Introduction to hierarchical clustering

UNSUPERVISED LEARNING IN R

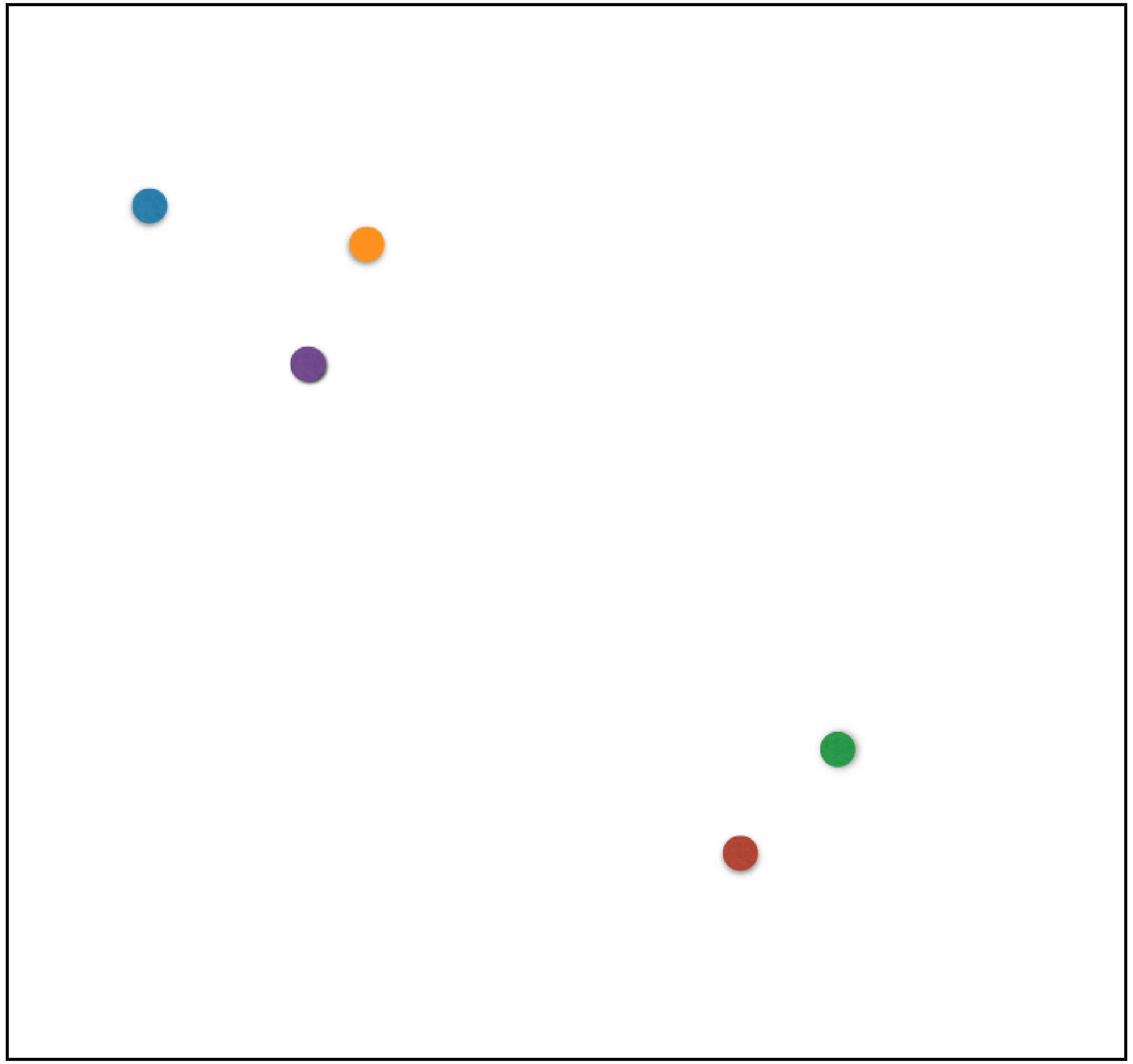
Hank Roark
Senior Data Scientist at Boeing

Hierarchical clustering

- Number of clusters is not known ahead of time
- Two kinds: bottom-up and top-down, this course bottom-up

