Unsupervised methods in machine learning

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Introduction

Presentation

In this project we will work with unsupervised machine learning models, with special emphasis on the modification of parameters to refine the results.

Objetives

The objectives are generation, interpretation, and evaluation of a k-means clustering model and a DBSCAN model. In doing so, we will not overlook the phases of data preparation, model quality, and initial knowledge extraction.

Example 1

k-means aggregation method with real data

We will use the 'Hawks' dataset, which is part of the 'Stat2Data' package that includes datasets used in the book 'Stat2: Building Models for a World of Data' by Cannon et al. (2013a)

The dataset originated from a research project as referenced earlier "Minería de Datos: PEC2" (2023) where measurements were taken on various characteristics of captured and subsequently released hawks. The data source is not clearly specified or documented in the book or on the Oberlin University website "Digital Commons at Oberlin" (n.d.) . The dataset package is used in the aforementioned book to provide an example of nonparametric statistics Cannon et al. (2013a), p. 86. It is widely used in statistics courses.

We have selected this dataset because of its potential for unsupervised data mining algorithms. The numerical variables on which we will be based are Wing, Weight, Culmen, Hallux

```
if (!require('Stat2Data')) install.packages('Stat2Data')
library(Stat2Data)
data("Hawks")
summary(Hawks)
```

```
##
                                              Year
                                                                          ReleaseTime
        Month
                             Day
                                                           CaptureTime
##
    Min.
            : 8.000
                       Min.
                               : 1.00
                                         Min.
                                                 :1992
                                                          11:35
                                                                 : 14
                                                                                 :842
                                         1st Qu.:1995
                                                                 : 14
                                                                                    2
##
    1st Qu.: 9.000
                       1st Qu.: 9.00
                                                          13:30
                                                                         11:00
##
    Median :10.000
                       Median :16.00
                                         Median:1999
                                                         11:45
                                                                 : 13
                                                                         11:35
            : 9.843
                                                                                    2
##
    Mean
                       Mean
                               :15.74
                                         Mean
                                                 :1998
                                                          12:10
                                                                 : 13
                                                                         12:05
    3rd Qu.:10.000
                       3rd Qu.:23.00
                                         3rd Qu.:2001
                                                          14:00
                                                                         12:50
##
                                                                 : 13
##
    Max.
            :11.000
                               :31.00
                                         Max.
                                                 :2003
                                                          13:05
                                                                : 12
                                                                         13:32
                                                                                    2
                       Max.
                                                          (Other):829
##
                                                                         (Other): 56
         {\tt BandNumber}
##
                                                        Wing
                                                                         Weight
                       Species
                                 Age
                                          Sex
                       CH: 70
##
                  2
                                 A:224
                                           :576
                                                   Min.
                                                           : 37.2
                                                                    Min.
                                                                            : 56.0
##
    1142-09240:
                       RT:577
                                 I:684
                                          F:174
                                                   1st Qu.:202.0
                                                                     1st Qu.: 185.0
                  1
    1142-09241:
                                                   Median :370.0
##
                  1
                       SS:261
                                          M:158
                                                                     Median: 970.0
    1142-09242:
                                                           :315.6
##
                                                   Mean
                                                                     Mean
                                                                             : 772.1
##
    1142-18229:
                  1
                                                   3rd Qu.:390.0
                                                                     3rd Qu.:1120.0
    1142-19209:
                  1
                                                           :480.0
##
                                                   Max.
                                                                     Max.
                                                                             :2030.0
##
    (Other)
               :901
                                                   NA's
                                                           :1
                                                                     NA's
                                                                            :10
##
        Culmen
                         Hallux
                                             Tail
                                                           StandardTail
##
            : 8.6
                             :
                                                :119.0
    Min.
                     Min.
                                9.50
                                       Min.
                                                         Min.
                                                                 :115.0
##
    1st Qu.:12.8
                     1st Qu.: 15.10
                                        1st Qu.:160.0
                                                         1st Qu.:162.0
                     Median: 29.40
##
    Median:25.5
                                        Median :214.0
                                                         Median :215.0
##
    Mean
            :21.8
                     Mean
                             : 26.41
                                        Mean
                                                :198.8
                                                         Mean
                                                                 :199.2
##
    3rd Qu.:27.3
                     3rd Qu.: 31.40
                                        3rd Qu.:225.0
                                                         3rd Qu.:226.0
    Max.
            :39.2
                             :341.40
                                                :288.0
                                                                 :335.0
##
                     Max.
                                        Max.
                                                         Max.
    NA's
##
            :7
                     NA's
                             :6
                                                         NA's
                                                                 :337
                        WingPitFat
                                            KeelFat
##
        Tarsus
                                                                Crop
##
    Min.
            :24.70
                      Min.
                              :0.0000
                                         Min.
                                                 :0.000
                                                          Min.
                                                                  :0.0000
##
    1st Qu.:55.60
                      1st Qu.:0.0000
                                         1st Qu.:2.000
                                                           1st Qu.:0.0000
##
    Median :79.30
                      Median :1.0000
                                         Median :2.000
                                                           Median : 0.0000
##
    Mean
            :71.95
                      Mean
                              :0.7922
                                         Mean
                                                :2.184
                                                           Mean
                                                                  :0.2345
##
    3rd Qu.:87.00
                      3rd Qu.:1.0000
                                         3rd Qu.:3.000
                                                           3rd Qu.:0.2500
##
    Max.
            :94.00
                              :3.0000
                                                 :4.000
                                                           Max.
                                                                   :5.0000
                      Max.
                                         Max.
##
    NA's
            :833
                      NA's
                              :831
                                         NA's
                                                 :341
                                                           NA's
                                                                   :343
```

