

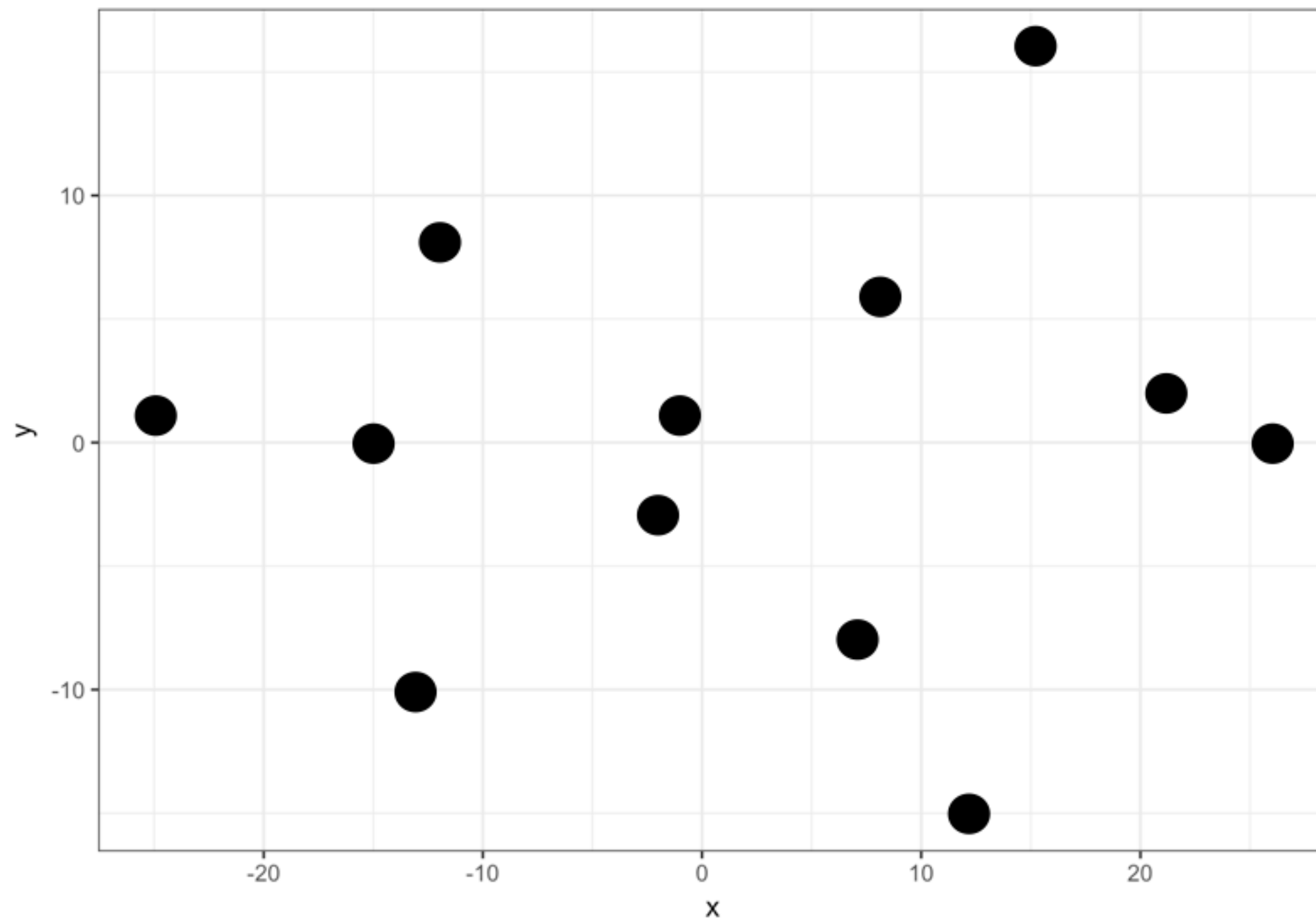
# Introduction to K-means

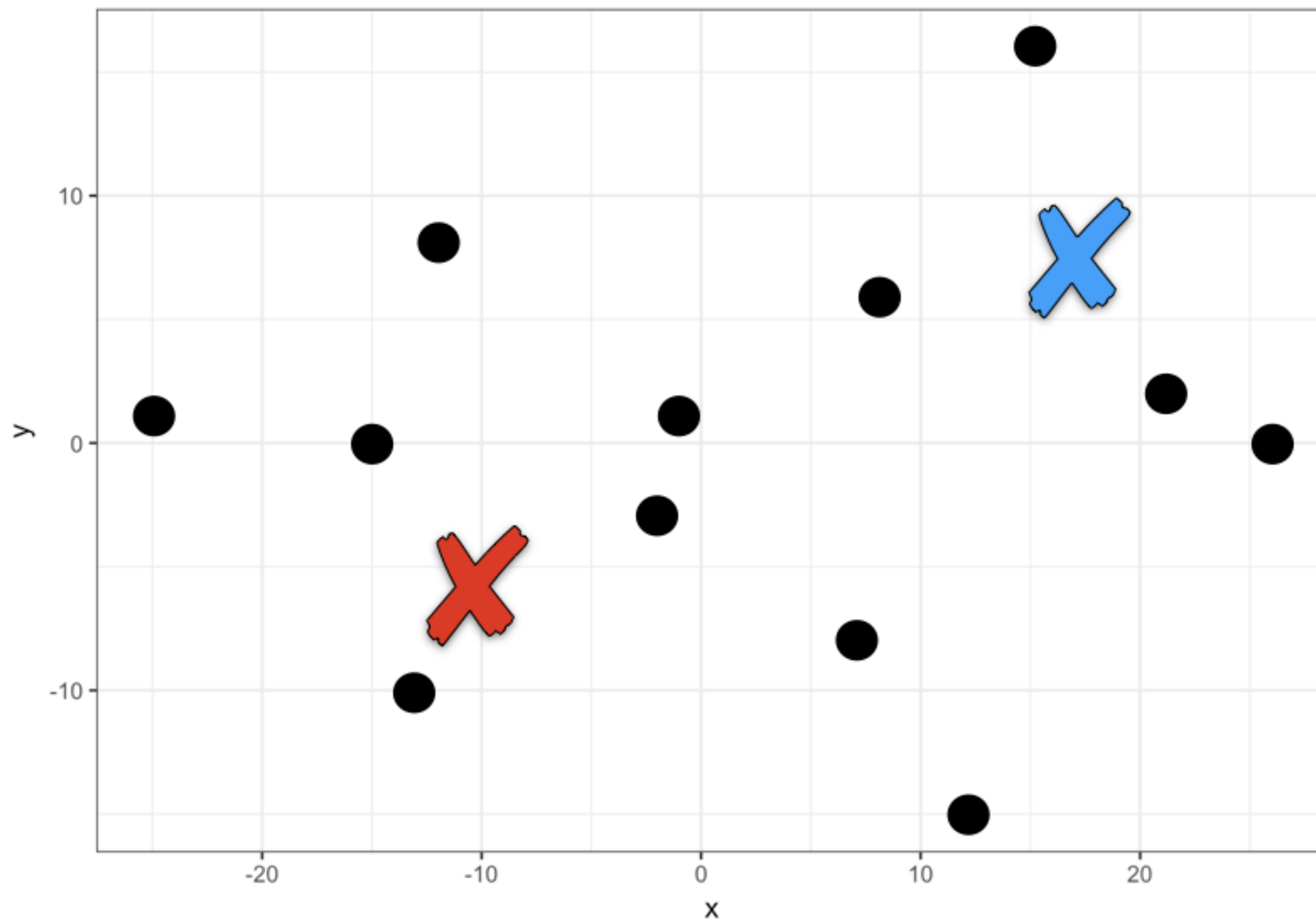
CLUSTER ANALYSIS IN R

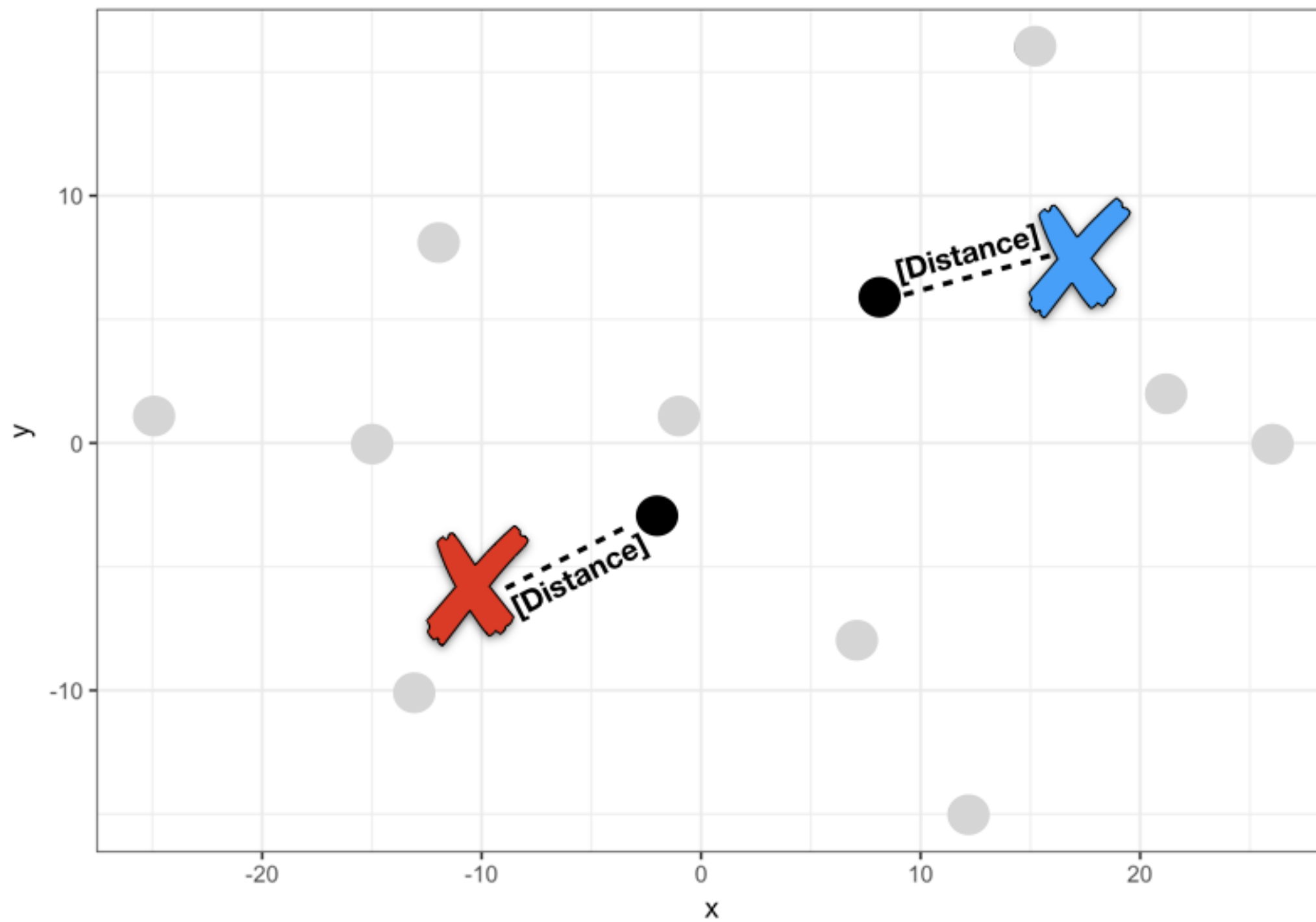


