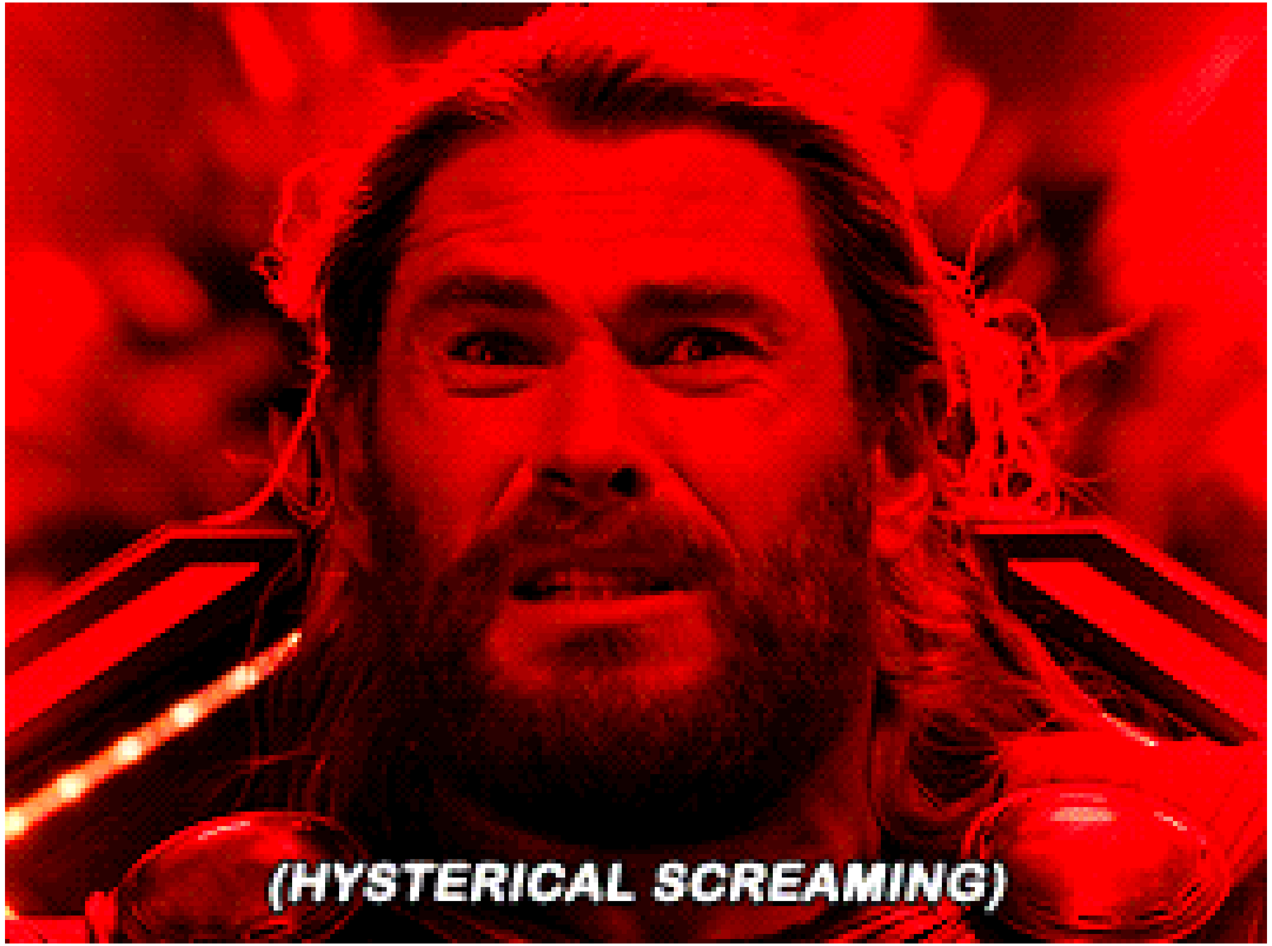
Clustering

K-means

June 14th, 2022

Brace yourselves



Into statistical learning with unsupervised learning

What is **statistical learning?** Preface of Introduction to Statistical Learning with Applications in R (ISLR):

> *refers to a set of tools for modeling and understanding complex datasets*

What is **unsupervised learning?**

We have p variables for n observations $x_1, \dots, x_n$, and for observation i:

$$x_{i1}, x_{i2}, \dots, x_{ip} \sim P$$

- P is a p-dimensional distribution that we might not know much about *a priori*.
- *unsupervised*: none of the variables are **response** variables, i.e., there are no labeled data

Think of unsupervised learning as **an extension of EDA...**

- $\Rightarrow$ **there is no unique right answer!**

What is clustering (aka cluster analysis)?

ISLR 10.3:

> *very broad set of techniques for finding subgroups, or clusters, in a dataset*

- observations **within** clusters are **more similar** to each other,
- observations **in different** clusters are **more different** from each other

How do we define **distance / dissimilarity** between observations?

- e.g. **Euclidean distance** between observations i and j

$$d(x_i, x_j) = \sqrt{(x_{i1} - x_{j1})^2 + \cdots + (x_{ip} - x_{jp})^2}$$

Units matter!

- one variable may *dominate* others when computing Euclidean distance because its range is much larger
- can standardize each variable / column of dataset to have mean 0 and standard divation 1 with `scale()`
- **but we may value the separation in that variable!** (so just be careful...)

What's the clustering objective?

