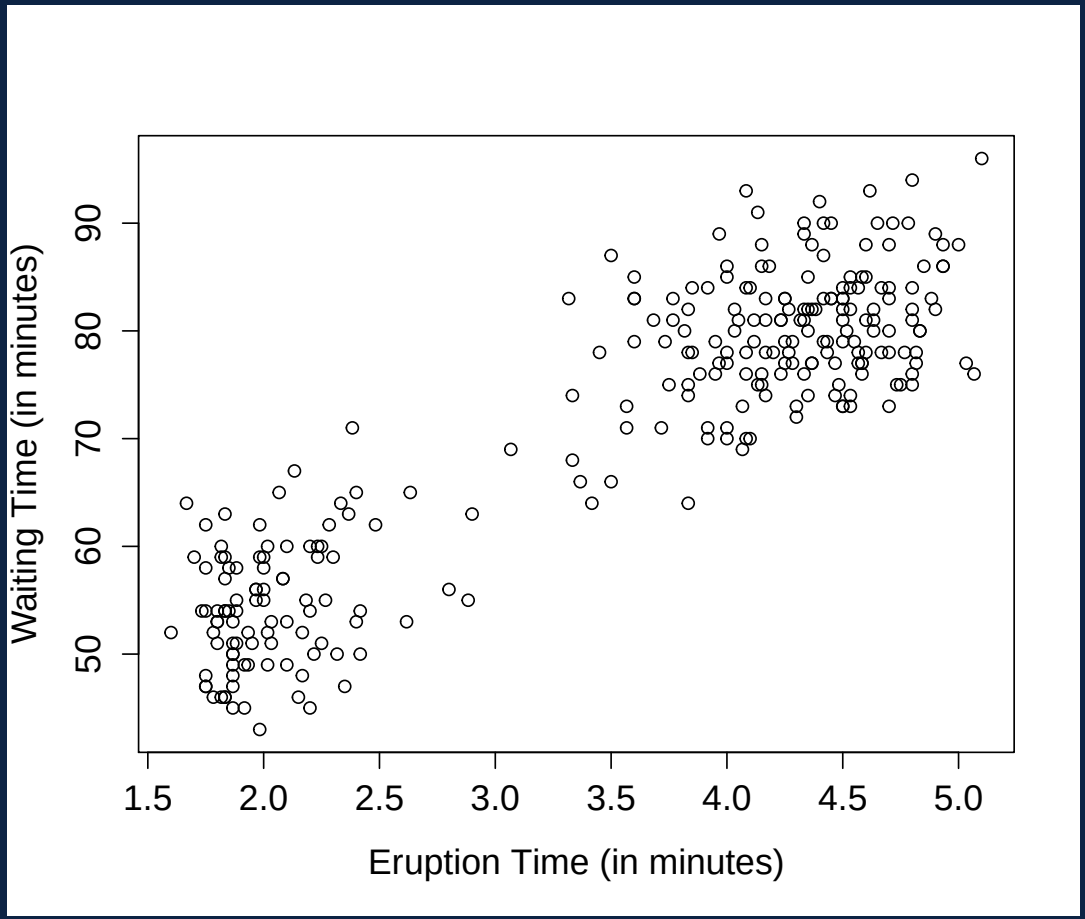
Clustering

UBCO MDS — DATA 573

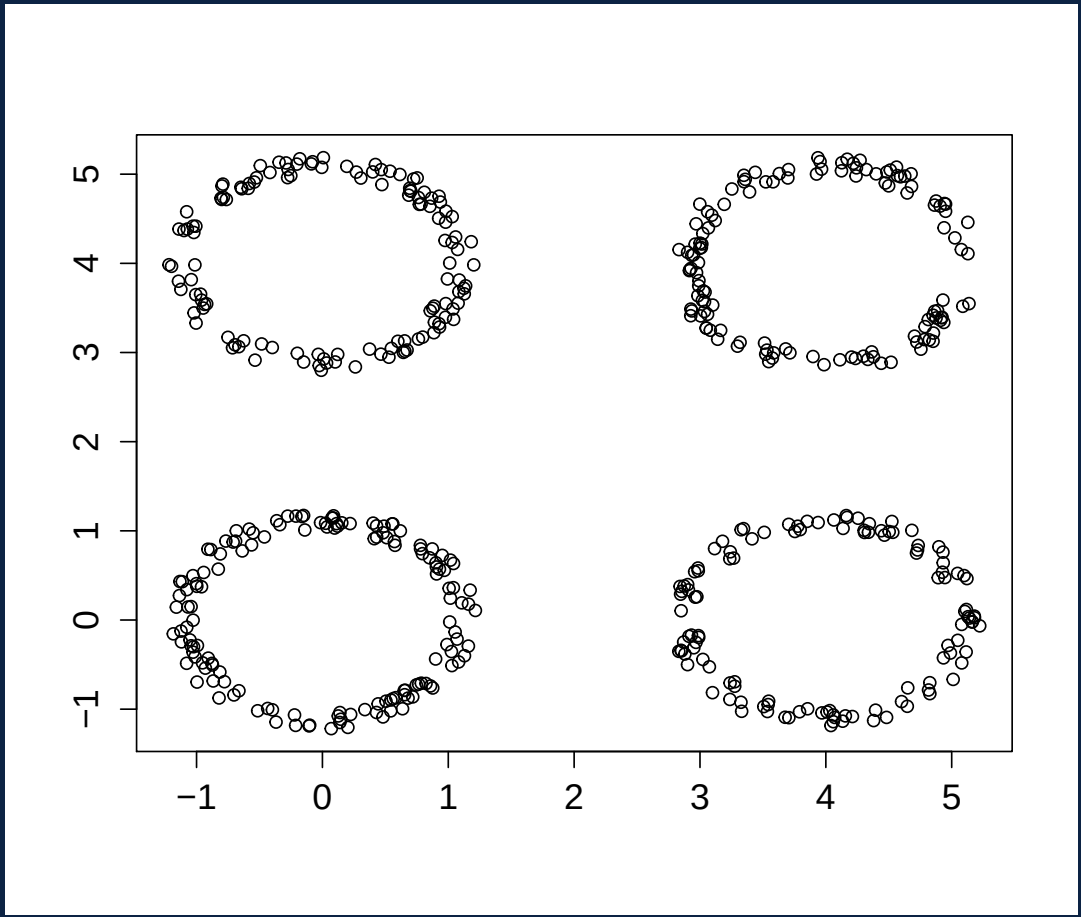
Clustering Motivation

- Measurements on time to eruption, and length of eruption time of the Old Faithful geyser in Yellowstone National Park.



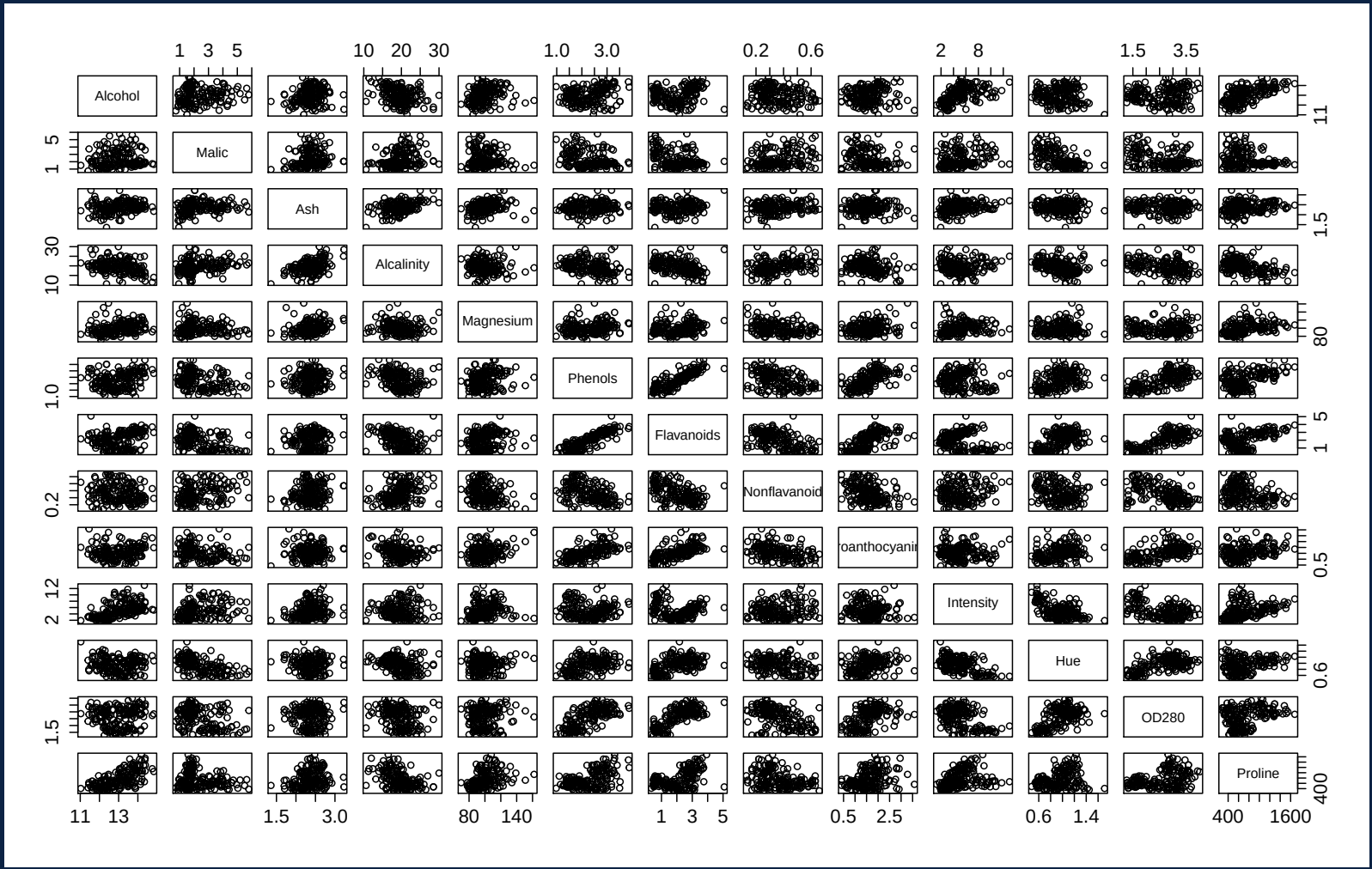
Clustering Motivation

- Simulated data



Clustering Motivation

- Scatterplot matrix of wine data (all 13 variables)



Motivation

- The goal of "clustering" (a form of unsupervised learning) is to find groups such that all observations are
  - more similar to observations inside their group and
  - more dissimilar to observations in other groups.

- Types of clustering algorithms:
  - Hierarchical
  - Partitioning
  - Mixture models

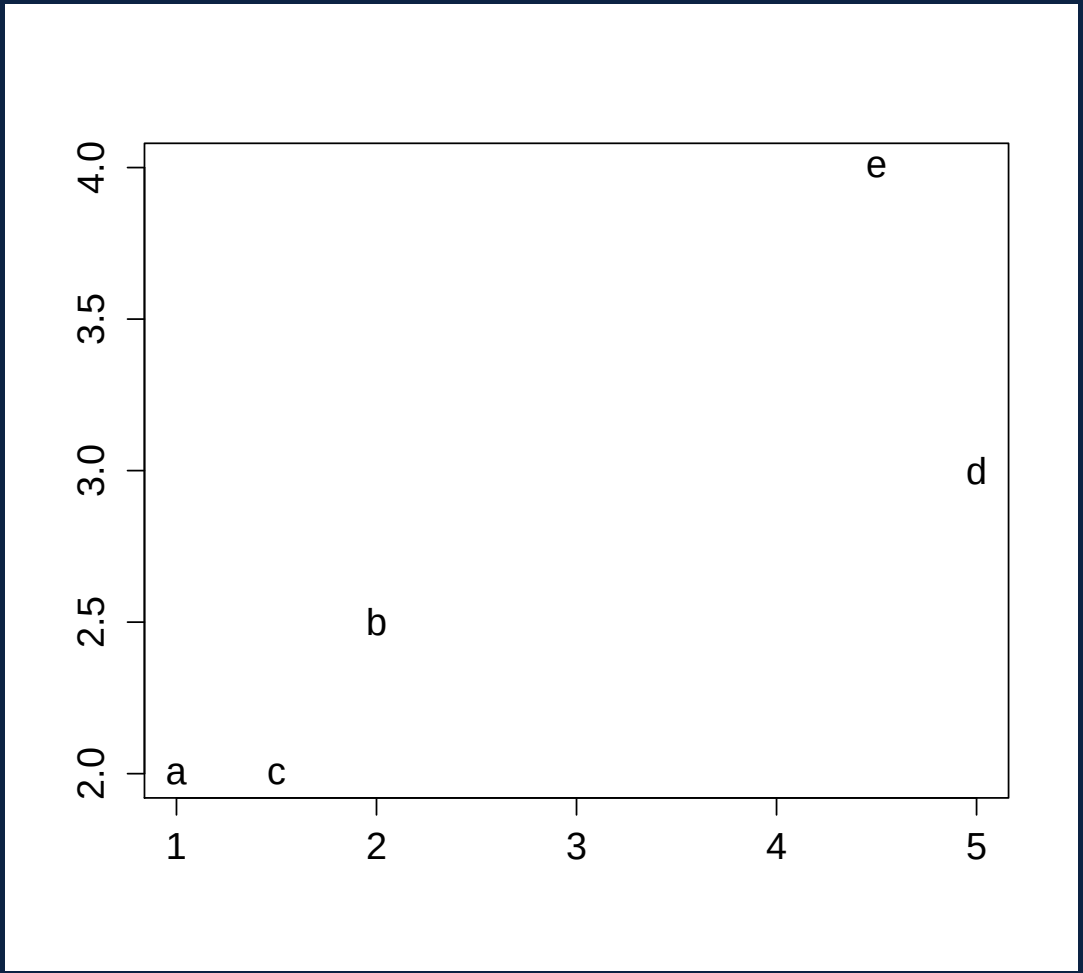
Hierarchical Clustering

- Once we have information on the distances between all observations in our data set, we're ready to come up with ways to group those observations.
- Hierarchical clustering, in many ways, is the most straightforward method for finding groups.

Hierarchical Clustering

- Hierarchical clustering can be boiled down to the following steps:
  1. Start with all observations in their own groups (n unique groups)
  2. Join the two closest observations (now there are $n - 1$ groups)
  3. Recalculate distances (more on this soon)
  4. Repeat 2) and 3) until you are left with only 1 group.

Simple Example



Example Distance Matrix

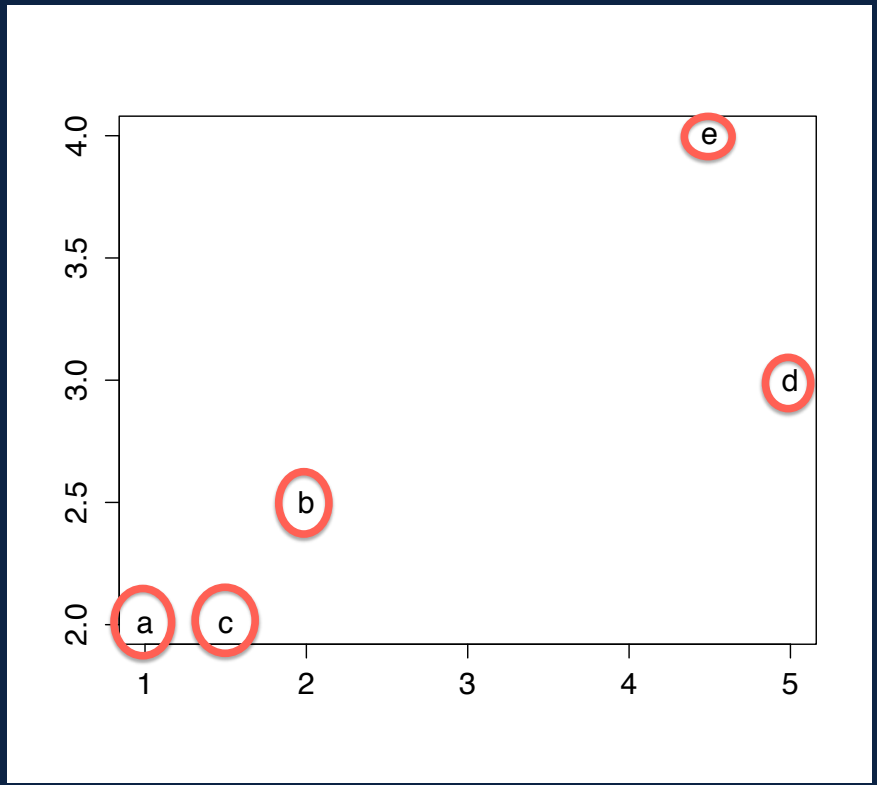
	a	b	c	d
b	1.12			
c	0.50	0.71		
d	4.12	3.04	3.64	
e	4.03	2.92	3.61	1.12

Example Distance Matrix

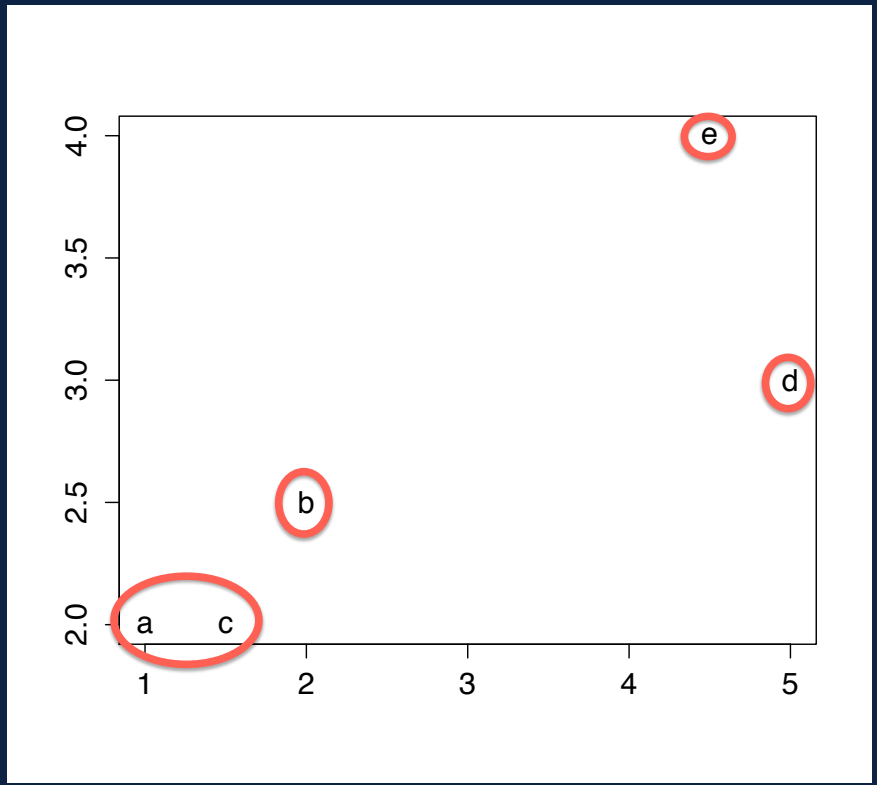
	a	b	c	d
b	1.12			
c	0.50	0.71		
d	4.12	3.04	3.64	
e	4.03	2.92	3.61	1.12

- So we join observation (a) with observation (c) at the second step of our process.