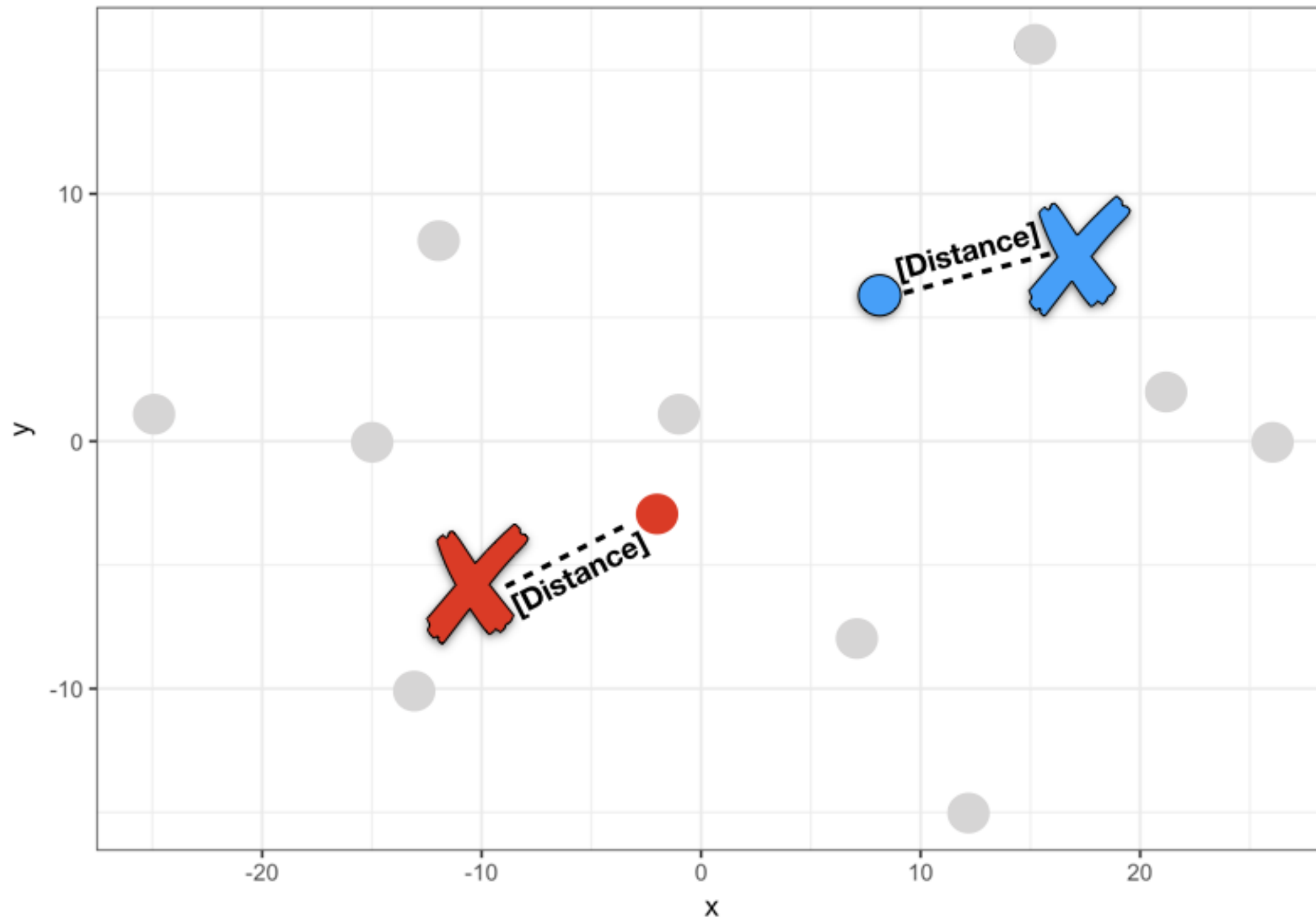
**Dmitriy (Dima) Gorenshteyn**

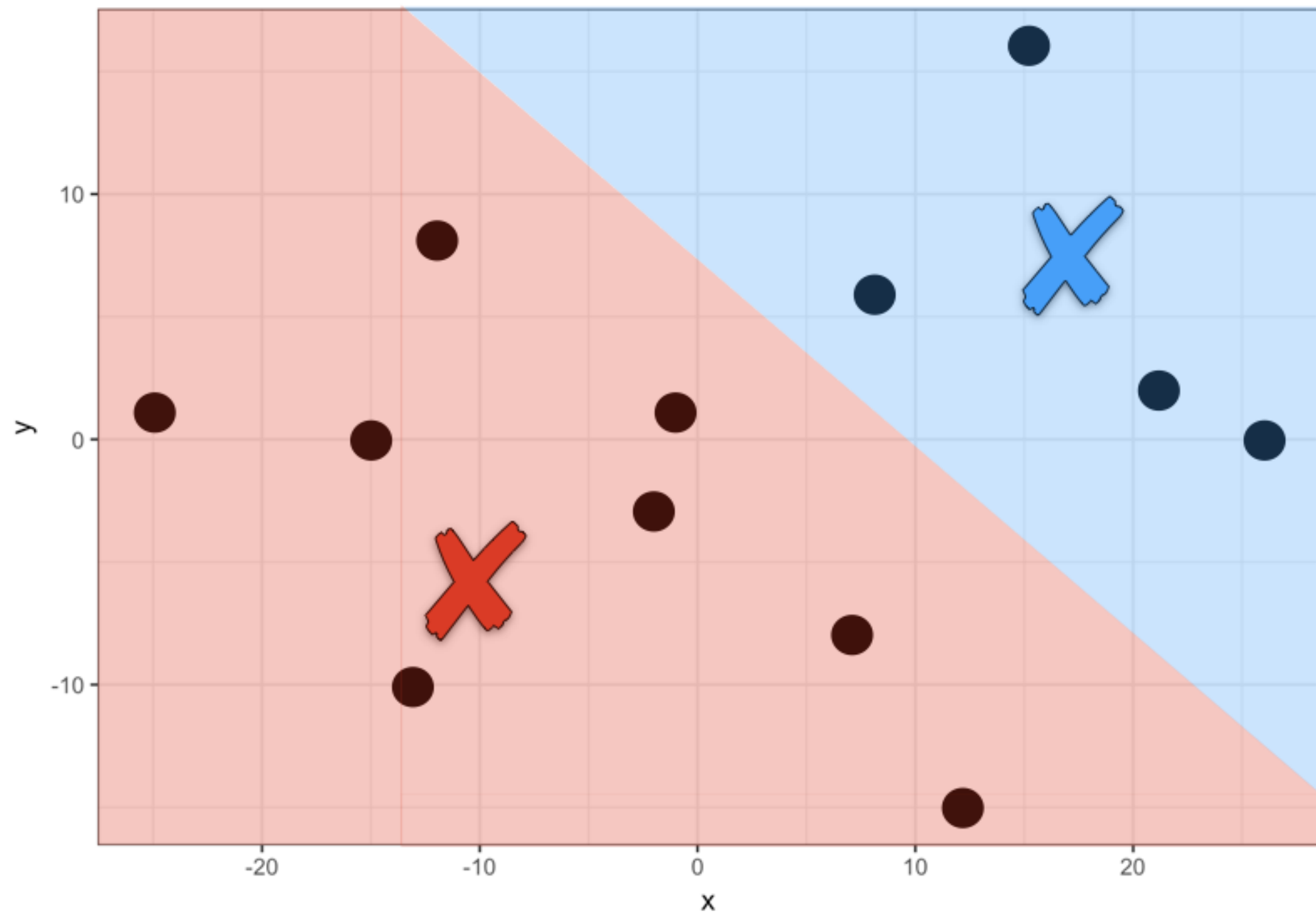
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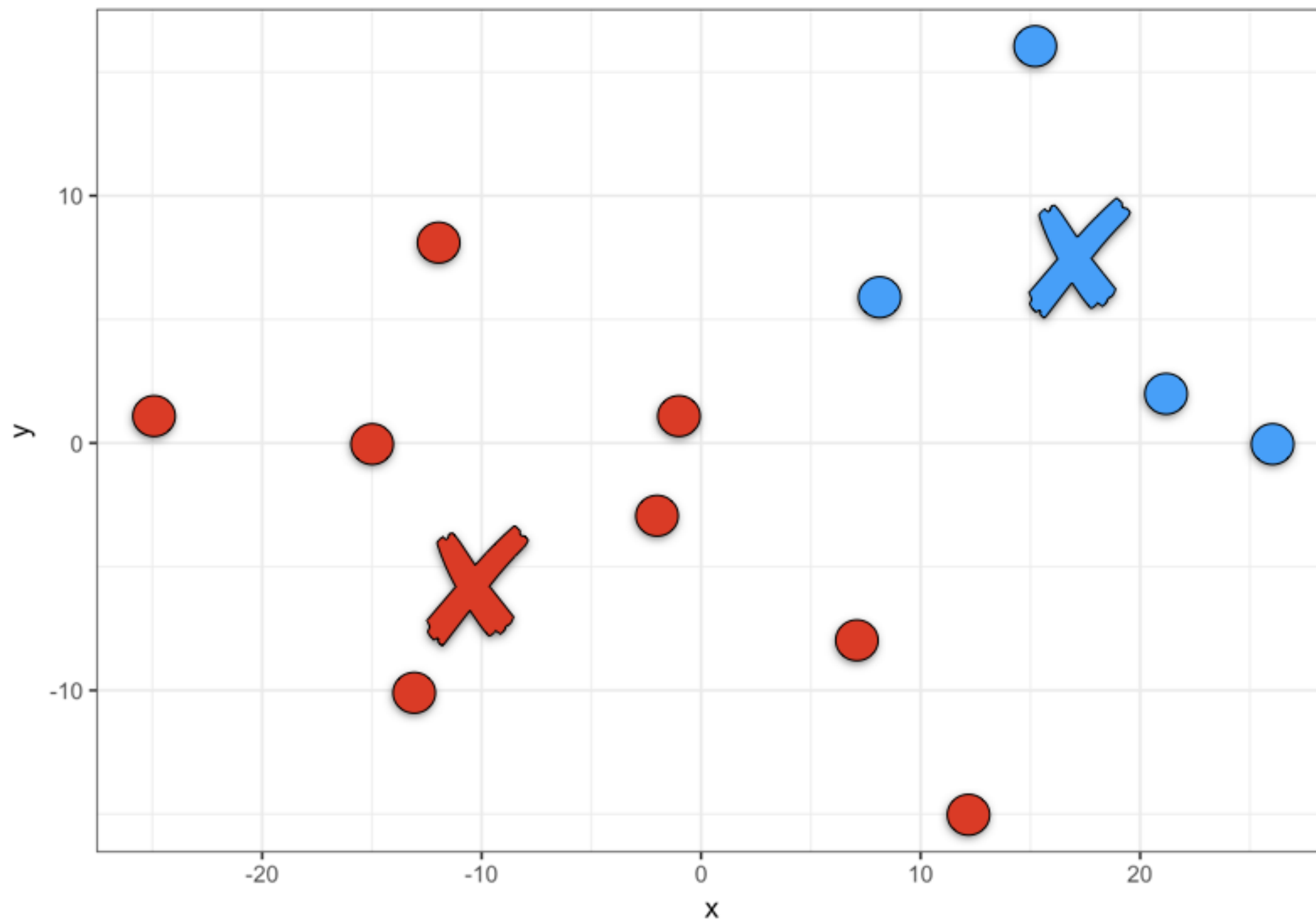


