



K-Means Clustering in R

RStudio Instructor Certification Teaching Exam

Uli Niemann

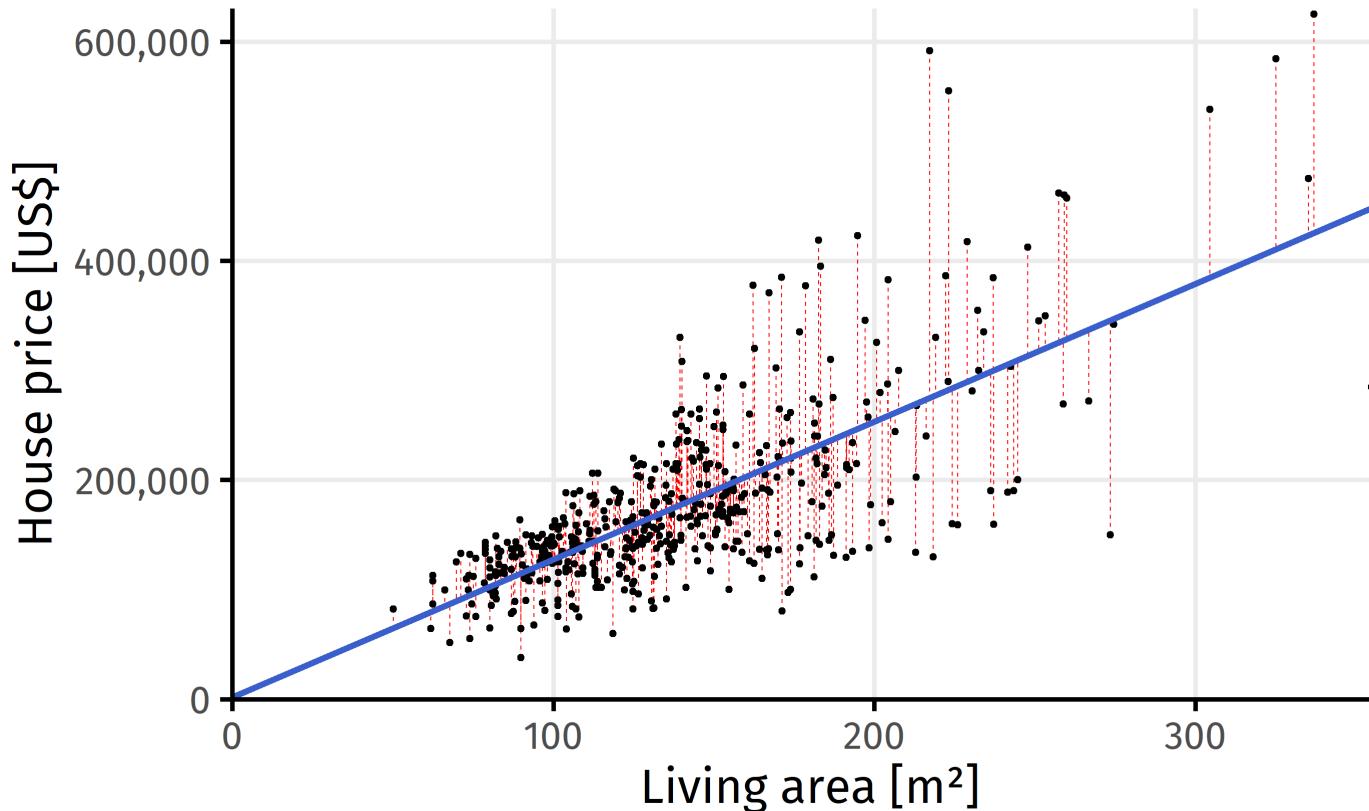
2020/08/21

<https://github.com/unmnn/sample-lesson-kmeans/>

Recap: Supervised Learning

General idea: train a model which estimates the value of the response based on the values of the predictors.

$$\hat{Y} = f(\mathbf{X})$$

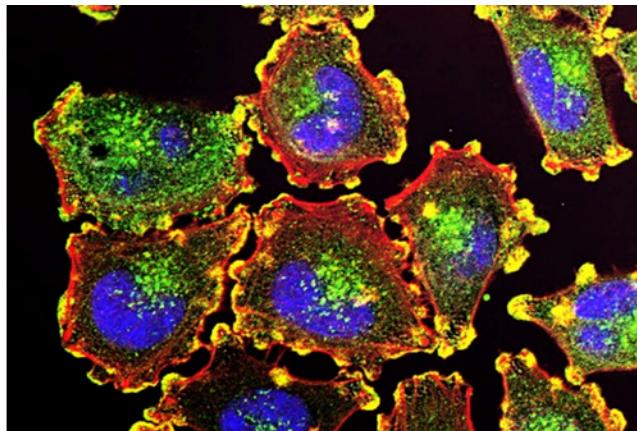


Unsupervised Learning

Goal: look for interesting patterns in the data without having a response



Customer Subgroups



Disease Phenotypes



Website Usage Patterns

Clustering: methods to find homogeneous subgroups in a dataset

Properties of a good clustering results:

- objects within a cluster are as **similar** as possible
- objects from different clusters are as **dissimilar** as possible

→ require: **similarity measure**

Photos: left: [Lucrezia Carnelos](#); center: [National Cancer Institute](#); right: [Agence Oolloweb](#)

K-Means Clustering

General idea: partition the observations into a pre-specified number of subgroups (clusters)

Centroid: mean vector of a cluster's observations

Objective: minimize total intra-cluster variation

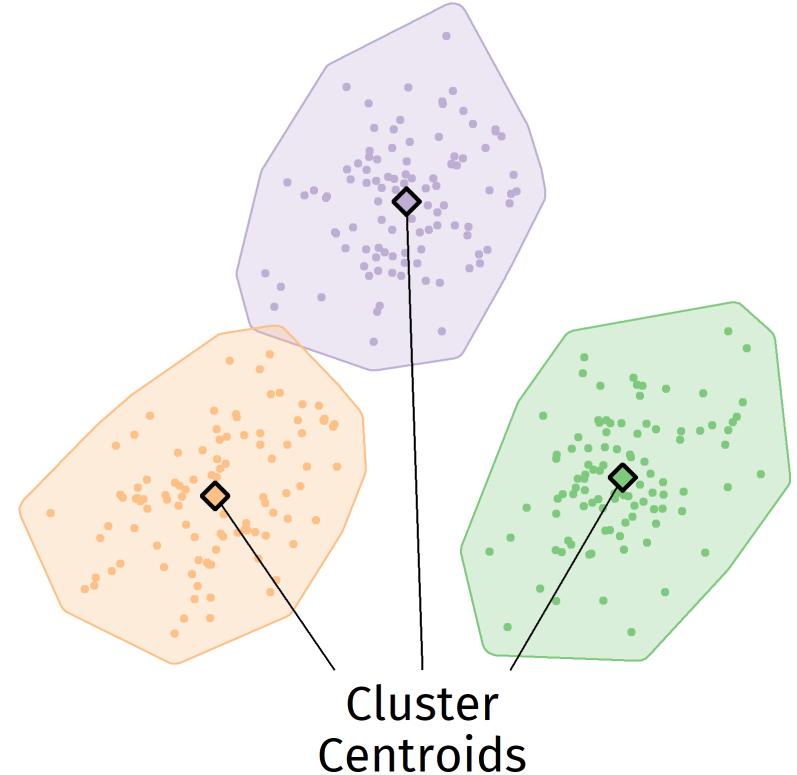
$$\min_{C_1, C_2, \dots, C_K} \left\{ \sum_k W(C_k) \right\}$$

Squared **Euclidean distance** is often used to measure the **within-cluster variation** W of a cluster C_k :

$$W(C_k) = \sum_{i \in C_k} \sum_j^p (x_{ij} - \bar{x}_{kj})^2$$

where

- i is the index of an observation assigned to C_k
- \bar{x}_k is the centroid of C_k