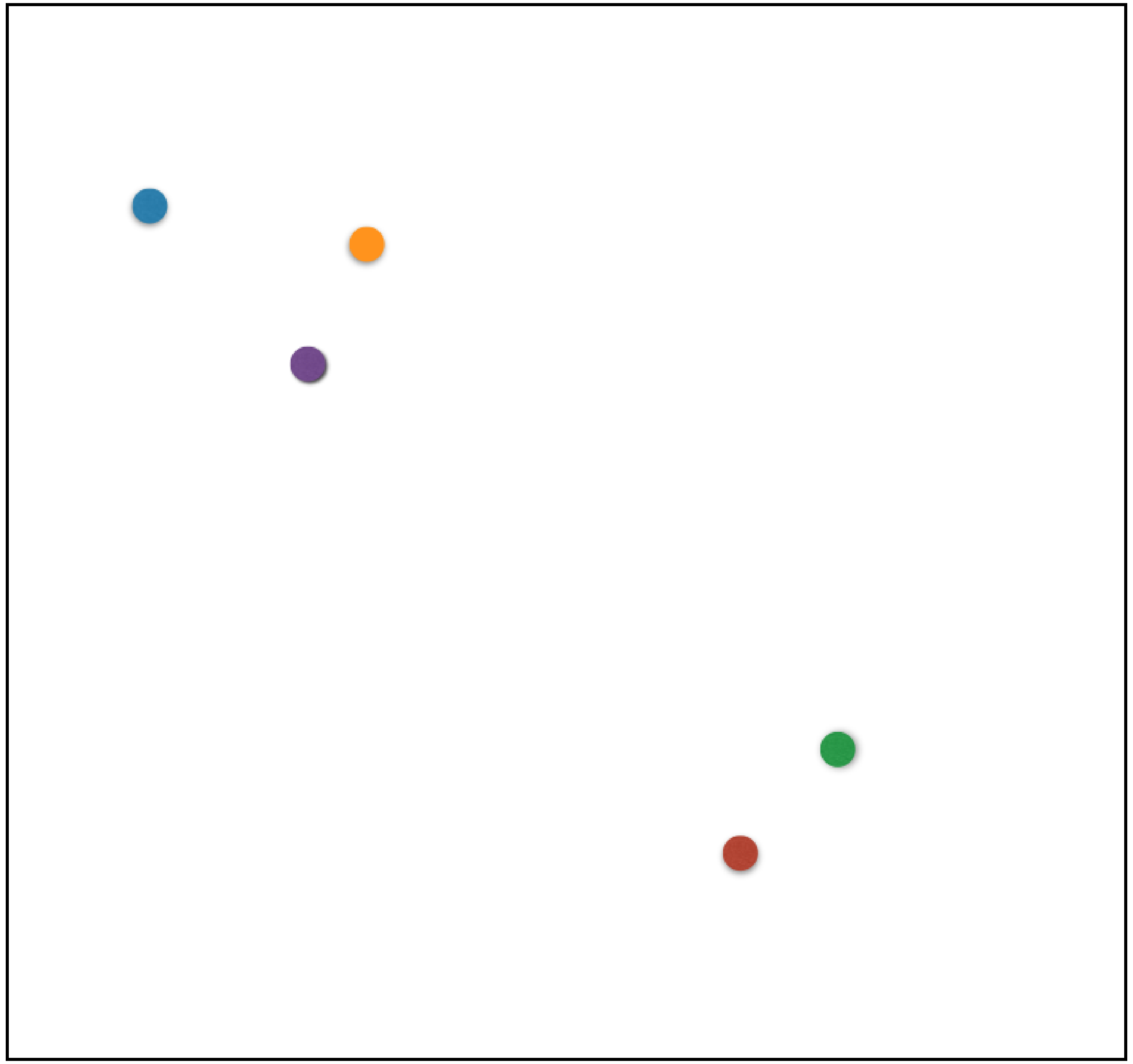
Simple example

Simple Example



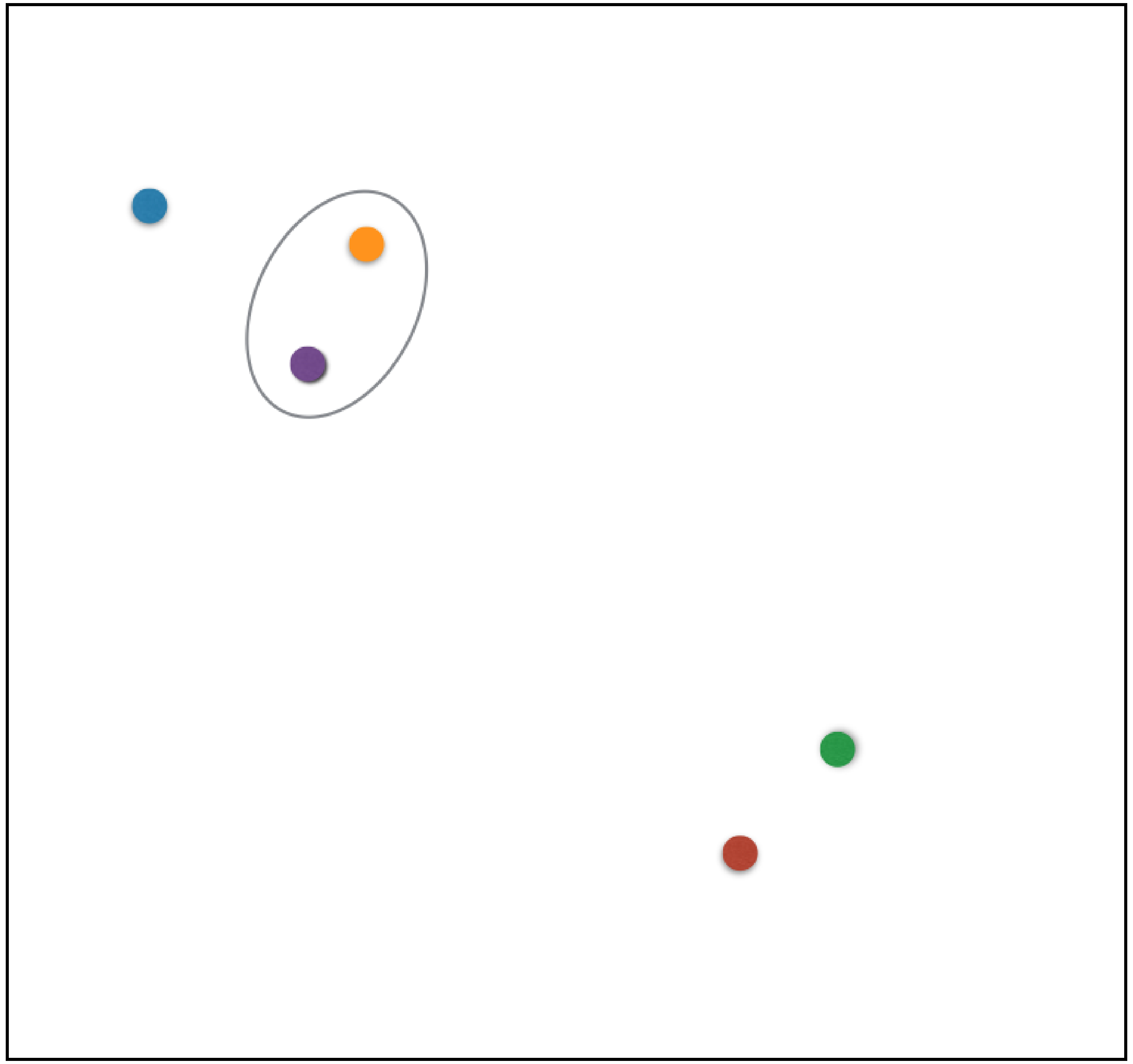
Five clusters

5 Clusters
Each point a cluster



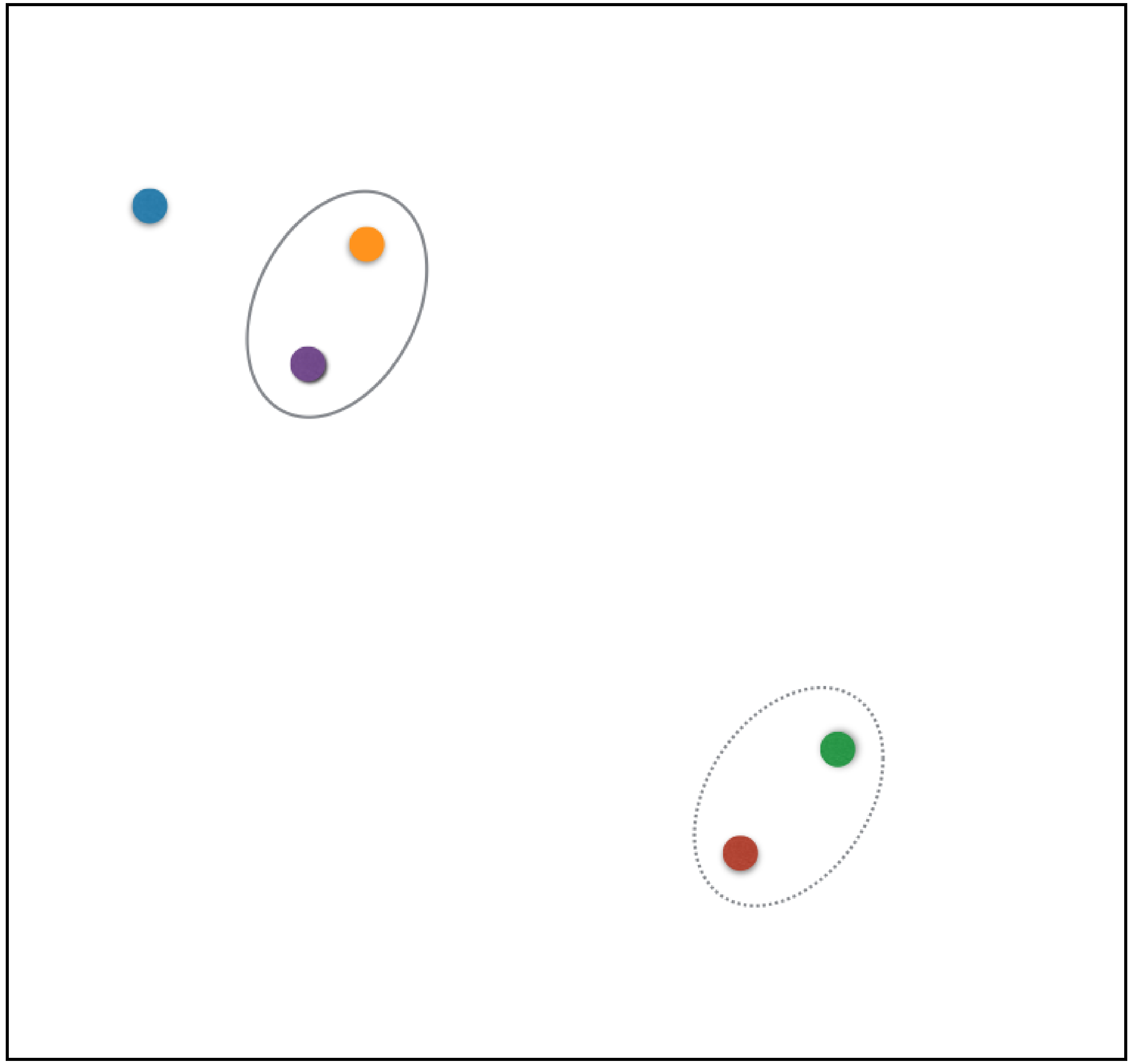
Four clusters

4 Clusters



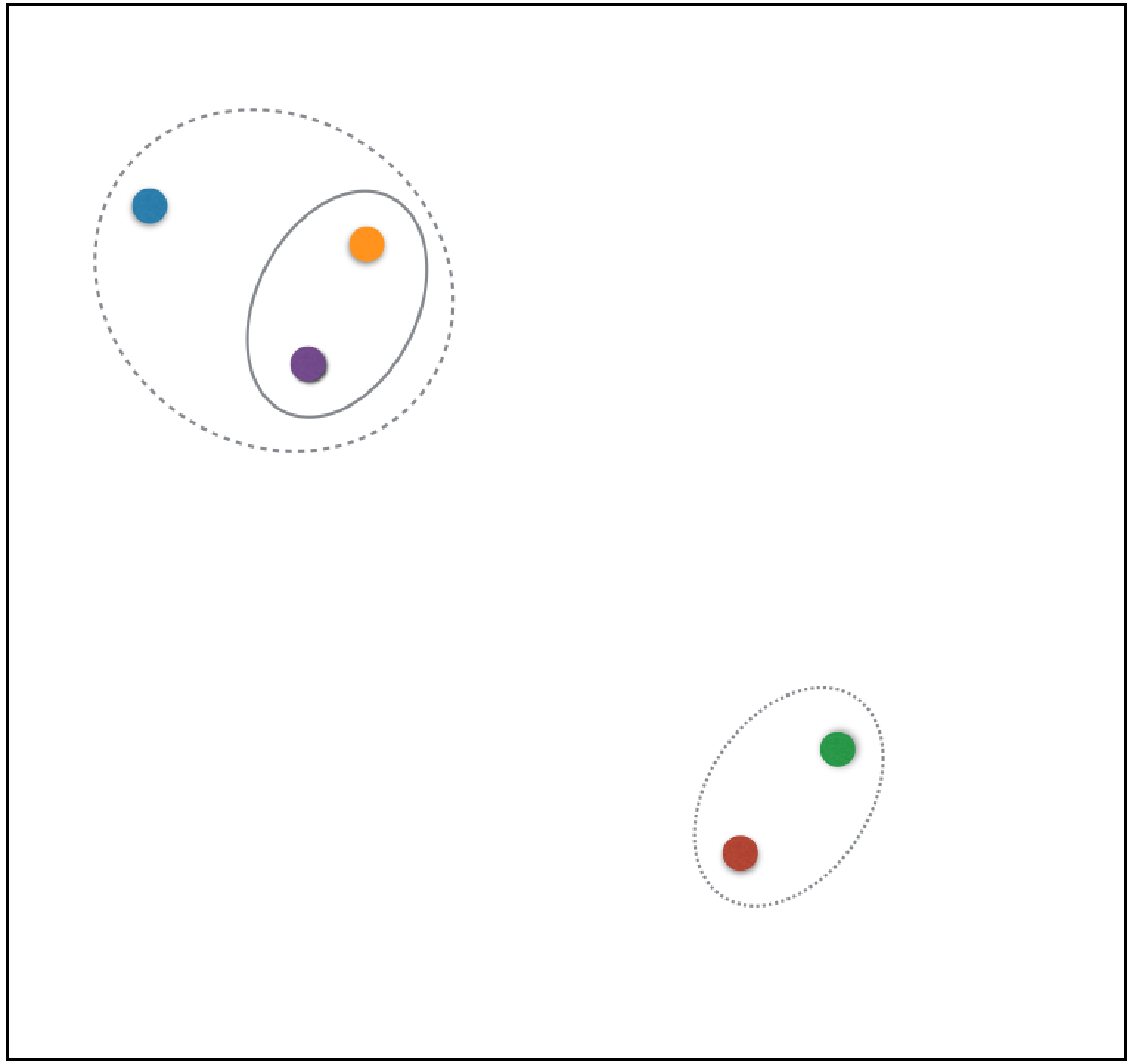
Three clusters

3 Clusters



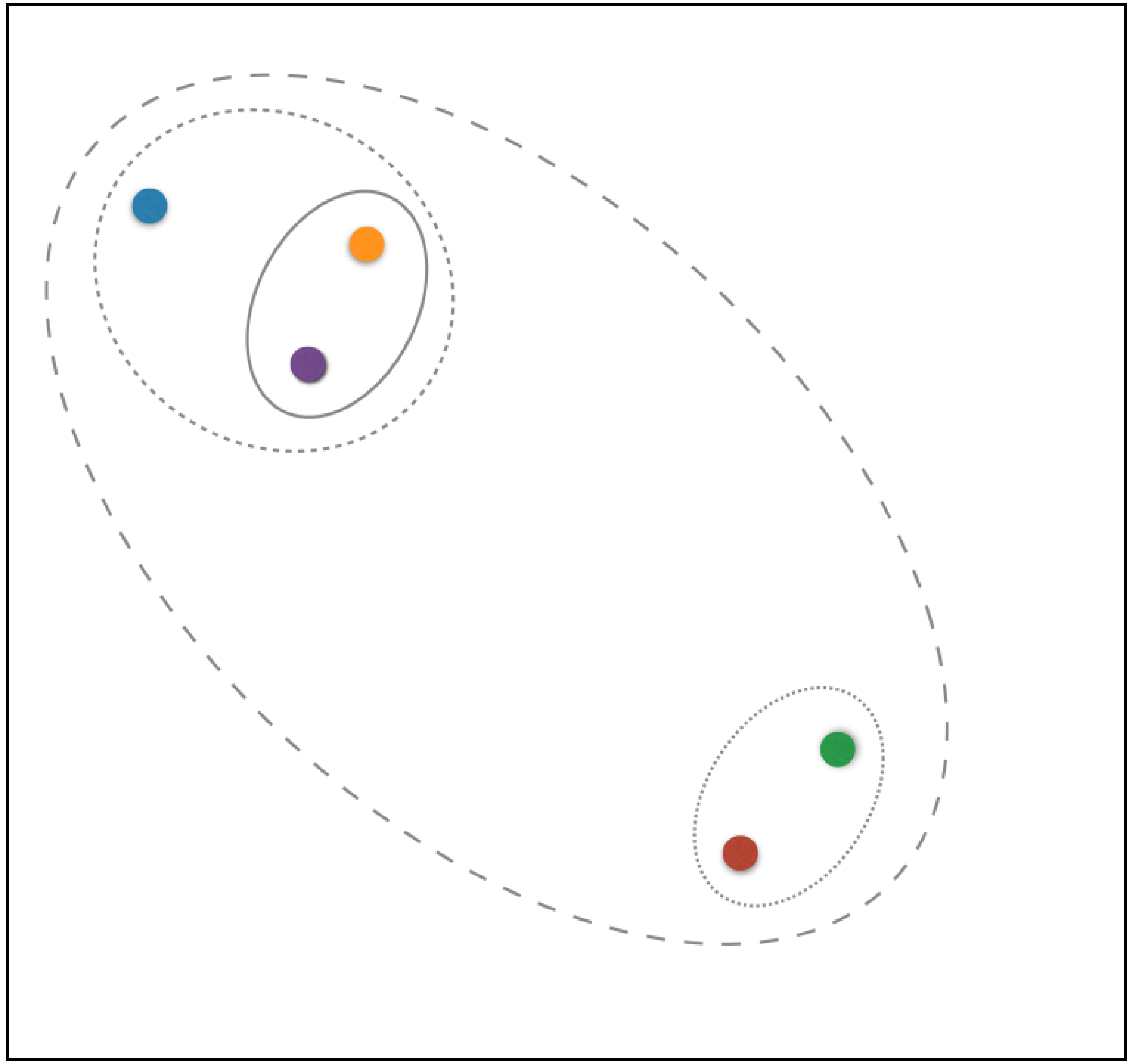
Two clusters

2 Clusters



One cluster

1 Cluster



Hierarchical clustering in R

```
# Calculates similarity as Euclidean distance
# between observations
dist_matrix <- dist(x)
# Returns hierarchical clustering model
hclust(d = dist_matrix)
```

```
Call:
hclust(d = s)

Cluster method   : complete
Distance         : euclidean
Number of objects: 50
```

Let's practice!

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Selecting number of clusters

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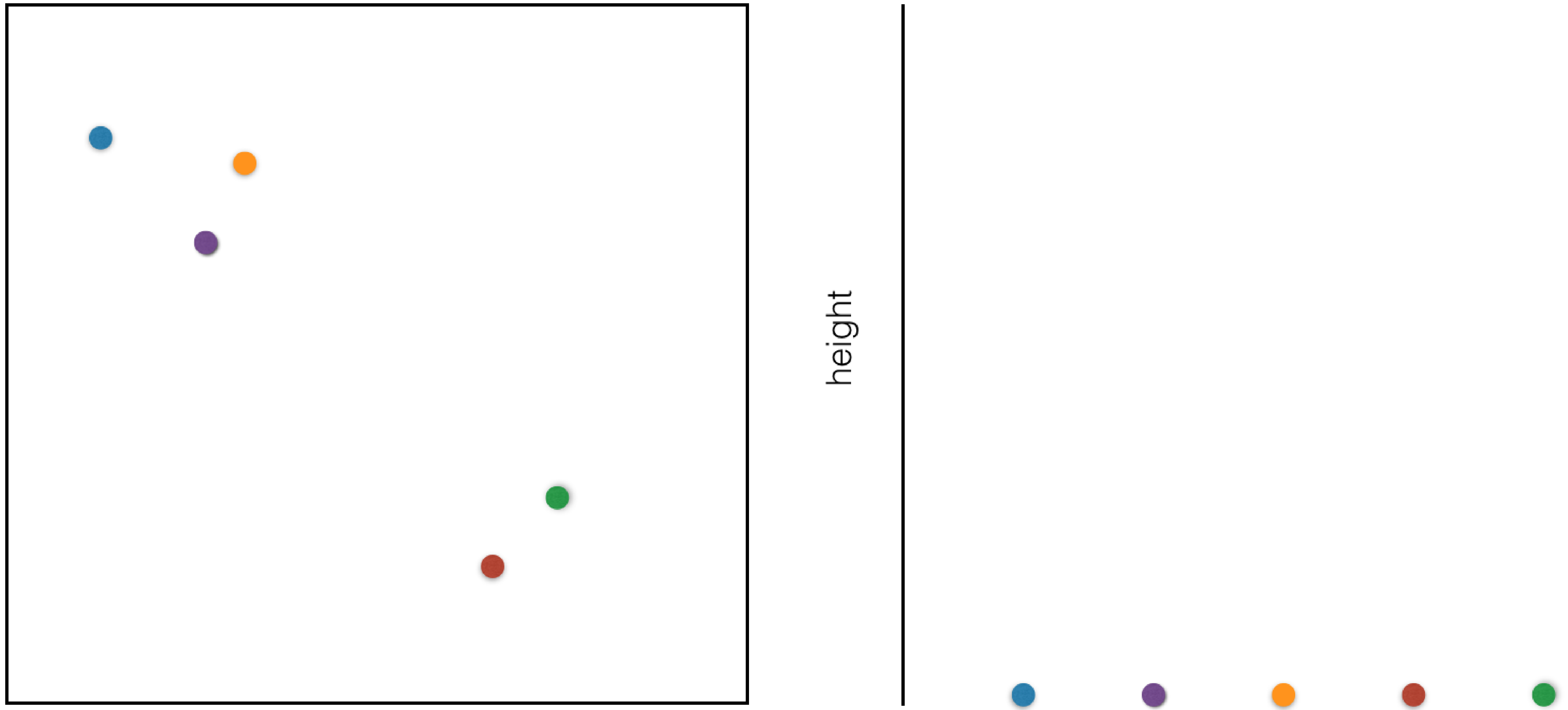
Interpreting results

```
# Create hierarchical cluster model: hclust.out
hclust.out <- hclust(dist(x))
# Inspect the result
summary(hclust.out)
```

```
            Length Class  Mode
merge       98     -none- numeric
height      49     -none- numeric
order       50     -none- numeric
labels       0     -none- NULL
method       1     -none- character
call         2     -none- call
dist.method  1     -none- character
```