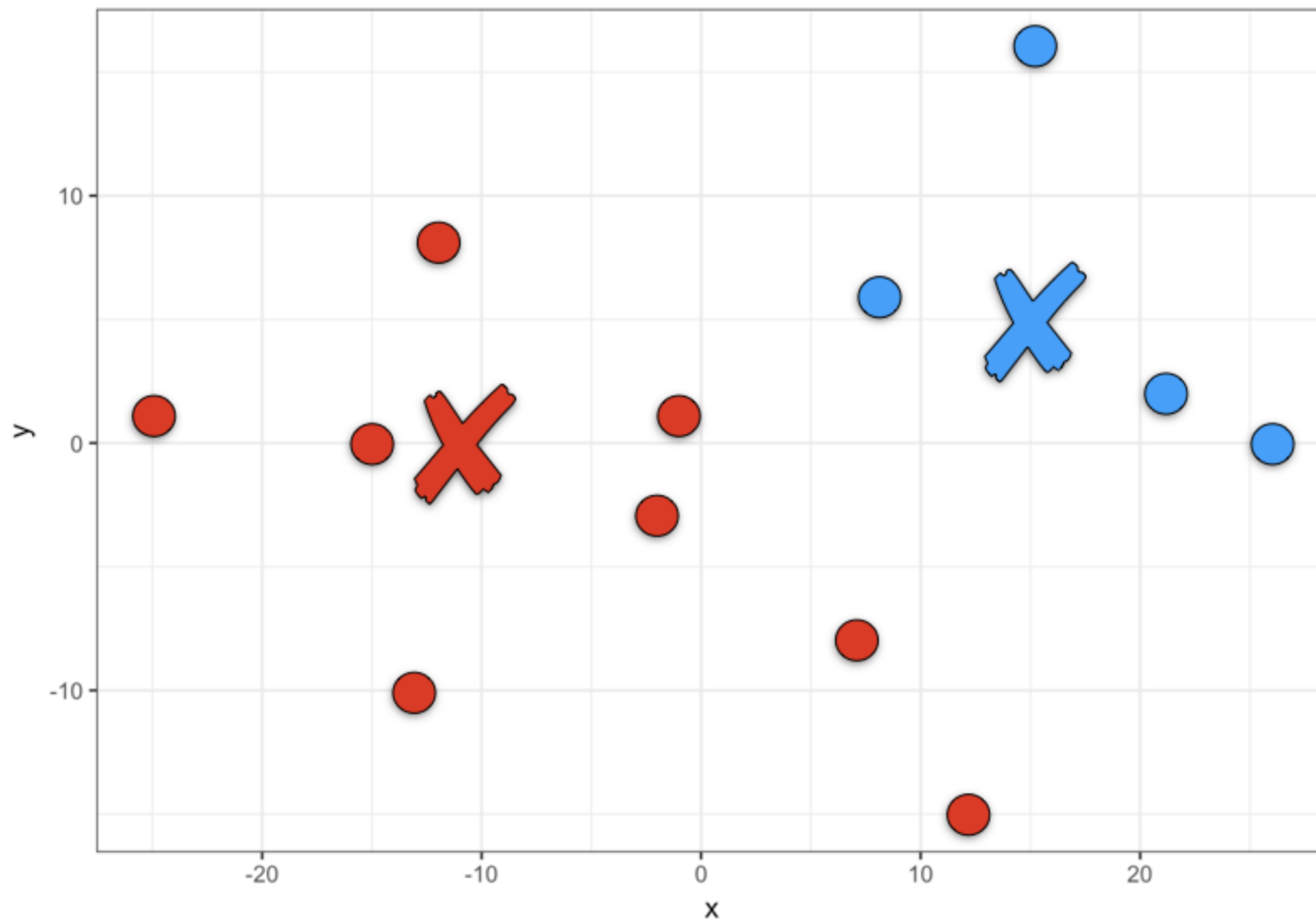




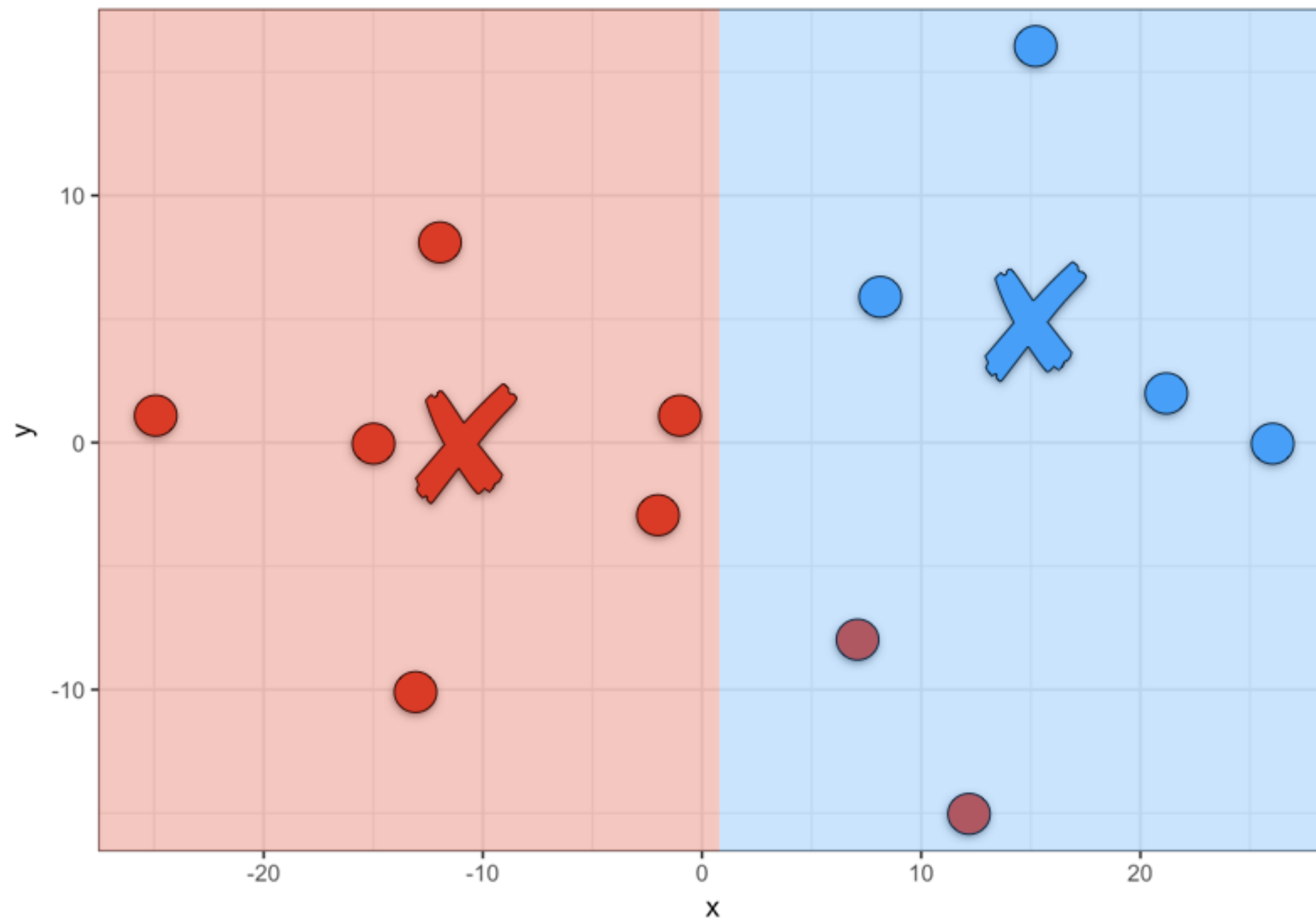


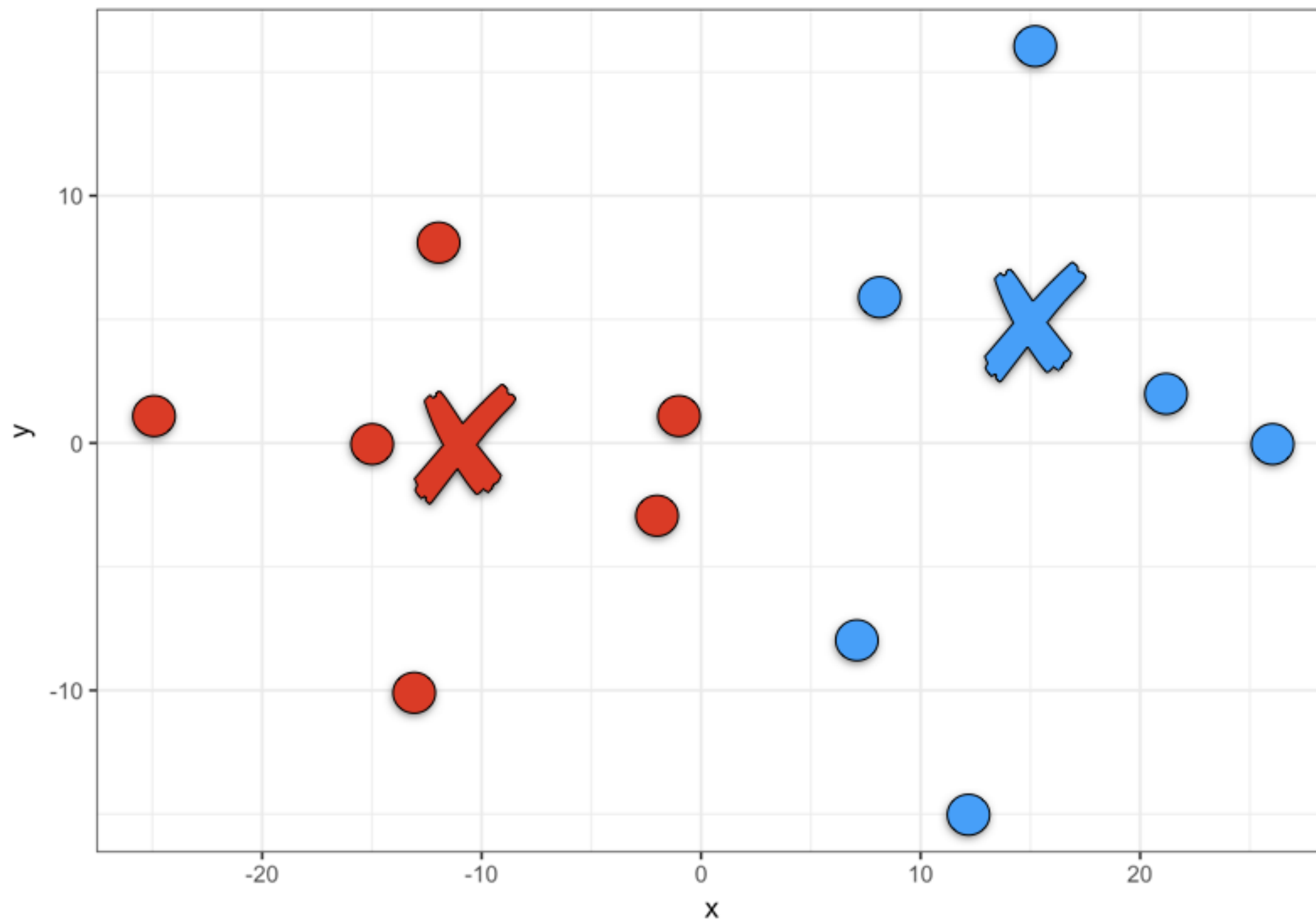


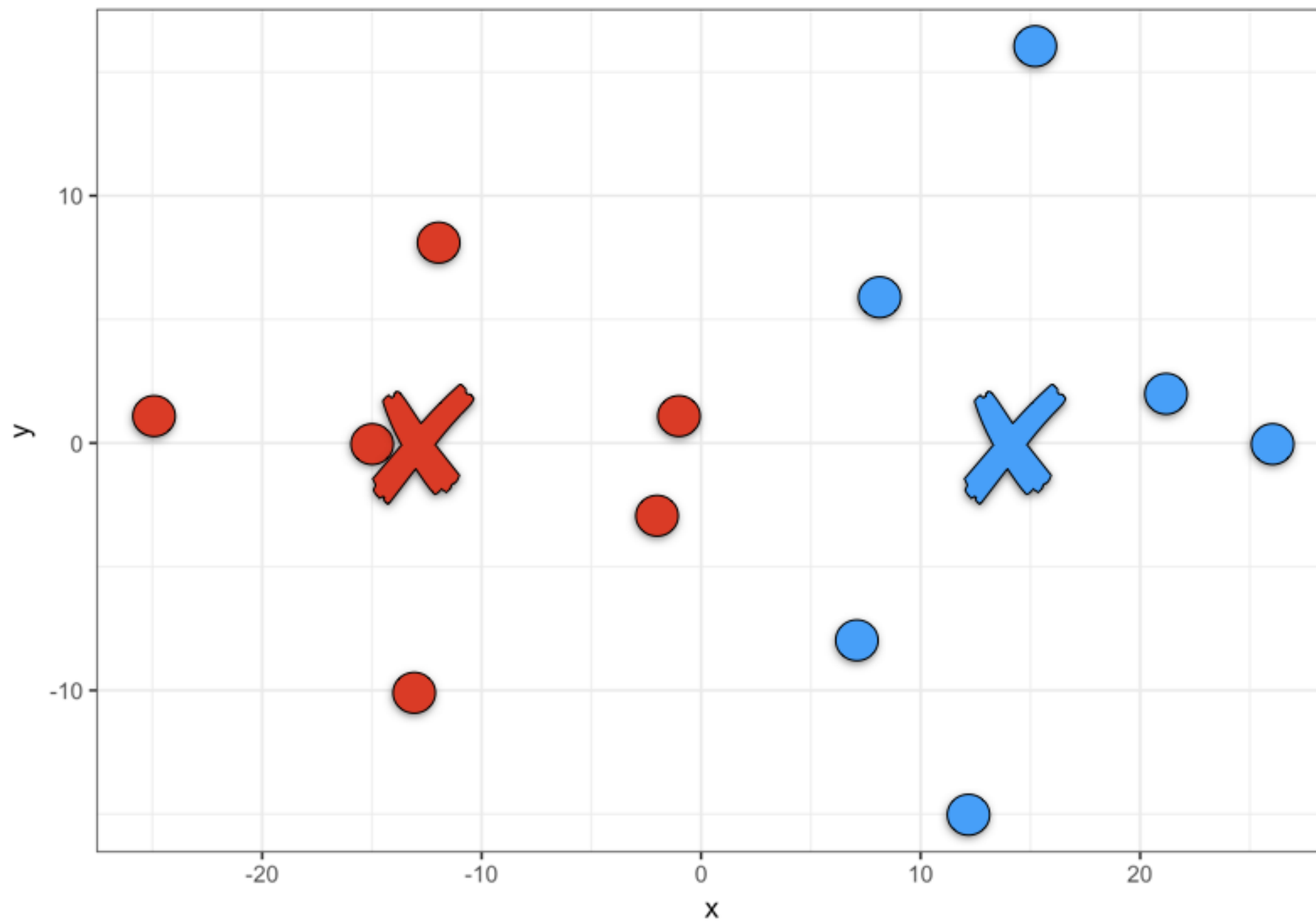












# kmeans()

```
print(lineup)
  x  y
1 -1  1
2 -2 -3
3  8  6
4  7 -8
... ..
model <- kmeans(lineup, centers = 2)
```

# Assigning clusters

```
print(model$cluster)
```

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

```
lineup_clustered <- mutate(lineup, cluster = model$cluster)
```

```
print(lineup_clustered)
```

	x	y	cluster
	<dbl>	<dbl>	<int>
1	-1	1	1
2	-2	-3	1
3	8	6	2
4	7	-8	2
...	...	...	...

# Let's practice!

CLUSTER ANALYSIS IN R

# Evaluating different values of $K$ by eye

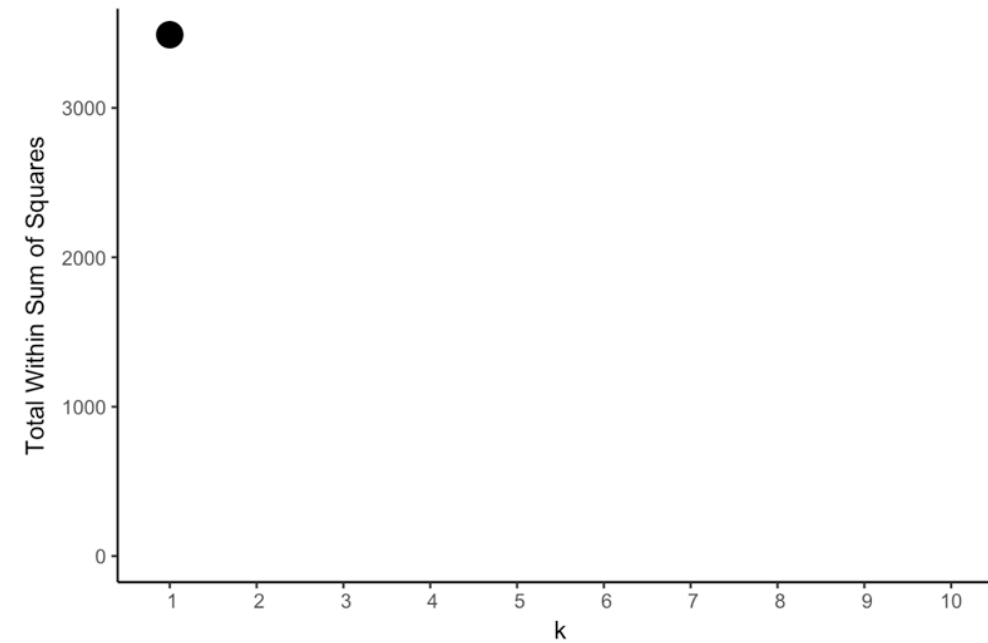
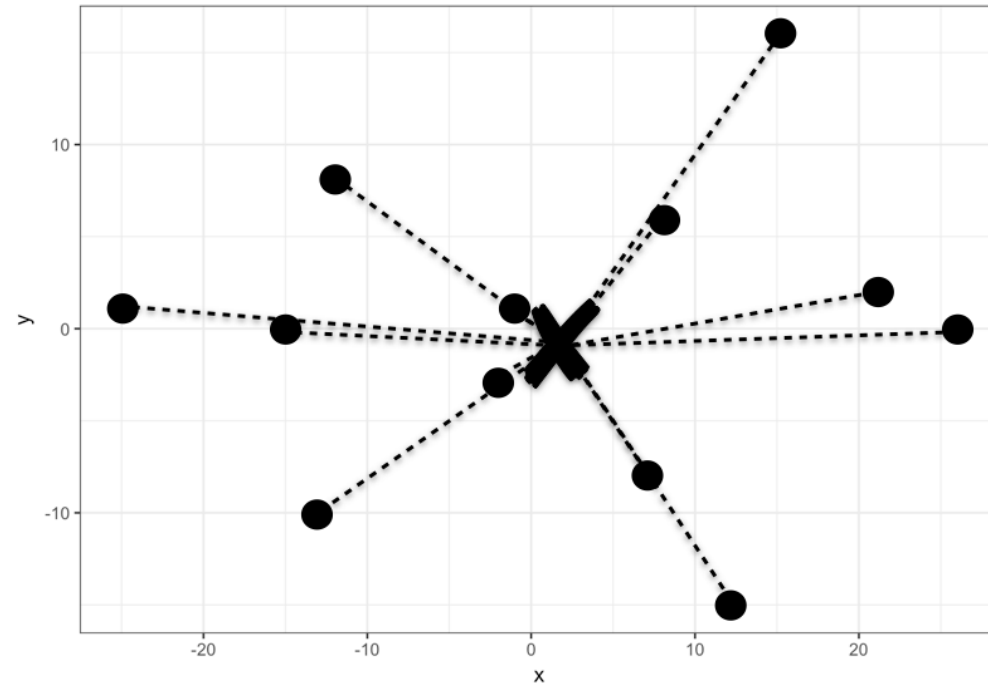
CLUSTER ANALYSIS IN R