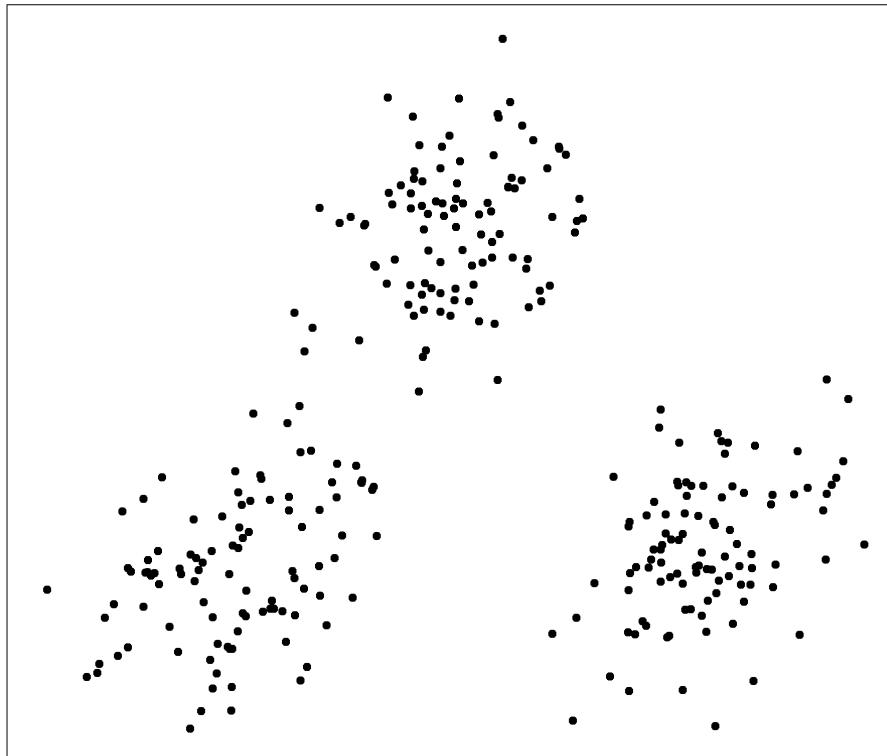


K-Means Algorithm

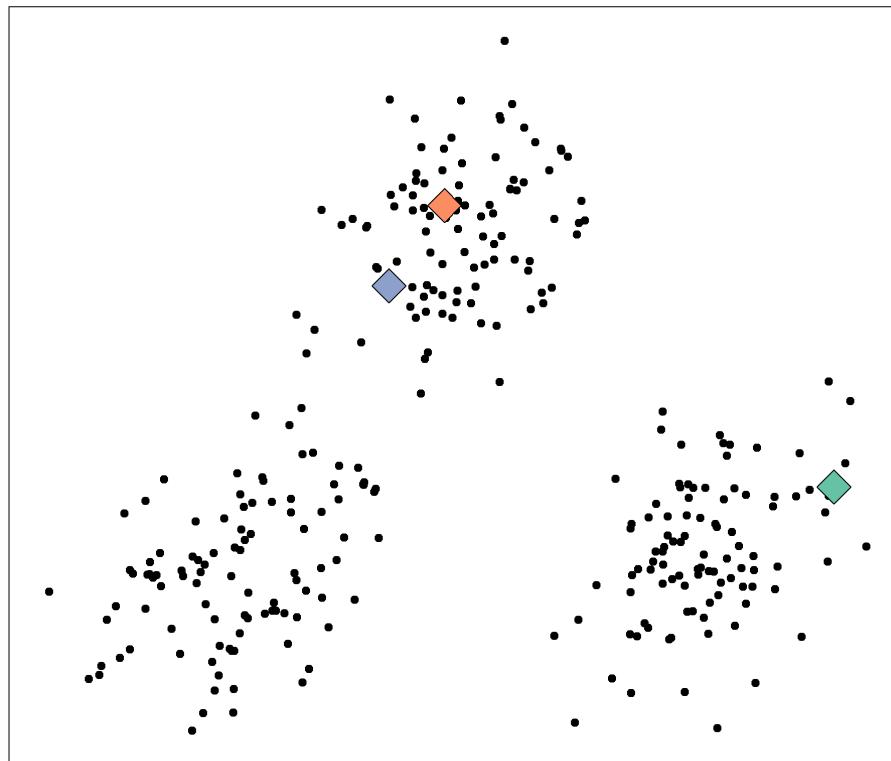
1. Select K initial centroids.
2. Repeat until the cluster assignments do not change anymore:
 - a. Assign each observation to the closest centroid.
 - b. Recompute the positions of all centroids.