- $C_1, \ldots, C_K$ are *sets* containing indices of observations in each of the K clusters
  - if observation i is in cluster k, then $i \in C_k$
- We want to minimize the **within-cluster variation** $W(C_k)$ for each cluster C_k and solve:

$$\underset{C_1, \ldots, C_K}{\text{minimize}} \Big\{ \sum_{k=1}^{K} W(C_k) \Big\}$$

- Can define using the **squared Euclidean distance** ($|C_k| = n_k =$ # observations in cluster k)

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,j \in C_k} d(x_i, x_j)^2$$

- Commonly referred to as the within-cluster sum of squares (WSS)

So how can we solve this?

Lloyd's algorithm

1) Choose K random centers, aka **centroids**

2) Assign each observation closest center (using Euclidean distance)

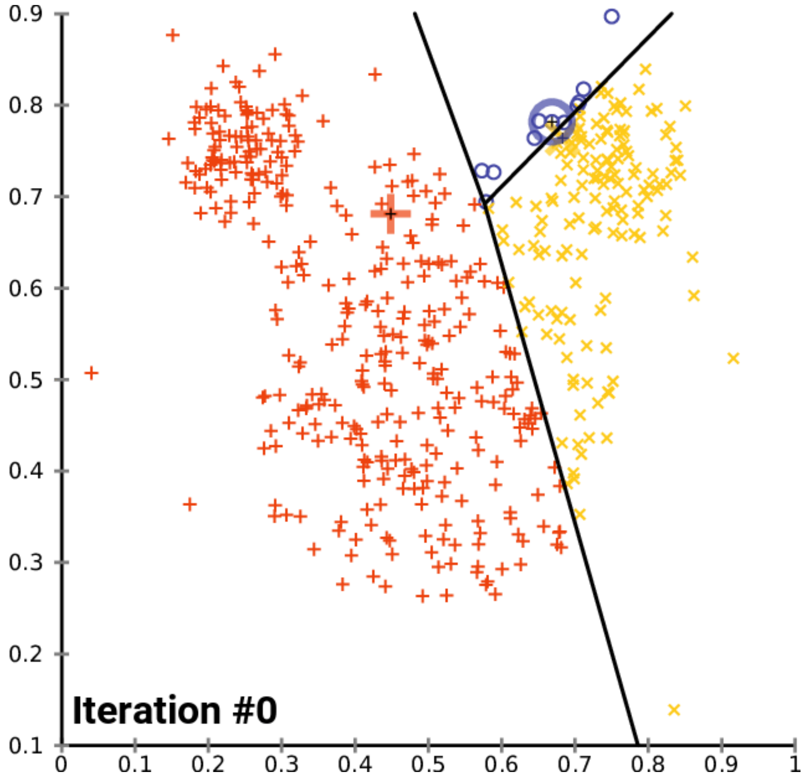
3) Repeat until cluster assignment stop changing:

- Compute new centroids as the averages of the updated groups
- Reassign each observations to closest center

Converges to a local optimum, not the global

Results will change from run to run (set the seed!)

Takes K as an input!



Gapminder data

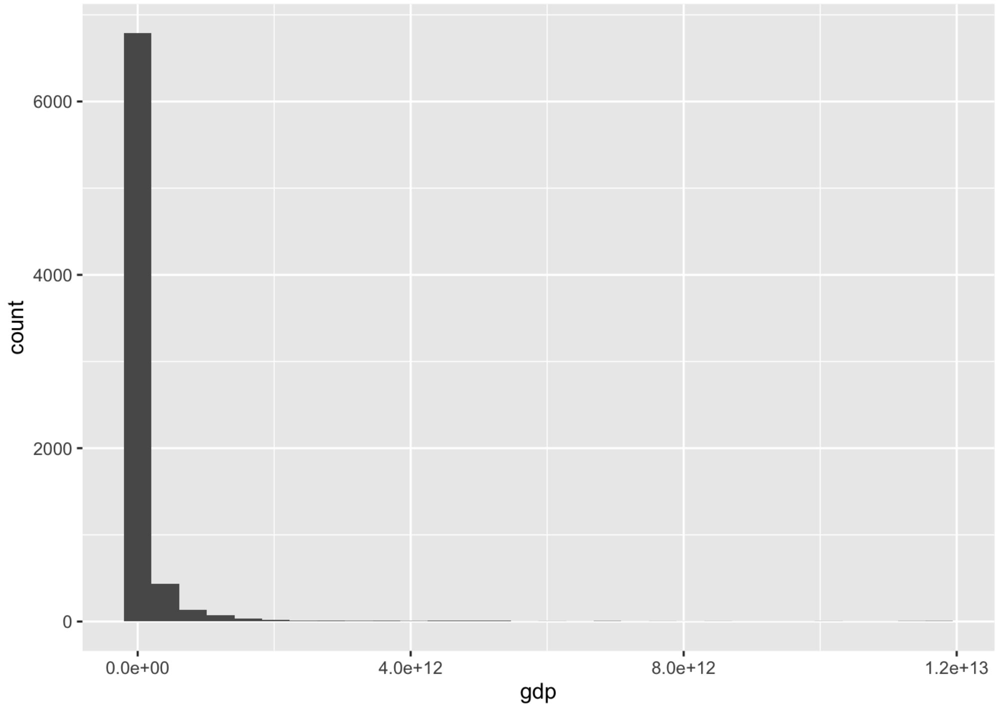
Health and income outcomes for 184 countries from 1960 to 2016 from the famous Gapminder project

```r
library(tidyverse)
library(dslabs)
gapminder <- as_tibble(gapminder)
head(gapminder)
```

```
## # A tibble: 6 × 9
##   country            year infan…¹ life_…² ferti…³ popul…⁴      gdp conti…⁵ region
##   <fct>             <int>   <dbl>   <dbl>   <dbl>   <dbl>    <dbl> <fct>   <fct>
## 1 Albania            1960   115.     62.9    6.19  1.64e6 NA       Europe  South…
## 2 Algeria            1960   148.     47.5    7.65  1.11e7  1.38e10 Africa  North…
## 3 Angola             1960   208      36.0    7.32  5.27e6 NA       Africa  Middl…
## 4 Antigua and Bar…   1960    NA      63.0    4.43  5.47e4 NA       Americ… Carib…
## 5 Argentina          1960    59.9    65.4    3.11  2.06e7  1.08e11 Americ… South…
## 6 Armenia            1960    NA      66.9    4.55  1.87e6 NA       Asia    Weste…
## # … with abbreviated variable names ¹infant_mortality, ²life_expectancy,
## #   ³fertility, ⁴population, ⁵continent
```