**Dmitriy (Dima) Gorenshteyn**

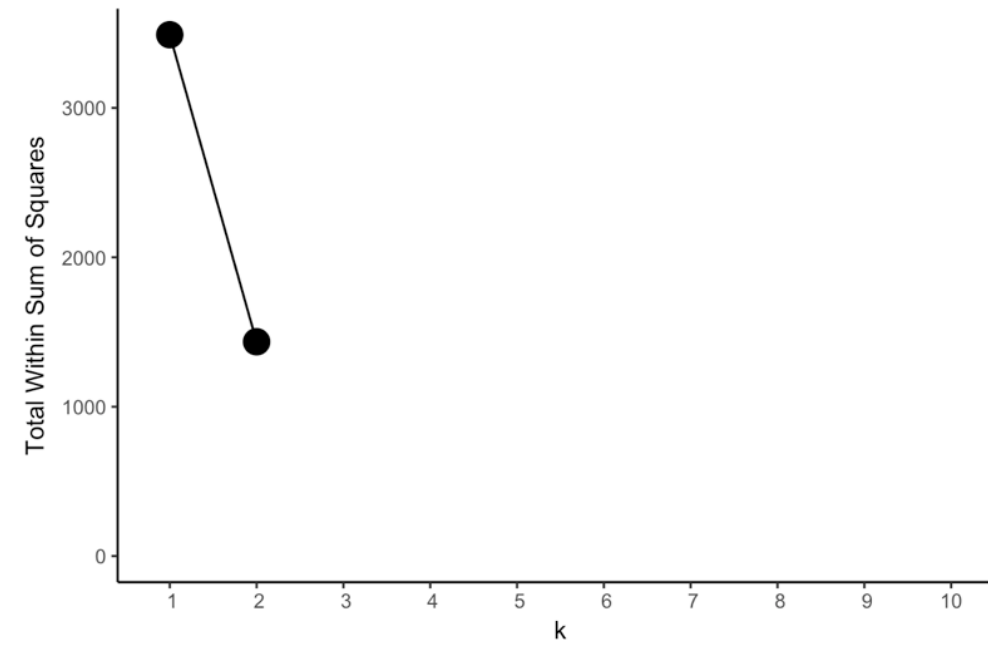
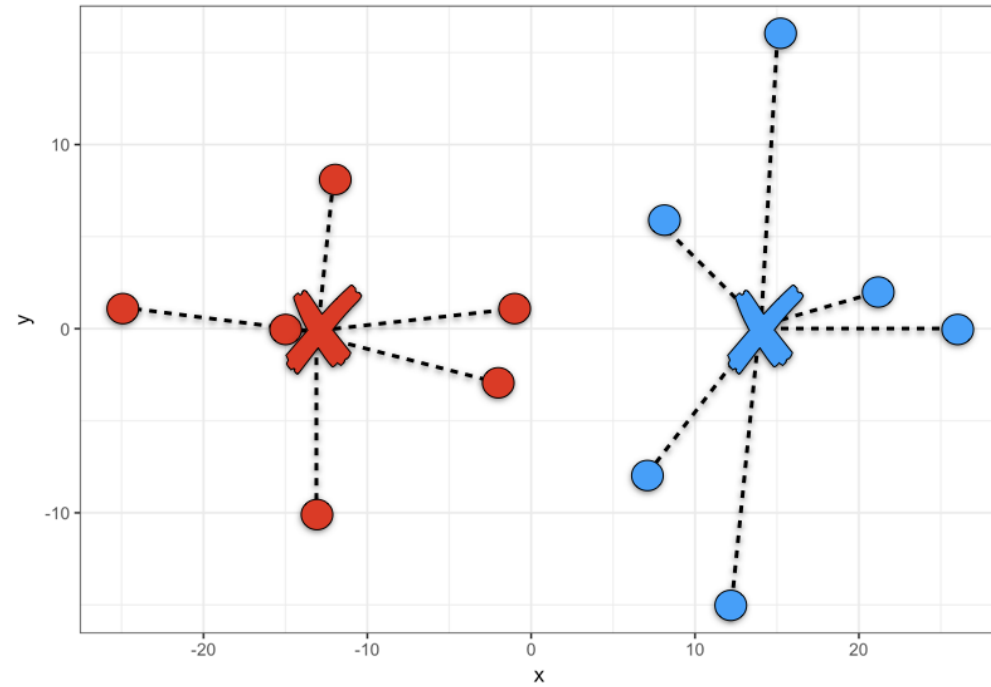
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# Total within-cluster sum of squares: $k = 1$

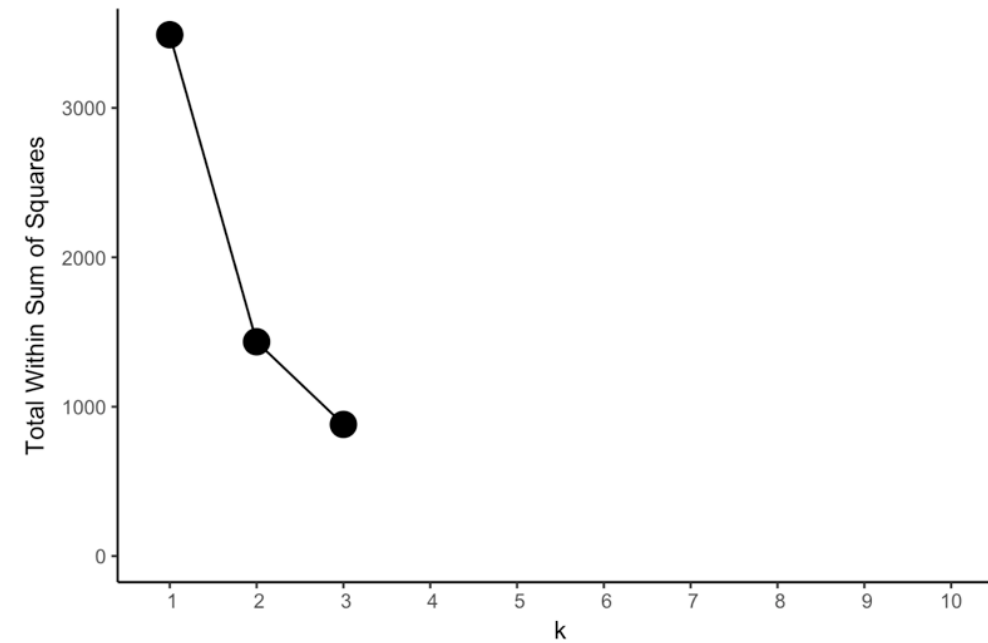
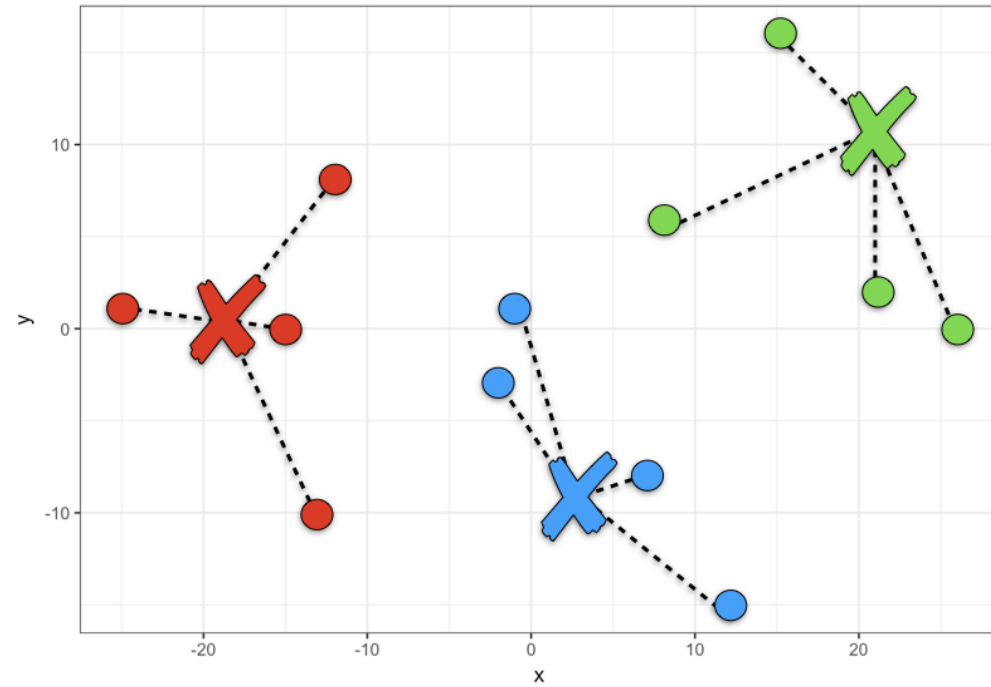




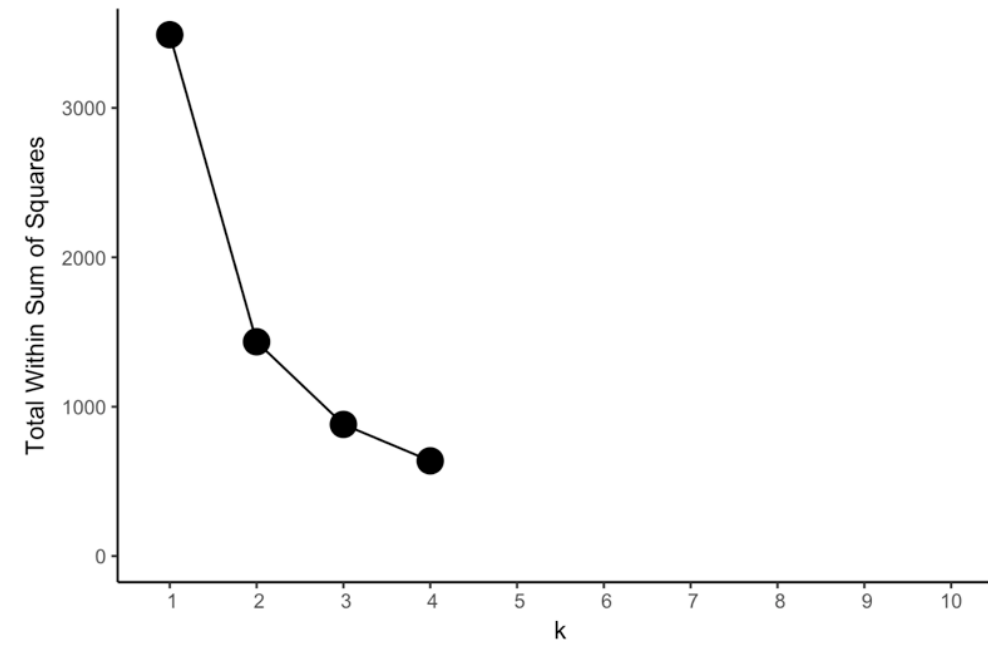
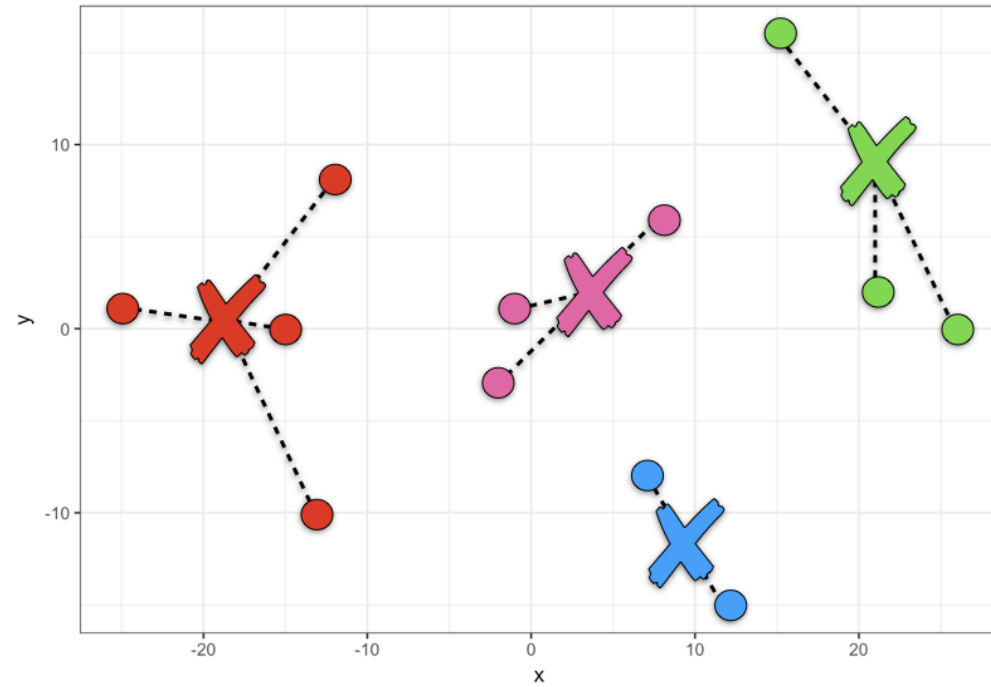
# Total within-cluster sum of squares: $k = 2$