Example: K=3

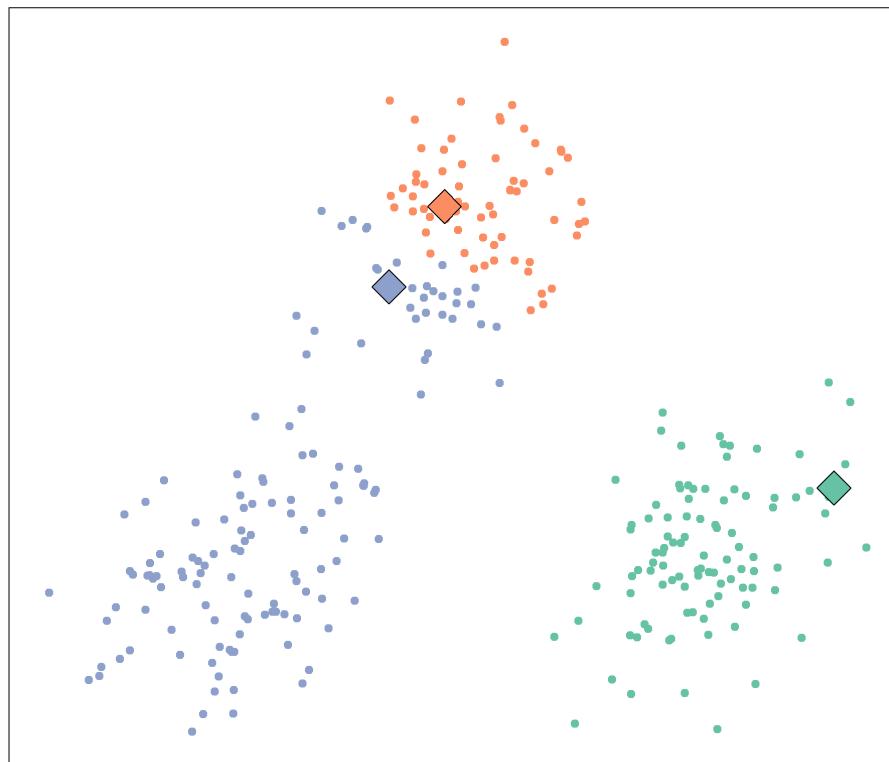
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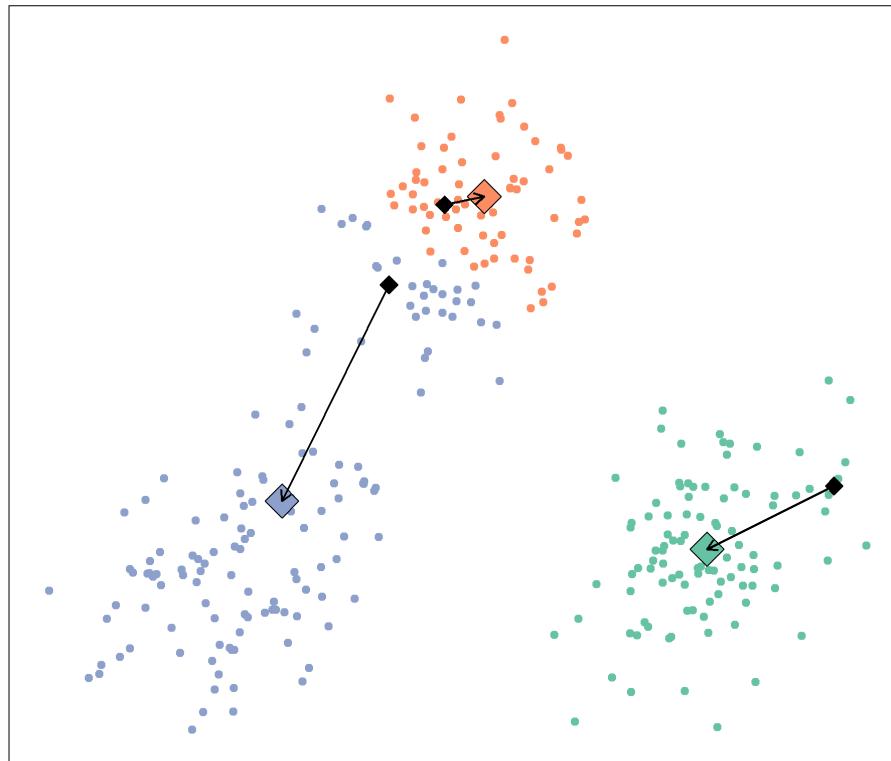
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