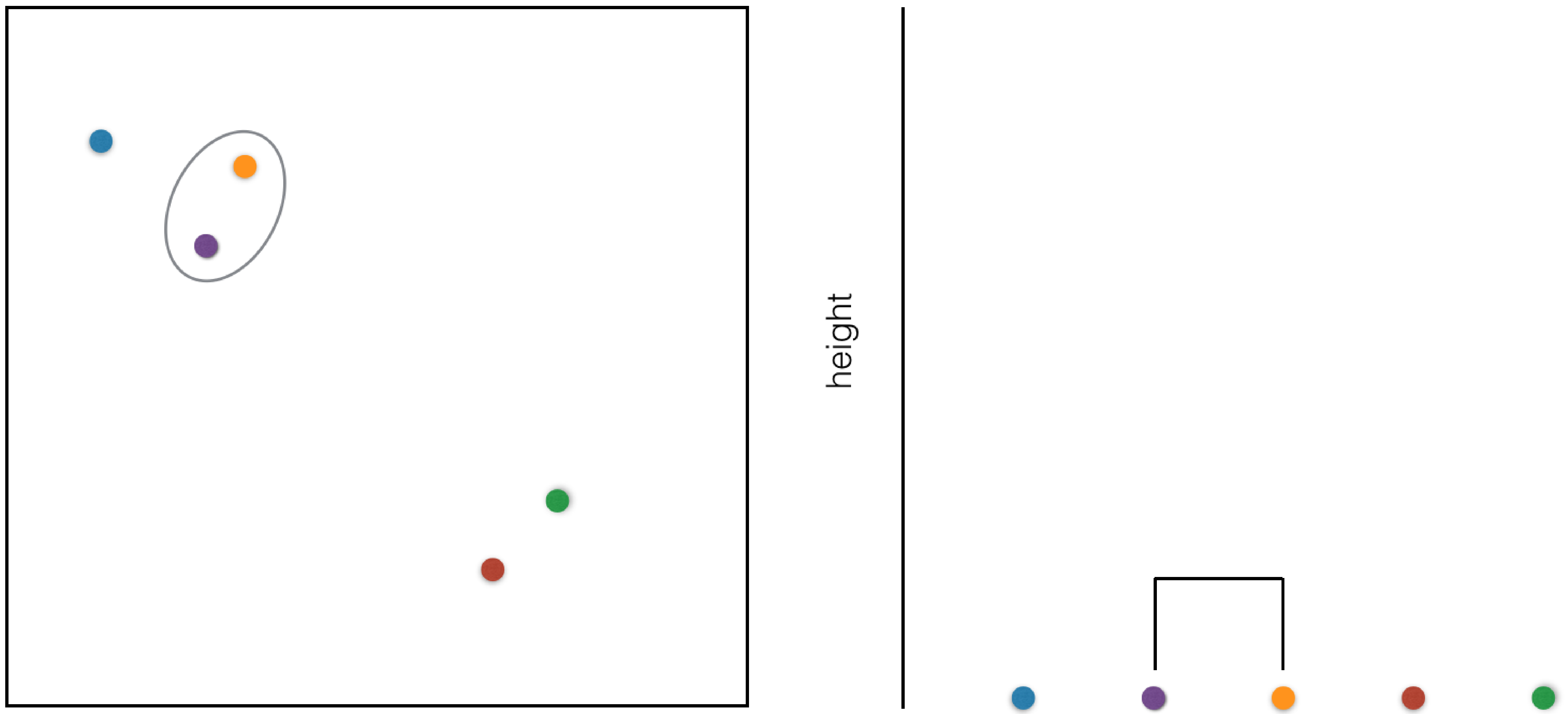
Dendrogram

- Tree shaped structure used to interpret hierarchical clustering models



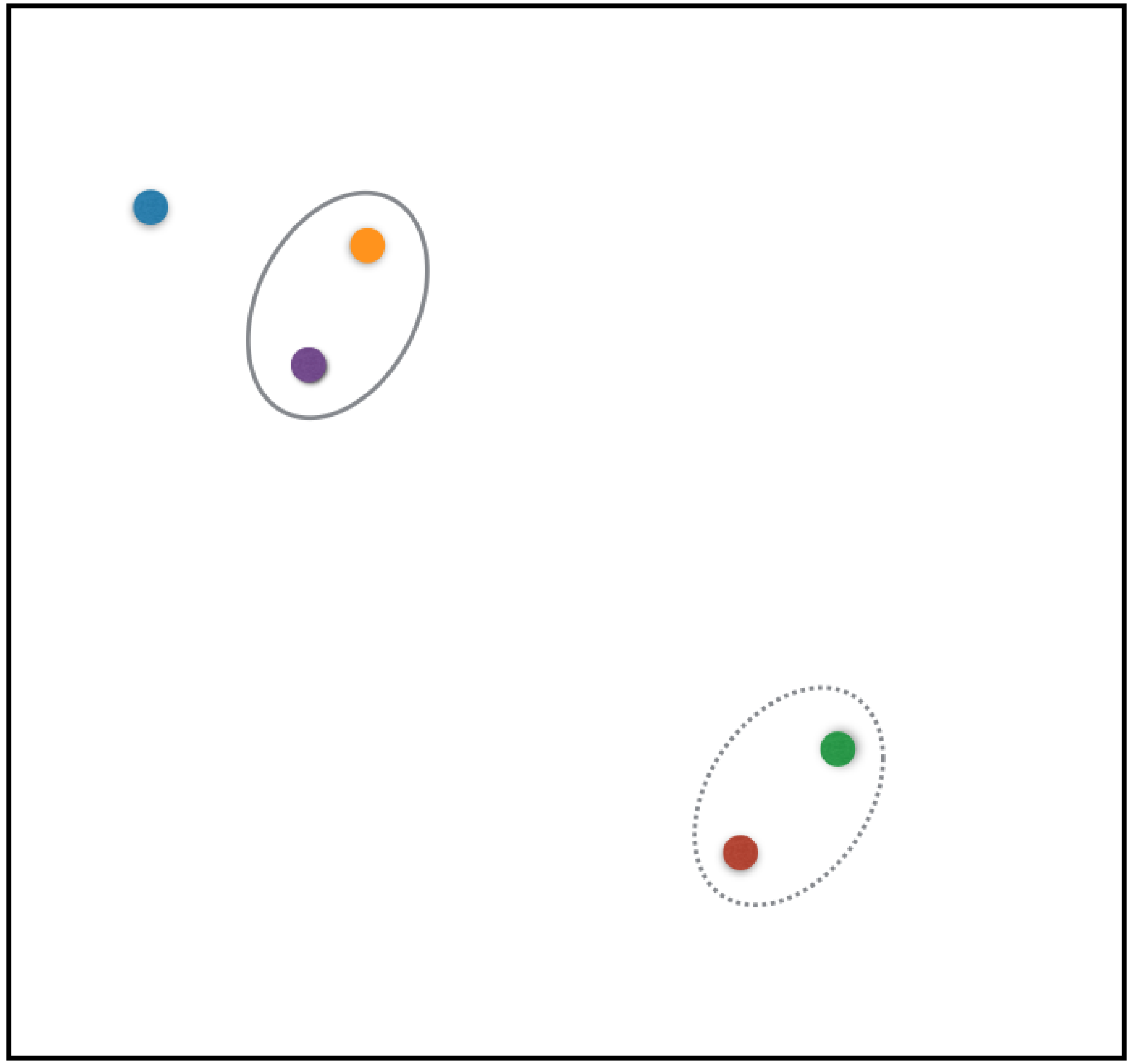
Dendrogram

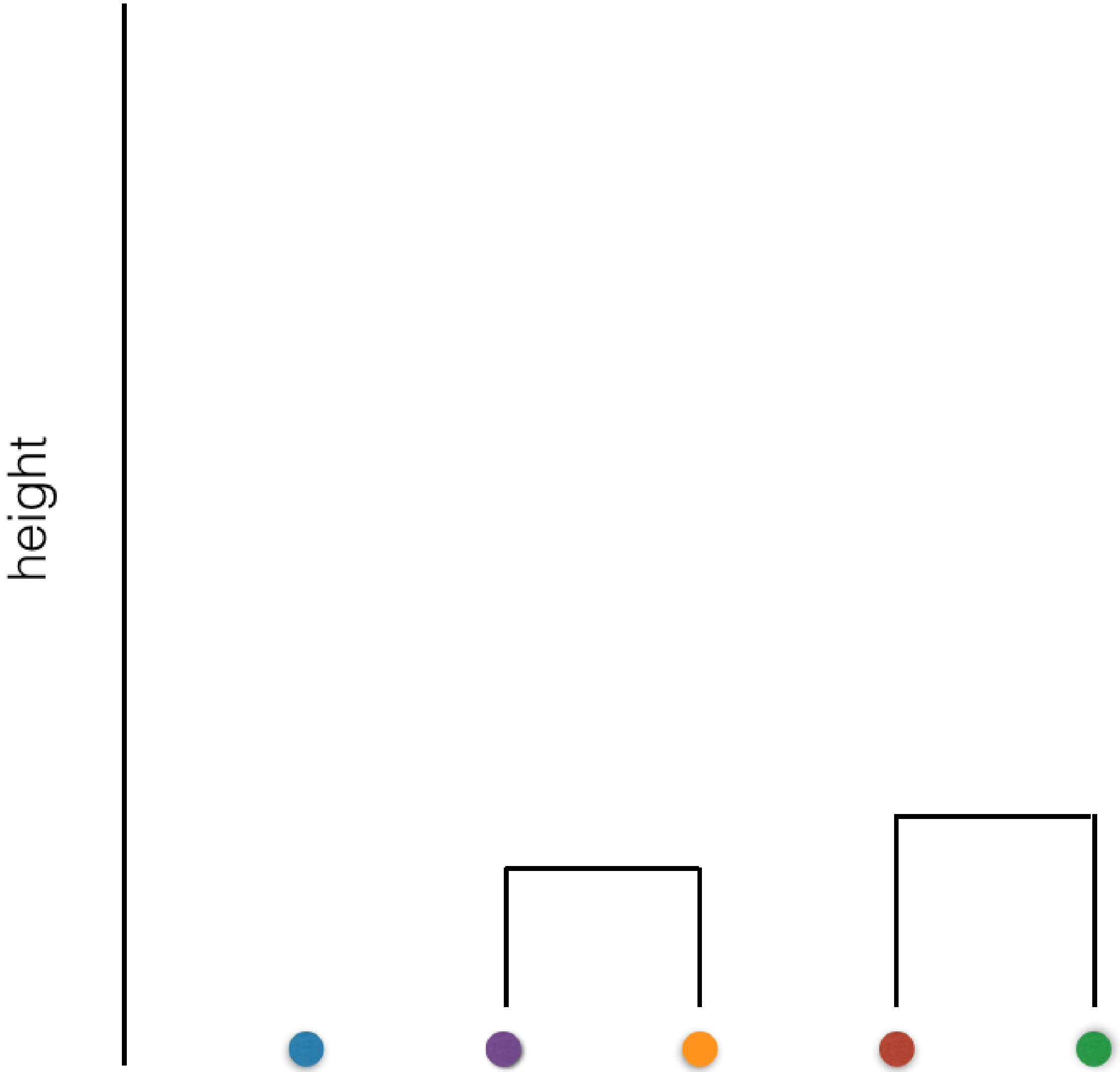
- Tree shaped structure used to interpret hierarchical clustering models