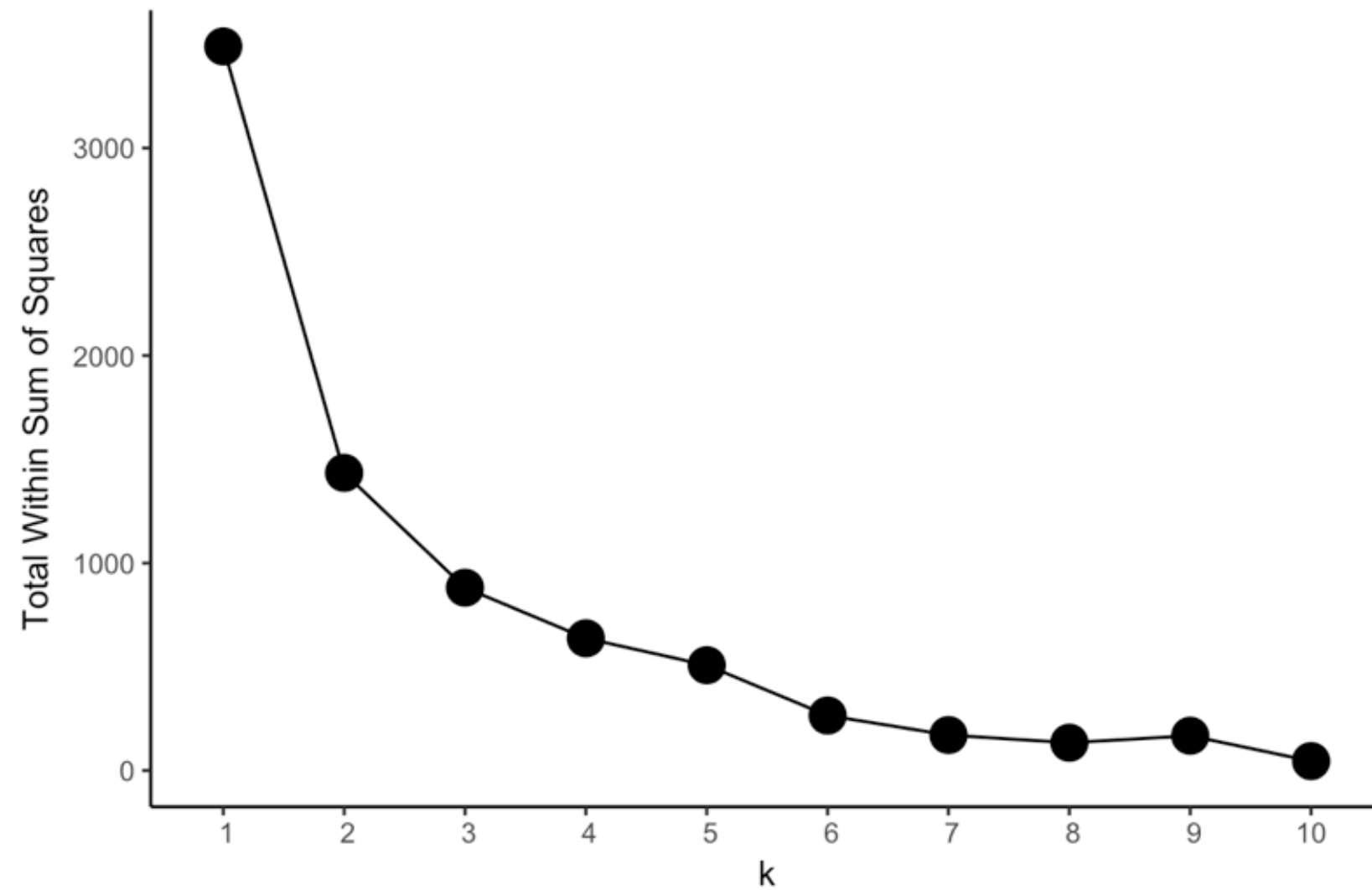
# Total within-cluster sum of squares: $k = 3$



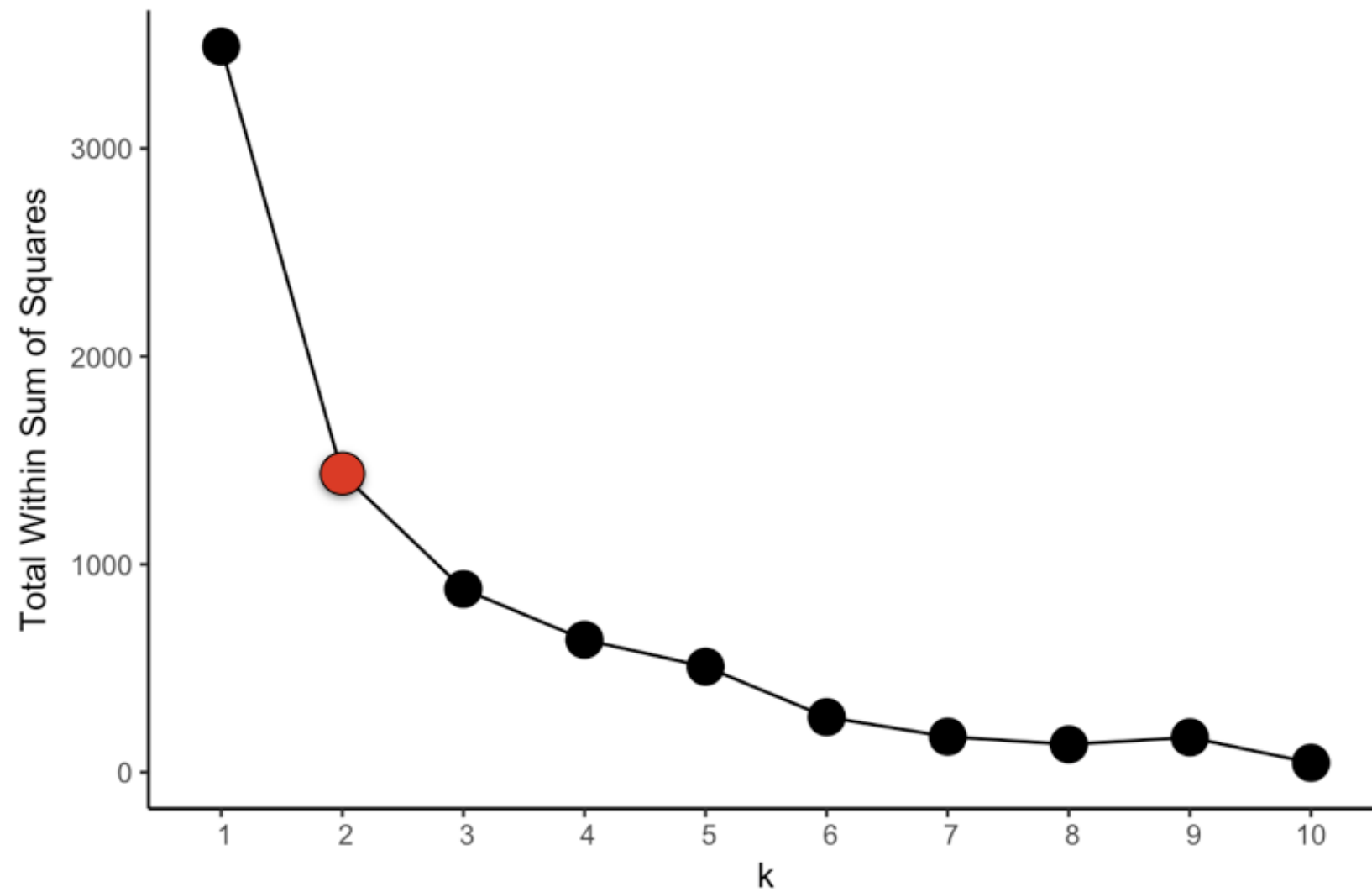
# Total within-cluster sum of squares: $k = 4$



# Elbow plot



# Elbow plot



# Generating the elbow plot

```
model <- kmeans(x = lineup, centers = 2)
```

```
model$tot.withinss
```

```
[1] 1434.5
```

# Generating the elbow plot

```
library(purrr)

tot_withinss <- map_dbl(1:10, function(k){
  model <- kmeans(x = lineup, centers = k)
  model$tot.withinss
})

elbow_df <- data.frame(
  k = 1:10,
  tot_withinss = tot_withinss
)

print(elbow_df)
```

	k	tot_withinss
1	1	3489.9167
2	2	1434.5000
3	3	881.2500
4	4	637.2500
...	...	...

# Generating the elbow plot

```
ggplot(elbow_df, aes(x = k, y = tot_withinss)) +  
  geom_line() +  
  scale_x_continuous(breaks = 1:10)
```