GDP is severely skewed right...

```
gapminder %>% ggplot(aes(x = gdp)) + geom_histogram()
```



Some initial cleaning...

- Each row is at the `country-year` level
- Will just focus on data for 2011 where gdp is not missing
- Take `log()` transformation of gdp

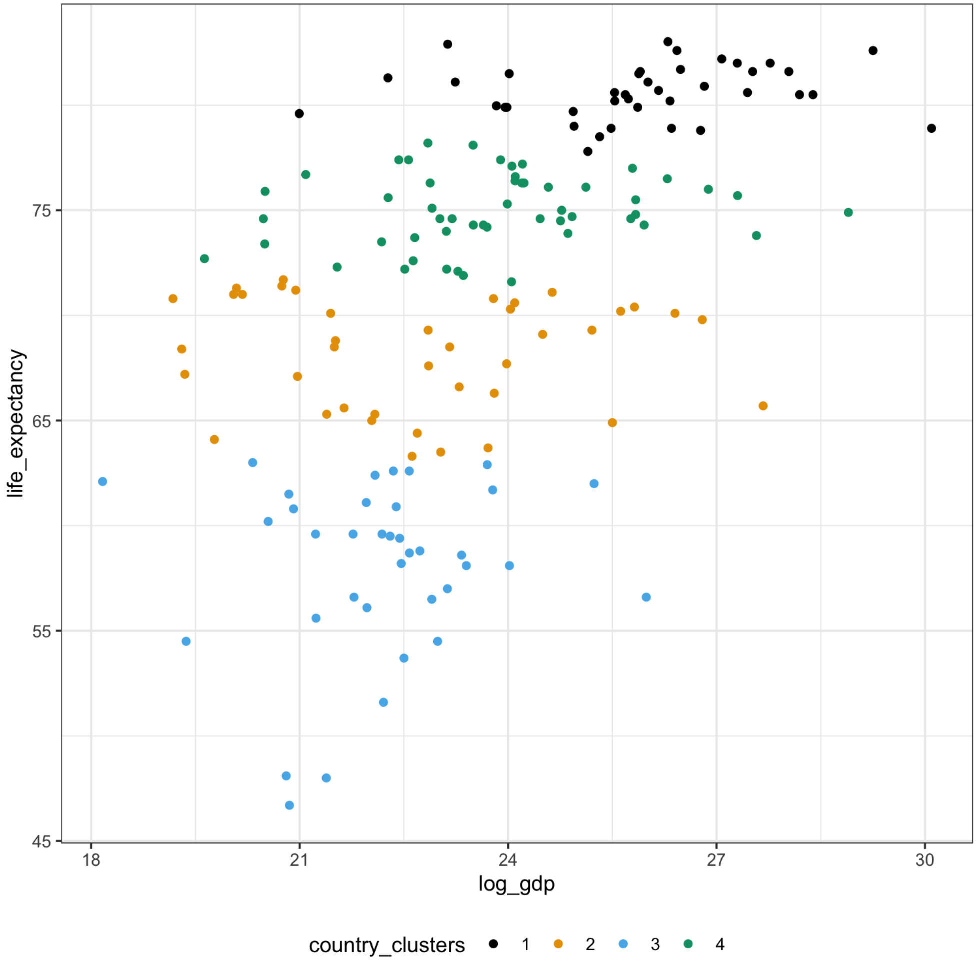
```
clean_gapminder <- gapminder %>%
  filter(year == 2011, !is.na(gdp)) %>%
  mutate(log_gdp = log(gdp))
clean_gapminder
```

```
## # A tibble: 168 × 10
##    country    year infan…¹ life_…² ferti…³ popul…⁴     gdp conti…⁵ region log_gdp
##    <fct>     <int>   <dbl>   <dbl>   <dbl>   <dbl>   <dbl> <fct>   <fct>    <dbl>
##  1 Albania    2011    14.3    77.4    1.75  2.89e6 6.32e 9 Europe  South…    22.6
##  2 Algeria    2011    22.8    76.1    2.83  3.67e7 8.11e10 Africa  North…    25.1
##  3 Angola     2011   107.     58.1    6.1   2.19e7 2.70e10 Africa  Middl…    24.0
##  4 Antigua…   2011     7.2    75.9    2.12  8.82e4 8.02e 8 Americ… Carib…    20.5
##  5 Argenti…   2011    12.7    76      2.2   4.17e7 4.73e11 Americ… South…    26.9
##  6 Armenia    2011    15.3    73.5    1.5   2.97e6 4.29e 9 Asia    Weste…    22.2
##  7 Austral…   2011     3.8    82.2    1.88  2.25e7 5.73e11 Oceania Austr…    27.1
##  8 Austria    2011     3.4    80.7    1.44  8.42e6 2.31e11 Europe  Weste…    26.2
##  9 Azerbai…   2011    32.5    70.8    1.96  9.23e6 2.14e10 Asia    Weste…    23.8
```