$n = 5$ Groups (our starting point)

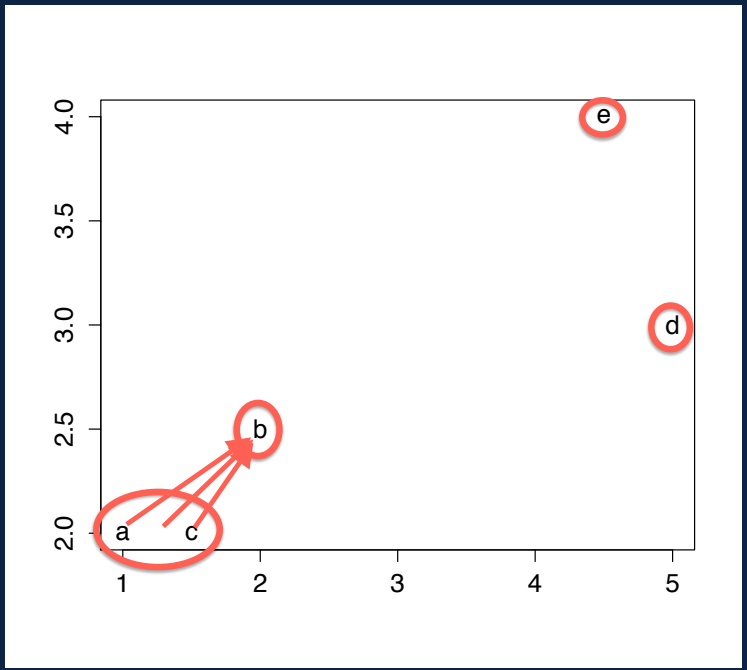


4 Groups (second step)



Recalculating Distances

- Now that we've joined the two closest observations...how do we determine the distance between that group and the others?



Recalculating Distances

- The arrows on the plot are three common ways of recalculating distances between groups, also called linkages
  - Single linkage - define distance as between closest observations.

    For this example, $d_{\{ac\}\{b\}} = d_{cb}$
  - Complete linkage - define distance as between furthest observations.

    For this example, $d_{\{ac\}\{b\}} = d_{ab}$.
  - Average linkage - define distance as the average distance between the observations inside group with those outside.

    For this example, $d_{\{ac\}\{b\}} = \frac{d_{ab}+d_{cb}}{2}$.

Distance Matrix - Single Linkage

	{ac}	b	d
b	0.71		
d	3.64	3.04	
e	3.61	2.92	1.12

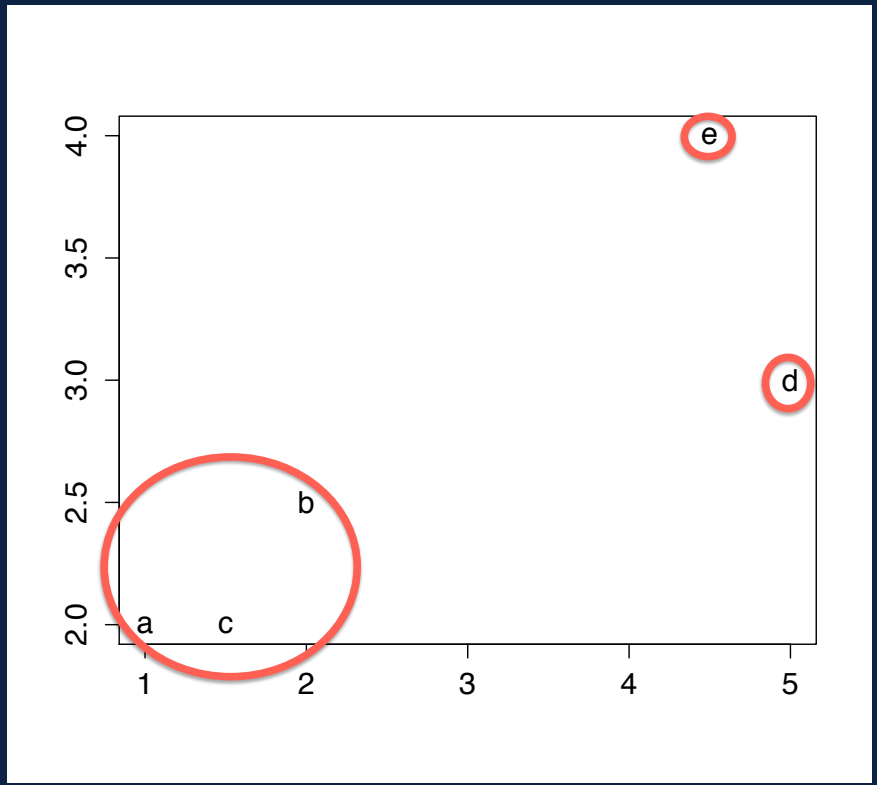
- We've updated the distances between our new group {ac} and the other remaining groups.

Distance Matrix - Single Linkage

	{ac}	b	d
b	0.71		
d	3.64	3.04	
e	3.61	2.92	1.12

- Closest groups are {ac} and {b}. We join those now.

3 Groups

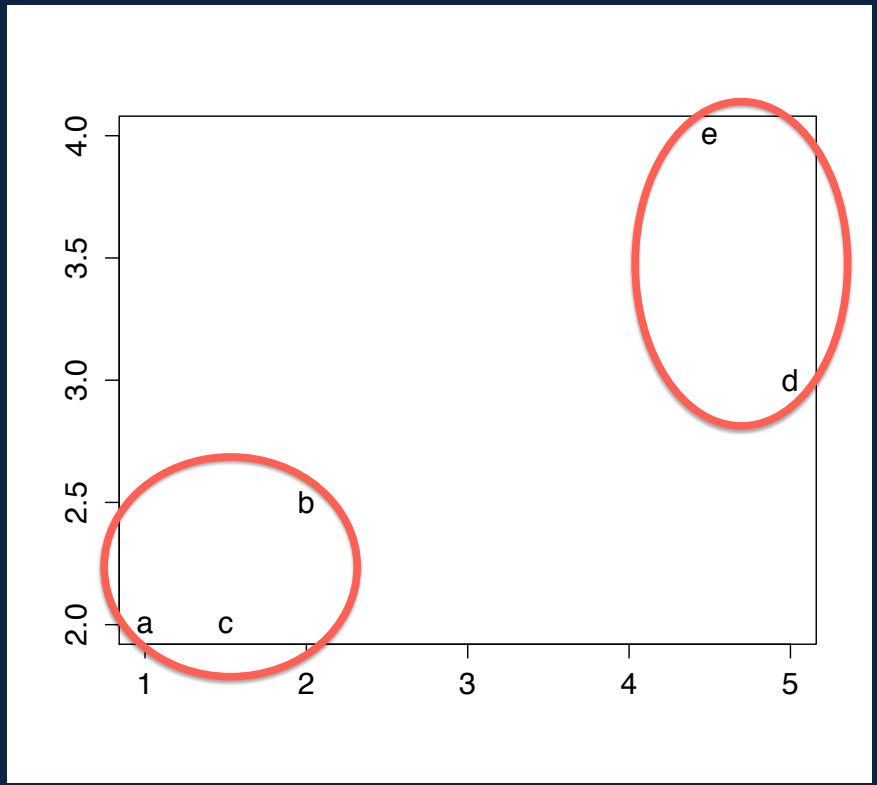


Distance Matrix - Single Linkage

	{abc}	d
d	3.04	
e	2.92	1.12

- Closest groups are {d} and {e}. We join those now.

2 Groups

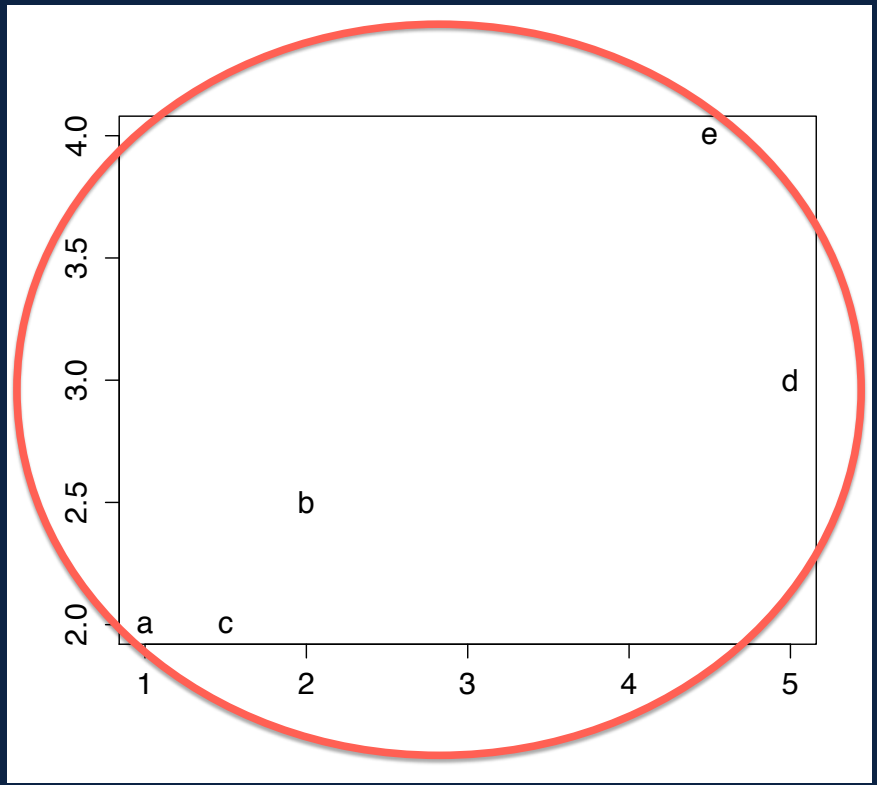


Distance Matrix - Single Linkage

	{abc}
{de}	2.92

- Closest groups are {abc} and {de} (only groups left to join). We join those now.

1 Group



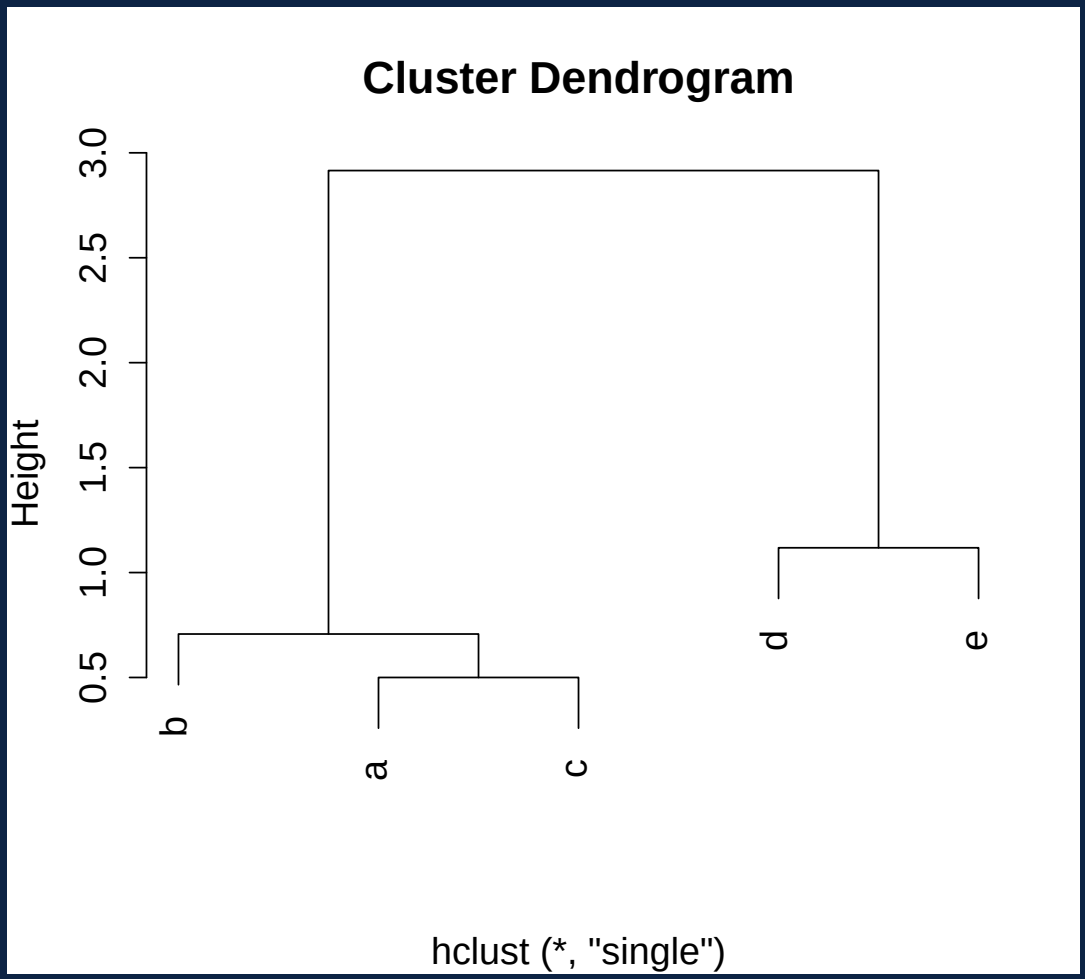
Hierarchical Clustering

- What have we accomplished?
- Technically, we've given potential solutions to the following non-trivial questions:
  - What would 2 groups look like in this data?
  - What would 3 groups look like in this data?
  - What would 4 groups look like in this data?
- This doesn't answer the more important question: how many groups are in this data and what do they look like?
- Also, do we really need to go through the algorithm step-by-step to see the process?

Hierarchical Clustering

- The solution to both issues is one in the same.
- We can summarize the algorithm graphically, using what's called a dendrogram.
- On the X-axis, we just have our observations
- On the Y-axis, we have the distance where the groups are combined

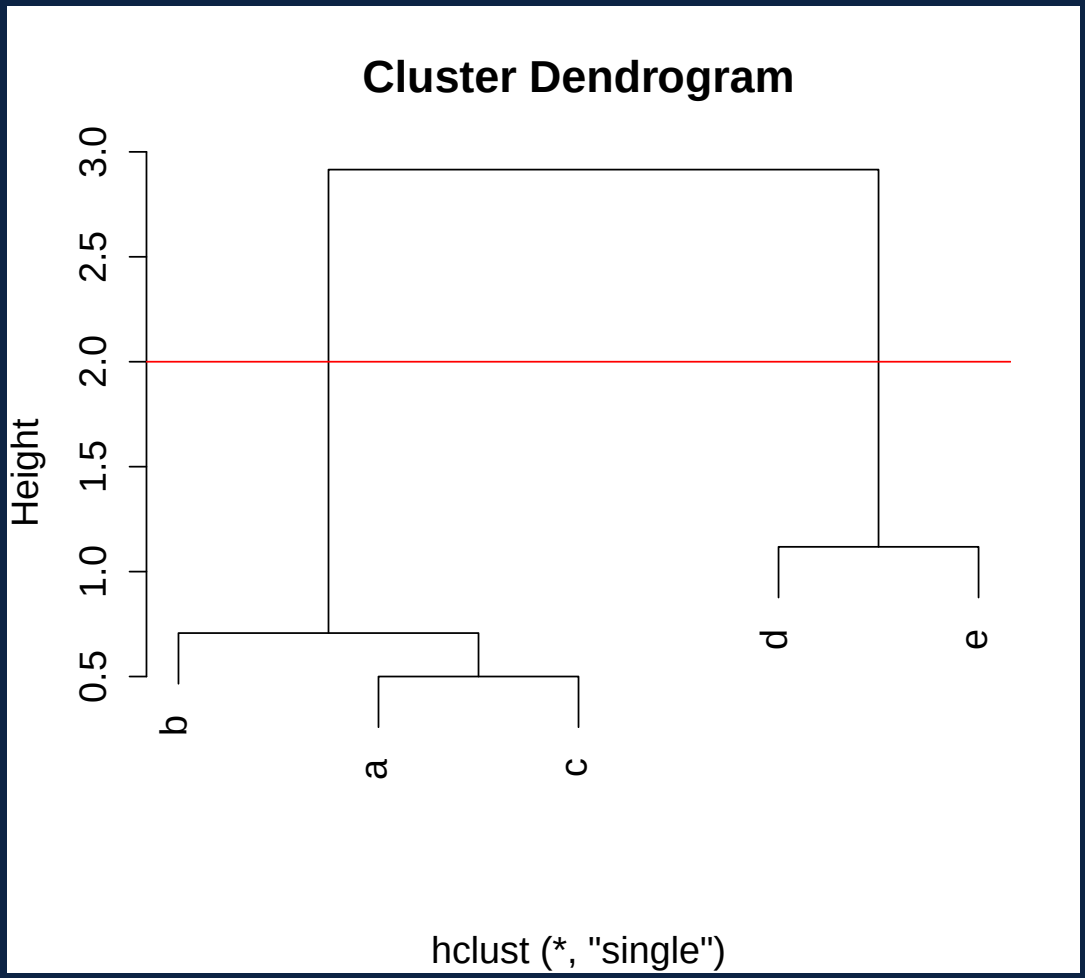
Dendrogram for our Simple Example



Hierarchical Clustering

- Dendrograms show what observations were joined at what distance.
- They can also be used to determine how many groups are present in the data.
- Large "jumps" between combining groups signify large distances between groups.
- So generally, we can "cut" at the largest jump in distance, and that will determine the number of groups, as well as each observation's group membership.