# Let's practice!

CLUSTER ANALYSIS IN R

# Silhouette analysis: observation level performance

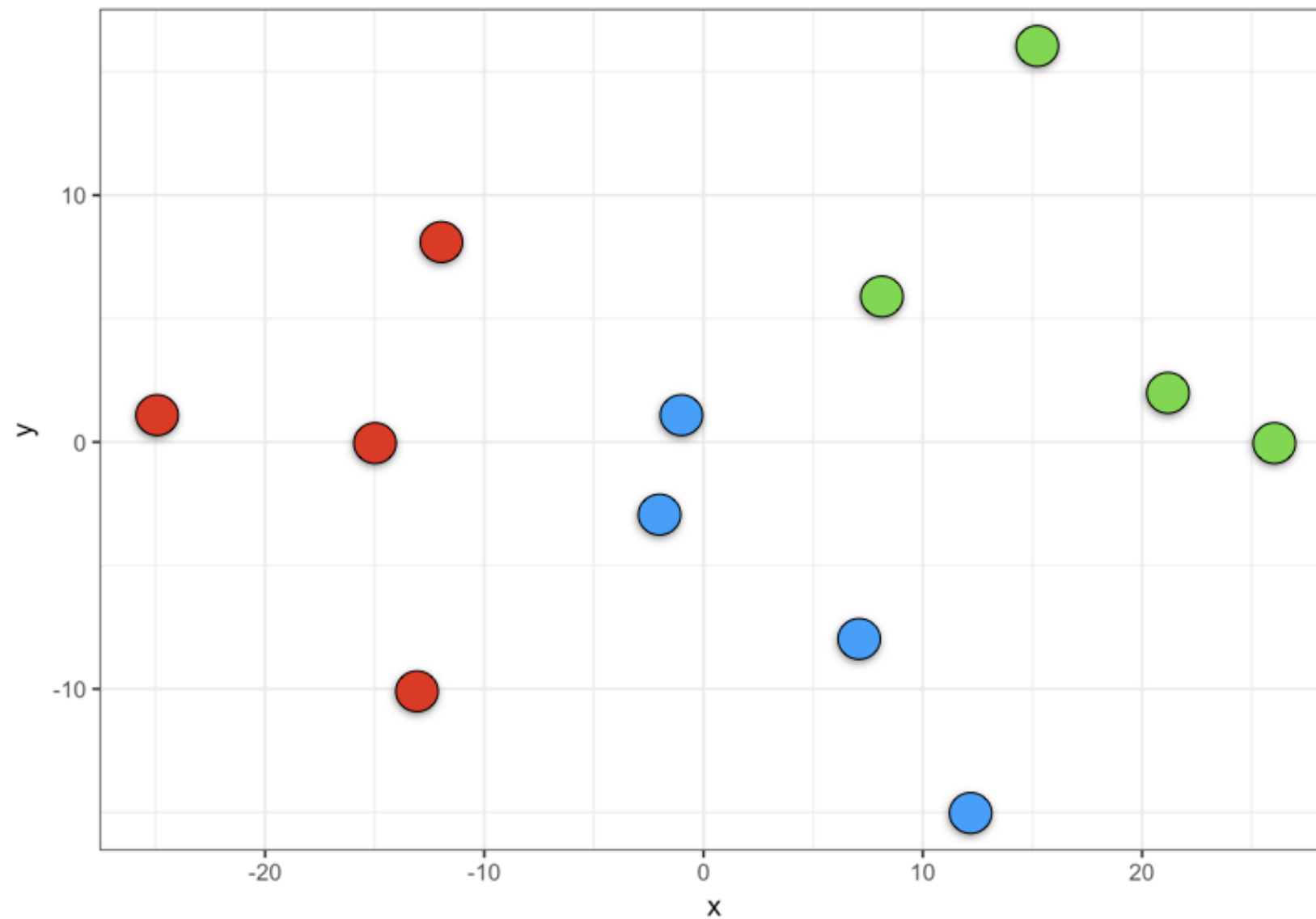
CLUSTER ANALYSIS IN R

**Dmitriy (Dima) Gorenshteyn**

Lead Data Scientist, Memorial Sloan  
Kettering Cancer Center



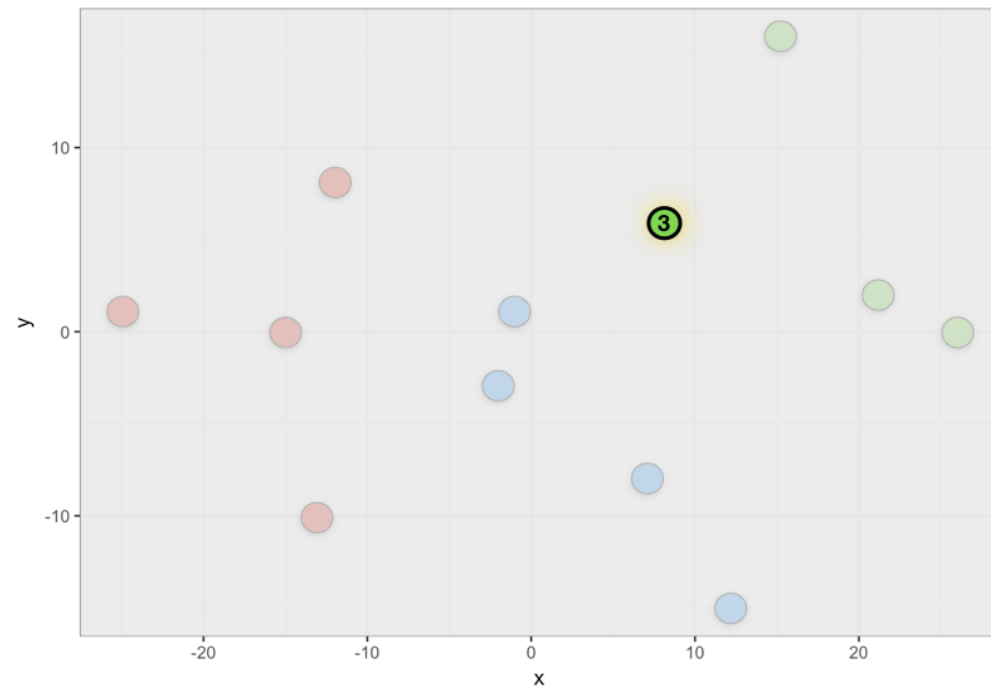
# Soccer lineup with $K = 3$



# Silhouette width

Within Cluster Distance:  $C(i)$

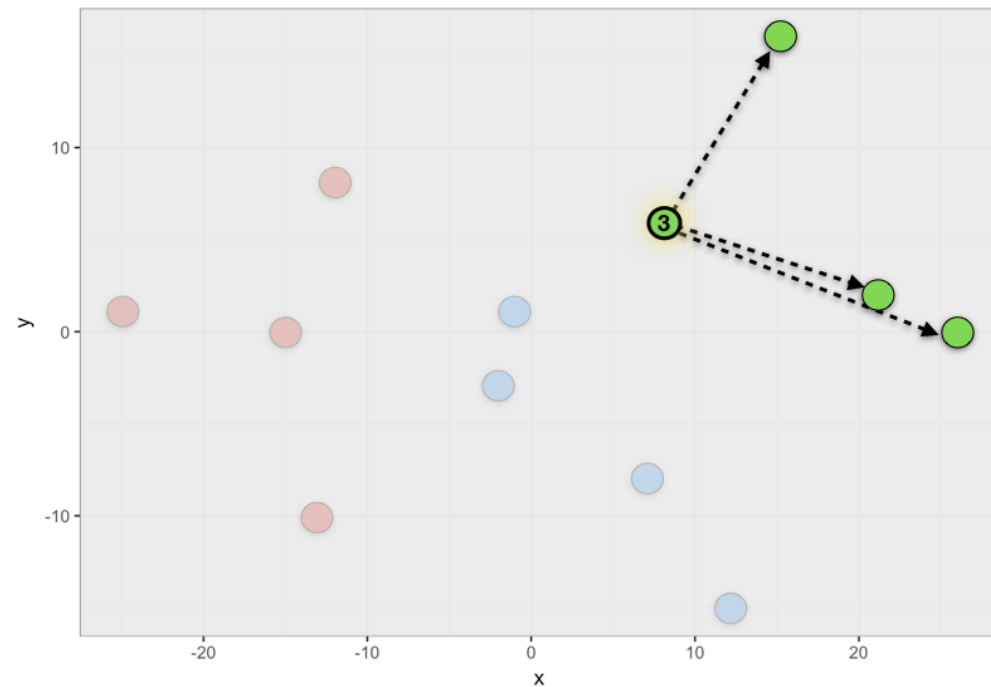
Closest Neighbor Distance:  $N(i)$



# Silhouette width

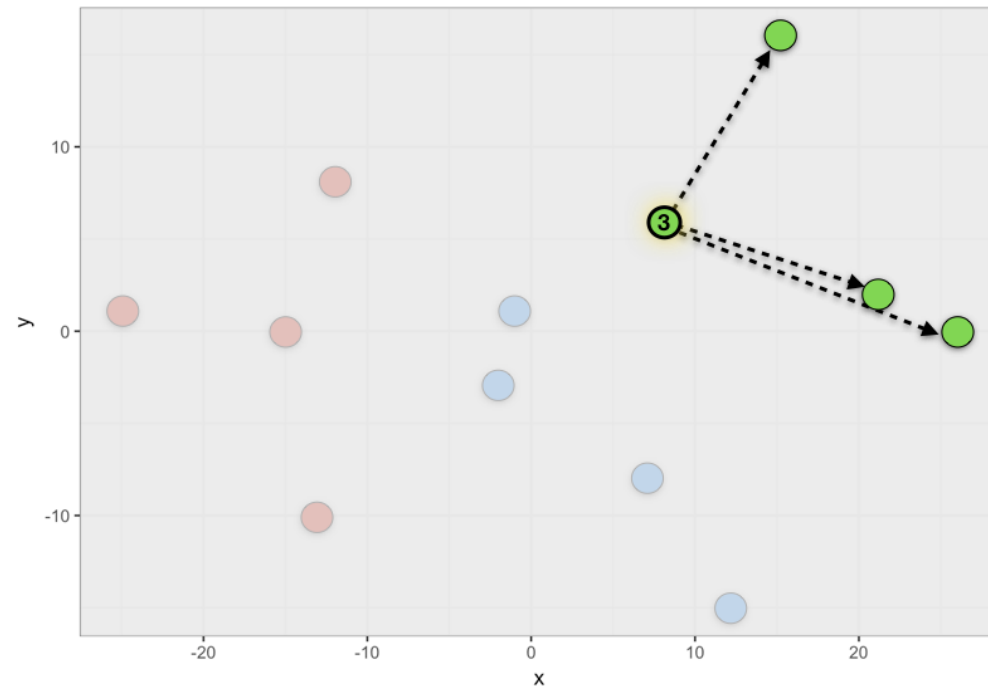
Within Cluster Distance:  $C(i)$

Closest Neighbor Distance:  $N(i)$

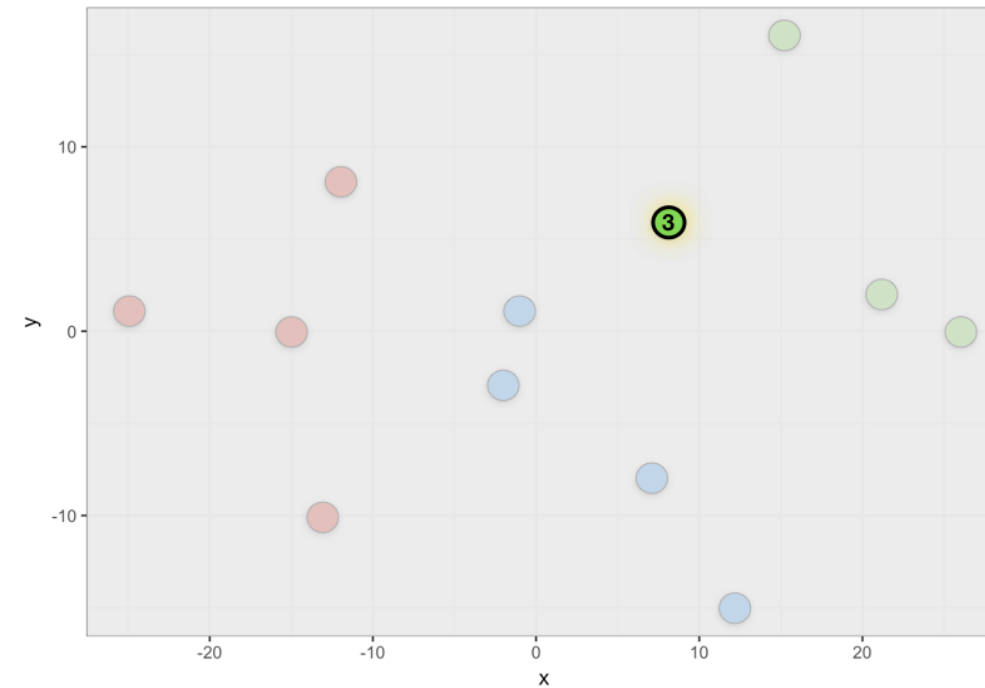


# Silhouette width

Within Cluster Distance:  $C(i)$

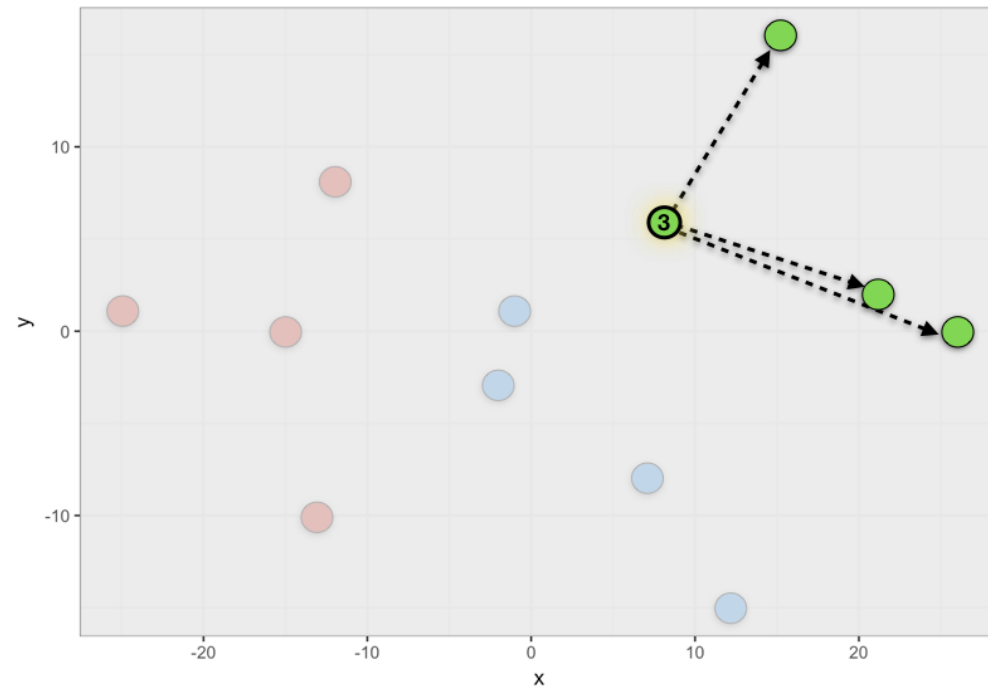


Closest Neighbor Distance:  $N(i)$

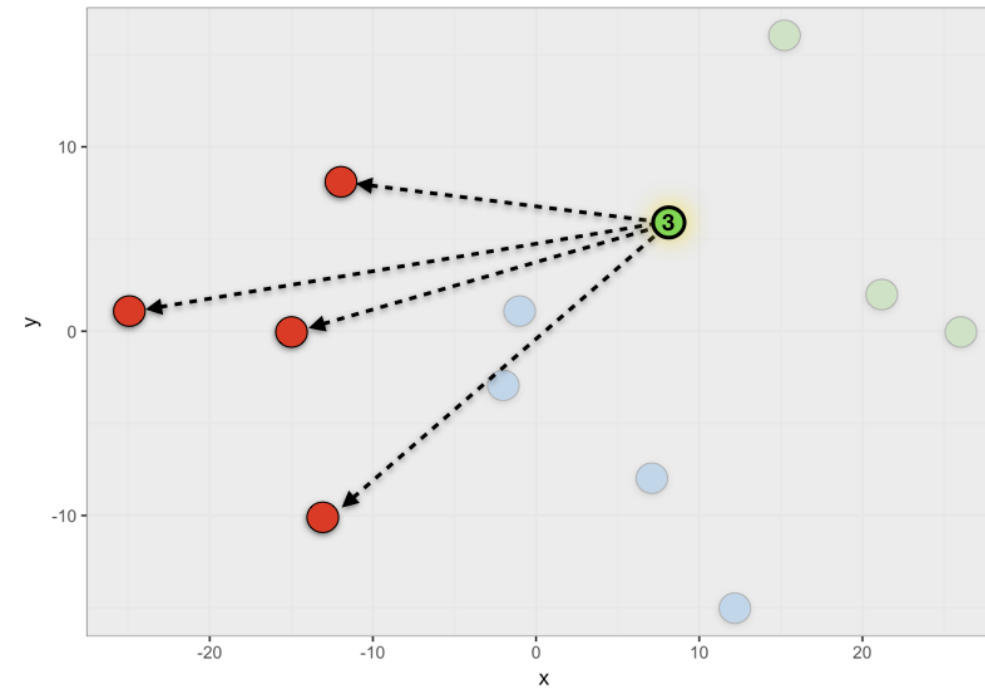


# Silhouette width

Within Cluster Distance:  $C(i)$