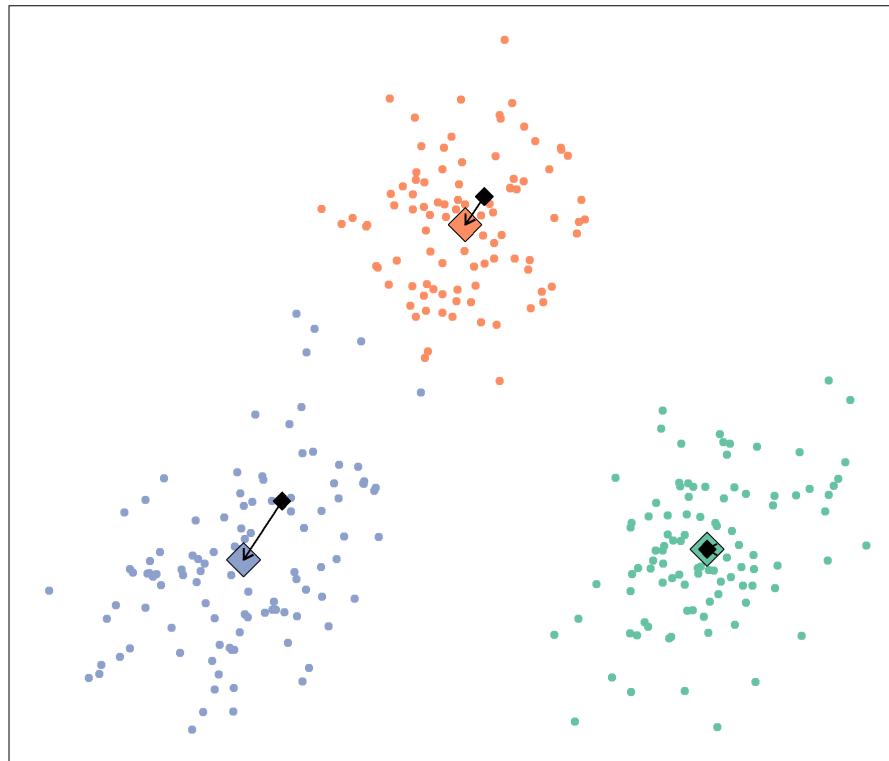
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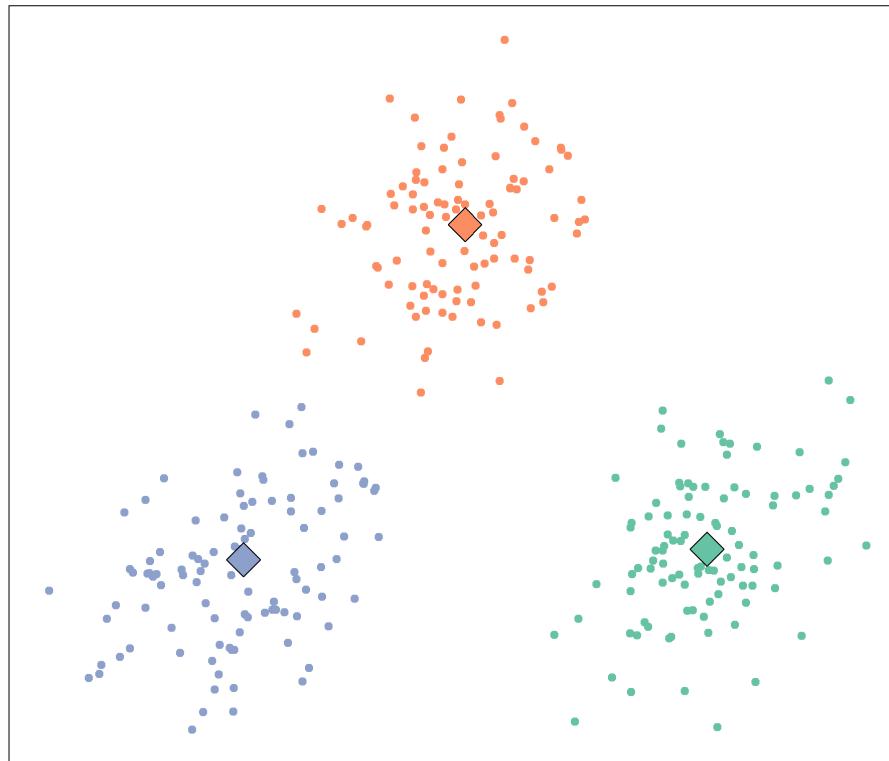
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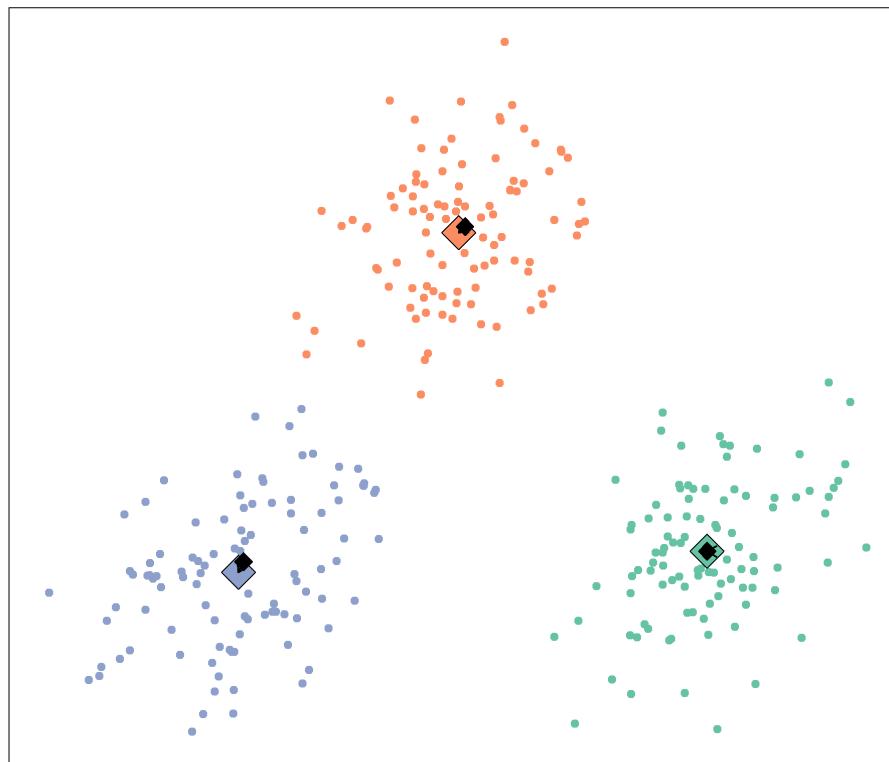