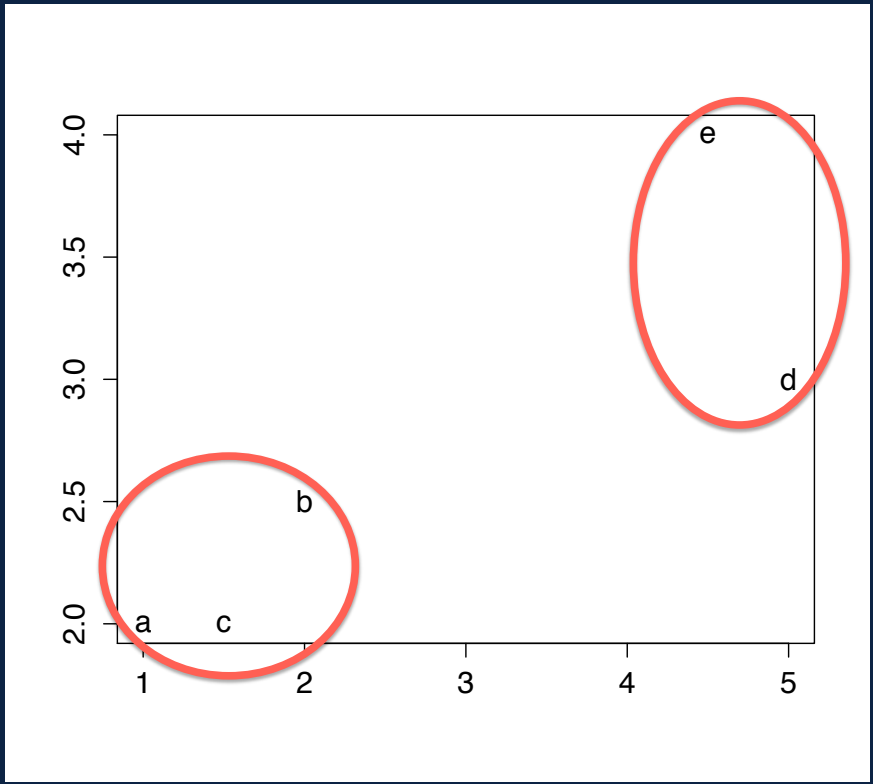
Dendrogram for our Simple Example



- This suggests a two group solution as "best" ...

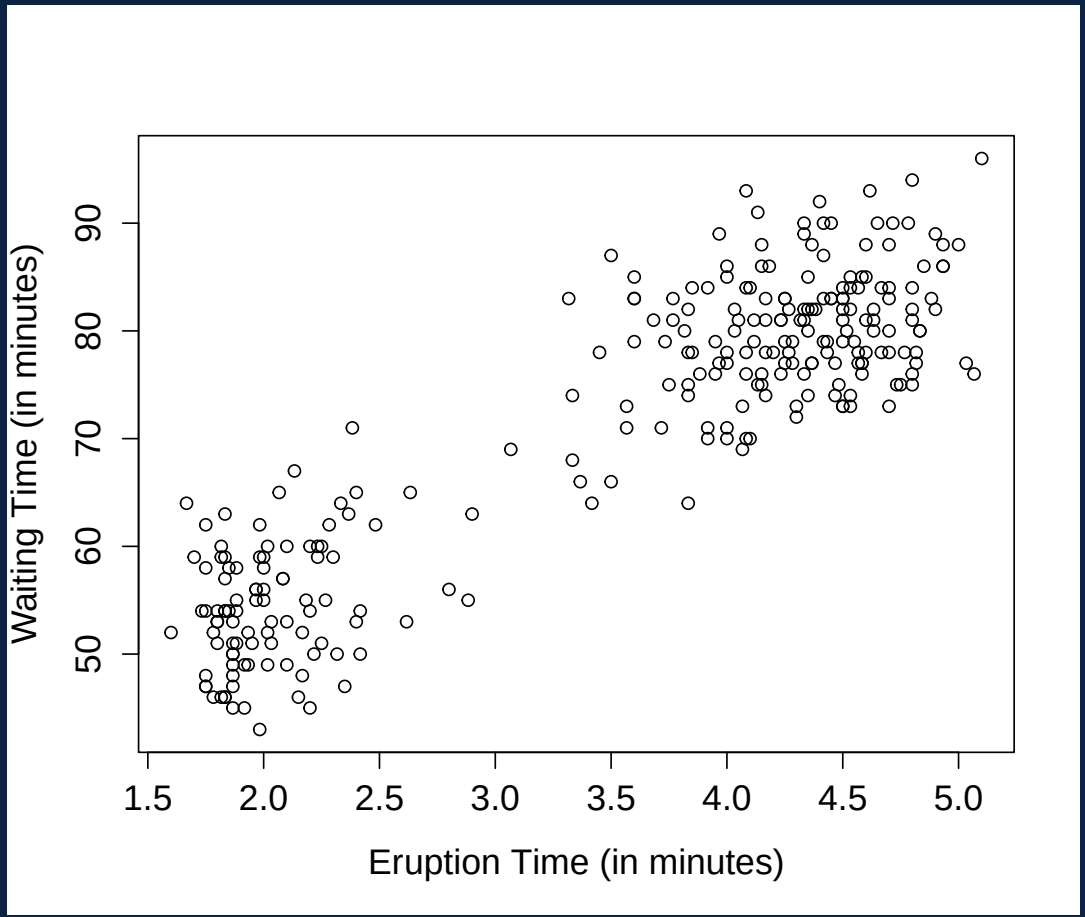
2 Groups

- Which should match our intuition...



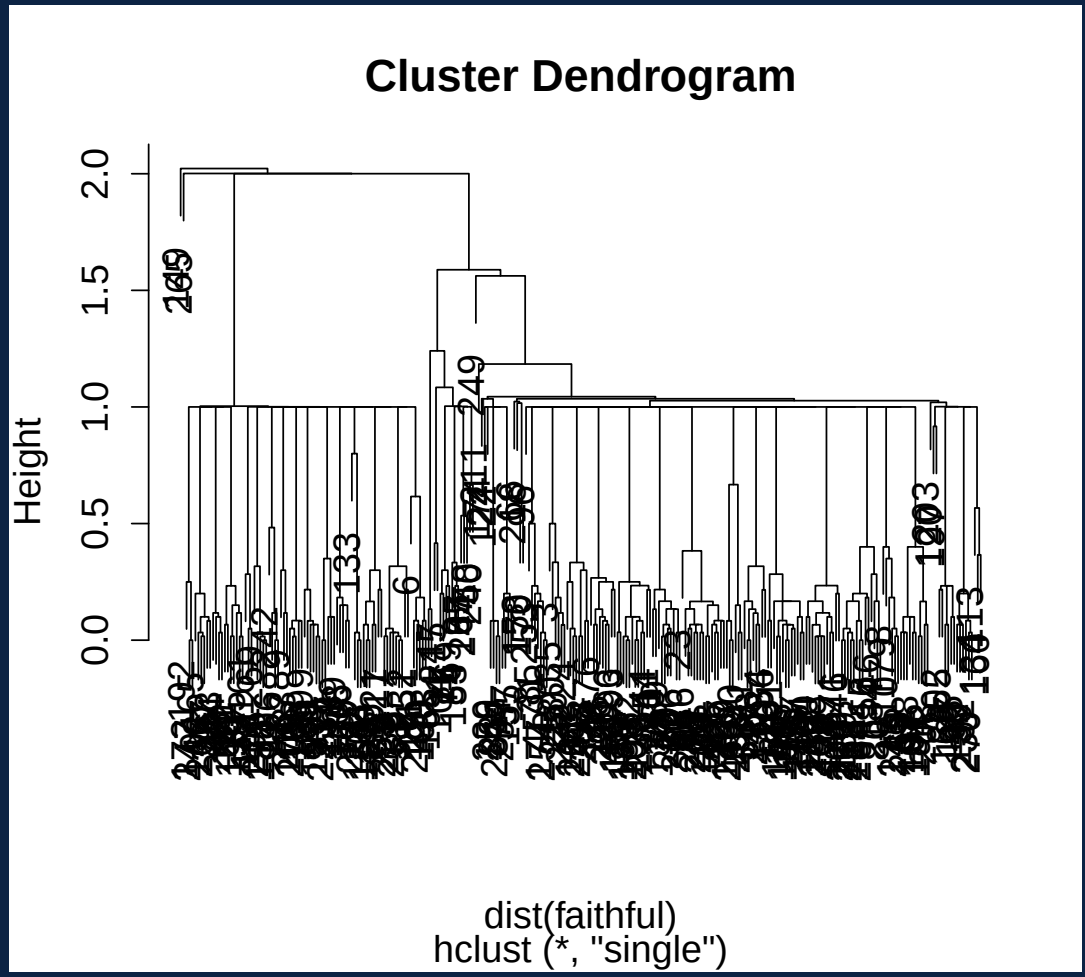
Old Faithful Data Set

- Let's apply HC to some more interesting data sets...



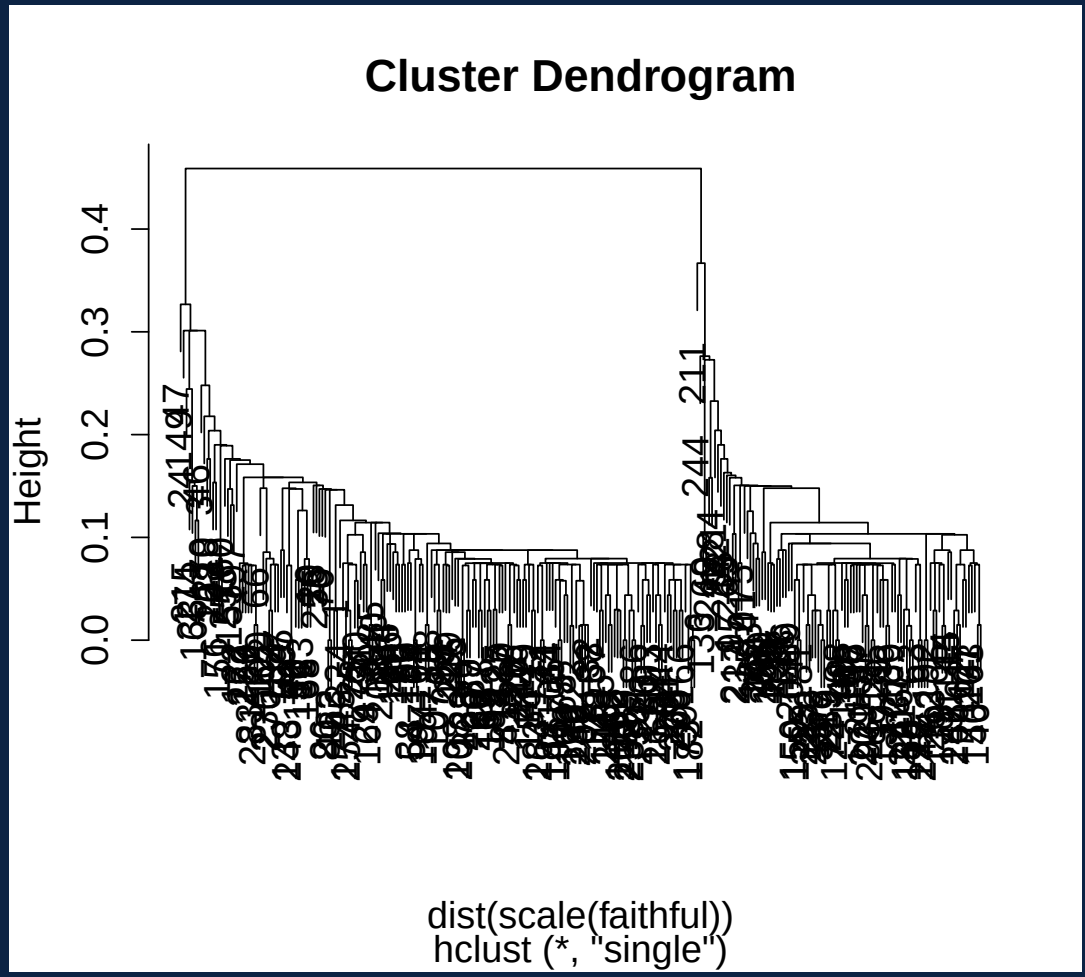
Old Faithful Data Set

- Here's HC on the raw distance matrix...



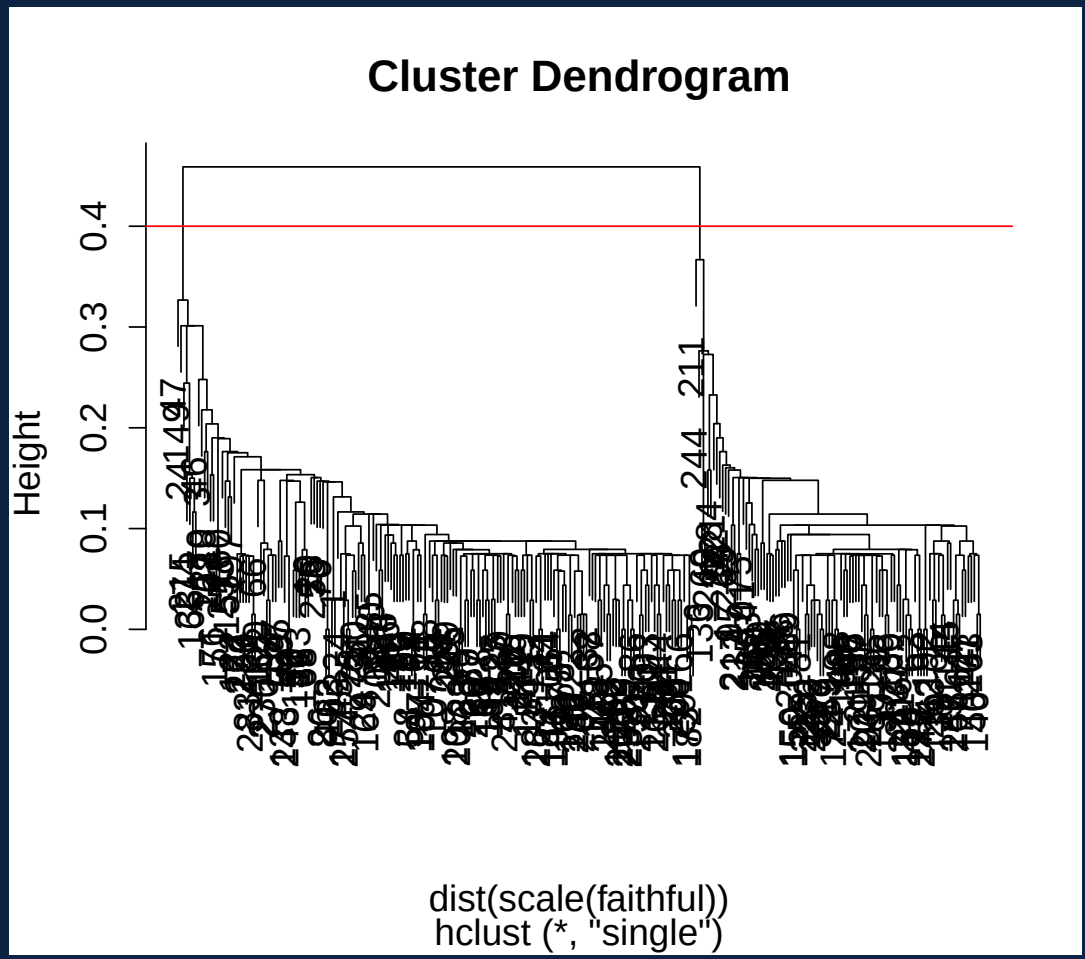
Old Faithful Data Set

- Here's HC on the standardized distance matrix...