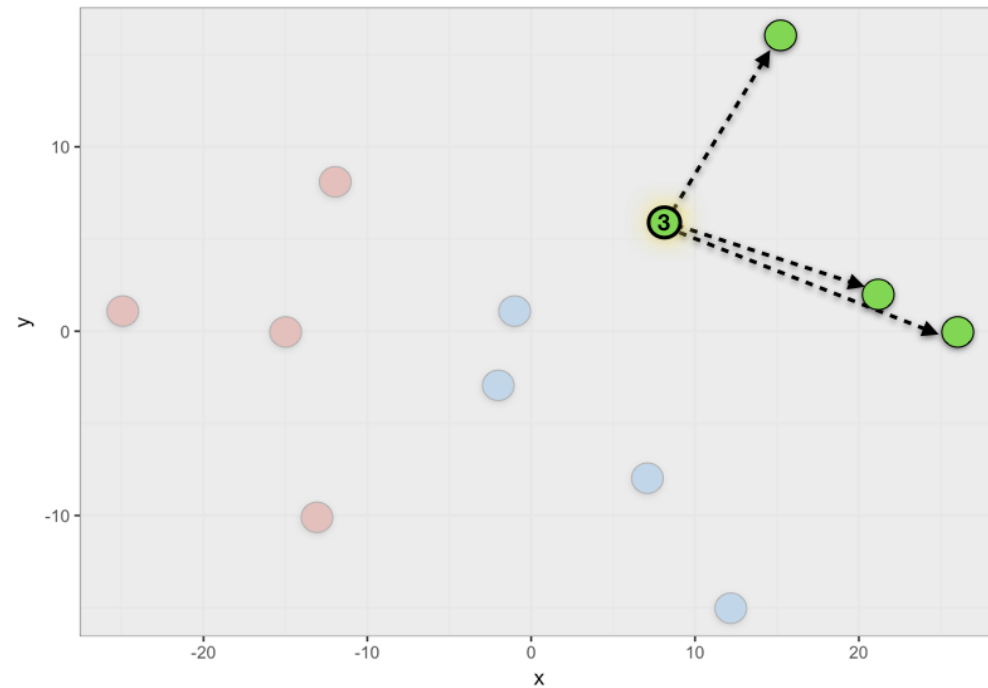


Closest Neighbor Distance:  $N(i)$

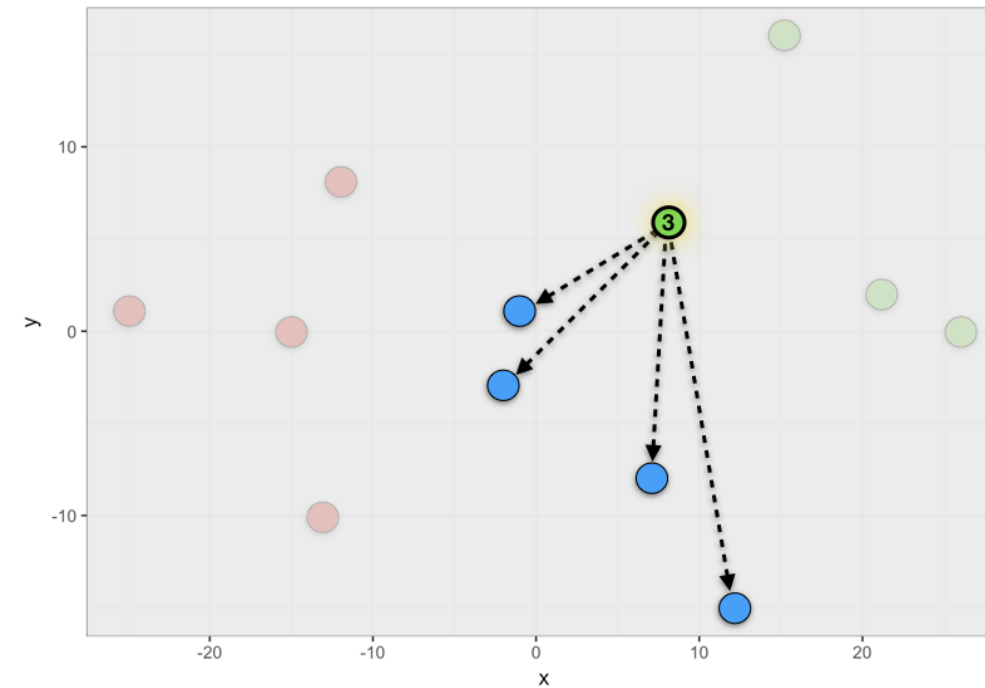


# Silhouette width

Within Cluster Distance:  $C(i)$

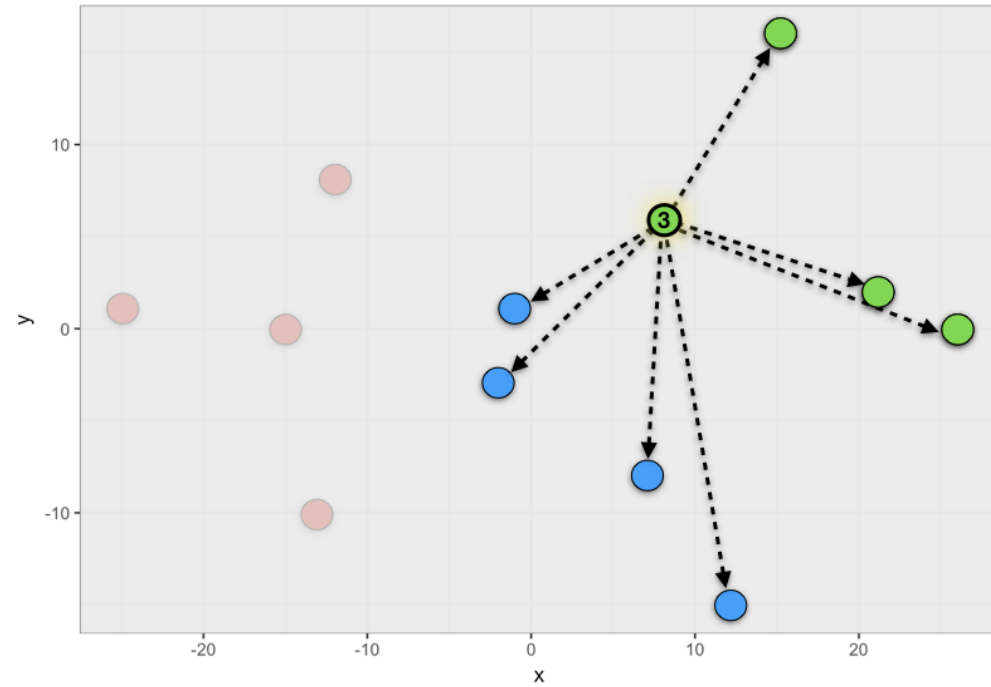


Closest Neighbor Distance:  $N(i)$



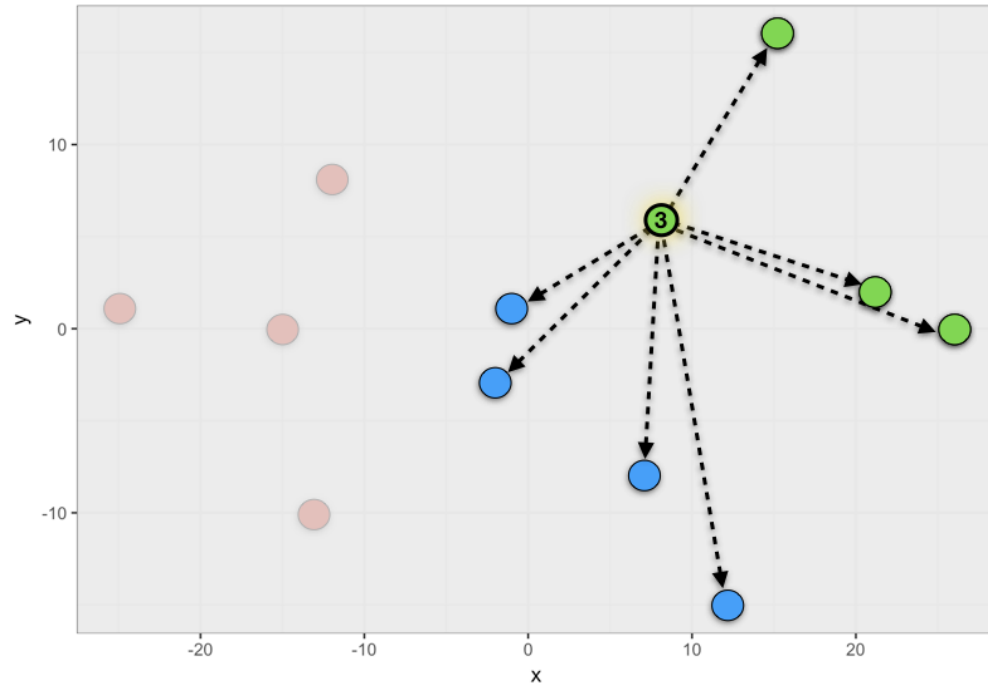


# Silhouette width: $S(i)$



$$s(i) = \begin{cases} 1 - C(i)/N(i), & \text{if } C(i) < N(i) \\ 0, & \text{if } C(i) = N(i) \\ N(i)/C(i) - 1, & \text{if } C(i) > N(i) \end{cases}$$

# Silhouette width: $S(i)$



- **1:** Well matched to cluster
- **0:** On border between two clusters
- **-1:** Better fit in neighboring cluster

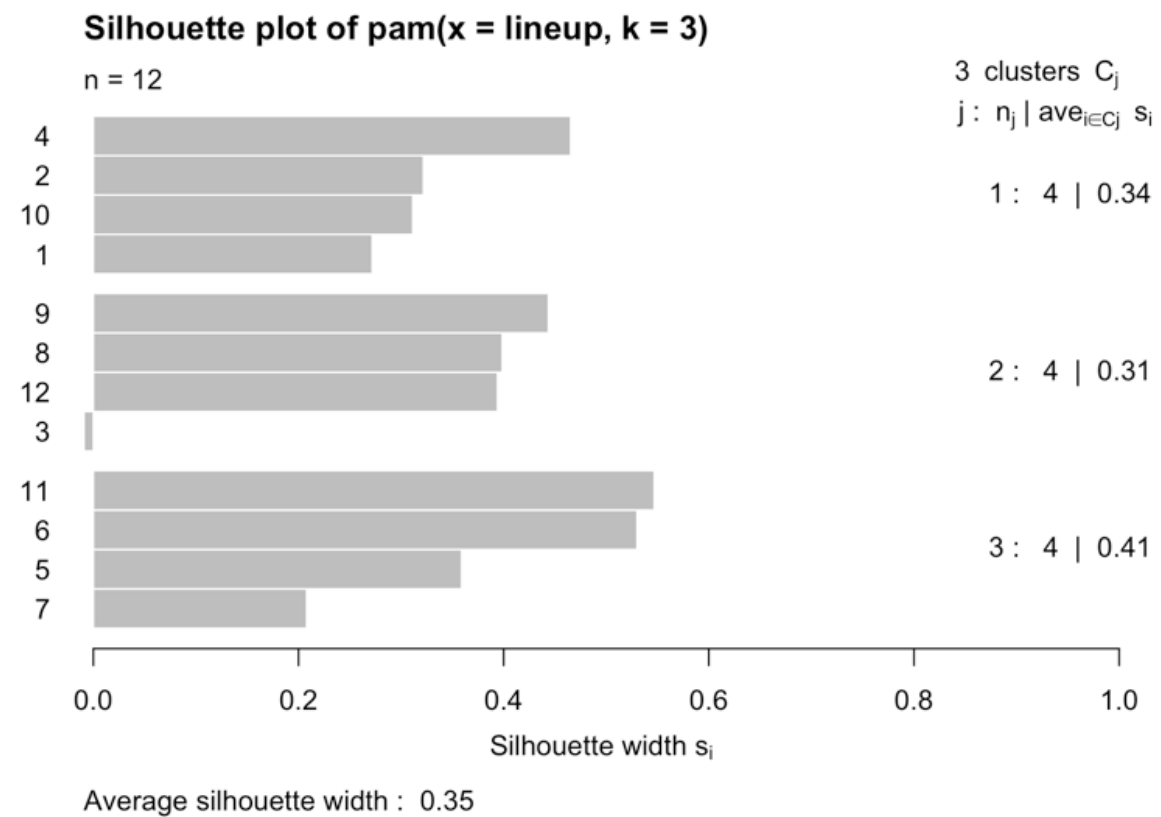
# Calculating $S(i)$

```
library(cluster)
pam_k3 <- pam(lineup, k = 3)
pam_k3$silinfo$widths
```

	cluster	neighbor	sil_width
4	1	2	0.465320054
2	1	3	0.321729341
10	1	2	0.311385893
1	1	3	0.271890169
9	2	1	0.443606497
...	...	...	...