K-means clustering example (`gdp` and `life_expectancy`)

- Use the `kmeans()` function, **but must provide number of clusters K**

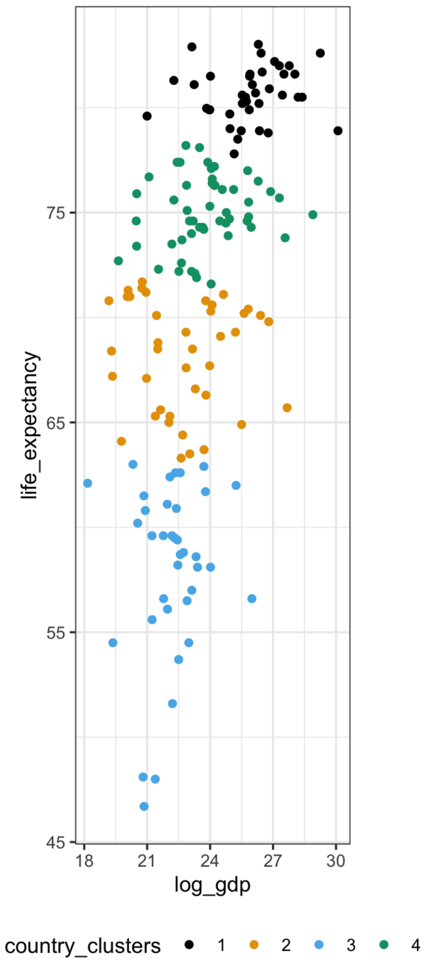
```
init_kmeans <-
  kmeans(dplyr::select(clean_gapminder,
                       log_gdp, life_expectan
         algorithm = "Lloyd", centers = 4,
         nstart = 1)

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(init_kmeans$cluster)) %>
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom")
```



Careful with units...

- Use the `coord_fixed()` so that the axes match with unit scales

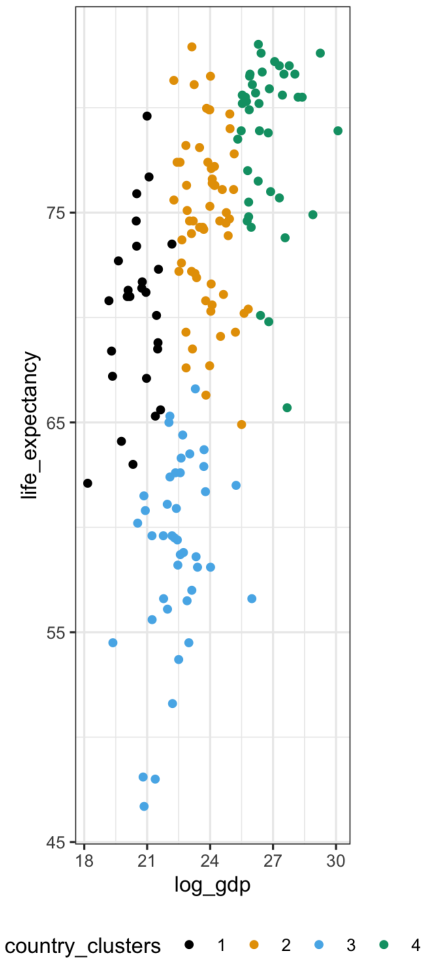
```
clean_gapminder %>%
  mutate(country_clusters =
             as.factor(init_kmeans$cluster)) %>
  ggplot(aes(x = log_gdp, y = life_expectancy
               color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom") +
  coord_fixed()
```



Standardize the variables!