Dendrogram

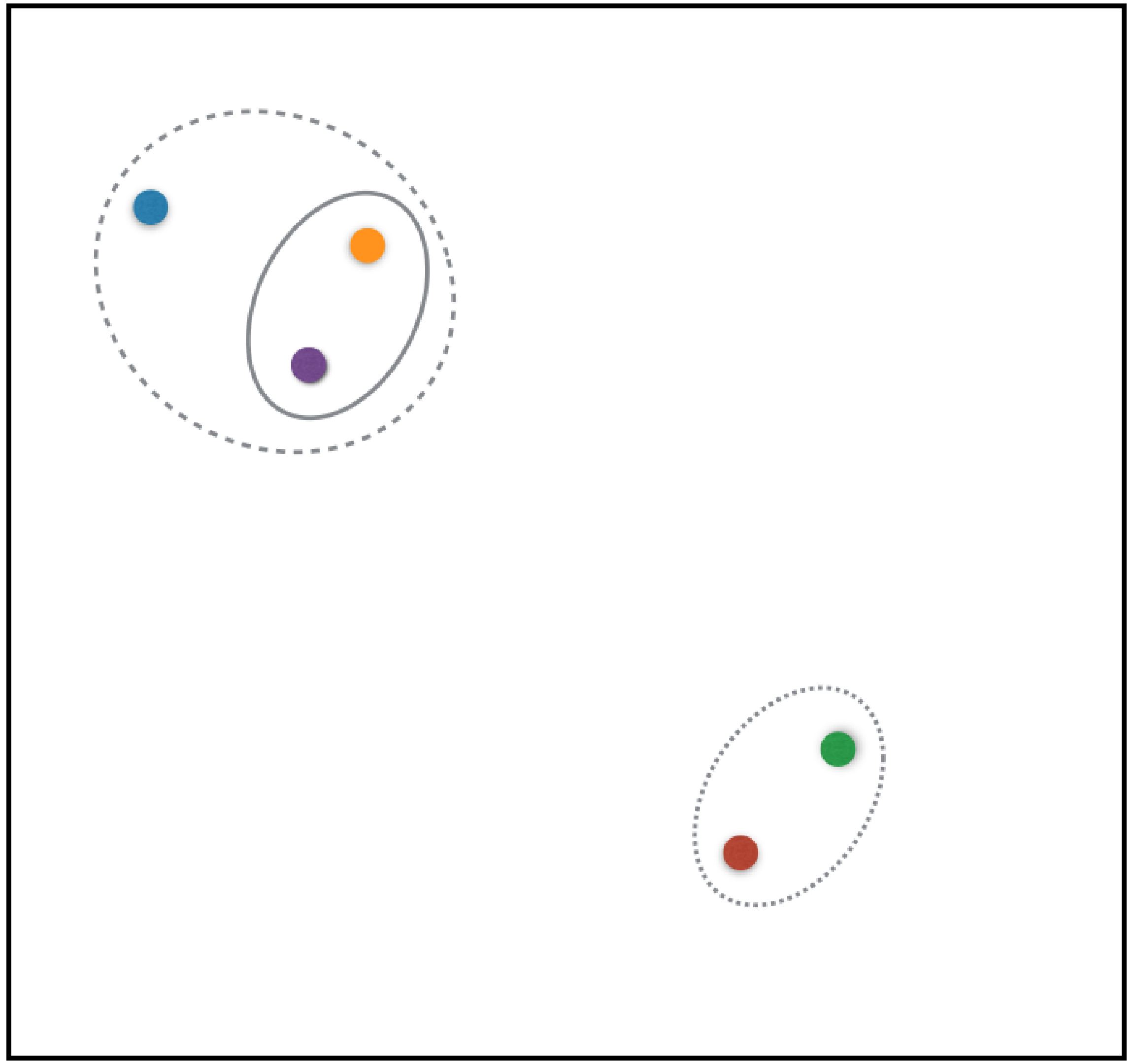
- Tree shaped structure used to interpret hierarchical clustering models

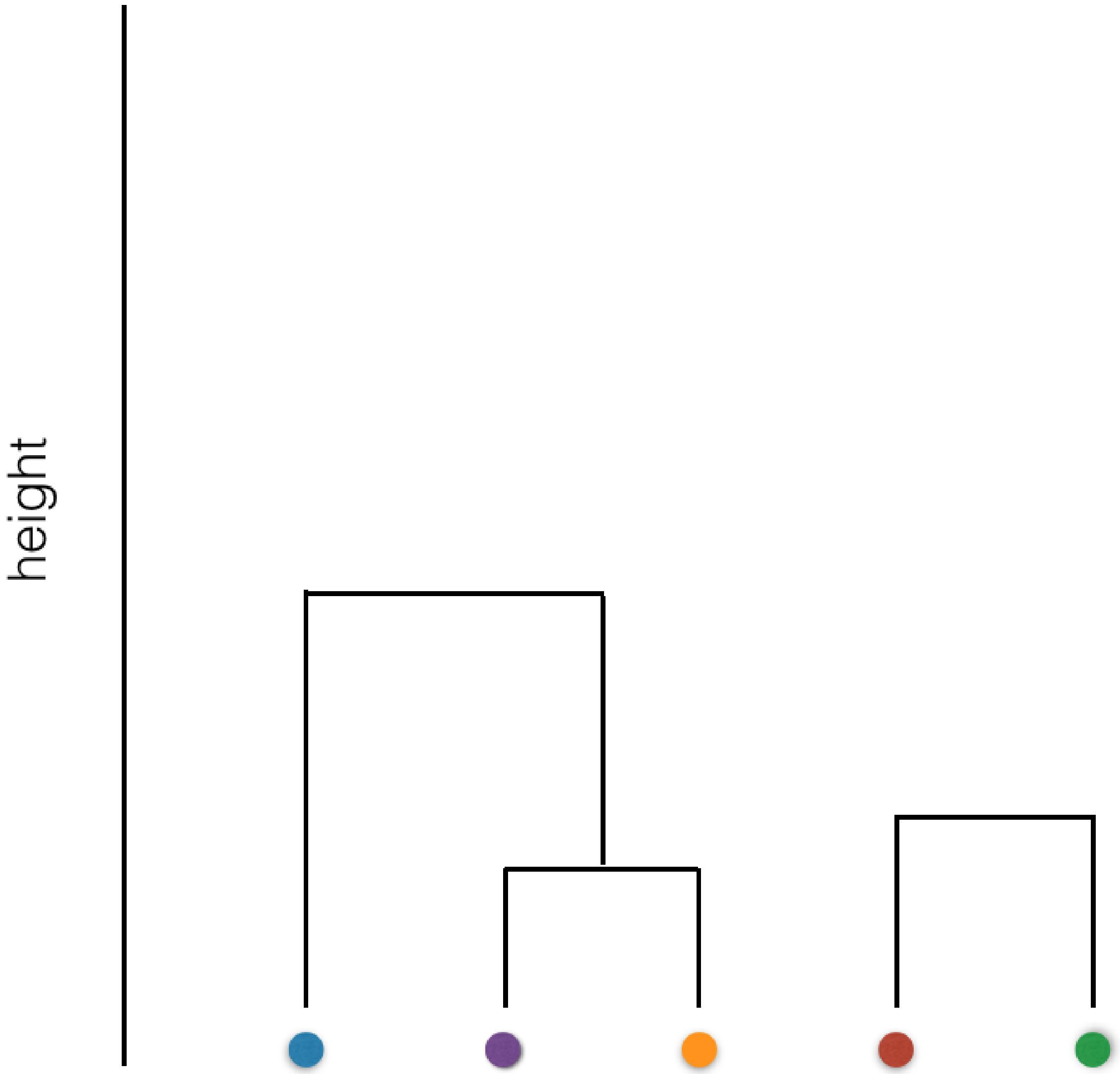




Dendrogram

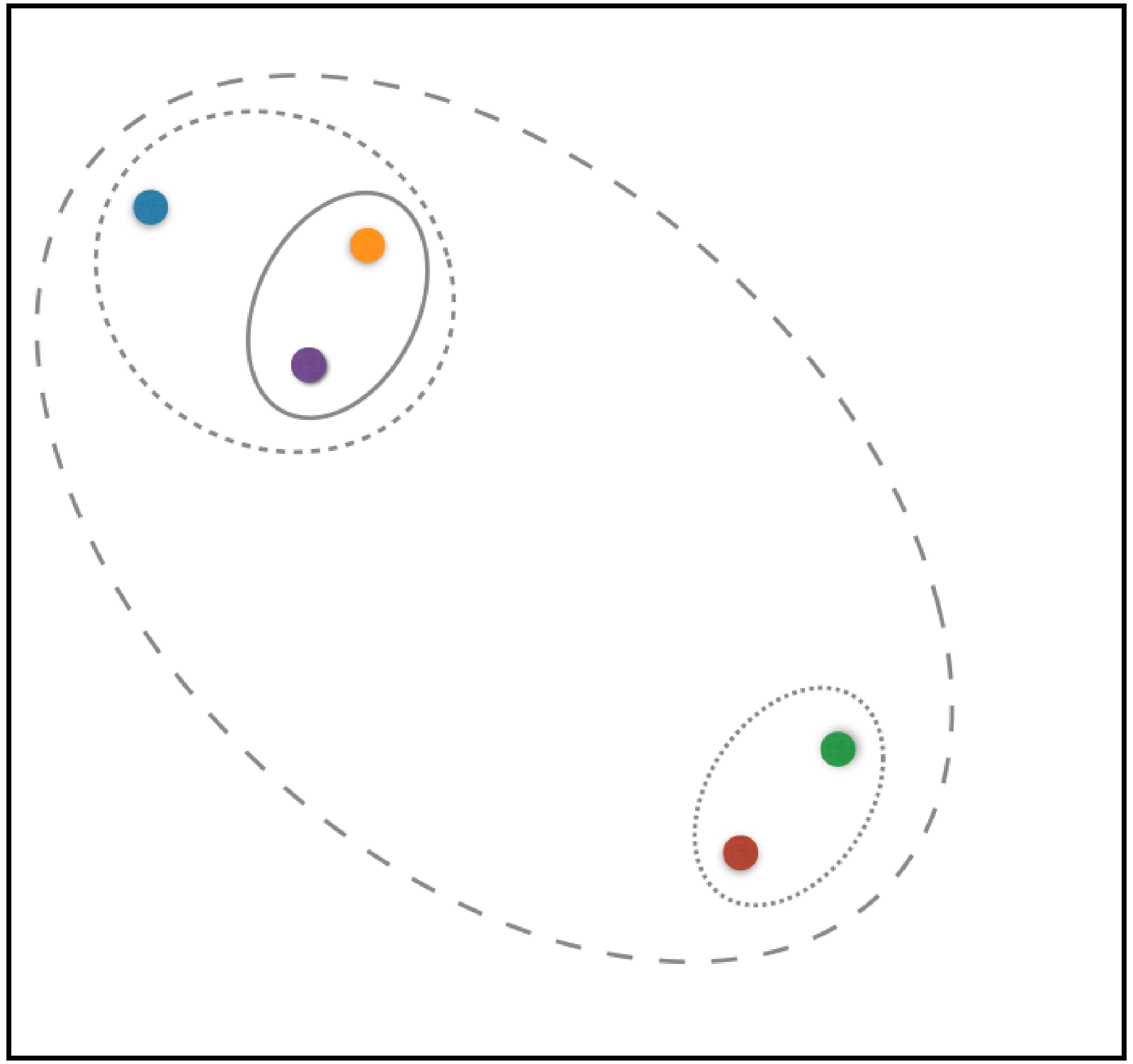
- Tree shaped structure used to interpret hierarchical clustering models