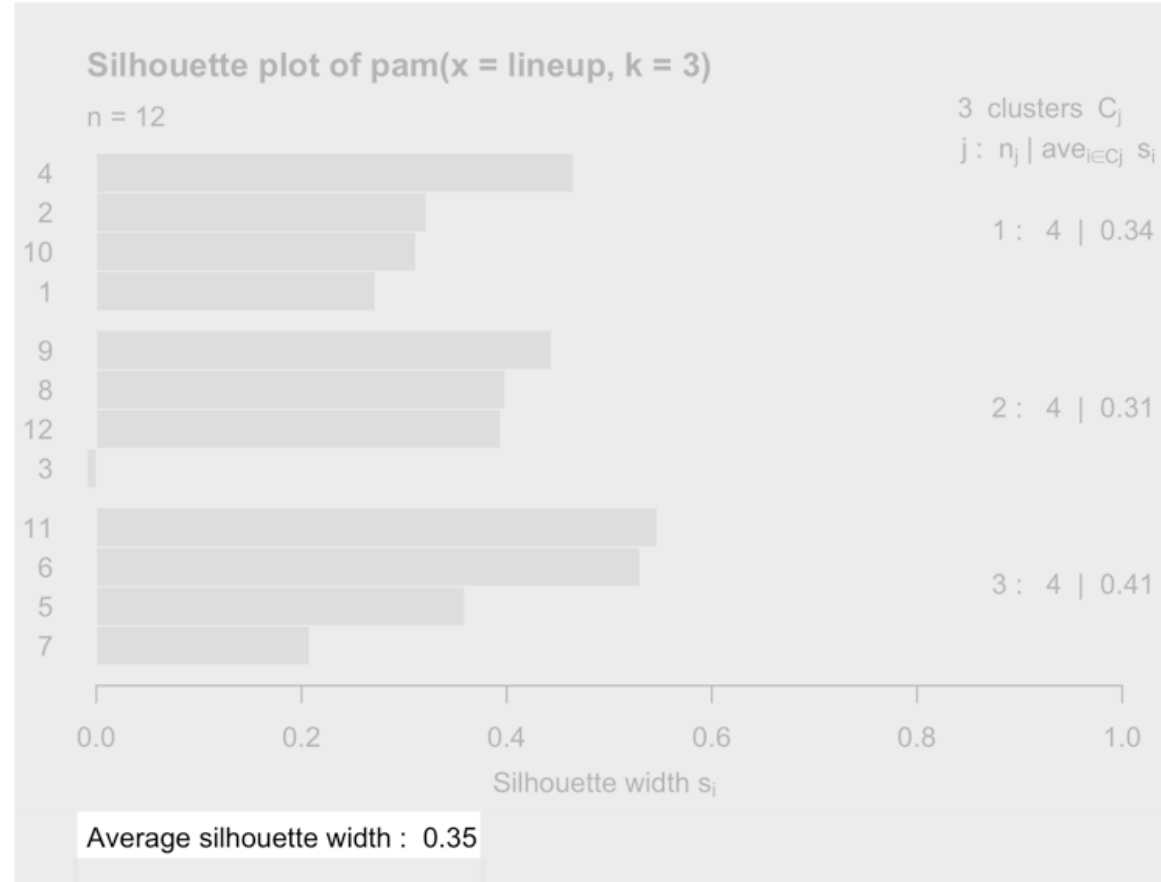
# Silhouette plot

```
sil_plot <- silhouette(pam_k3)  
plot(sil_plot)
```



# Silhouette plot

```
sil_plot <- silhouette(pam_k3)  
plot(sil_plot)
```



# Average silhouette width

```
pam_k3$silinfo$avg.width  
[1] 0.353414
```

- **1:** Well matched to each cluster
- **0:** On border between clusters
- **-1:** Poorly matched to each cluster

# Highest average silhouette width

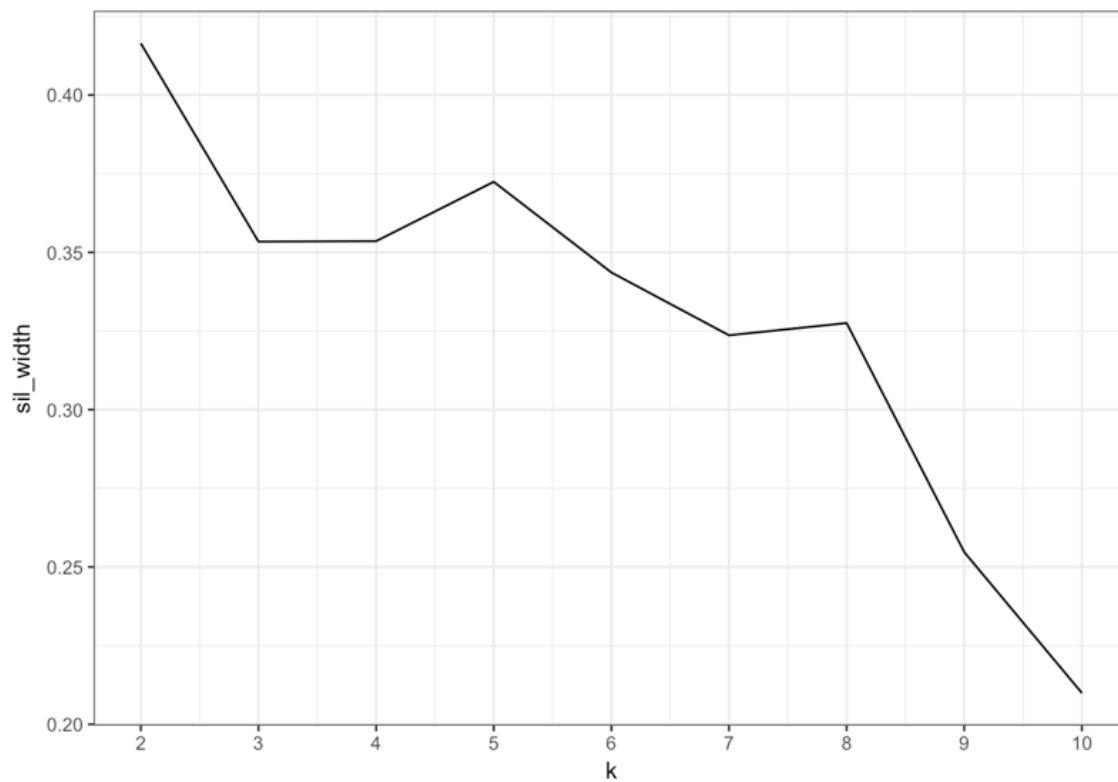
```
library(purrr)

sil_width <- map_dbl(2:10, function(k){
  model <- pam(x = lineup, k = k)
  model$silinfo$avg.width
})
sil_df <- data.frame(
  k = 2:10,
  sil_width = sil_width
)
print(sil_df)
```

	k	sil_width
1	2	0.4164141
2	3	0.3534140
3	4	0.3535534
4	5	0.3724115
...	...	...

# Choosing K using average silhouette width

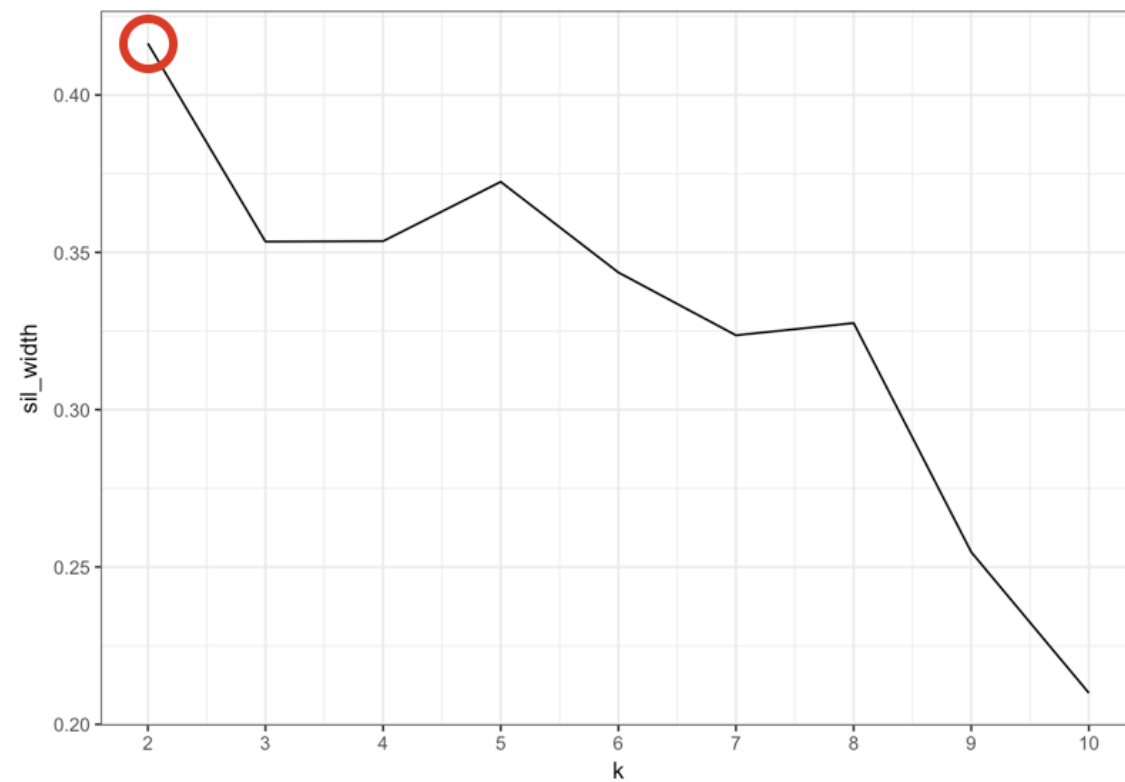
```
ggplot(sil_df, aes(x = k, y = sil_width)) +  
  geom_line() +  
  scale_x_continuous(breaks = 2:10)
```





# Choosing K using average silhouette width

```
ggplot(sil_df, aes(x = k, y = sil_width)) +  
  geom_line() +  
  scale_x_continuous(breaks = 2:10)
```



# Let's practice!

CLUSTER ANALYSIS IN R

# Making sense of the K-means clusters

CLUSTER ANALYSIS IN R



**Dmitriy (Dima) Gorenshteyn**

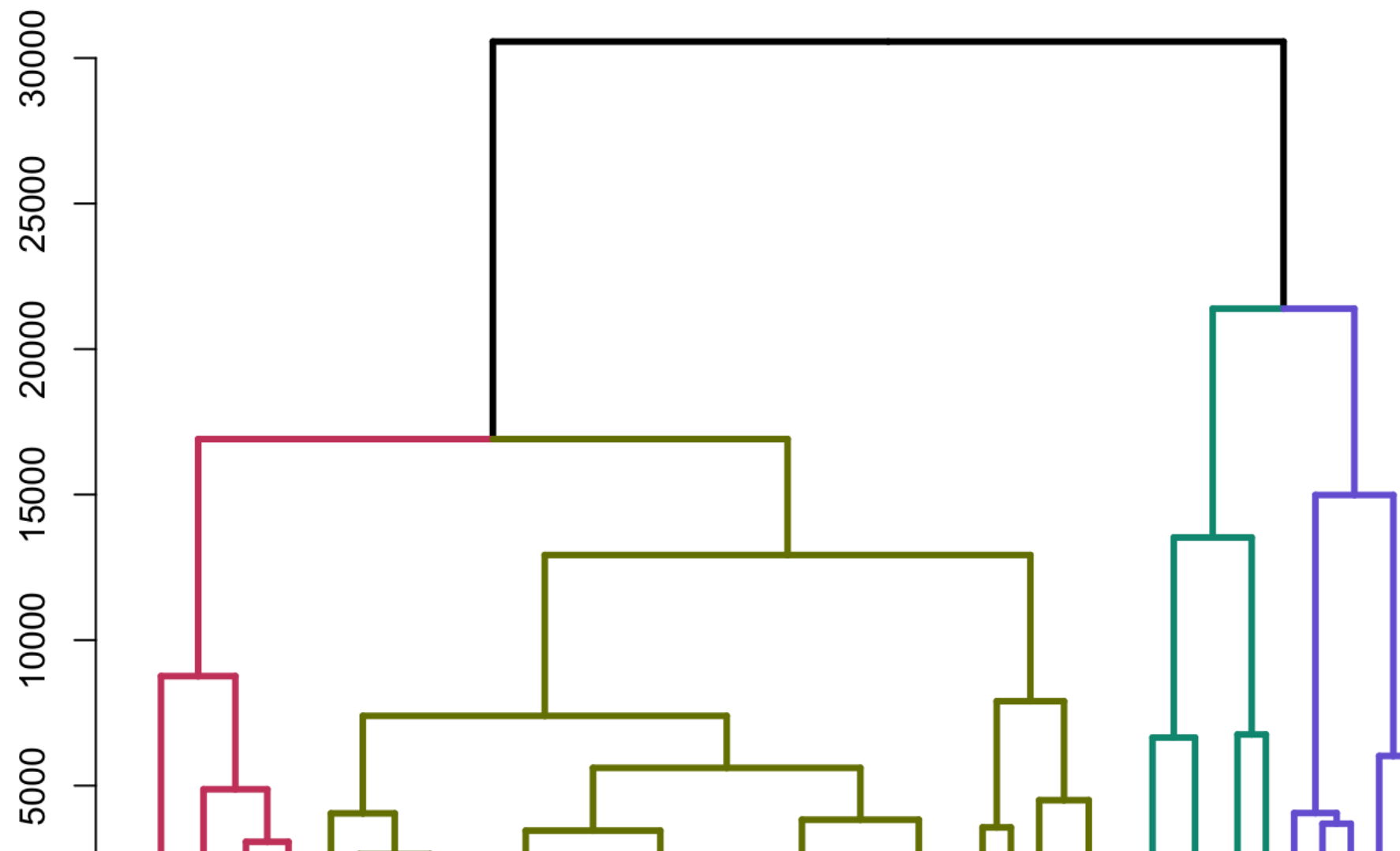
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# Wholesale dataset

- 45 observations
- 3 features:
  - Milk Spending
  - Grocery Spending
  - Frozen Food Spending

```
print(customers_spend)
      Milk Grocery Frozen
1  11103   12469    902
2   2013    6550    909
3   1897    5234    417
4   1304    3643   3045
5   3199    6986   1455
...     ...     ...     ...
```

# Segmenting with hierarchical clustering



# Segmenting with hierarchical clustering

cluster	Milk	Grocery	Frozen	cluster size
1	<b>16950</b>	12891	991	5
2	2512	5228	1795	29
3	10452	<b>22550</b>	1354	5
4	1249	3916	<b>10888</b>	6

# Segmenting with K-means

- Estimate the "best"  $k$  using average silhouette width
- Run k-means with the suggested  $k$
- Characterize the spending habits of these clusters of customers

# Let's cluster!

CLUSTER ANALYSIS IN R