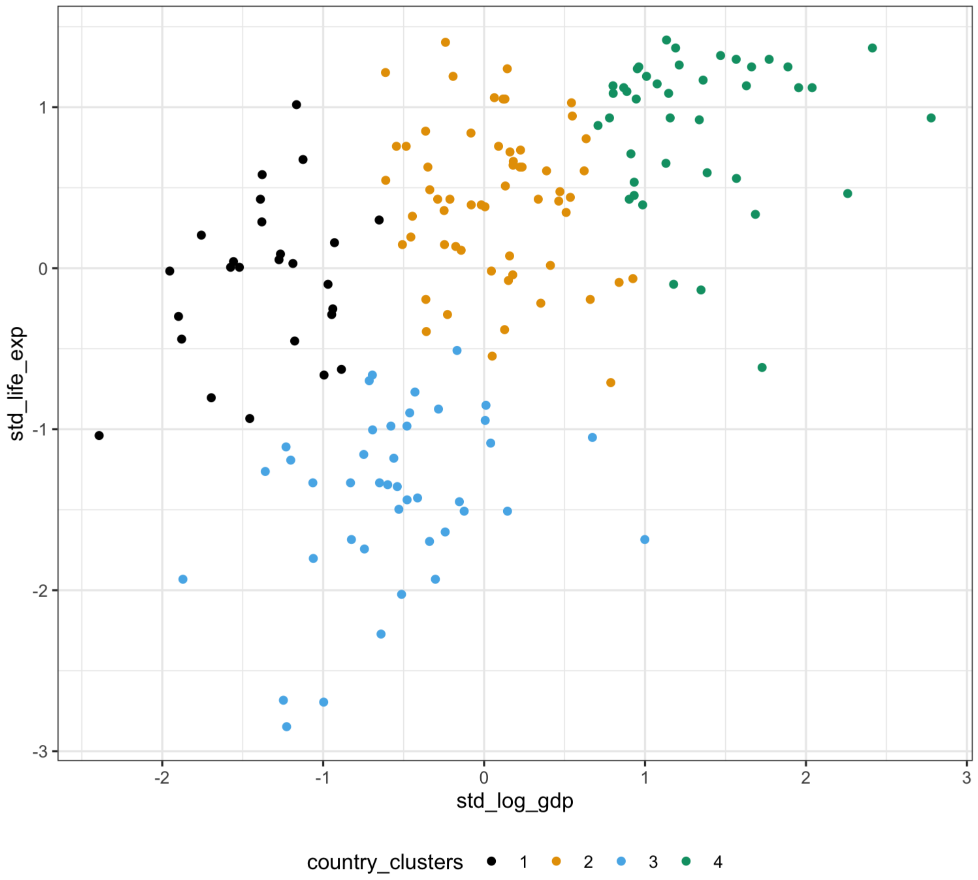
- Use the `scale()` function to first **standardize the variables**, $\frac{value - mean}{standard\ deviation}$

```
clean_gapminder <- clean_gapminder %>%
  mutate(std_log_gdp = as.numeric(scale(log_g
         std_life_exp = as.numeric(scale(life
std_kmeans <-
  kmeans(dplyr::select(clean_gapminder, std_l
         algorithm = "Lloyd", centers = 4, ns

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(std_kmeans$cluster)) %>%
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom") +
  coord_fixed()
```



Standardize the variables!

```
clean_gapminder %>%
  mutate(country_clusters =
           as.factor(std_kmeans$cluster)) %>%
  ggplot(aes(x = std_log_gdp, y = std_life_ex
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom") +
  coord_fixed()
```



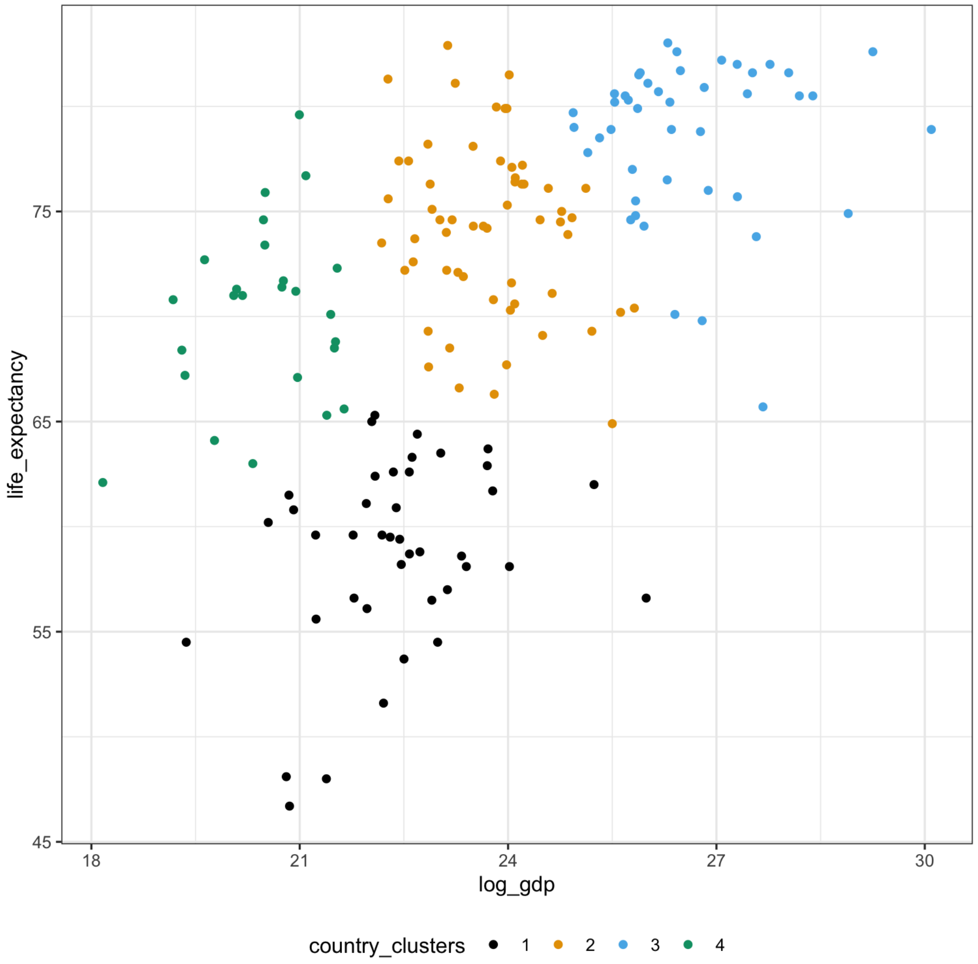
And if we run it again?