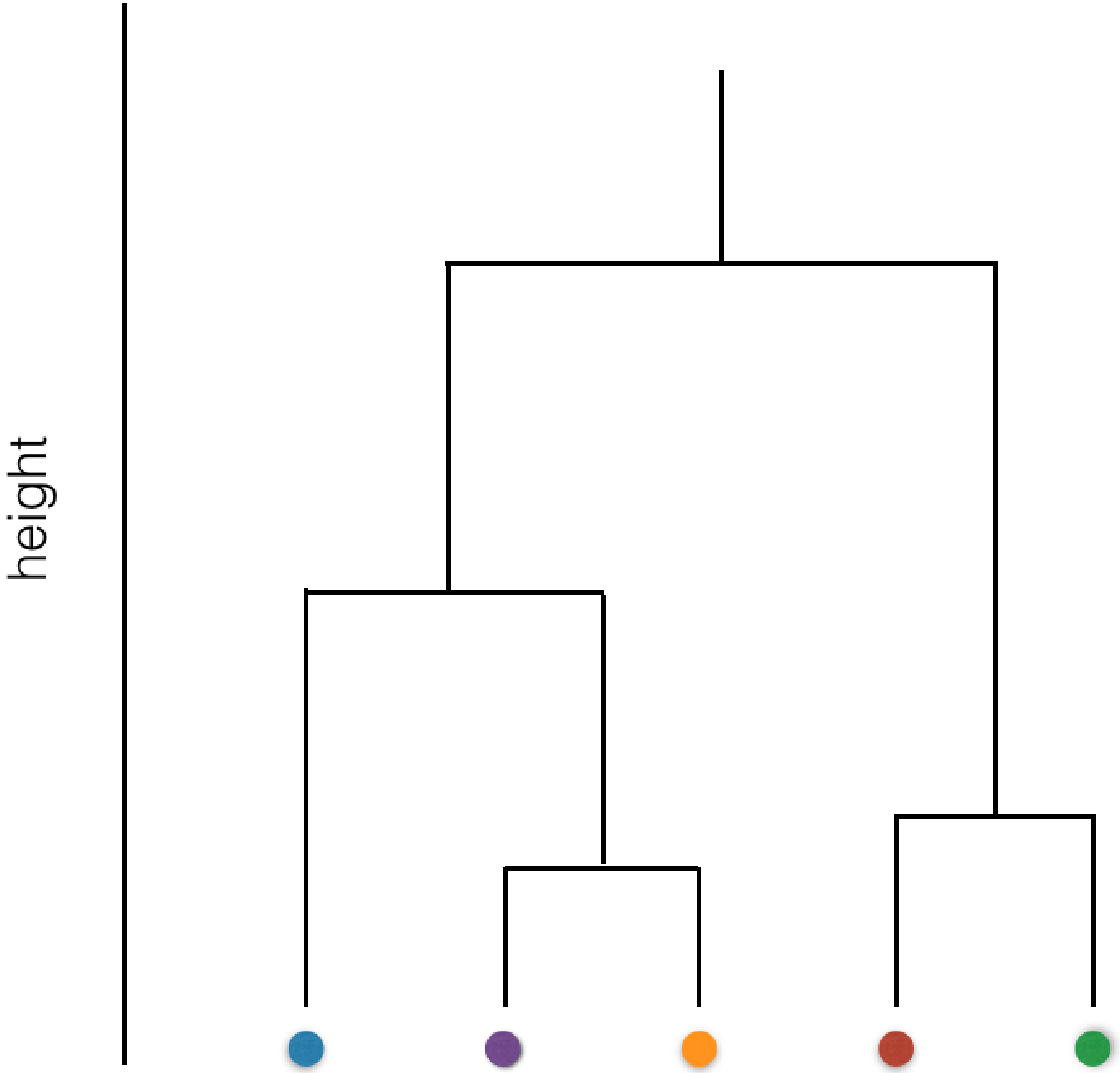




Dendrogram

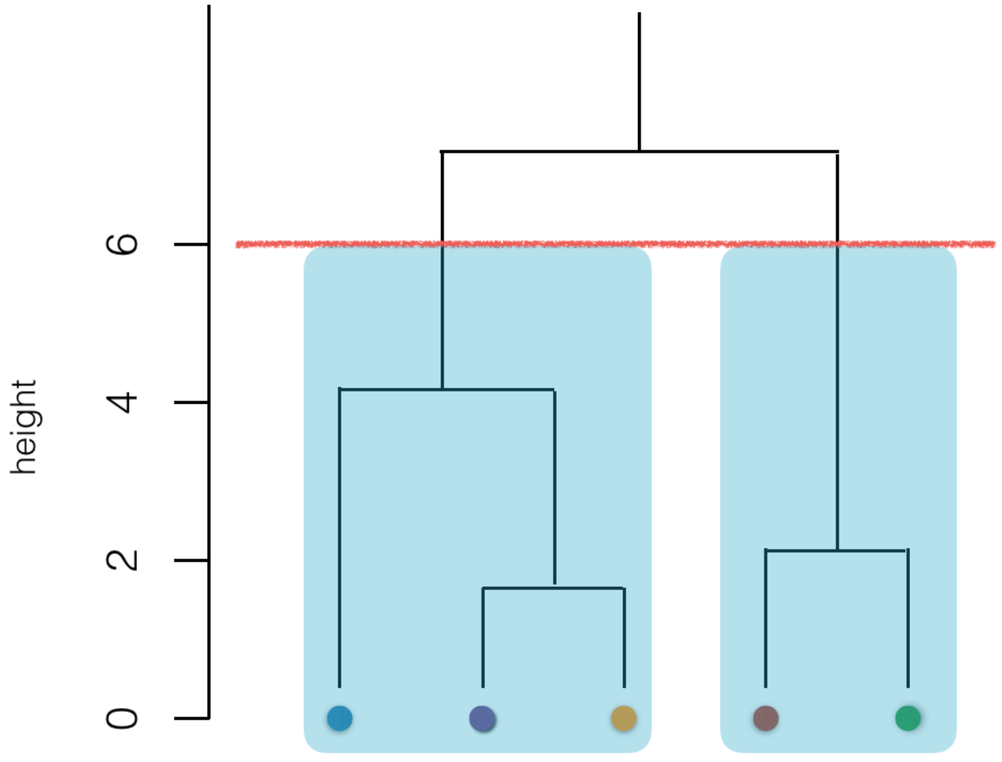
- Tree shaped structure used to interpret hierarchical clustering models





Dendrogram plotting in R

```
# Draws a dendrogram
plot(hclust.out)
abline(h = 6, col = "red")
```



Tree "cutting" in R

```
# Cut by height h
cutree(hclust.out, h = 6)
```

```
1 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3 3 3
3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4 2 4 2 4 4
```

```
# Cut by number of clusters k
cutree(hclust.out, k = 2)
```

```
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2
2 2 2 2 2 2 2 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1 1
```

Let's practice!

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Clustering linkage and practical matters

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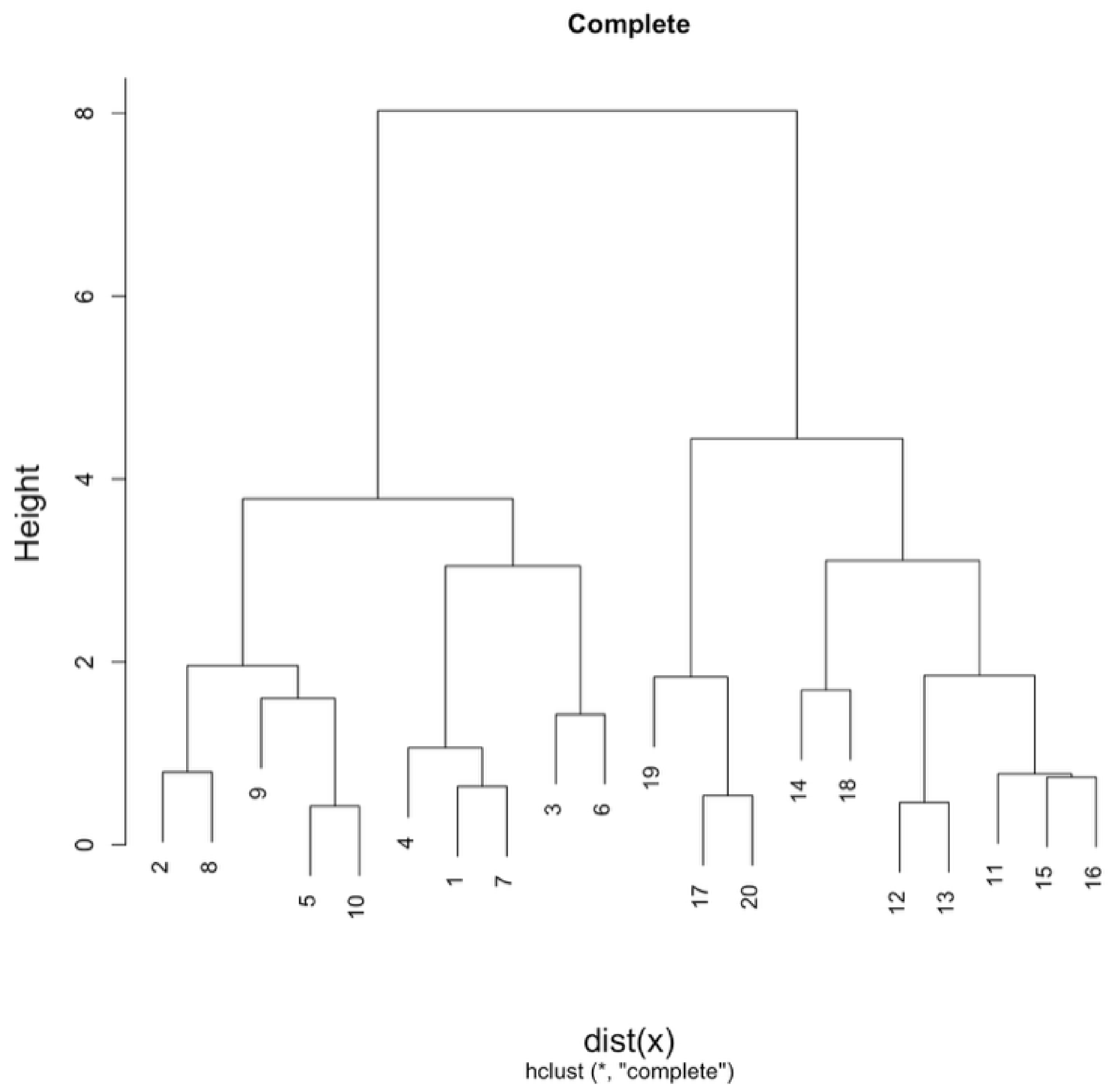
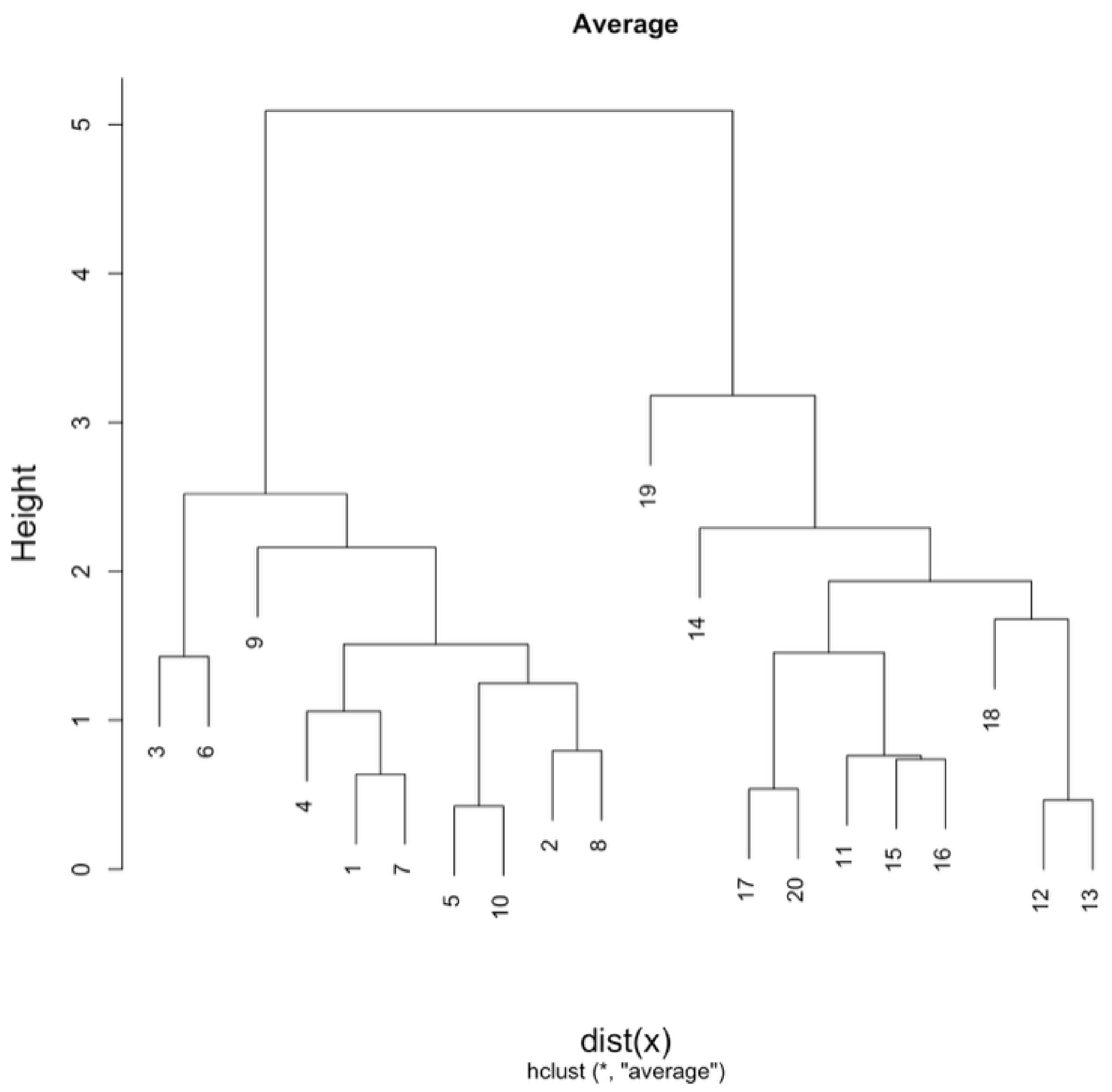
Hank Roark
Senior Data Scientist at Boeing