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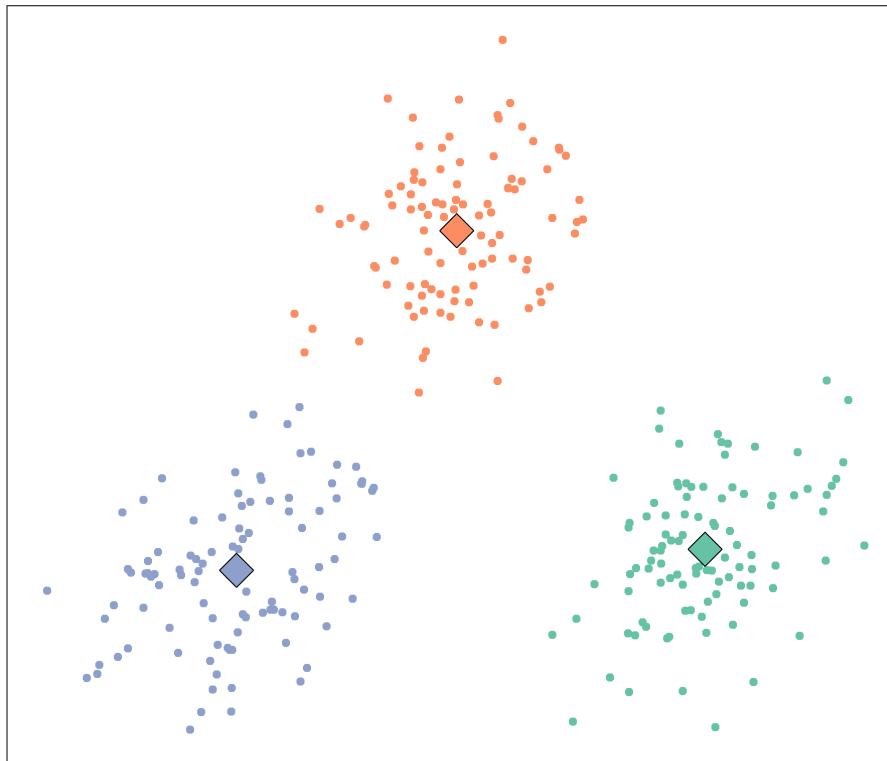
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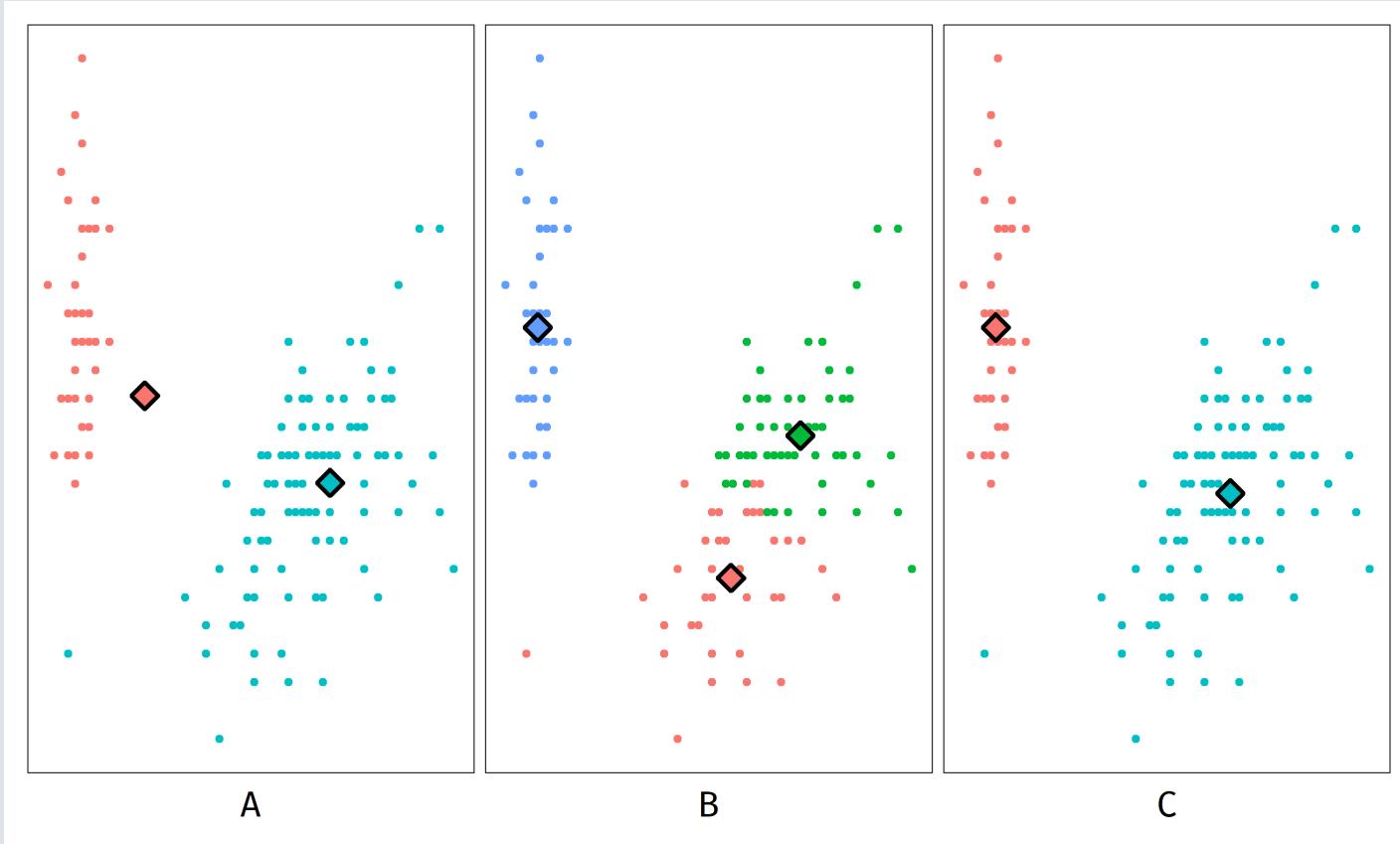