We get different clustering results!

```
another_kmeans <-
  kmeans(dplyr::select(clean_gapminder, std_l
         algorithm = "Lloyd", centers = 4, ns

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(another_kmeans$cluster))
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom")
```

Results depend on initialization

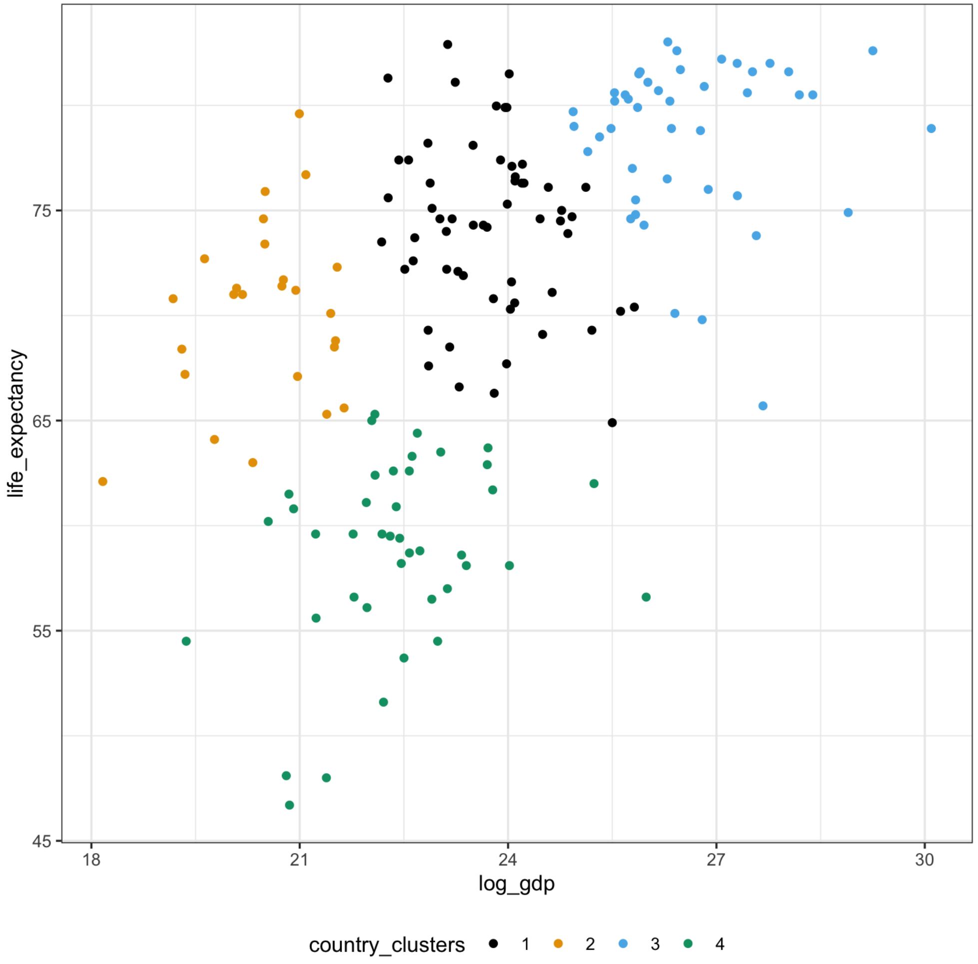
Keep in mind: **the labels / colors are arbitrary**



Fix randomness issue with `nstart`

Run the algorithm `nstart` times, then **pick the results with lowest total within-cluster variation** (total WSS $= \sum_k^K W(C_k)$)

```
nstart_kmeans <-
  kmeans(dplyr::select(clean_gapminder,
                       std_log_gdp, std_life_
         algorithm = "Lloyd", centers = 4,
         nstart = 30)

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(nstart_kmeans$cluster))
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom")
```