Linking clusters in hierarchical clustering

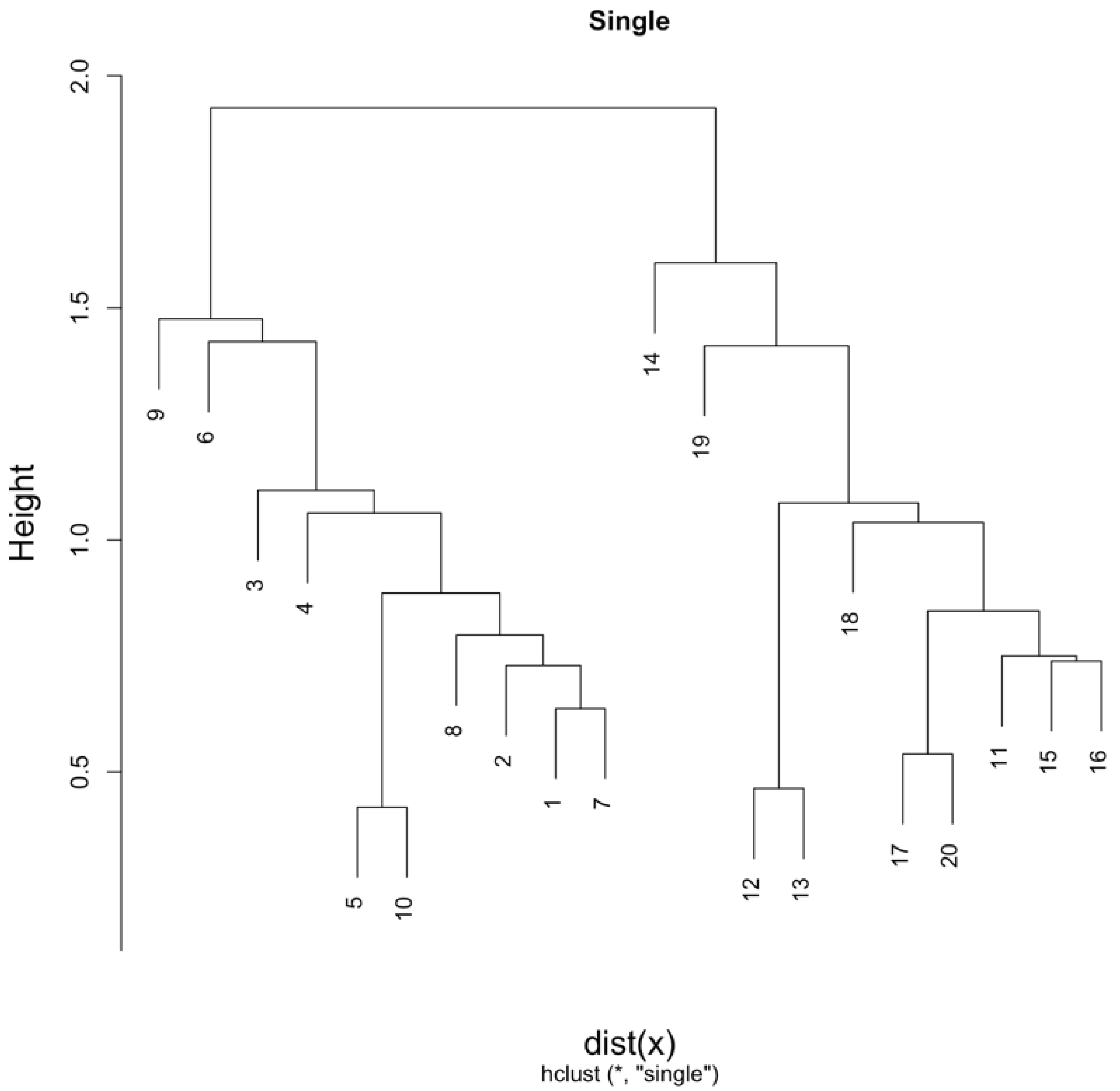
- How is distance between clusters determined? Rules?
- Four methods to determine which cluster should be linked
  - *Complete*: pairwise similarity between all observations in cluster 1 and cluster 2, and uses **largest of similarities**
  - *Single*: same as above but uses **smallest of similarities**
  - *Average*: same as above but uses **average of similarities**
  - *Centroid*: finds centroid of cluster 1 and centroid of cluster 2, and uses **similarity between two centroids**

Linking methods: complete and average

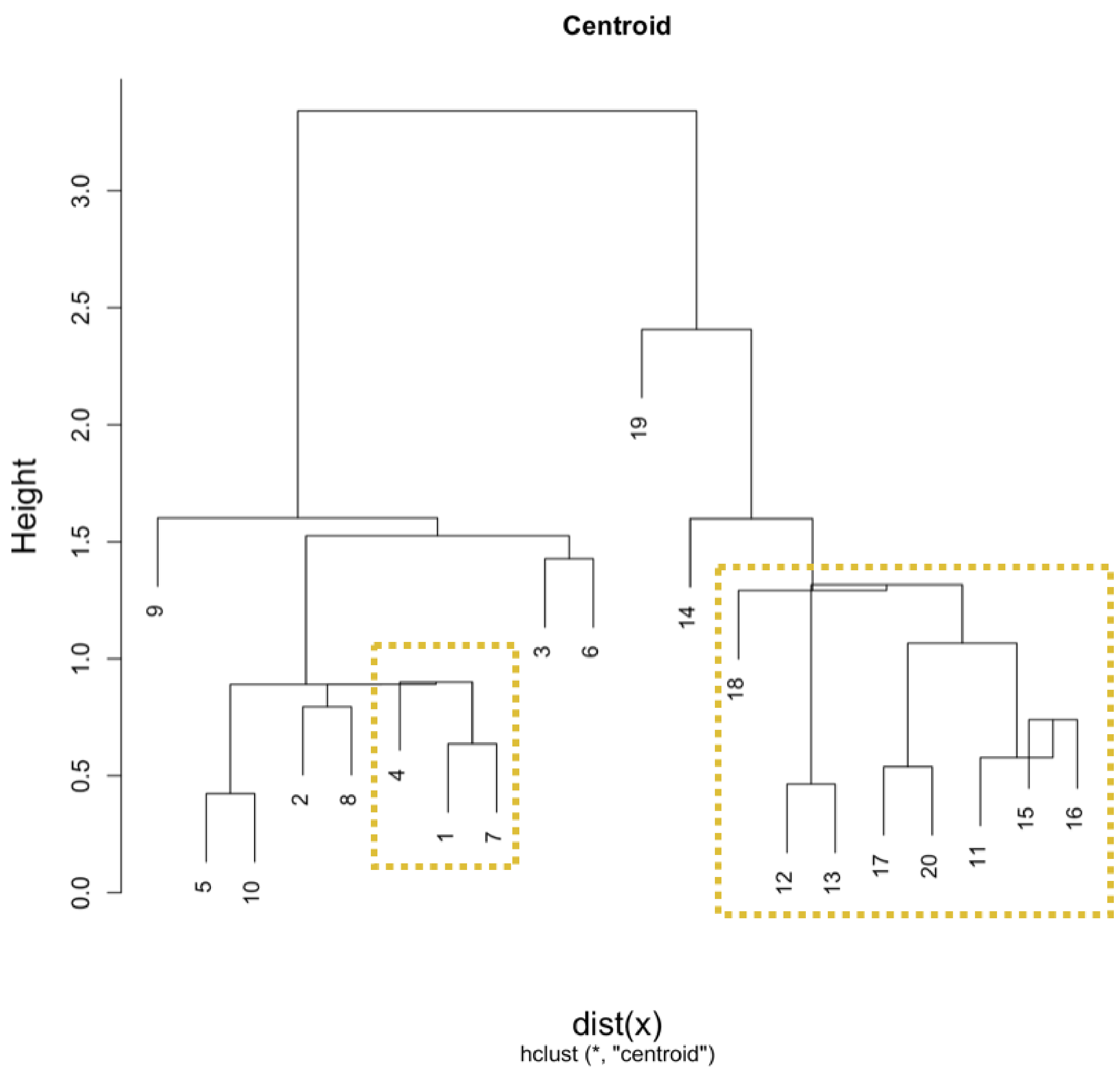




Linking method: single



Linking method: centroid



Linkage in R

```
# Fitting hierarchical clustering models using different methods
hclust.complete <- hclust(d, method = "complete")
hclust.average <- hclust(d, method = "average")
hclust.single <- hclust(d, method = "single")
```

Practical matters

- Data on different scales can cause undesirable results in clustering methods
- Solution is to scale data so that features have same mean and standard deviation
  - Subtract mean of a feature from all observations
  - Divide each feature by the standard deviation of the feature
  - Normalized features have a mean of zero and a standard deviation of one

Practical matters

```
# Check if scaling is necessary
colMeans(x)
```

```
-0.1337828  0.0594019
```

```
apply(x, 2, sd)
```

```
1.974376 2.112357
```

Practical matters

```
# Produce new matrix with columns of mean of 0 and sd of 1
scaled_x <- scale(x)
colMeans(scaled_x)
```

```
2.775558e-17 3.330669e-17
```

```
apply(scaled_x, 2, sd)
```

```
1 1
```

Let's practice!

Review of hierarchical clustering

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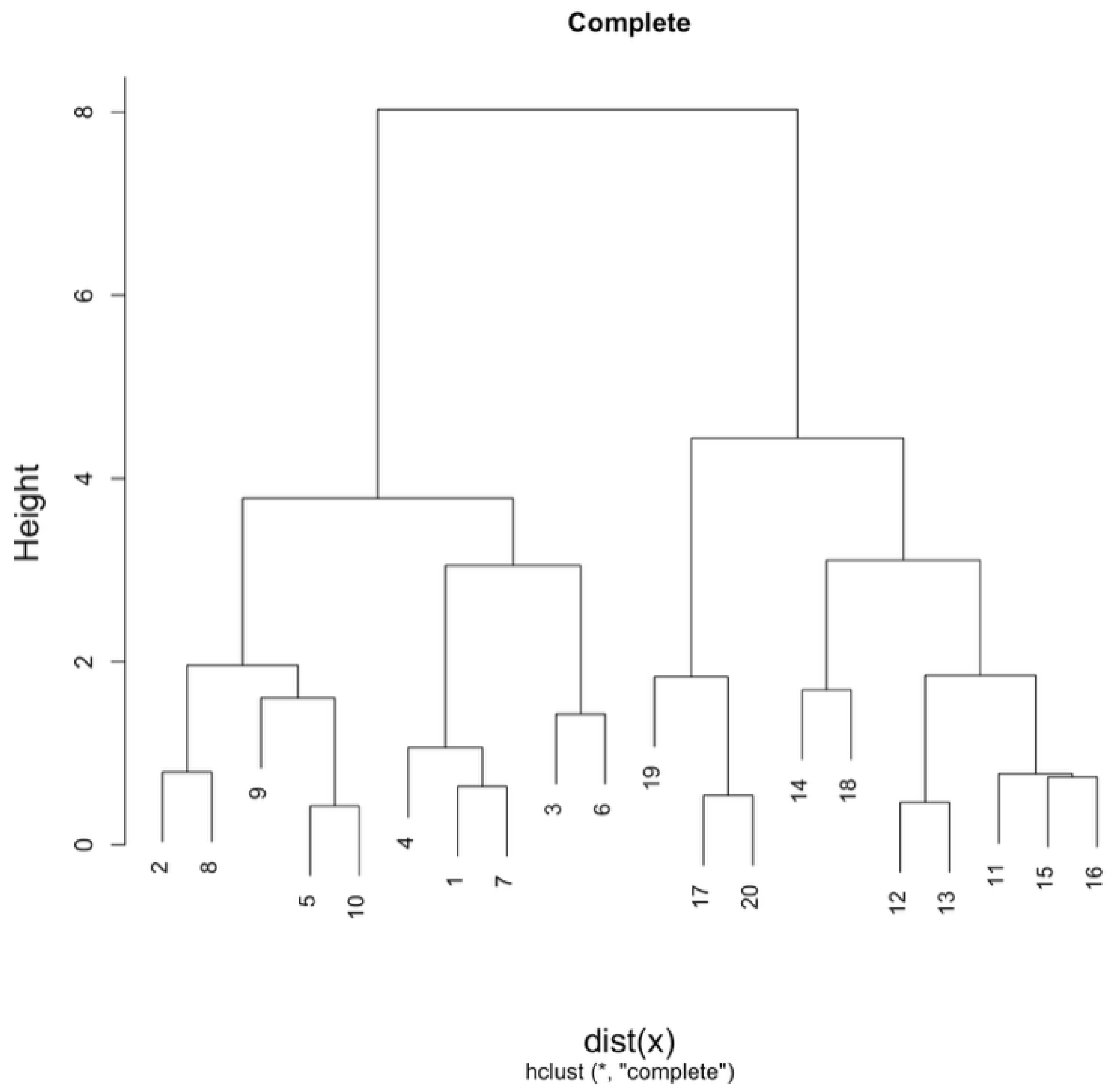
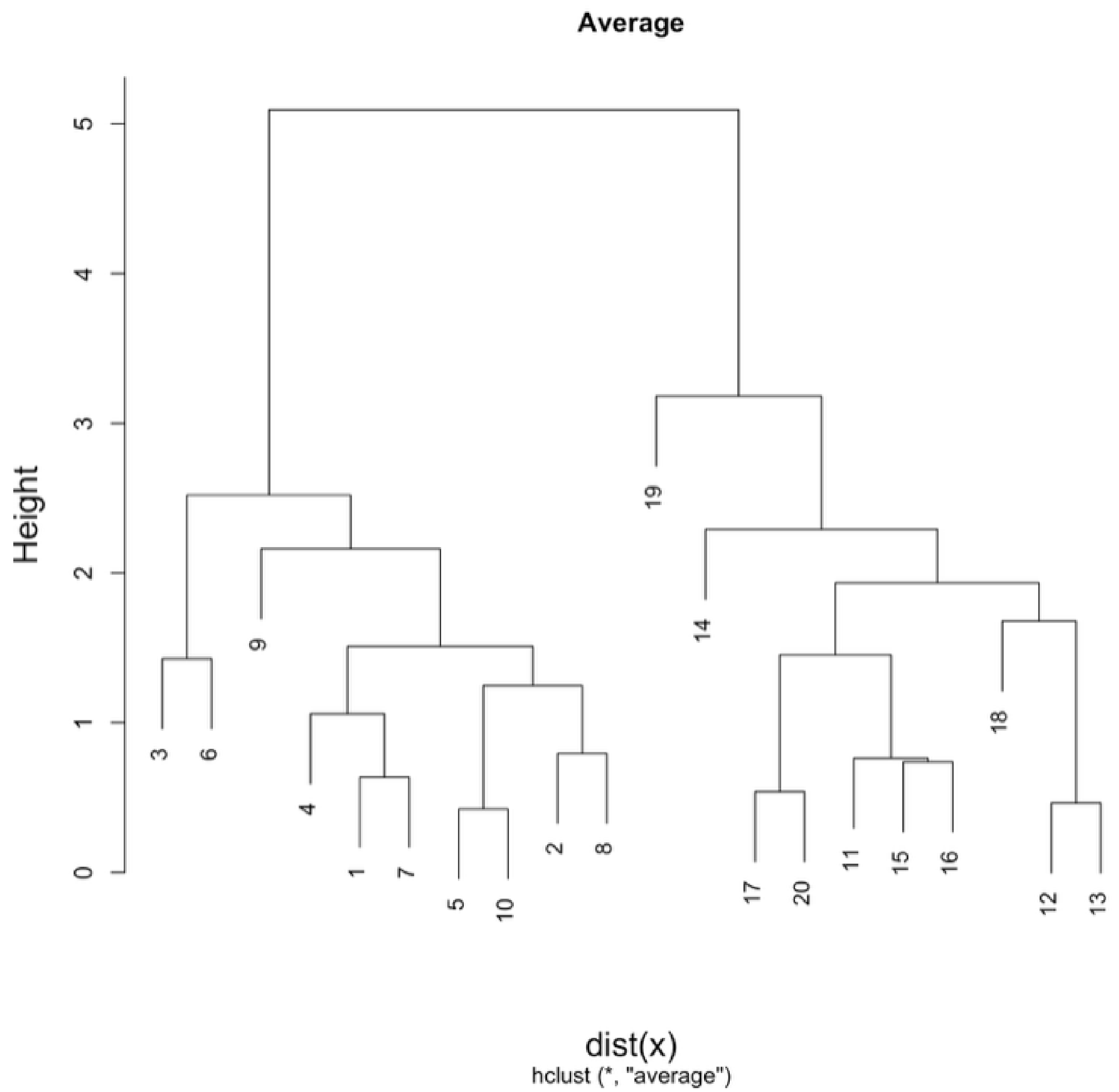
Hank Roark
Senior Data Scientist at Boeing