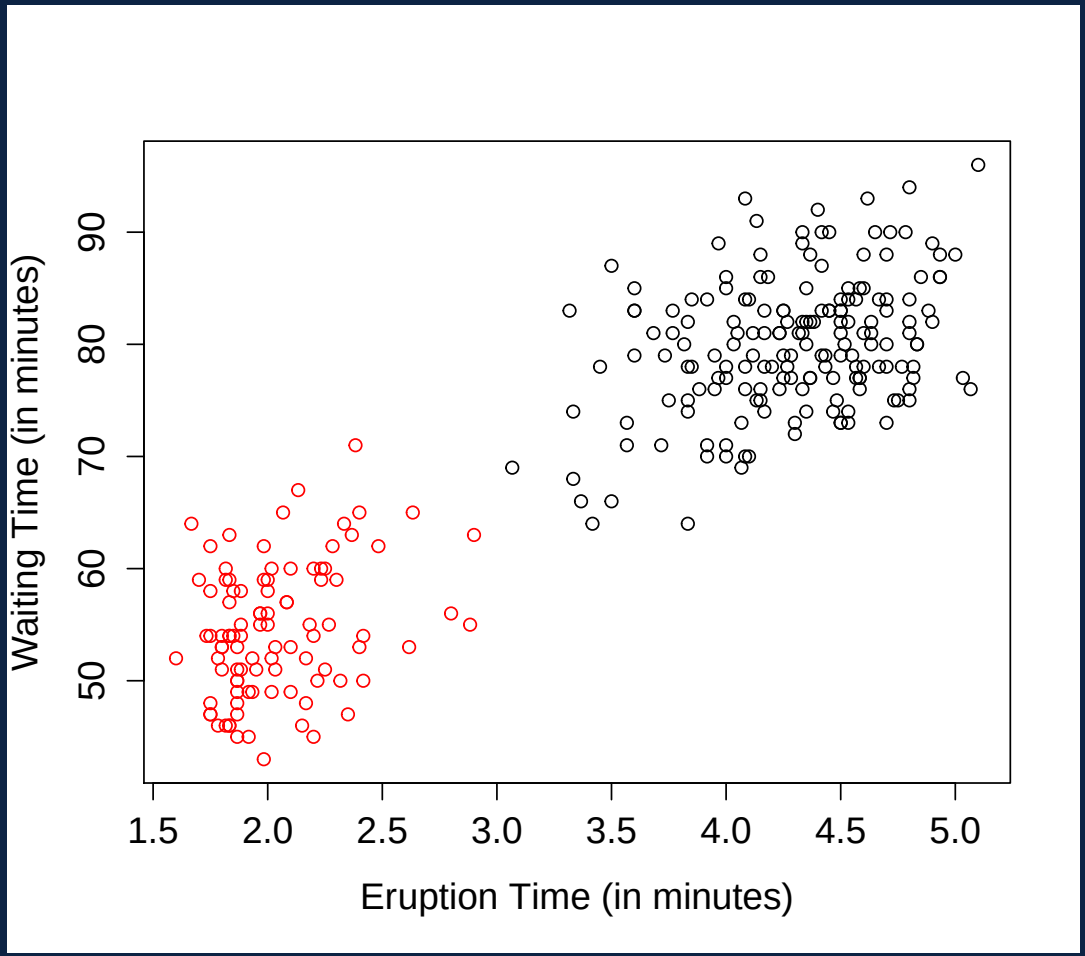
Old Faithful Data Set

- Here's HC on the standardized distance matrix...

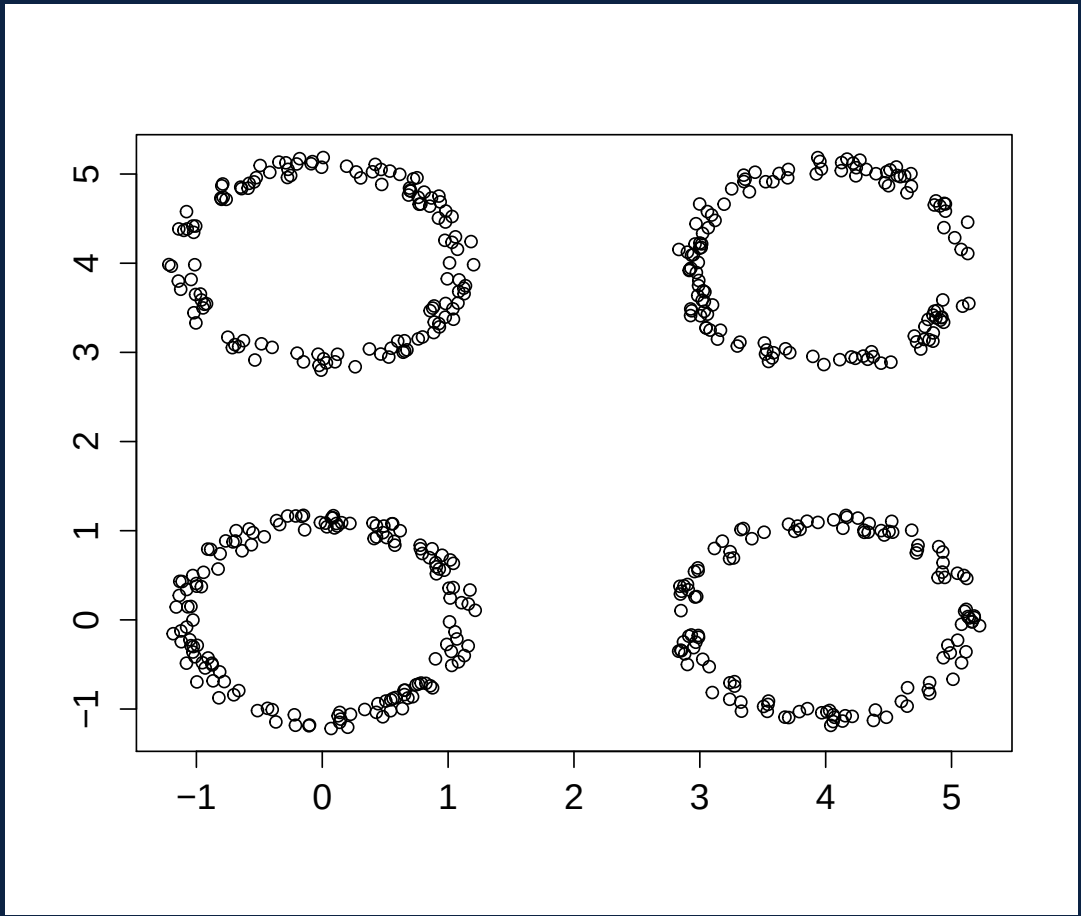


Old Faithful Data Set

- Which gives the following solution...



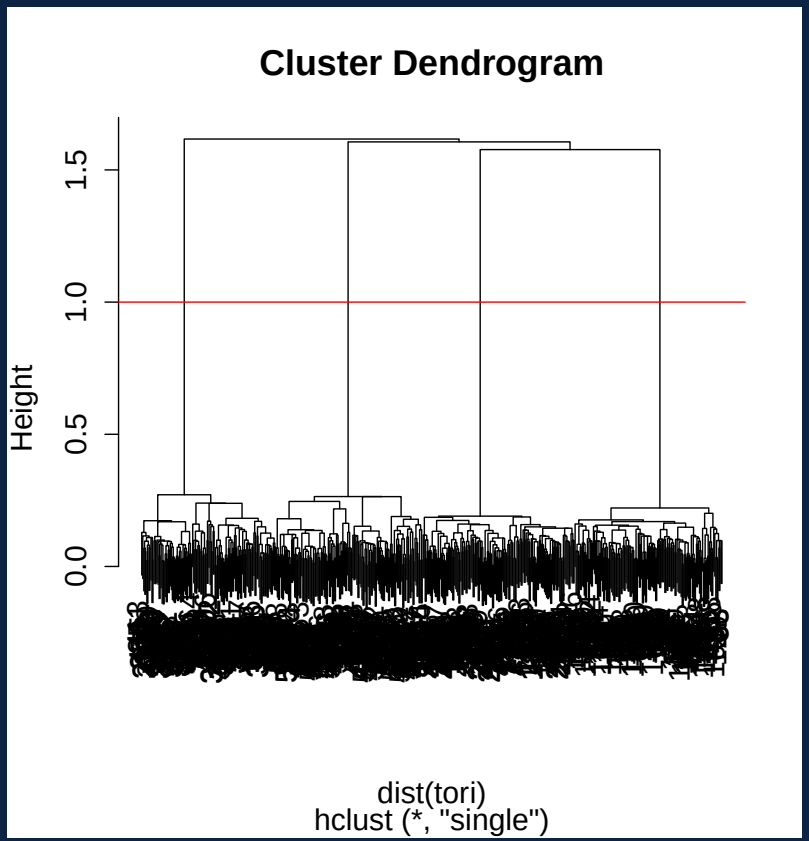
Tori! Data Set



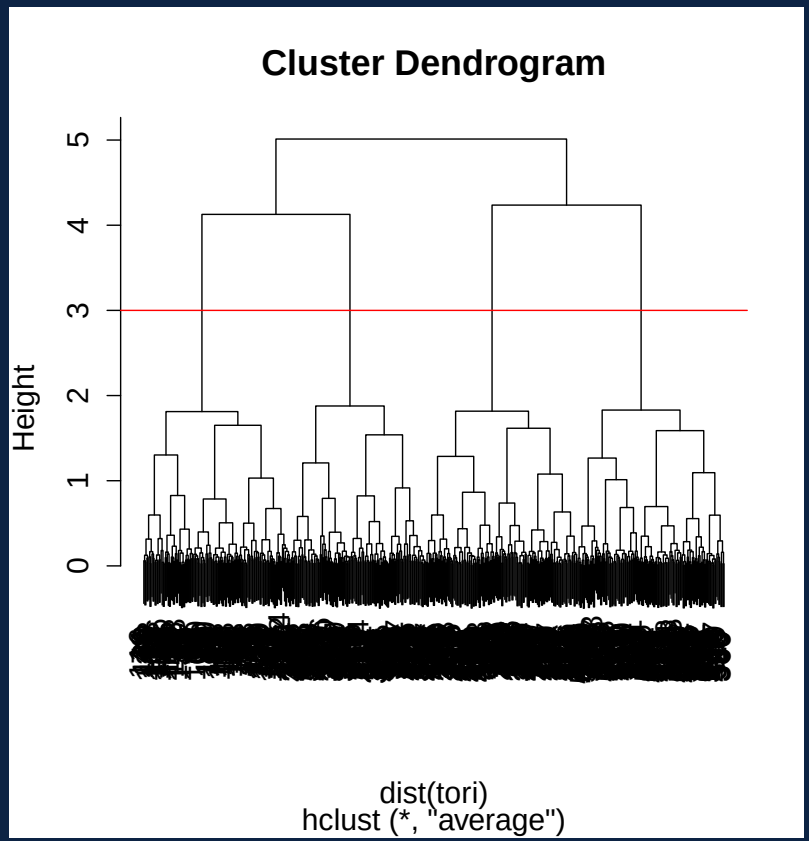
Tori Data Set

- For "easy" data sets, linkage method doesn't affect the end result...

Single

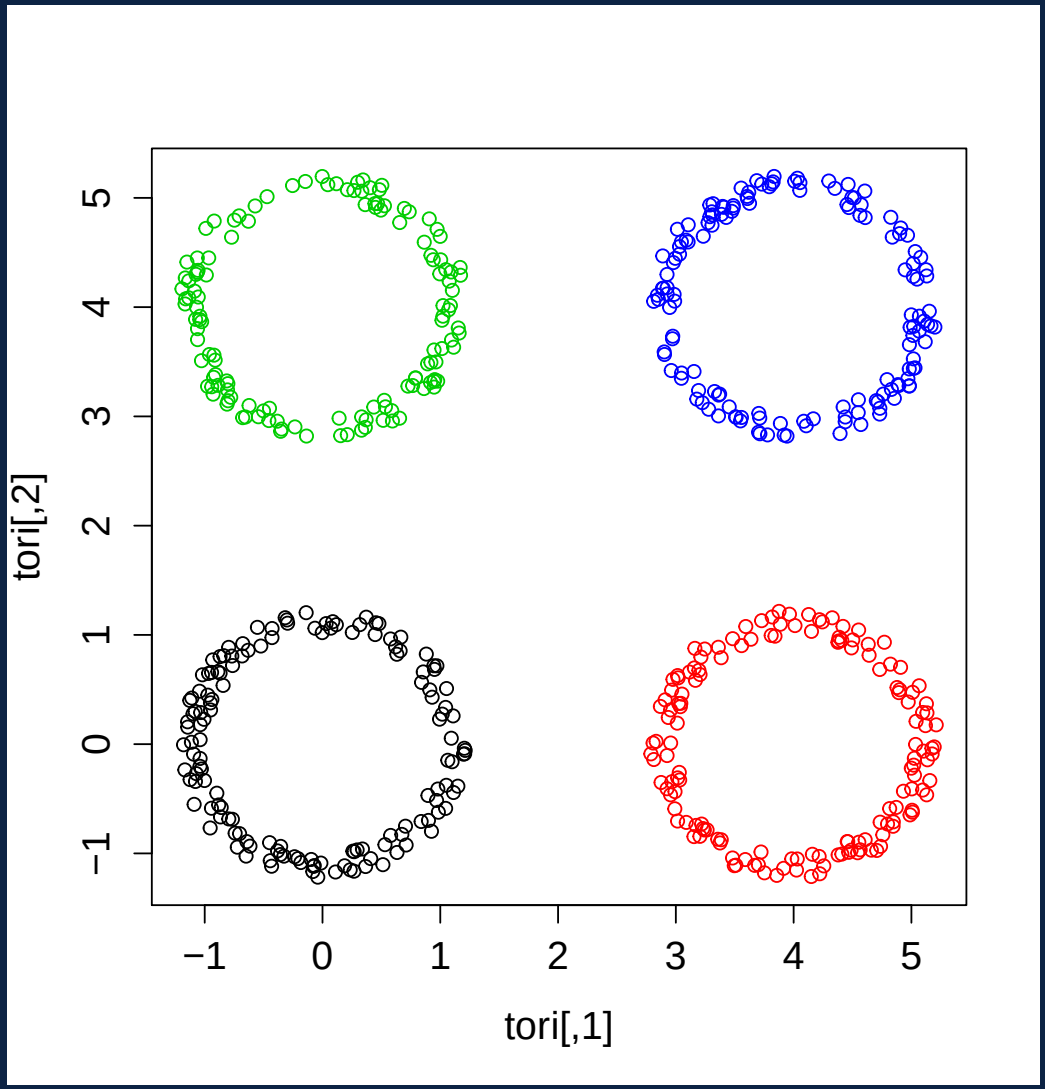


Average



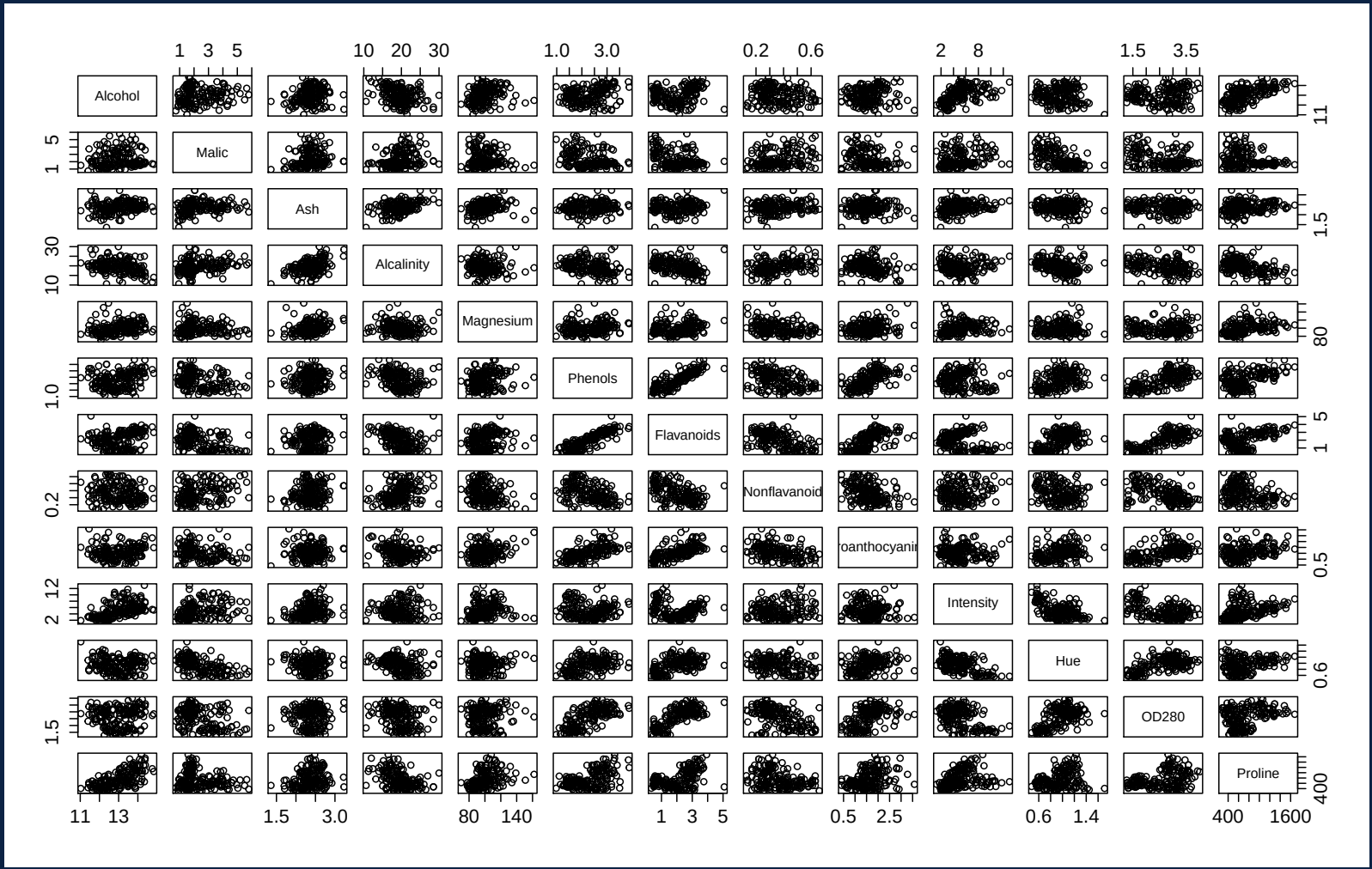
Tori Data Set

- Which, again, gives the solution we expect...