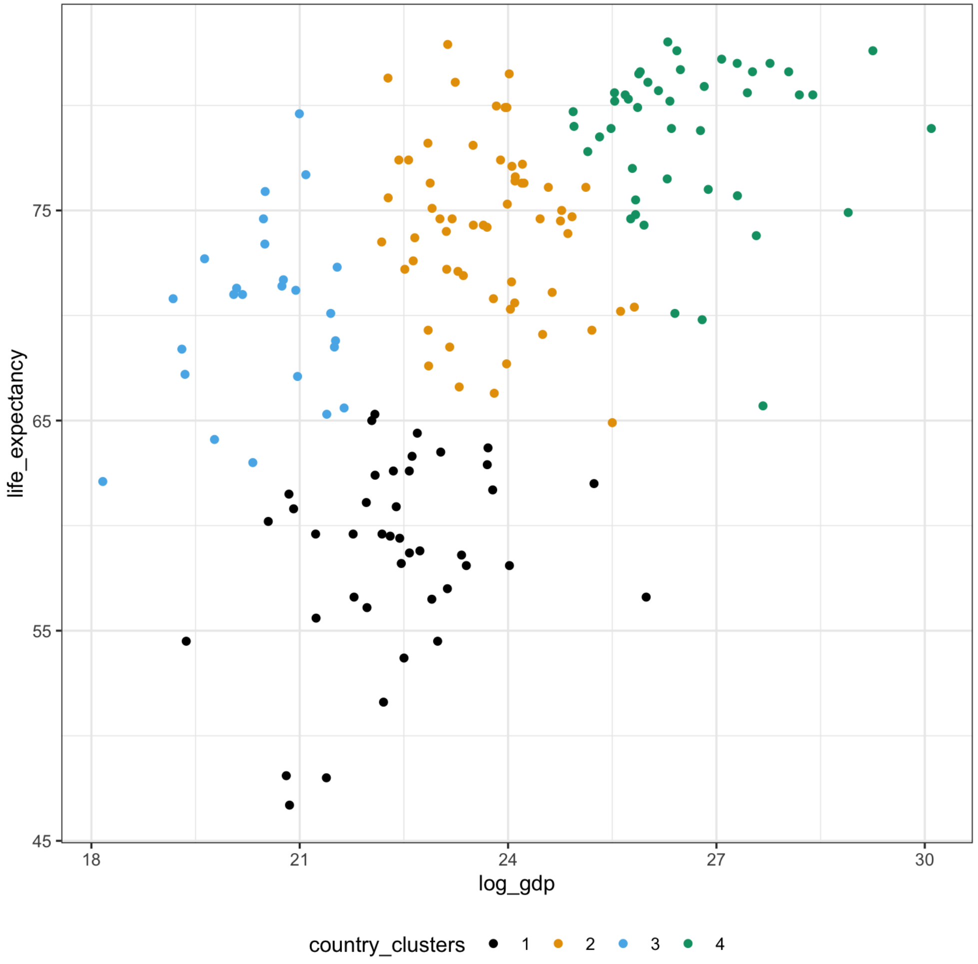


By default R uses Hartigan and Wong algorithm

Updates based on changing a single observation

Computational advantages over re-computing distances for every observation

```
default_kmeans <-
  kmeans(dplyr::select(clean_gapminder,
                       std_log_gdp, std_life_
         algorithm = "Hartigan-Wong",
         centers = 4, nstart = 30)

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(default_kmeans$cluster))
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom")
```



Very little differences for our purposes...

Better alternative to `nstart`: **K-means++**

Pick a random observation to be the center c_1 of the first cluster C_1

- This initializes a set $Centers = \{c_1\}$

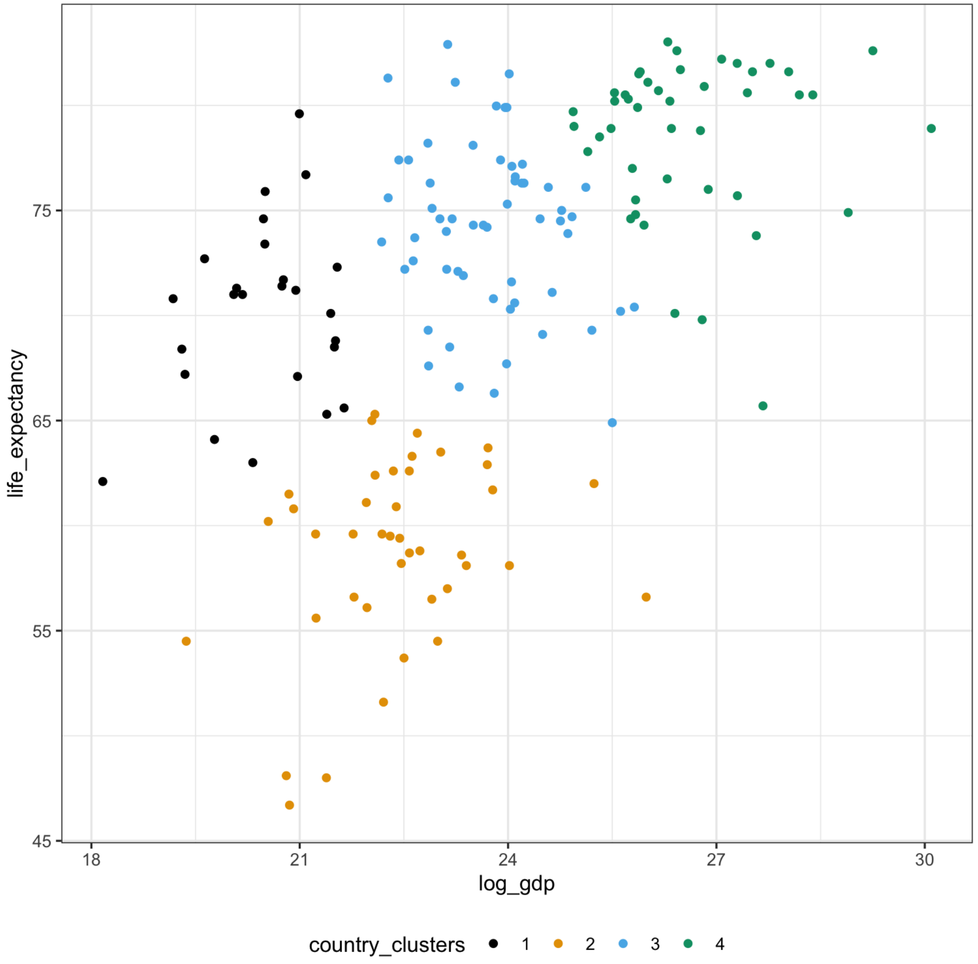
Then for each remaining cluster $c^* \in 2, \ldots, K$:

- For each observation (that is not a center), compute $D(x_i) = \min_{c \in Centers} d(x_i, c)$
  - Distance between observation and its closest center $c \in Centers$
- Randomly pick a point x_i with probability: $p_i = \frac{D^2(x_i)}{\sum_{j=1}^{n} D^2(x_j)}$
- As distance to closest center increases $\Rightarrow$ probability of selection increases
- Call this randomly selected observation c^*, update $Centers = Centers \cup c^*$
  - Same as `centers = c(centers, c_new)`

Then run K-means using these $Centers$ as the starting points

K-means++ in R using `flexclust`

```
library(flexclust)
init_kmeanspp <-
  kcca(dplyr::select(clean_gapminder,
                     std_log_gdp, std_life_ex
       control = list(initcent = "kmeanspp"))

clean_gapminder %>%
  mutate(country_clusters =
           as.factor(init_kmeanspp@cluster))
  ggplot(aes(x = log_gdp, y = life_expectancy
             color = country_clusters)) +
  geom_point() +
  ggthemes::scale_color_colorblind() +
  theme_bw() +
  theme(legend.position = "bottom")
```



Note the use of `@` instead of `$`...