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Your Turn

Which of the plots below shows the correct result of K-means clustering with K=2? A, B or C?



K-Means in R

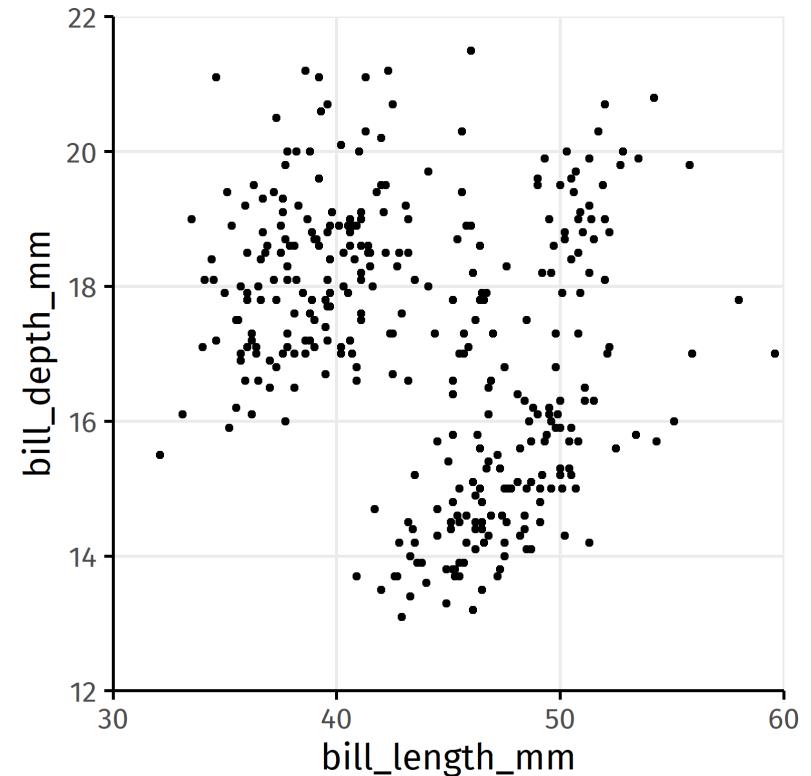
The `kmeans()` function takes two mandatory arguments:

- `x`: the data (data frame or numeric matrix)
- `centers`: number of clusters K or a set of initial centroids

Example: Clustering Palmer Penguins Bill Sizes

```
library(tidyverse)
(df <- palmerpenguins::penguins %>%
  select(bill_length_mm, bill_depth_mm) %>%
  drop_na())

## # A tibble: 342 x 2
##       bill_length_mm bill_depth_mm
##              <dbl>          <dbl>
## 1            39.1          18.7
## 2            39.5          17.4
## 3            40.3           18
## 4            36.7          19.3
## 5            39.3          20.6
## 6            38.9          17.8
## 7            39.2          19.6
## 8            34.1          18.1
## 9             42            20.2
## 10           37.8          17.1
## # ... with 332 more rows
```



K-Means in R

Components of a `kmeans` object

```
str(clustering)
```

```
## List of 9
## $ cluster      : int [1:342] 2 2 2 2 2 2 2 2 2 ...
## $ centers       : num [1:3, 1:2] 45.5 38.4 50.9 15.6 18.3 ...
##   ..- attr(*, "dimnames")=List of 2
##     ...$ : chr [1:3] "1" "2" "3"
##     ...$ : chr [1:2] "bill_length_mm" "bill_depth_mm"
## $ totss         : num 11494
## $ withinss      : num [1:3] 755 944 618
## $ tot.withinss: num 2317
## $ betweenss     : num 9177
## $ size          : int [1:3] 116 141 85
## $ iter          : int 2
## $ ifault        : int 0
## - attr(*, "class")= chr "kmeans"
```

```
str(clustering)
```

```
## List of 9
## $ cluster      : int [1:342] 2 2 2 2 2 2 2 2 2 ...
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```

- `cluster`: cluster ID for each observation
- `centers`: centroid positions

```
df %>%
  mutate(cluster = as.factor(clustering$cluster)) %>%
  ggplot(aes(bill_length_mm, bill_depth_mm)) +
  geom_point(aes(color = cluster)) +
  geom_point(data = as_tibble(clustering$centers),
             pch = 18, size = 5) +
  guides(color = FALSE)
```

```
str(clustering)
```

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## List of 9
## $ cluster      : int [1:342] 2 2 2 2 2 2 2 2 2 ...
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## $ size         : int [1:3] 116 141 85
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## $ ifault       : int 0
## - attr(*, "class")= chr "kmeans"
```

- `totss`: total sum of squares (sum of squared distances to global mean over all observations)
- `withinss`: within sum of squares (sum of squared distances to cluster centroid)
- `tot.withinss`: sum of `withinss`
- `betweenss`: `totss - tot.withinss` (reduction in sum of squares)
- `size`: number of cluster members
- `iter`: number of iterations until convergence

Your Turn (exercise.R)

Run K-means clustering on the Palmer penguins data with K=3.

Instead of initializing the centroids randomly, use the provided custom coordinates.

Return the number of observations for each cluster.

```
library(dplyr)
library(tidyr)
library(palmerpenguins)

# Prepare 2-dimensional data for clustering
df <- penguins %>%
  select(bill_length_mm, bill_depth_mm) %>%
  drop_na()

# Run K-means clustering using custom initial centroids
clustering <- kmeans(____,
  _____ = tibble(
    bill_length_mm = c(40, 50, 60),
    bill_depth_mm = c(15, 18, 21)
  )
)
clustering

# Return cluster sizes
clustering$_____
```

Learner Persona*

Meet Nathalie...

1. Background: Nathalie is a 22-year-old undergraduate student pursuing a Bachelor's degree in "Operations Research and Business Analytics". She is born in Turkey, and moved to Germany to take up her study.

2. Relevant Experience: Currently, Nathalie is in her 5th semester. Until now, she has been analyzing data mainly with Excel, and has some working knowledge of SPSS, but she has never programmed in R prior to taking this course. This is also her first course on data science.

3. Needs: Nathalie is enrolled in this course which is required for her degree, so she needs to pass it. However, she is also interested in this course because she knows that showing data science and R proficiency on her CV will increase her value on the job market. She needs a gentle introduction to these topics which doesn't require familiarity with R.

4. Special considerations: Nathalie has little experience in programming and she doesn't have a very powerful laptop.



Photo: [Andrew Neel](#)

* This lesson on "K-Means Clustering in R" is meant to be a part of the (fictional) undergraduate course "Data Mining with R".

Concept Map