Wine Data Set

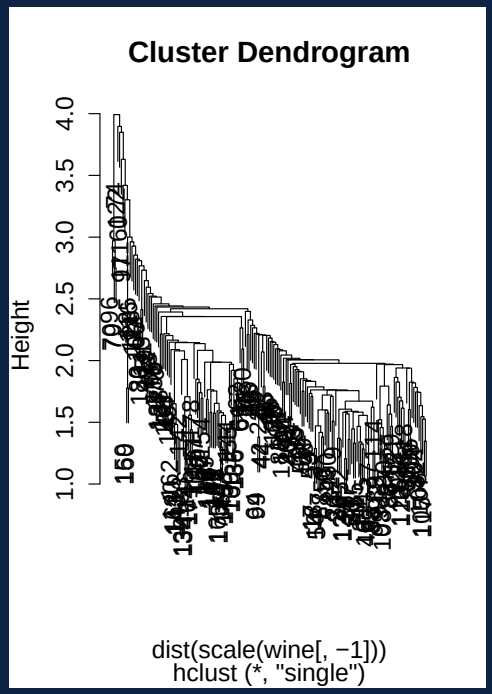
- Back to the wine!



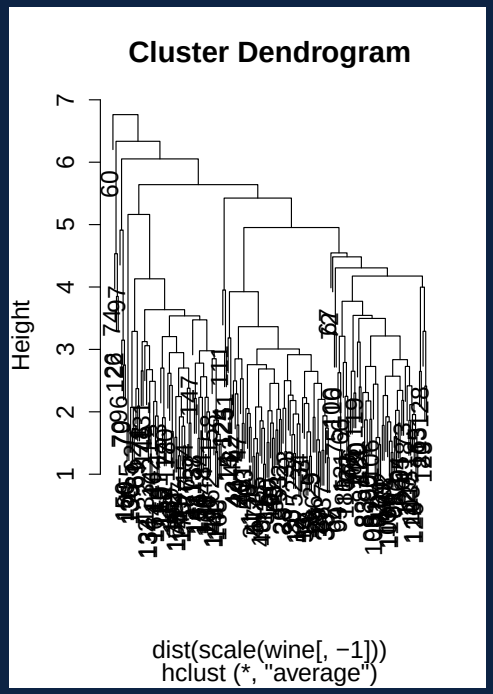
Wine Data Set

- Linkage method will affect more difficult clustering problems...

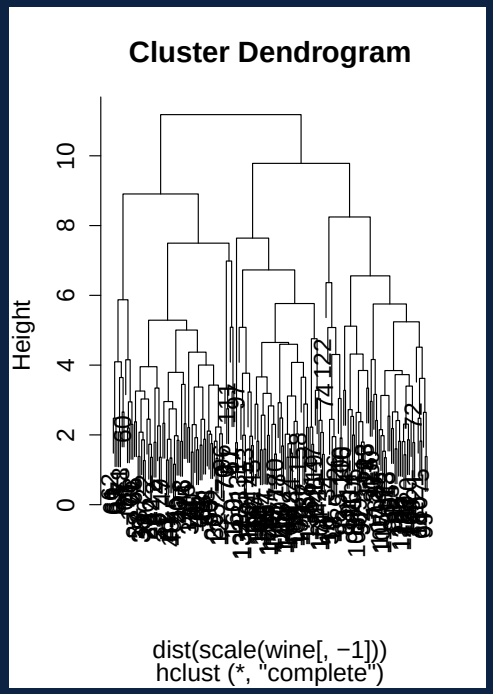
Single



Average

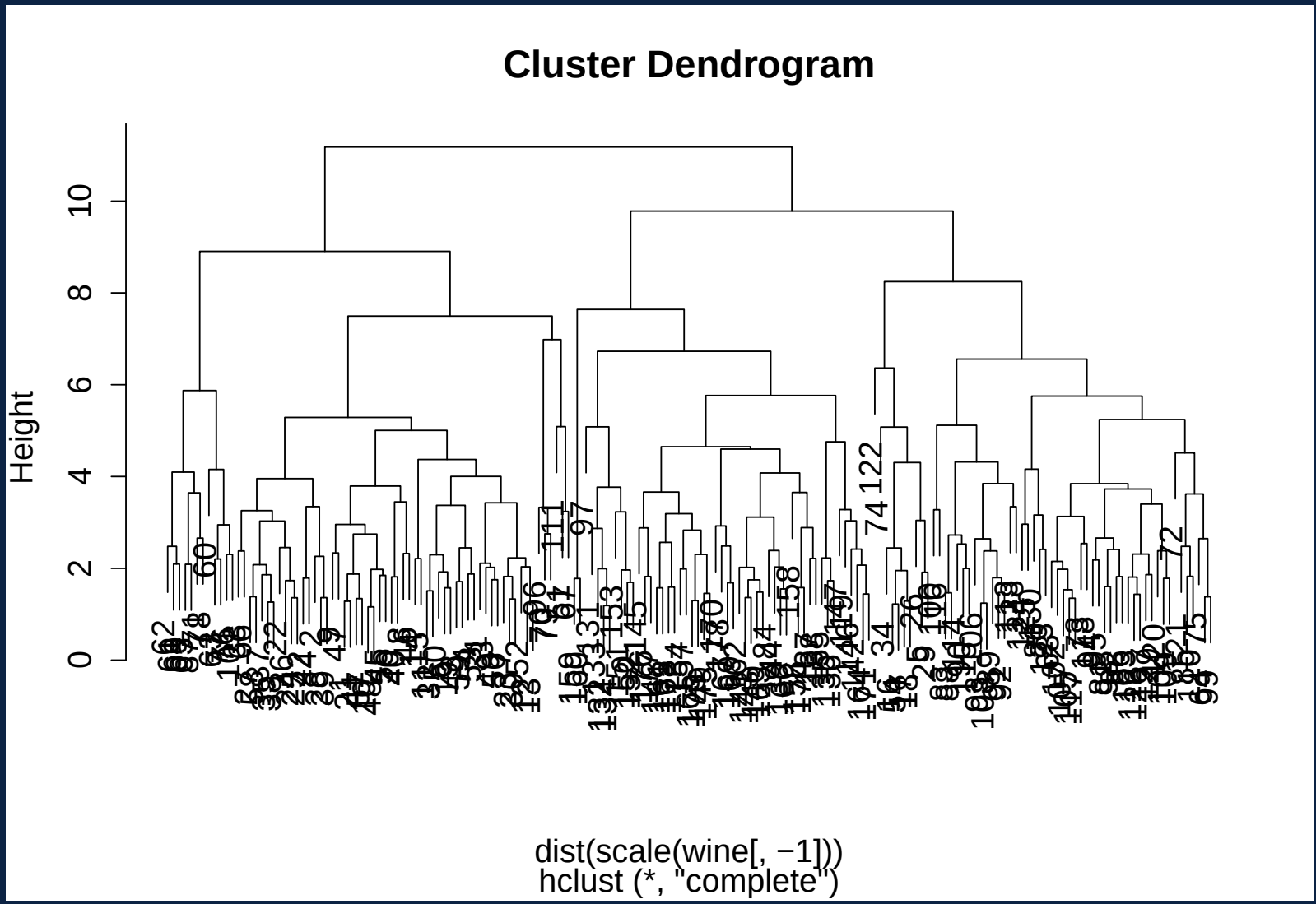


Complete



Wine Data Set

- Complete linkage gives the only clear-ish clustering result, suggesting probably 2 or 3 groups. We'll come back to this later.



Hierarchical Clustering: Problems

- Some cons of HC...
- Distance matrices (of size $n \times n$, symmetric) must be calculated. For very large samples, this can be time consuming (even for computers).
- Results are often sensitive to what distance type and what linkage method are used.

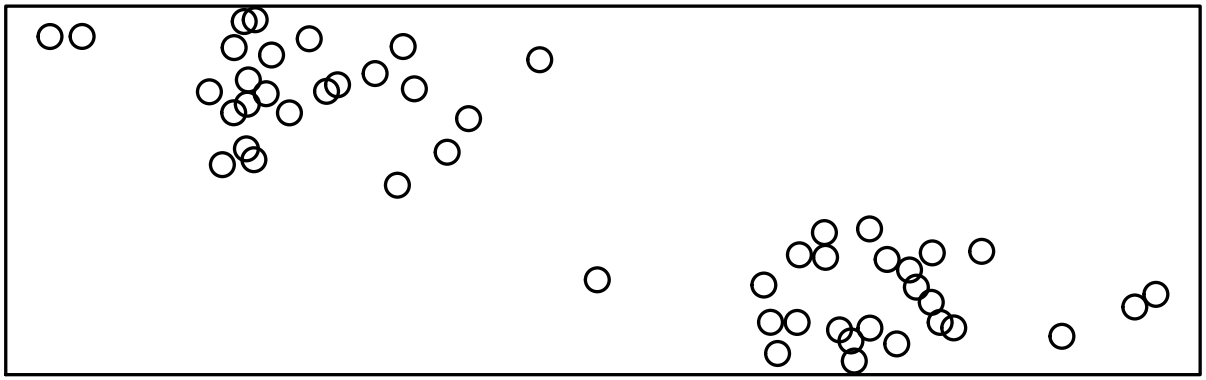
k-means Clustering

- Moving on from hierarchical methods, we'll now consider a method based on partitioning data.
- k-means clustering is a popular method that requires the user to provide the number of groups they are looking for — though we will discuss one way of seeking evidence for the number of groups.

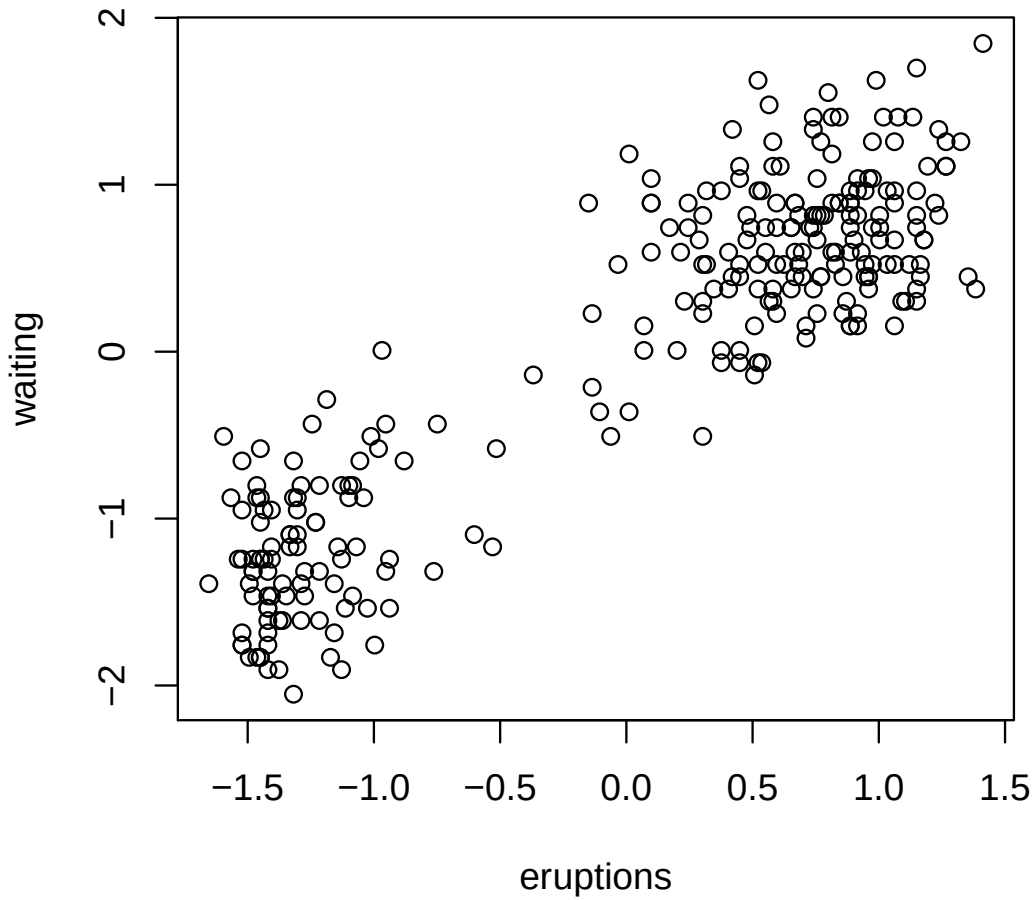
k-means Algorithm

- The k-means algorithm has the following steps:
  1. Randomly select k (the number of groups) points in your data. These will serve as the first centroids.
  2. Assign all observations to their closest centroid. You now have k groups.
  3. Calculate the means of each group. These are your new centroids.
  4. Repeat 2) and 3) until nothing changes anymore.

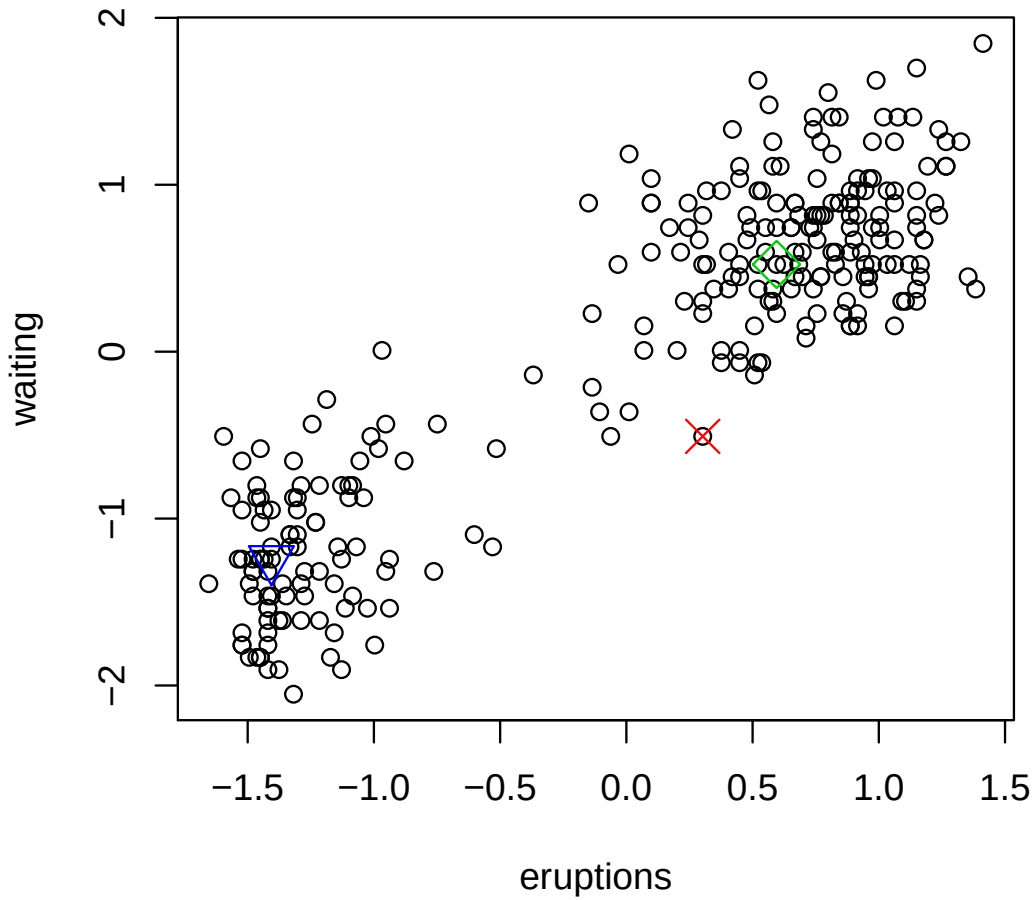
k-means on Simulated Data



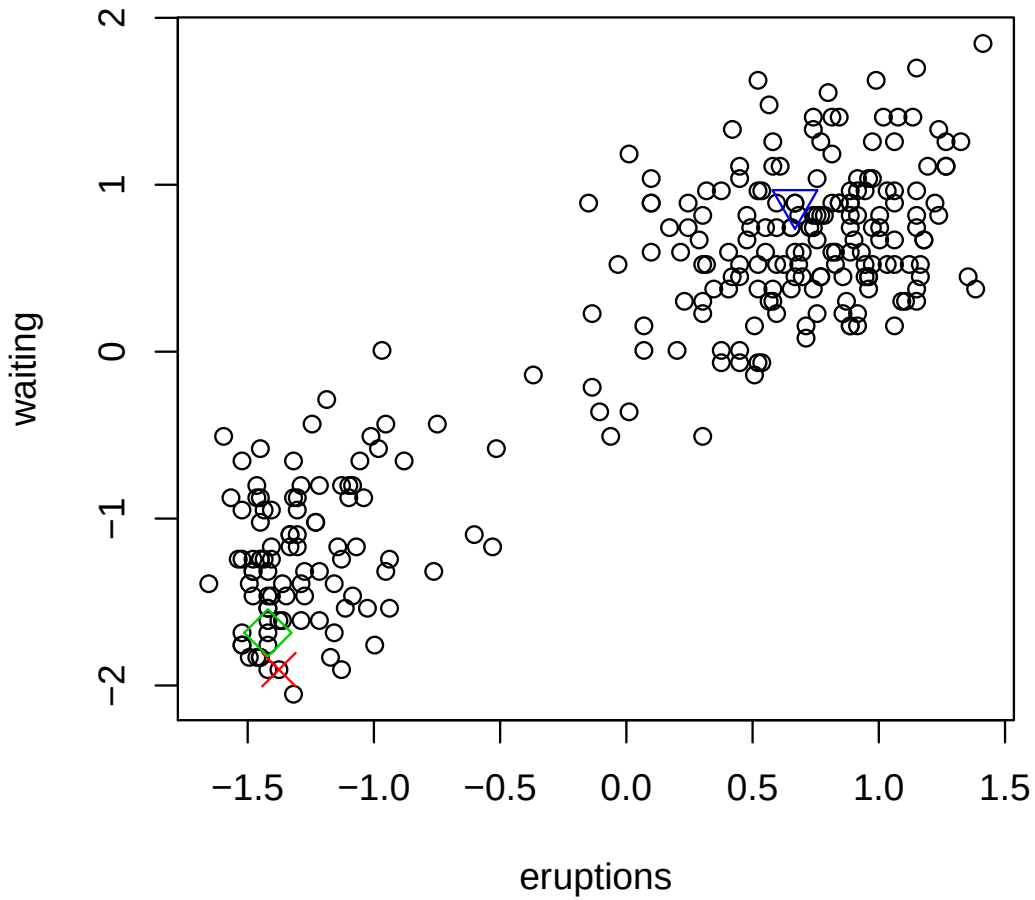
k-means on Old Faithful (2 groups)



k-means on Old Faithful (3 groups)