So, how do we choose the number of clusters?!

There is no universally accepted way to conclude that a particular choice of K is optimal!

Popular heuristic: elbow plot (use with caution)

Look at the total within-cluster variation as a function of the number of clusters

```
# Initialize number of clusters to search over
n_clusters_search <- 2:12
tibble(total_wss =
         # Compute total WSS for each number by looping with sapply
         sapply(n_clusters_search,
                function(k) {
                  kmeans_results <- kmeans(dplyr::select(clean_gapminder,
                                                         std_log_gdp,
                                                         std_life_exp),
                                           centers = k, nstart = 30)
                  # Return the total WSS for choice of k
                  return(kmeans_results$tot.withinss)
                })) %>%
  mutate(k = n_clusters_search) %>%
  ggplot(aes(x = k, y = total_wss)) +
  geom_line() + geom_point() +
  labs(x = "Number of clusters K", y = "Total WSS") +
  theme_bw()
```

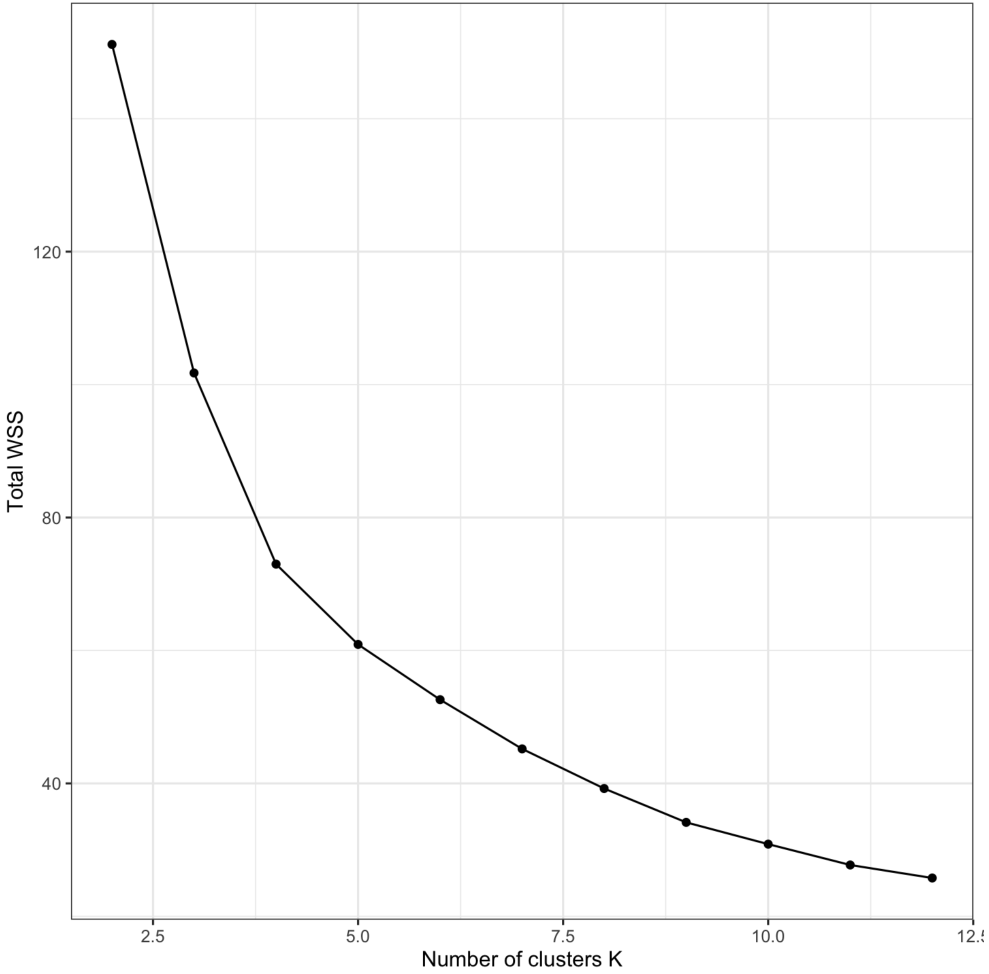
Popular heuristic: elbow plot (use with caution)

Choose K where marginal improvements is low at the bend (hence the elbow)

This is just a guideline and should not dictate your choice of K!

Gap statistic is a popular choice (see `clusGap` function in `cluster` package)

Next Tuesday: model-based approach to choosing the number of clusters!



Appendix: elbow plot with `flexclust`

```r
# Initialize number of clusters to search over
n_clusters_search <- 2:12
tibble(total_wss =
         # Compute total WSS for each number by looping with sapply
         sapply(n_clusters_search,
                function(k_choice) {
                  kmeans_results <- kcca(dplyr::select(clean_gapminder,
                                                       std_log_gdp,
                                                       std_life_exp),
                                         k = k_choice,
                                         control = list(initcent = "kmeanspp"))
                  # Return the total WSS for choice of k
                  return(sum(kmeans_results@clusinfo$size *
                               kmeans_results@clusinfo$av_dist))
                })) %>%
  mutate(k = n_clusters_search) %>%
  ggplot(aes(x = k, y = total_wss)) +
  geom_line() + geom_point() +
  labs(x = "Number of clusters K", y = "Total WSS") +
  theme_bw()
```

Appendix: elbow plot with `flexclust`