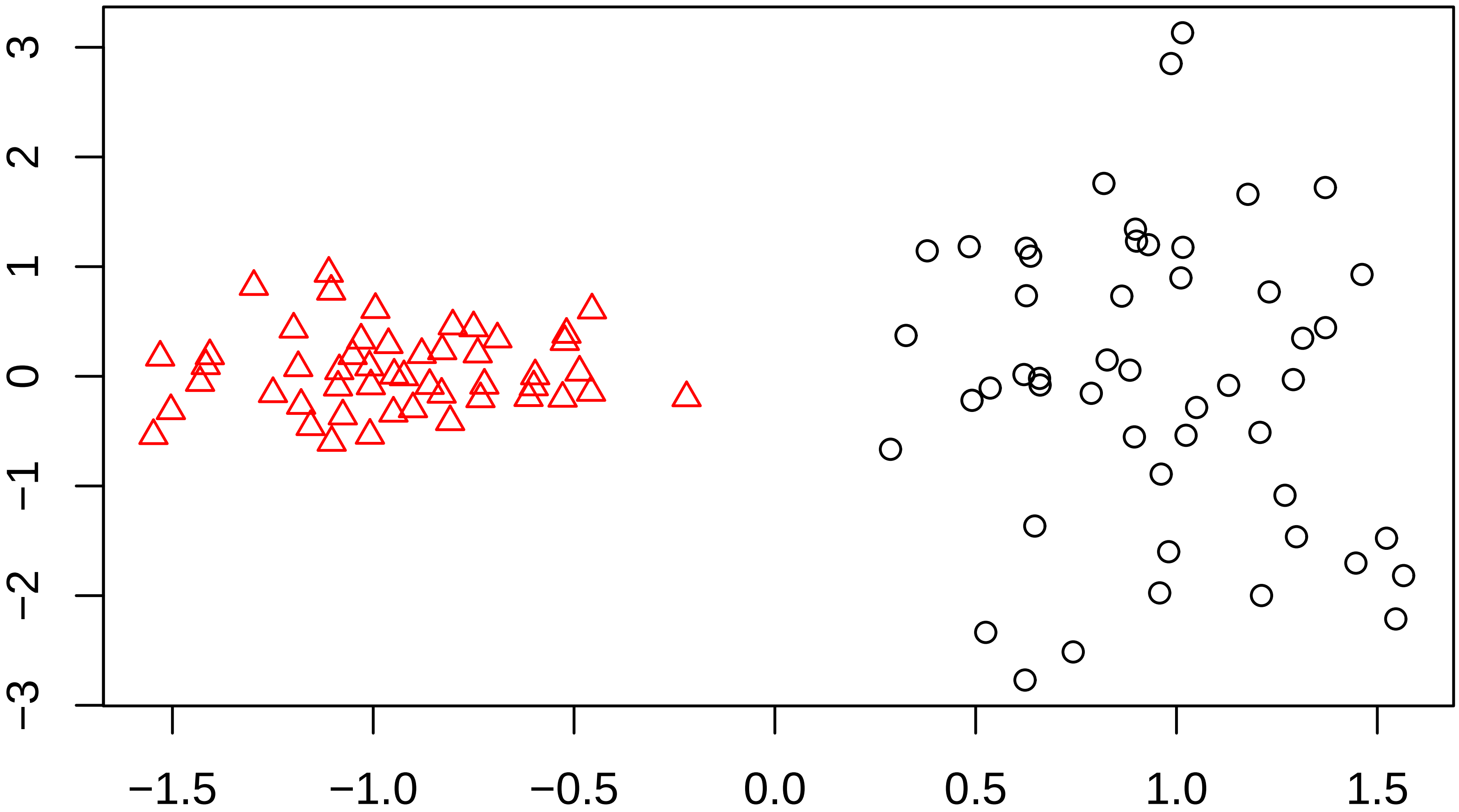
Tricky Data

- Recall the tricky data from earlier.
- If we cluster it into two groups, we get:



Tricky Data

- But if we ran k-means from a different and specific starting point:



Local Minima

- The k-means algorithm can give different answers when initiated at different starting values.
- This means that the algorithm does not always find the minimum value for the Total Within Sum of Squares.
- The Total Within Sum of Squares for the first clustering is 82.4+36.3=118.7.
- The Total Within Sum of Squares for the second clustering is 11.0+98.1=109.1.
- Therefore, the second set of results is better.