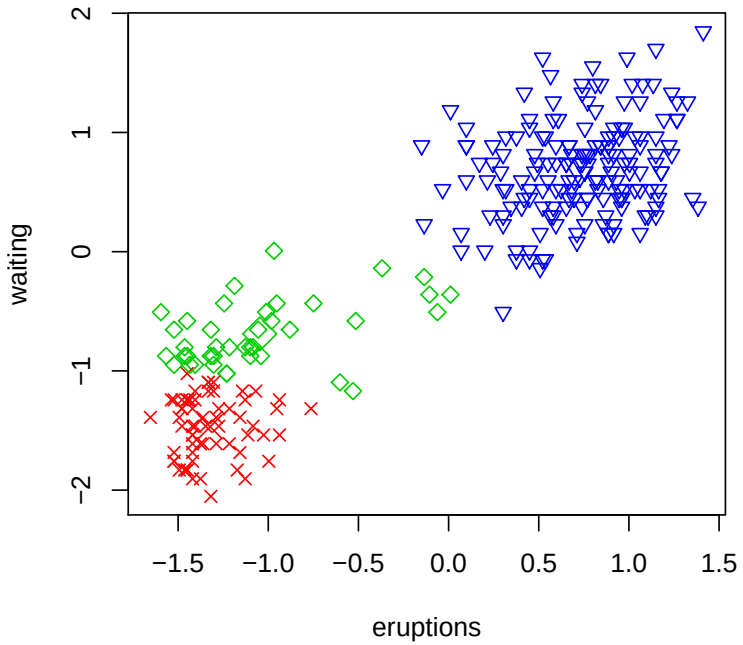


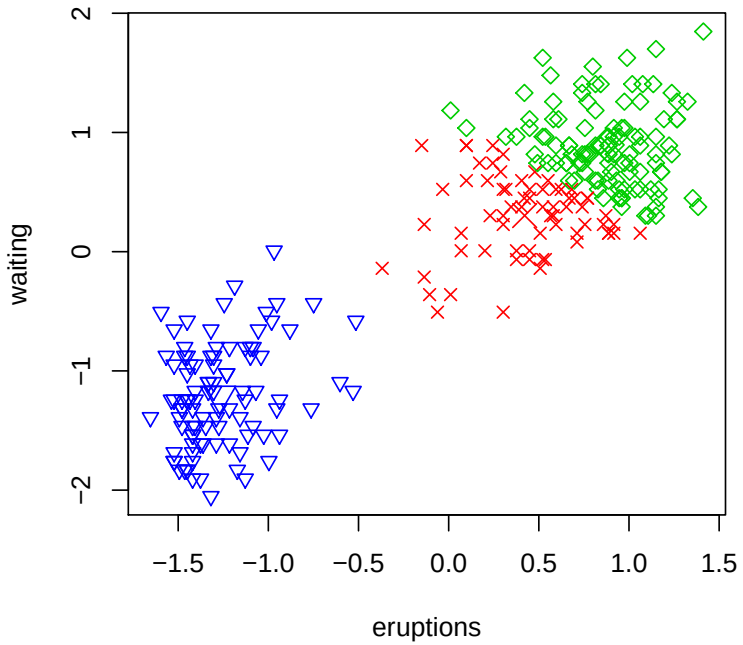
k-means on Old Faithful (3 groups again)



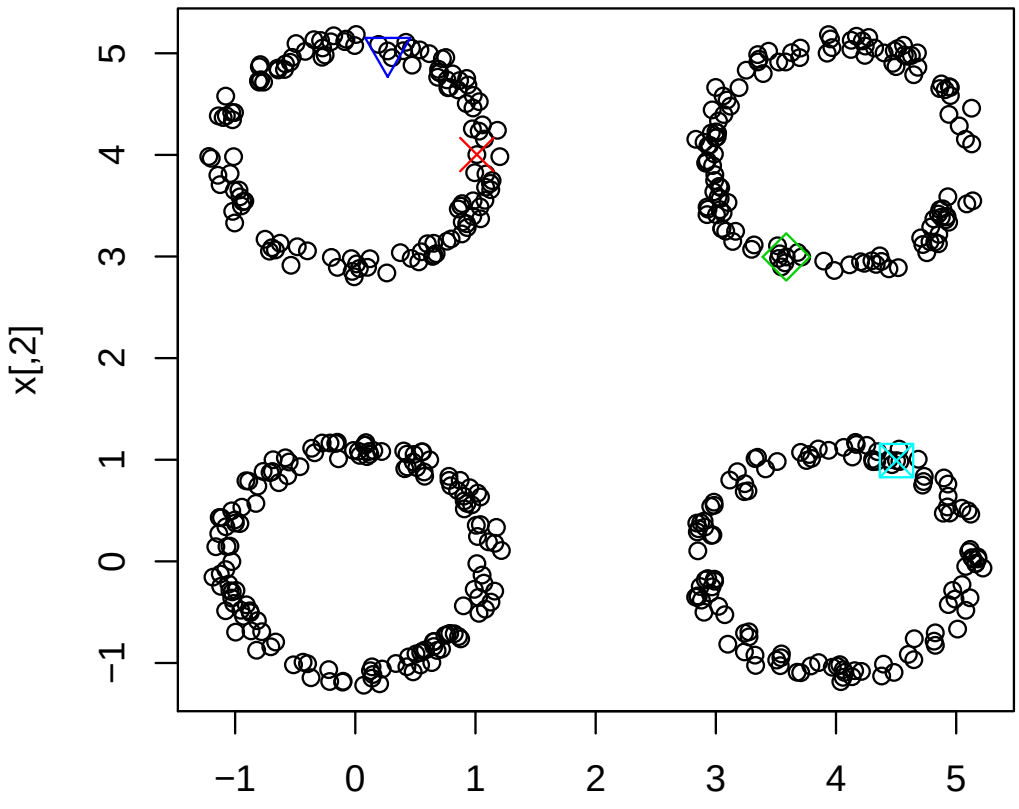
k-means on Old Faithful (3 group comparison)

- This should make the difference in results more clear...





k-means on Tori



k-means Algorithm

- Why does the k-means algorithm work?
  1. Randomly select k (the number of groups) points in your data. These will serve as the first centroids.
  2. Assign all observations to their closest centroid. You now have k groups.
  3. Calculate the means of each group. These are your new centroids.
  4. Repeat 2) and 3) until nothing changes anymore.

- Both 2) and 3) are recursively finding the minimum within-group sum of squared distances between observations and their centroids.

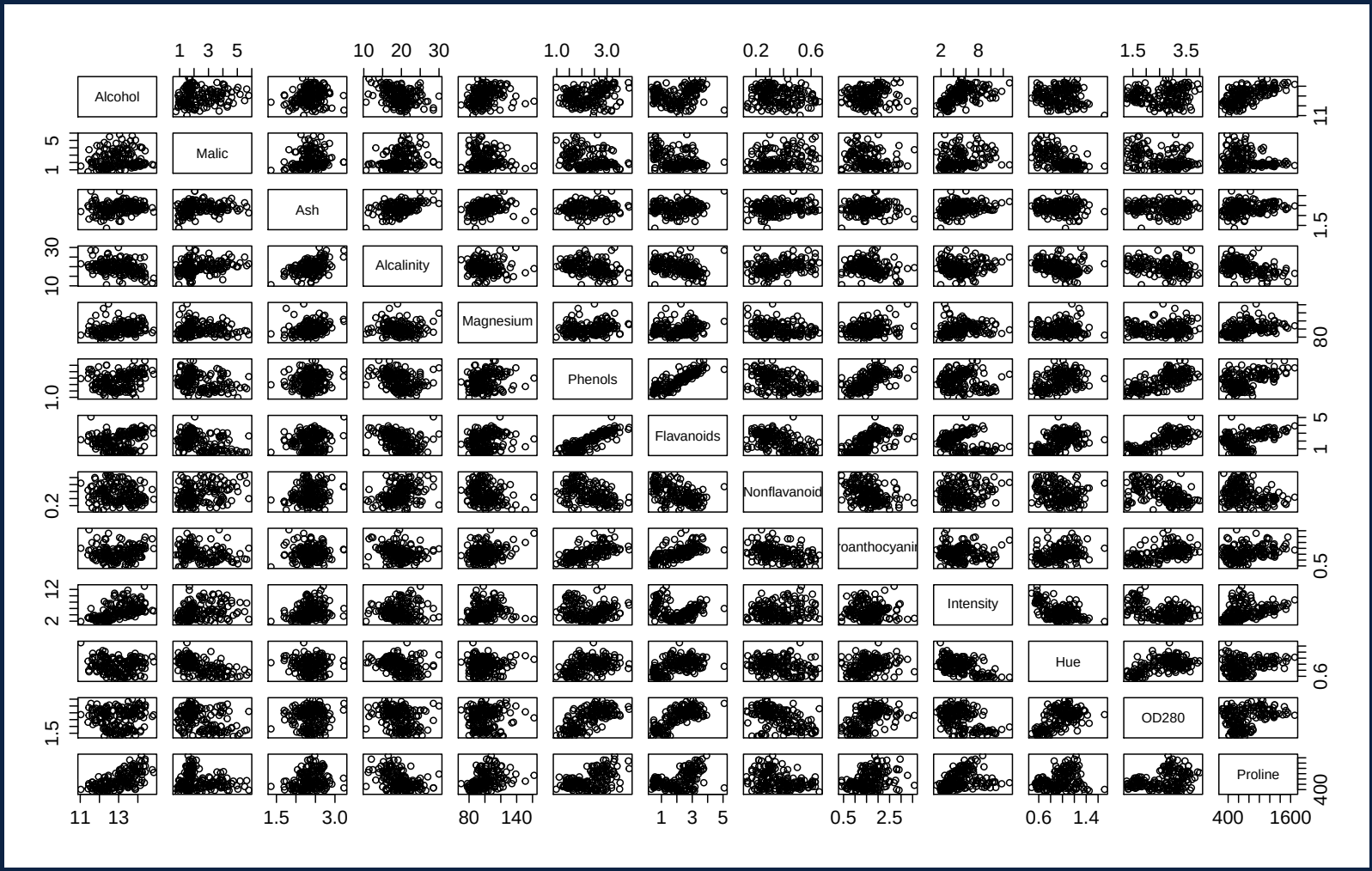
k-means Algorithm: Pros and Cons

- Pros
  - Computationally efficient (fast to run), even for large data sets.
  - Only $n \times k$ distance matrices needed (distances between n observations and k centroids).
  - Relatively straightforward concept.
  - Often provides clearer groups than HC.

- Cons
  - As we saw, where the algorithm (randomly) starts can affect the results (local optimization rather than global)
  - Groups will be found no matter what — even if there are no groups present in the data.

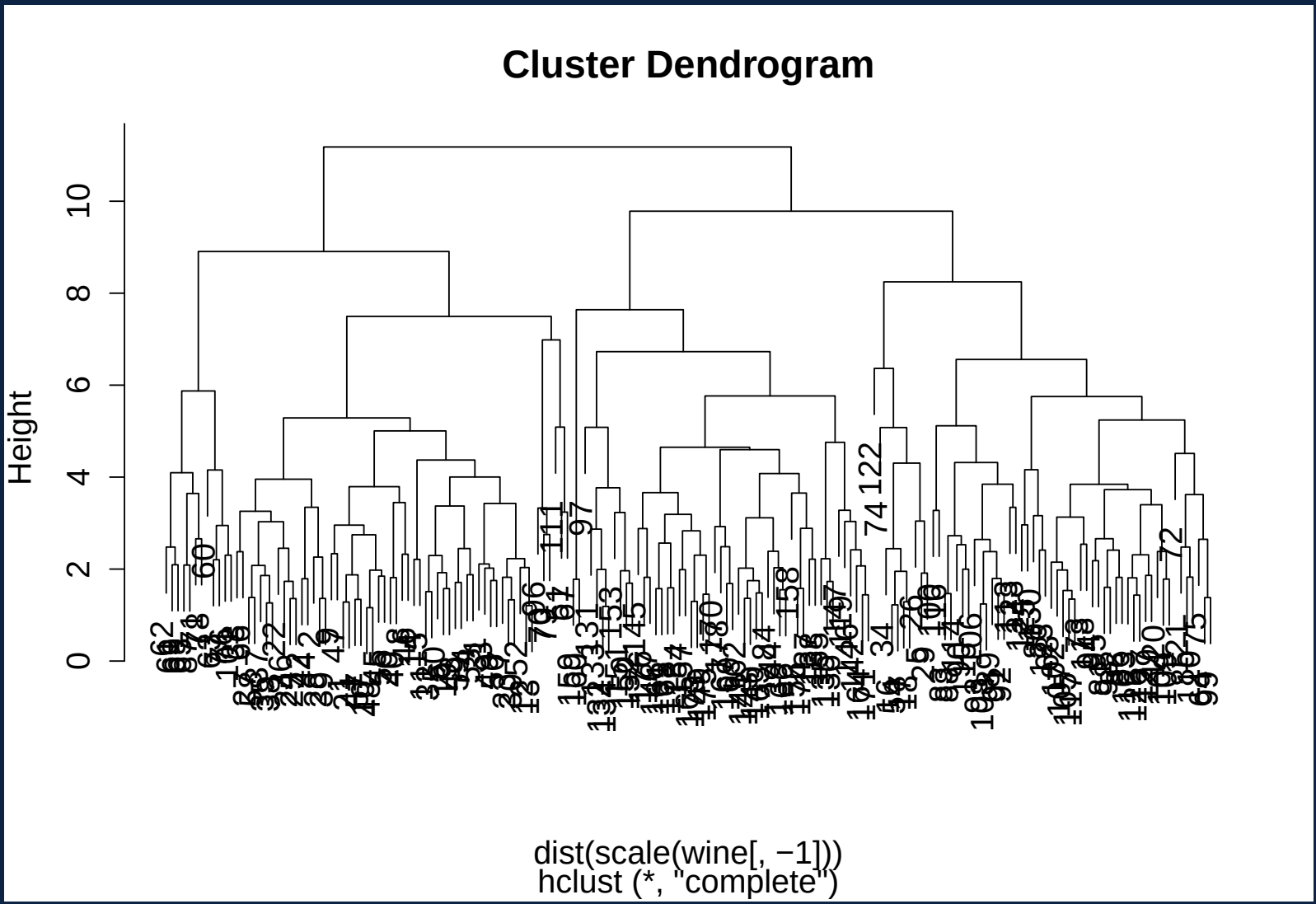
Application to Wine Data Set

- Back to the wine again. Let's apply HC and k-means and then investigate the results...