Hierarchical clustering review

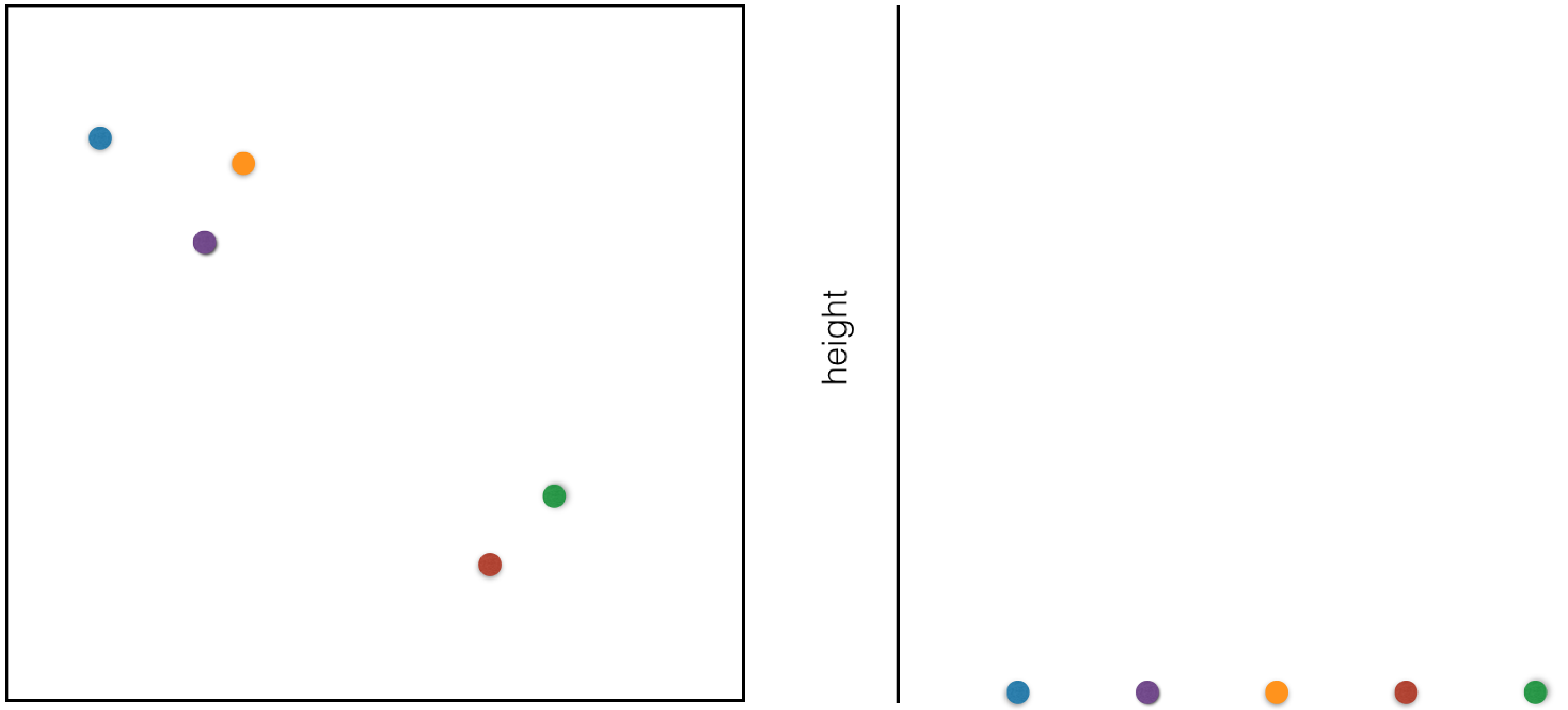
```
# Fitting various hierarchical clustering models
hclust.complete <- hclust(d, method = "complete")
hclust.average <- hclust(d, method = "average")
hclust.single <- hclust(d, method = "single")
```