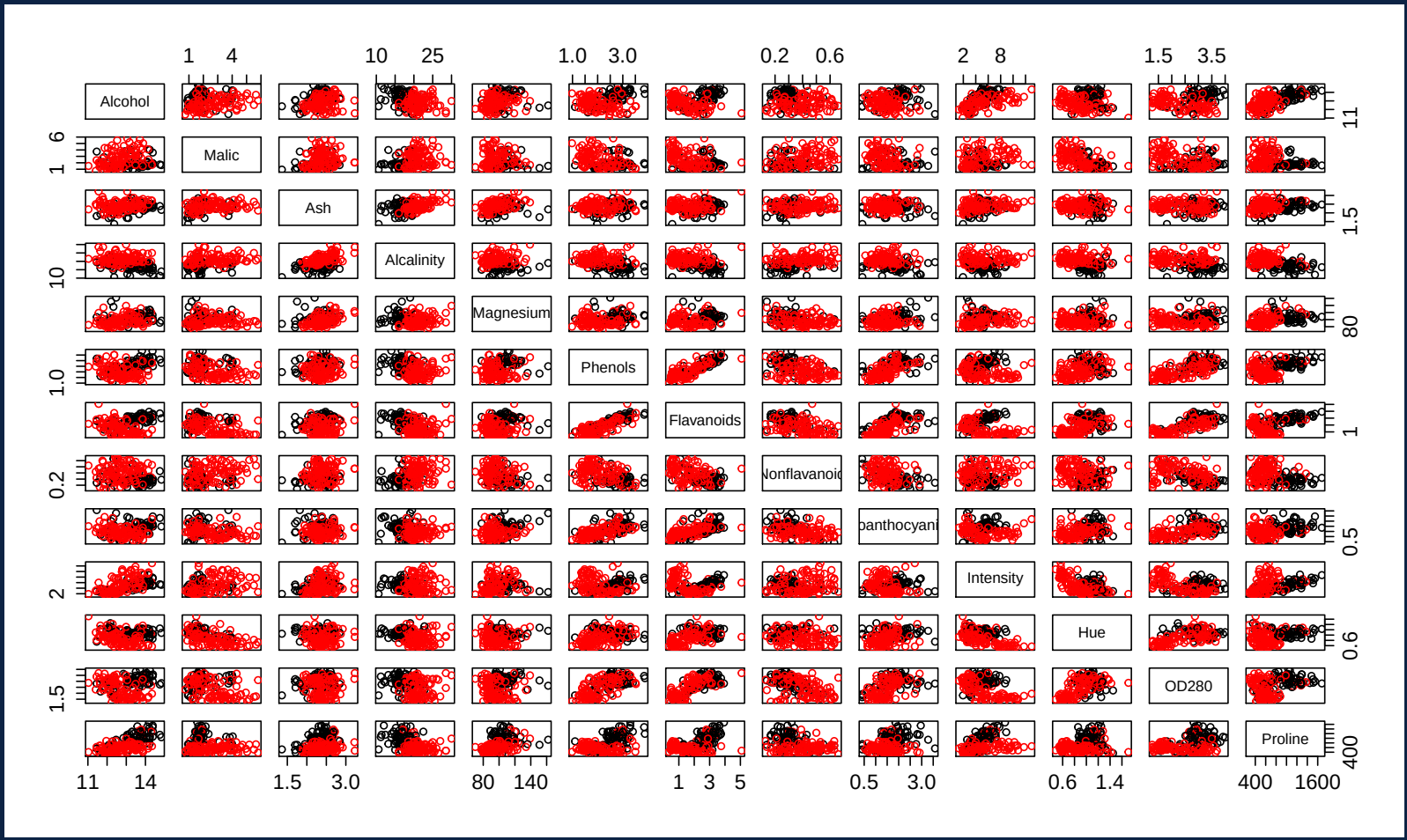
Wine Data Set

- Complete linkage suggested probably 2 or 3 groups.



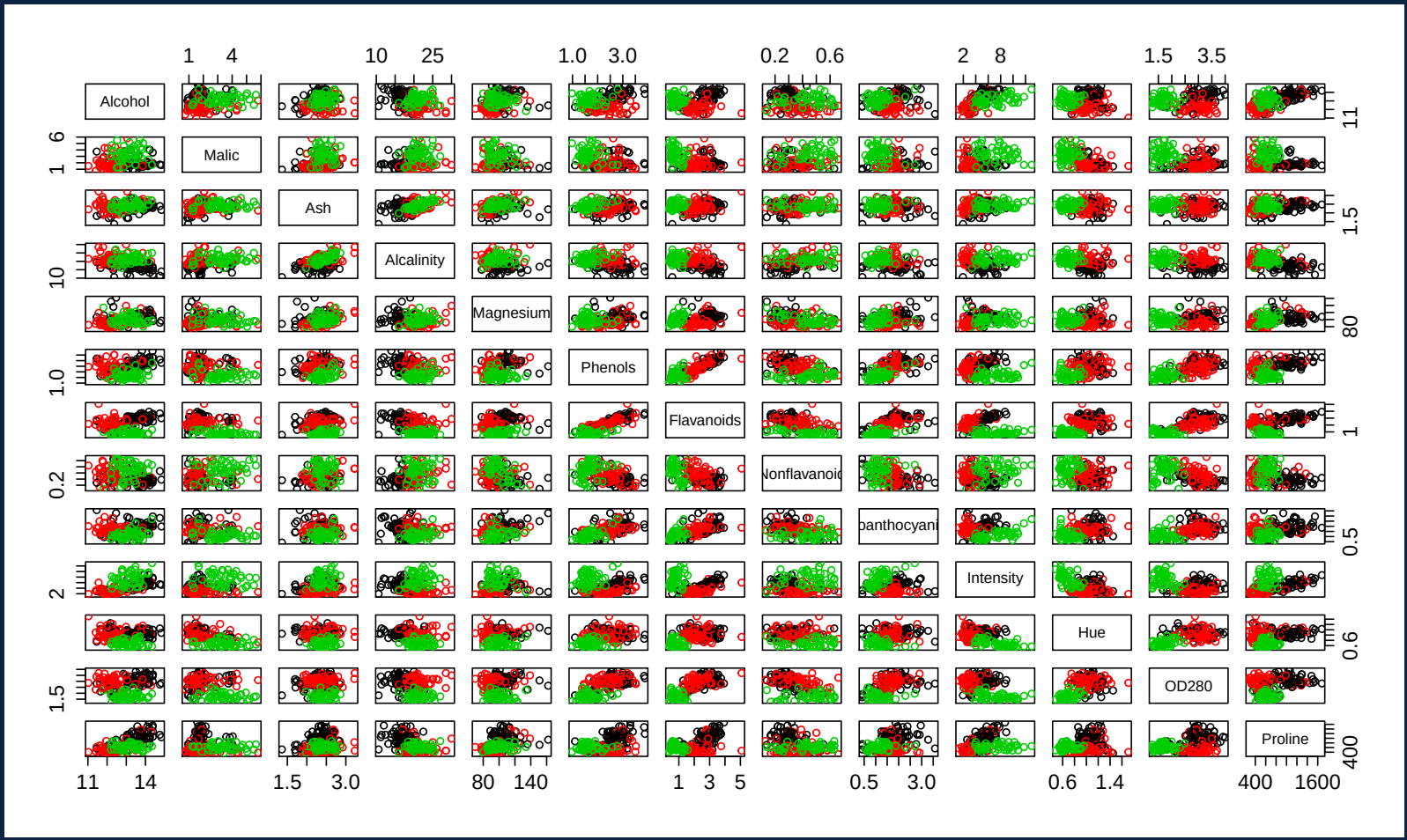
Wine Data Set

- HC 2 groups



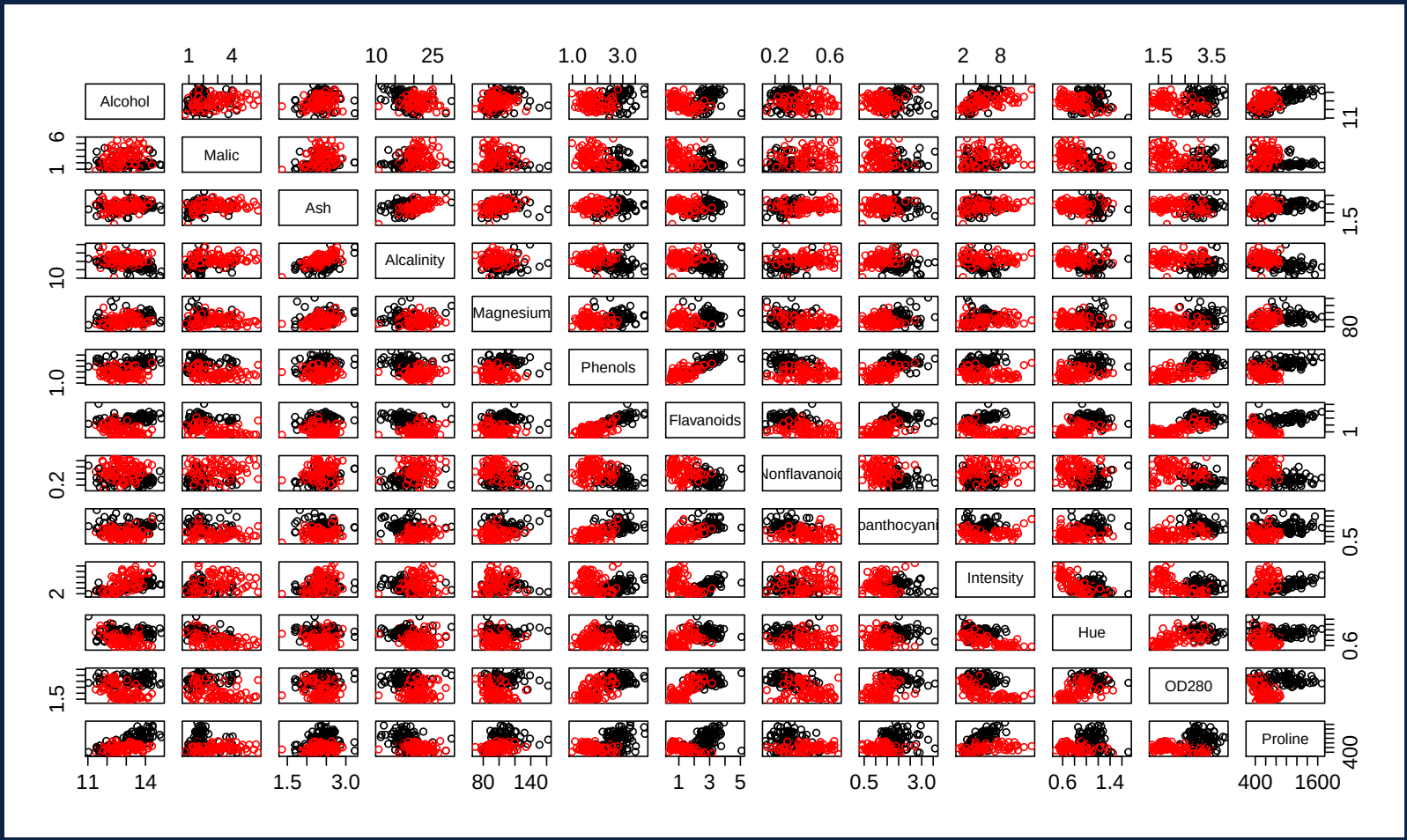
Wine Data Set

- HC 3 groups



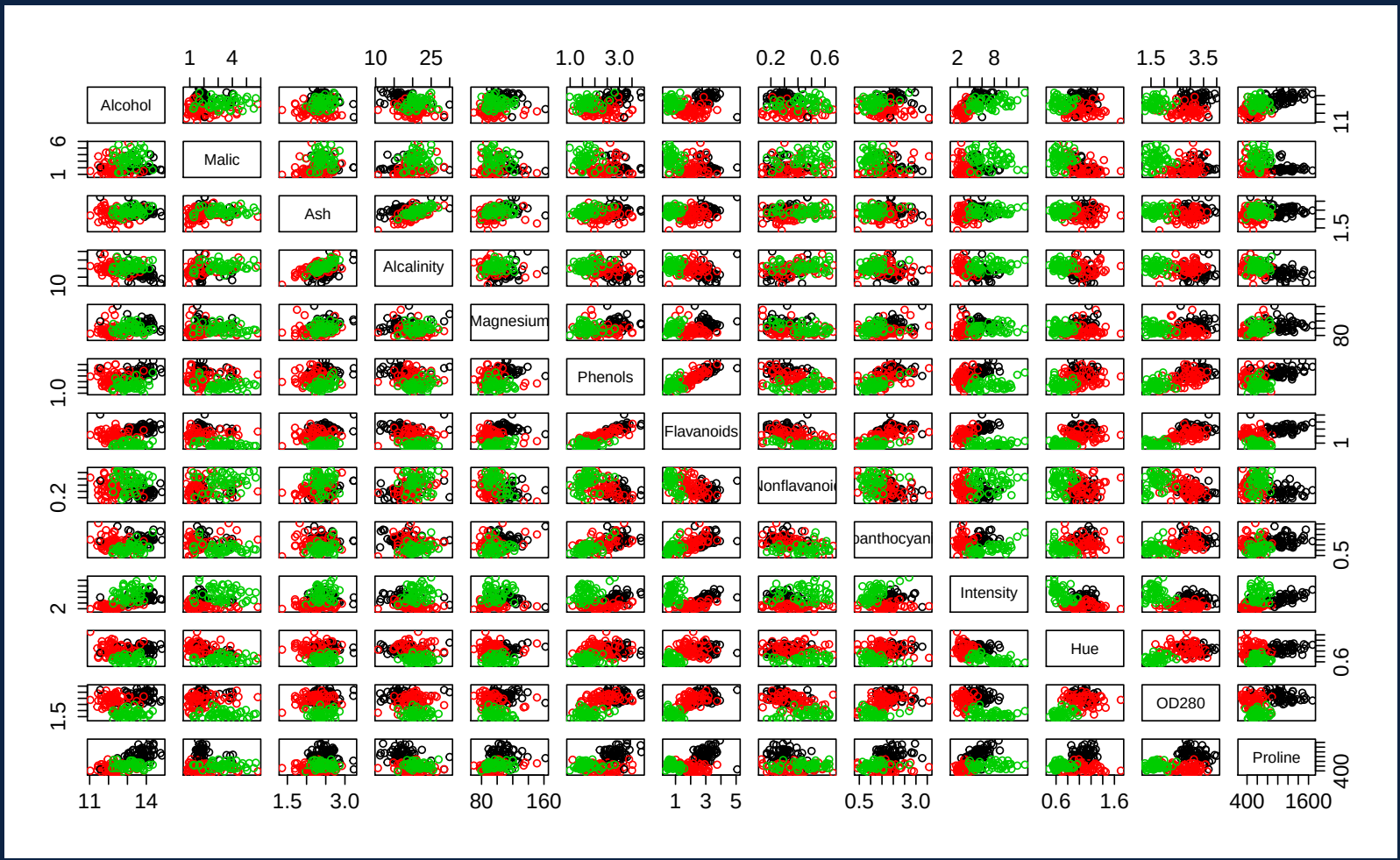
Wine Data Set

- *k*-means 2 groups



Wine Data Set

- *k*-means 3 groups



Comparing Results

- By looking at the plots, it seems as though the results are pretty similar between k-means and HC.
- The resolution makes it tough to tell, but the solutions are not identical.

Comparing Results

- Classification tables

	k-M			HC		
	1	2	3	1	2	3
Barolo	59	0	0	51	8	0
Grignolino	3	65	3	18	50	3
Barbera	0	0	48	0	0	48

- Both methods are finding most of the group structure, but...
  - k-means only misclassifies 6 of the 178 wines
  - HC misclassifies 29 of them

Dealing with Random Starts

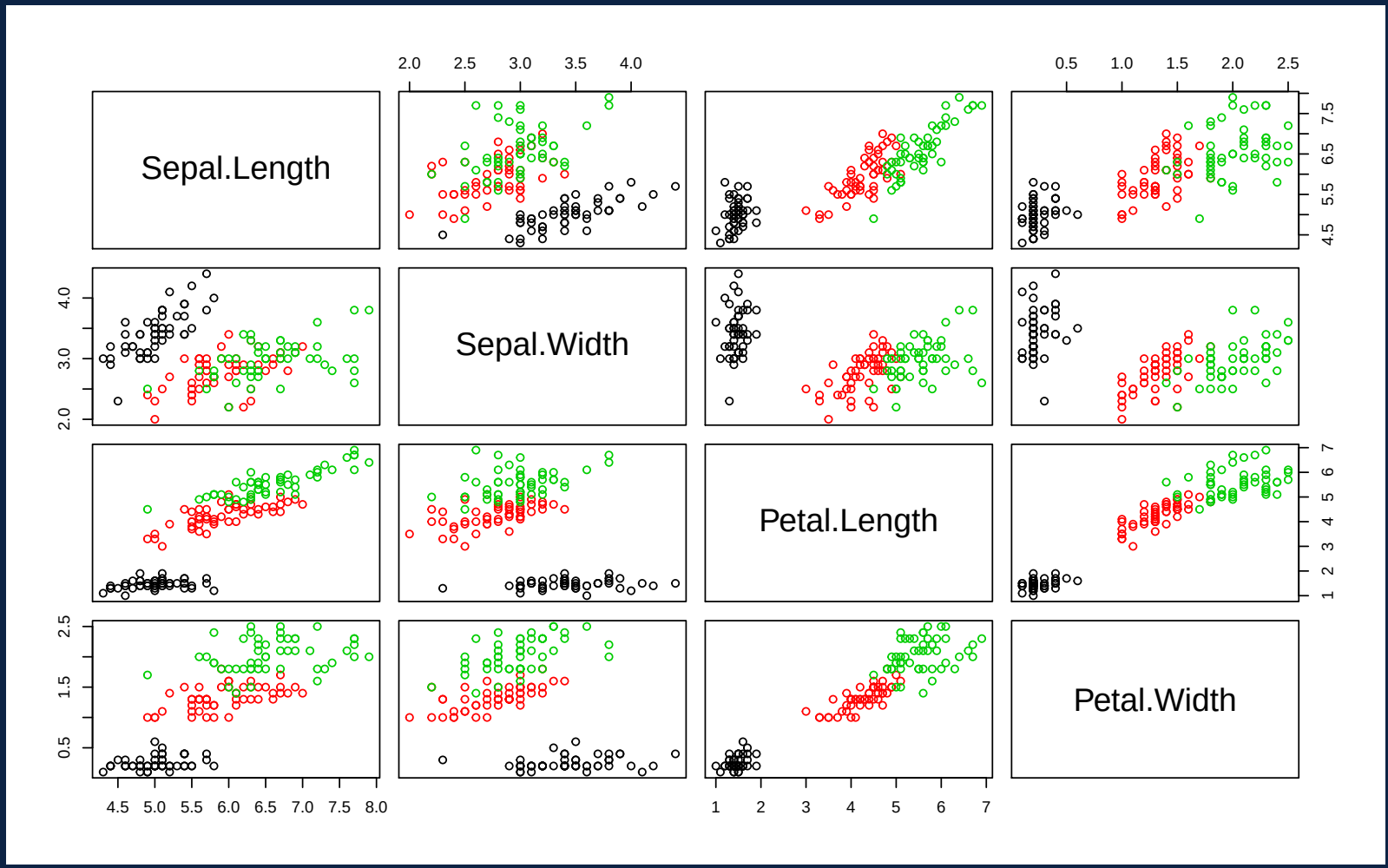
- As mentioned, k-means minimizes the within group sum of squares (WSS).
- But it does so as a local minimizer, not global.
- Further, since it's initlialized randomly, results change from run to run.

Dealing with Random Starts

- Importantly: it's fast!
- So we can run it many times, and choose the solution with the smallest within-group sum of squares for those runs.
- In fact, there's a built in argument in R...

Example

- Famous Iris data set!



Example

```
kiris <- kmeans(iris[,-5], 3)
table(iris[,5], kiris$cluster)
              1  2  3
  setosa      0 50  0
  versicolor 48  0  2
  virginica  14  0 36

kiris <- kmeans(iris[,-5], 3)
table(iris[,5], kiris$cluster)

              1  2  3
  setosa      0 50  0
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Example

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kiris <- kmeans(iris[,-5], 3)
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              1  2  3
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  versicolor  0  4 46
  virginica   0  0 50

kiris <- kmeans(iris[,-5], 3)
table(iris[,5], kiris$cluster)
              1  2  3
  setosa      0  0 50
  versicolor 48  2  0
  virginica  14 36  0
```

Example

```
kiris <- kmeans(iris[,-5], 3, nstart=25)
table(iris[,5], kiris$cluster)
             1  2  3
  setosa     0 50  0
  versicolor 2  0 48
  virginica 36  0 14
```

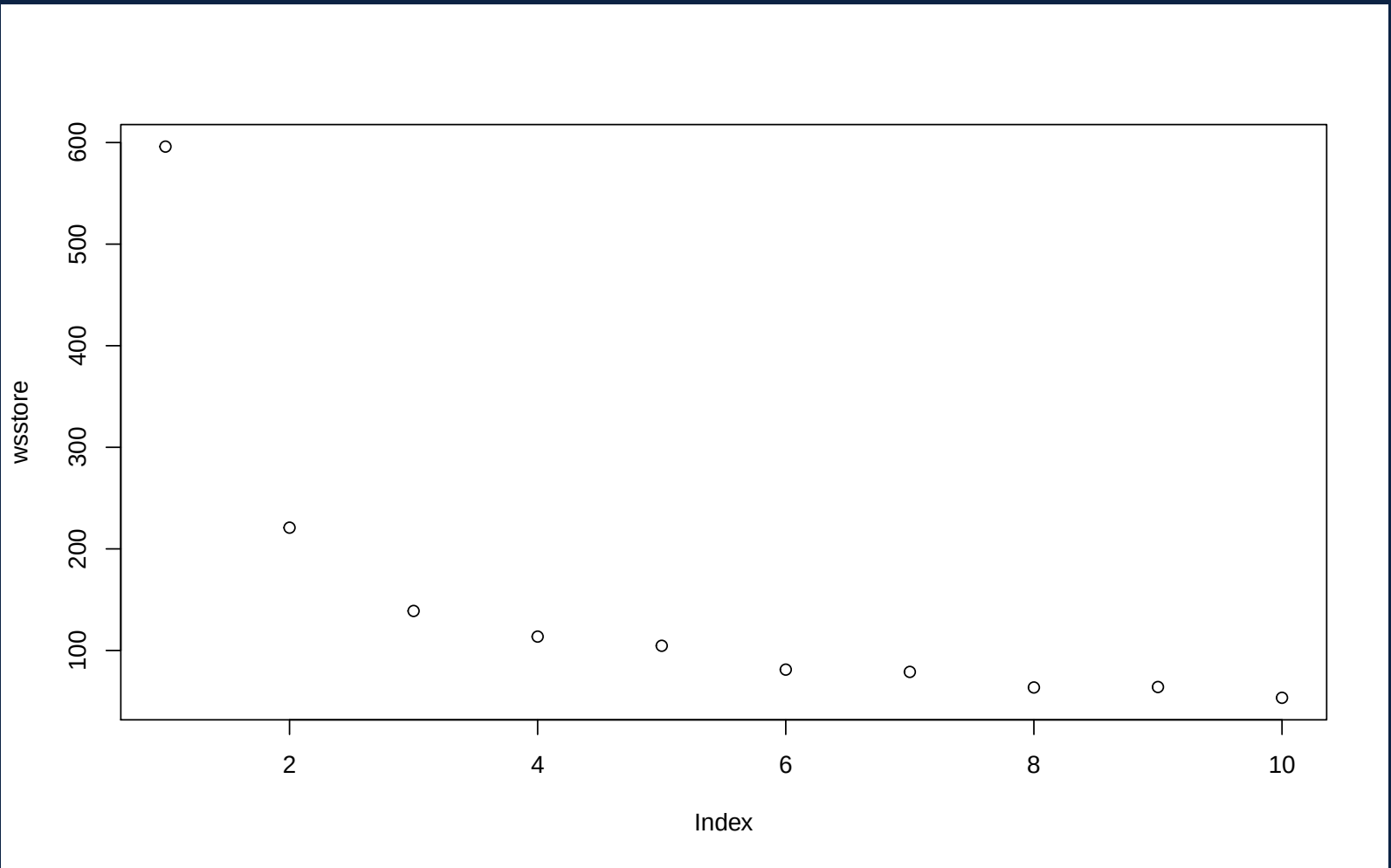
Determining Number of Groups

- For heirarchical, we have an argument for the number of groups present in the data (largest jump in dendrogram).
- For k-means, we need to specify k but can still provide some guidance
- We can plot the WSS for differing numbers of groups

Example

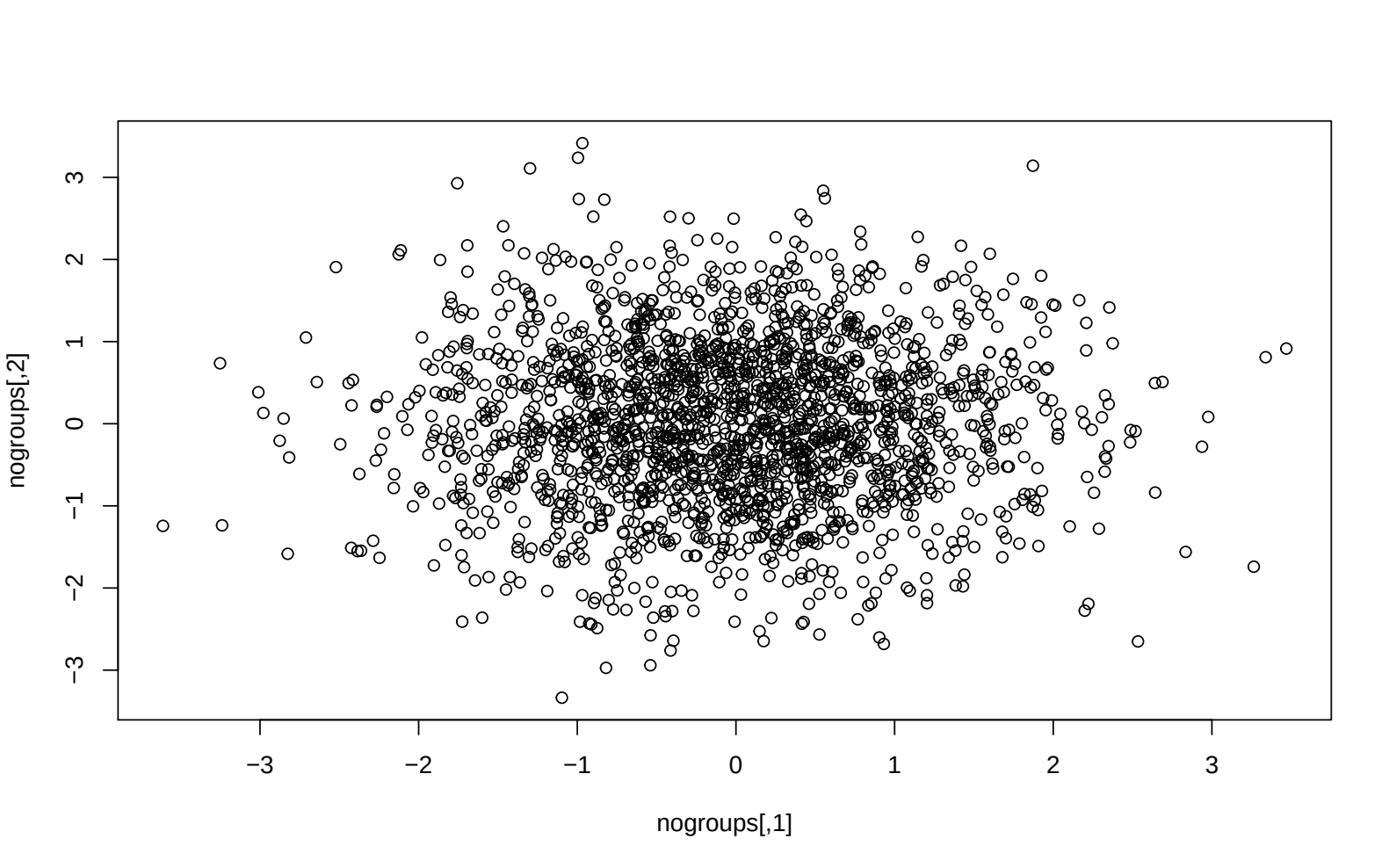
```
clustore <- matrix(0, nrow=150, ncol=10)
wsstore <- NULL
for(i in 1:10){
  dum <- kmeans(scale(iris[,-5]), i, nstart=25)
  clustore[, i] <- dum$cluster
  wsstore[i] <- dum$tot.withinss
}
plot(wsstore)
```

Example



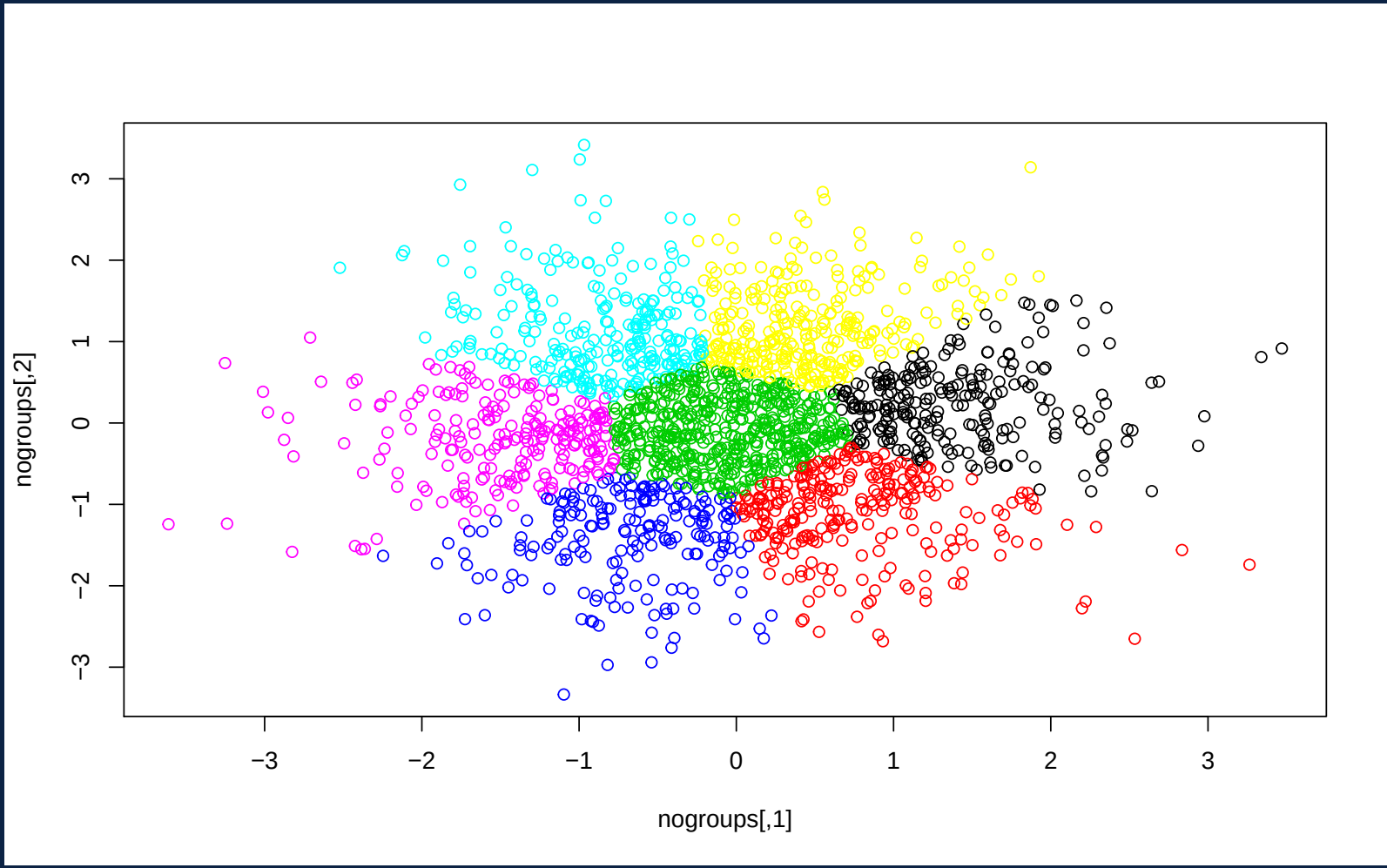
No groups?

- Also as previously noted, k-means can seem like it finds groups, even when they may not exist.



No groups?

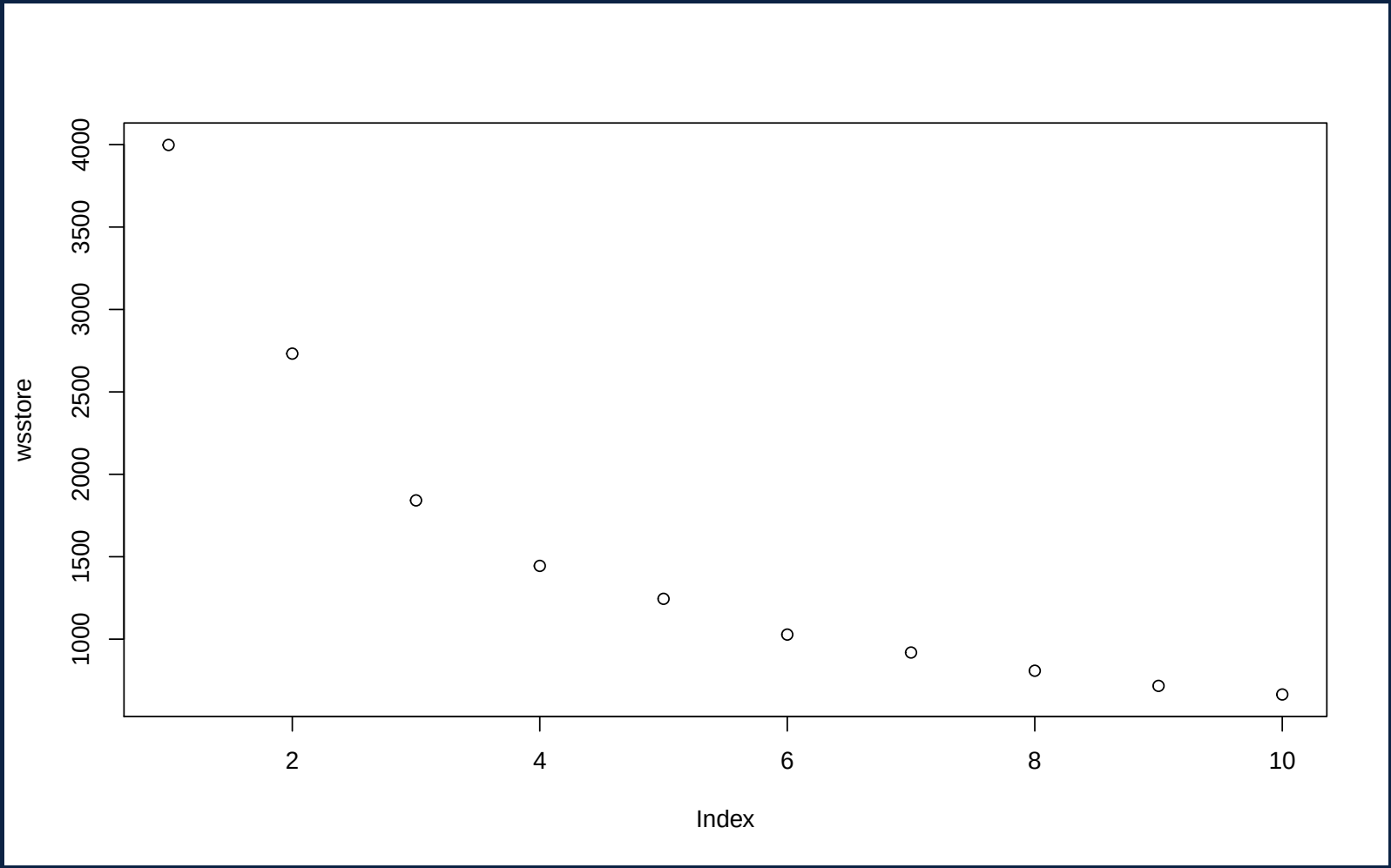
- See...



Example

```
clustore <- matrix(0, nrow=2000, ncol=10)
wsstore <- NULL
for(i in 1:10){
  dum <- kmeans(scale(nogroups), i)
  clustore[, i] <- dum$cluster
  wsstore[i] <- dum$tot.withinss
}
plot(wsstore)
```

No groups?



Partitioning and Hierarchical

- Neither HC or k-means can really be considered "statistical," in the sense of:
  - What model are we assuming?
  - How can we test whether the model is accurate?

- They are basically *ad hoc* methods that mostly follow from intuition and tend to perform alright.

- Next, we'll scrape the surface of clustering via mixture models — the unsupervised equivalent of discriminant analysis.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