Linking methods: complete and average

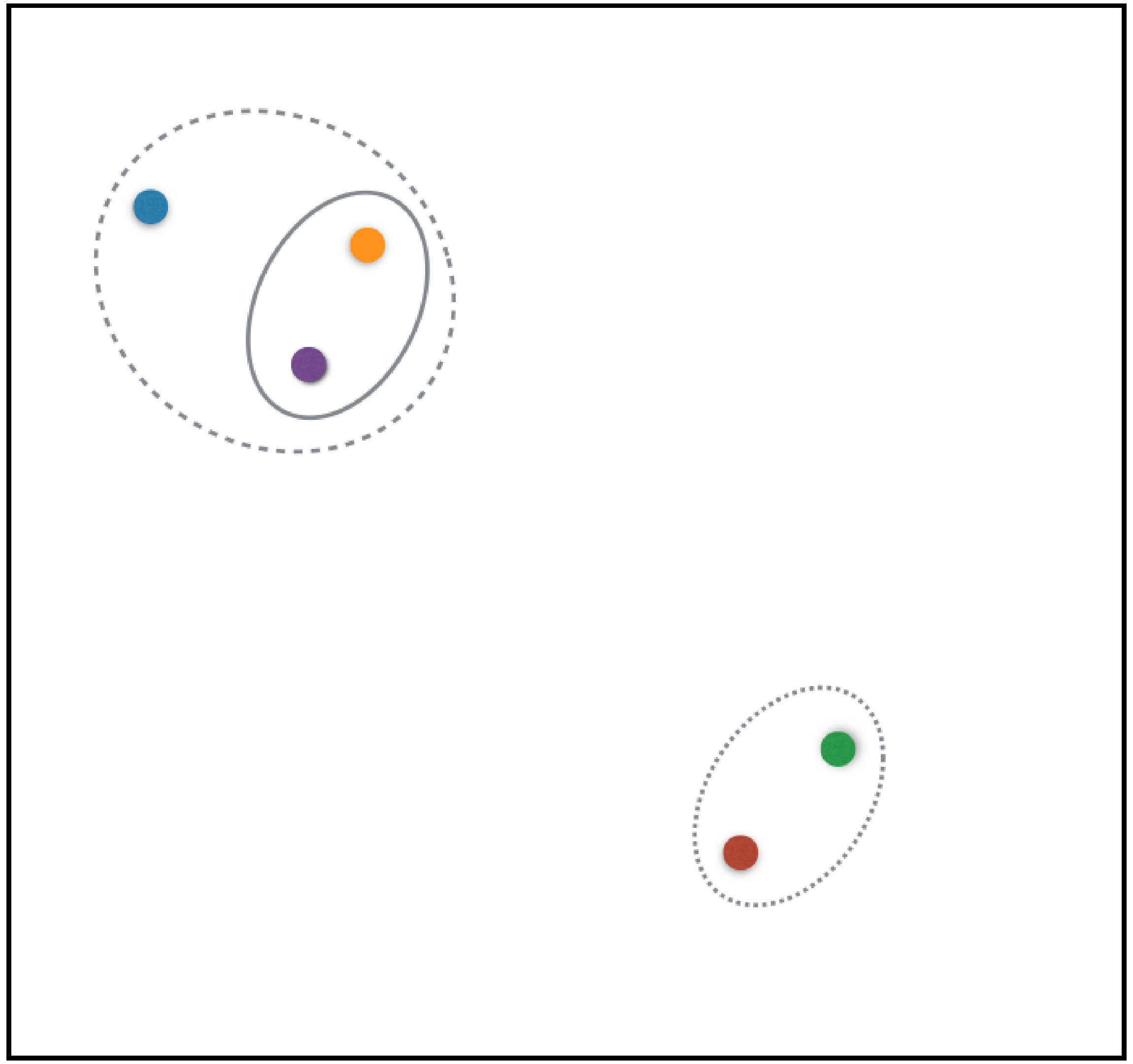


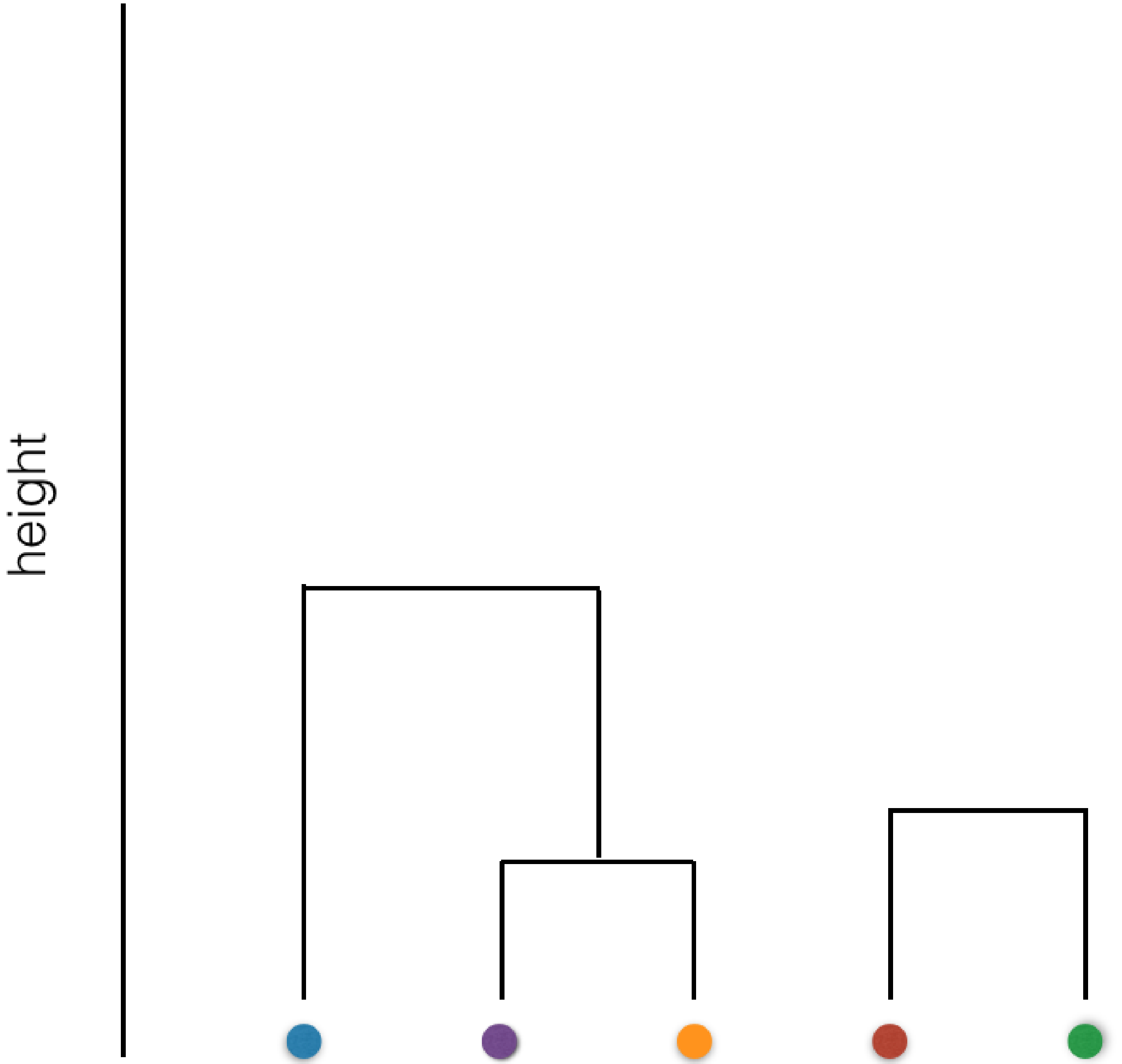


Hierarchical clustering

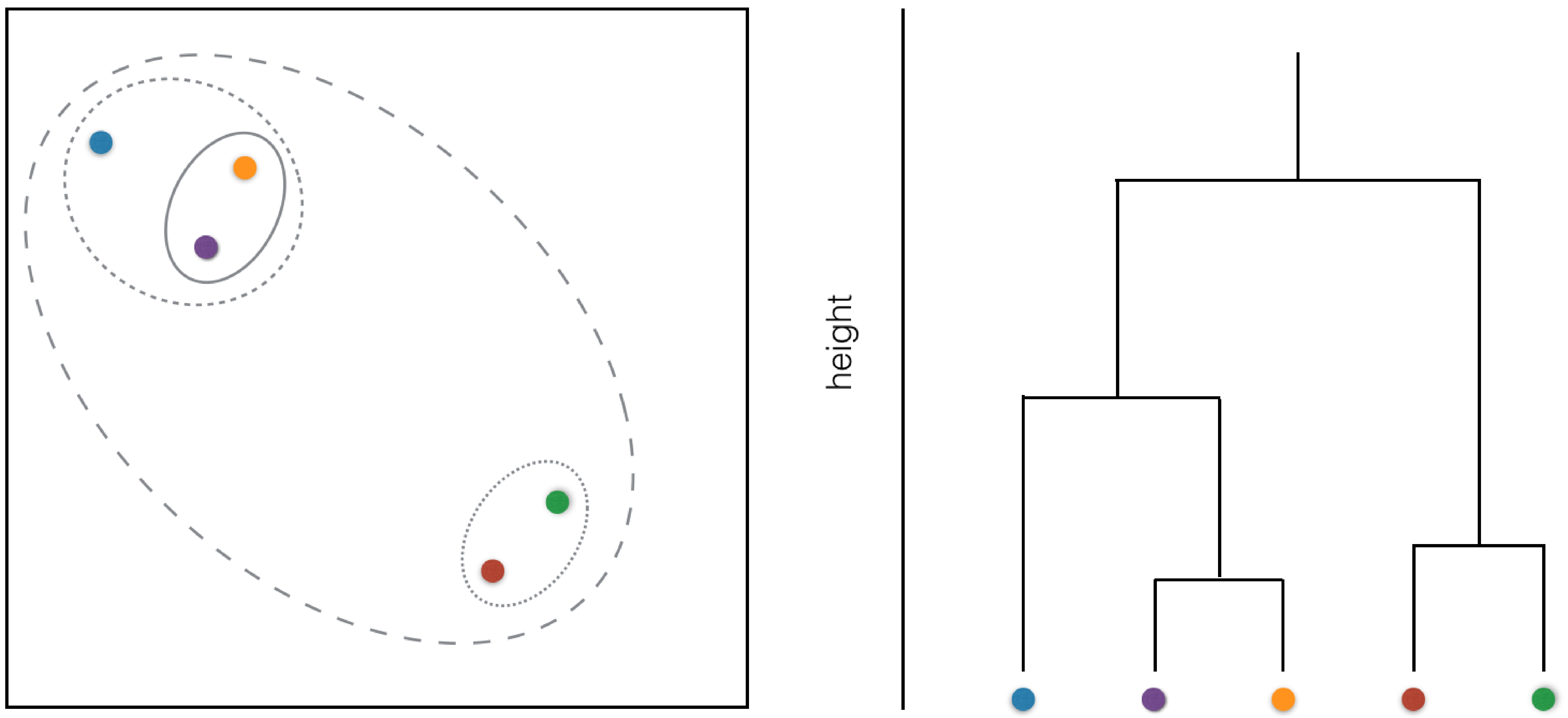


Iterating

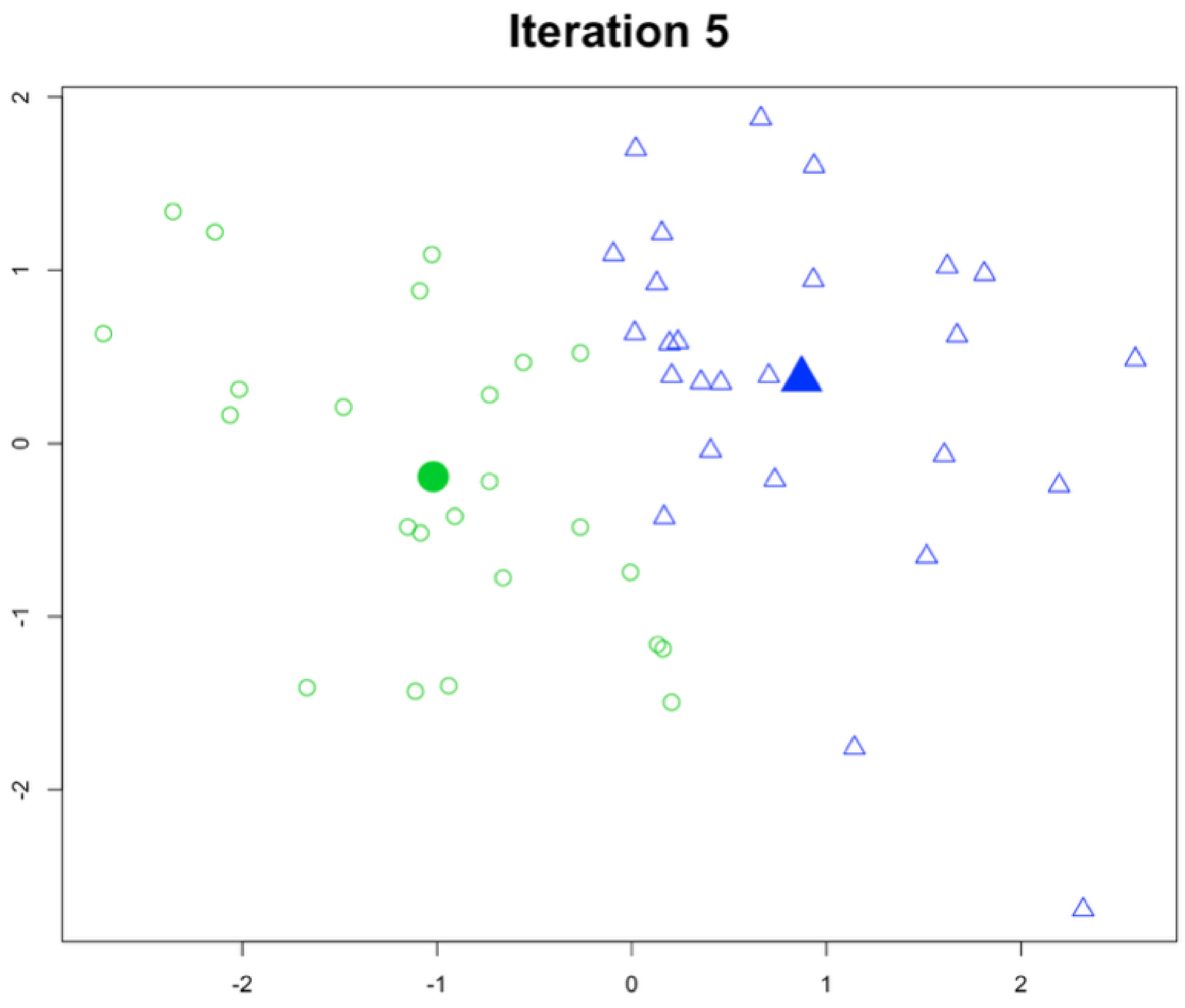


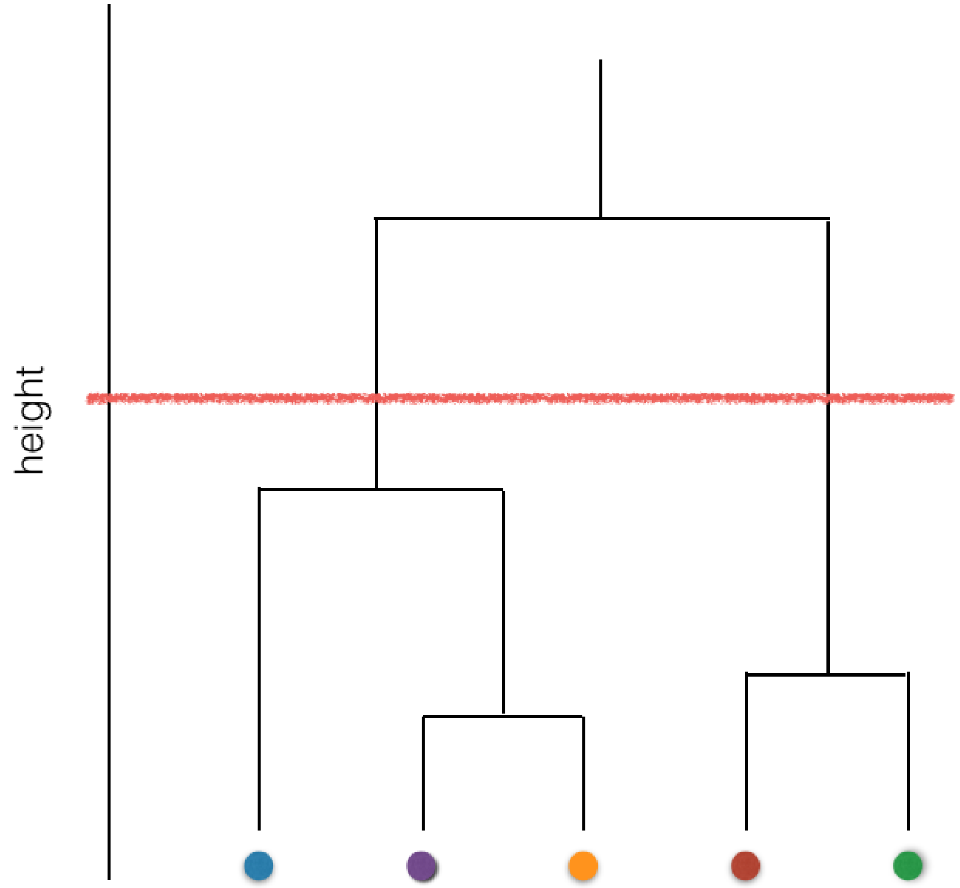


Dendrogram



How k-means and hierarchical clustering differ





Practical matters

```
# Scale the data
pokemon.scaled <- scale(pokemon)

# Create hierarchical and k-means clustering models
hclust.pokemon <- hclust(dist(pokemon.scaled), method = "complete")
km.pokemon <- kmeans(pokemon.scaled, centers = 3,
                     nstart = 20, iter.max = 50)

# Compare results of the models
cut.pokemon <- cutree(hclust.pokemon, k = 3)
table(km.pokemon$cluster, cut.pokemon)
cut.pokemon
```

```
    1   2   3
1 242   1   0
2 342   1   0
3 204   9   1
```

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