The 'summary()' function in the R language provides a basic statistical summary of variables in a dataset. For numeric variables, it returns statistics such as minimum, first quartile (Q1), median, mean, third quartile (Q3), and maximum. For categorical variables, it returns a frequency table.

We will complete a first analysis using the head() function that will allow us to obtain a snapshot of the first records in the database:

head(Hawks)

##		Month	Day	Year	Captu	reTime	ReleaseTime	BandNu	mber	Species	s Age	Sex	Wing
##	1	9	19	1992		13:30		877-7	6317	R	ΓΙ		385
##	2	9	22	1992		10:30		877-7	6318	R	ΓΙ		376
##	3	9	23	1992		12:45		877-7	6319	R	ΓΙ		381
##	4	9	23	1992		10:50		745-4	9508	CH	I H	F	265
##	5	9	27	1992		11:15		1253-9	8801	SS	S I	F	205
##	6	9	28	1992		11:25		1207-55	910	R	ΓΙ		412
##		Weight	Cul	Lmen	Hallux	Tail	StandardTail	Tarsus	WingF	PitFat H	KeelFa	at C	rop
##	1	920) 2	25.7	30.1	219	NA	NA		NA	I	ΙA	NA
##	2	930)	NA	NA	221	NA	NA		NA	N	ΙA	NA
##	3	990) 2	26.7	31.3	235	NA	NA		NA	N	ΙA	NA
##	4	470) :	18.7	23.5	220	NA	NA		NA	N	ΙA	NA
##	5	170) :	12.5	14.3	157	NA	NA		NA	I	ΙA	NA
##	6	1090) 2	28.5	32.2	230	NA	NA		NA	N	ΙA	NA

From the analysis of the attributes, we obtain the following information about the variables:

- Age: Age of the hawk young (I) or adult (A) -.
- Species: Species of the hawk Cooper's Hawk (CH), Red-Tailed Hawk (RT), or Sharp-Shinned Hawk (SS) -.
- Sex: Gender of the hawk male (M) or female (F) -.
- Wing: Wing length of the hawk in millimeters -.
- Weight: Weight of the hawk in grams -.
- Culmen: Culmen length of the hawk's beak in millimeters -.
- Hallux: Hallux length of the hawk's claw in millimeters -.

At this point, there are other variables or columns in the dataset that are irrelevant for the requirements of this work, so we will filter them later.

Additionally, thanks to the information provided by the summary function, we know the following:

- 1. The 'BandNumber' variable contains unique records that help identify specific individuals and can be used as a primary key. We observe that there are two blank records without a number, so we will opt to create a new numeric variable.
- 2. The 'Wing' variable contains 1 infinite or NA value. Considering that there are noticeable size differences depending on the age and species of the specimens, but this data does not correspond to a continuous variable but a discrete one, we will assign the mean wing size based on the age of the specific specimen and its species.
- 3. The 'Weight' variable also has 10 instances with NA values. We will apply the same criterion as the 'Wing' variable. That is, we will assign the mean weight corresponding to its age group to each record.

- 4. The 'Culmen' variable contains 7 records with NA values. We will apply the previously described criterion of assigning means according to age.
- 5. The 'Hallux' variable also contains 6 NA records to which we will apply the corrective policies described earlier.

We will select the dataset of interest from the current dataset.

```
# We select only the variables that we are interested in working with.

hawks_select <- Hawks %>% select(BandNumber, Year, Month, Day, Species, Age, Wing, Weight, Culmen, Hall
```

Point 1. We correct the primary key according to the parameters set in the plan:

```
# creating a new record with numbers from 1 to the total number of rows in the dataset.
hawks_select$Num_id <- 1:nrow(hawks_select)

# Verifying that all values are unique
if (length(unique(hawks_select$Num_id)) == nrow(hawks_select)) {
   cat("The values in the column 'Num_ID' are unique.\n")
} else {
   cat("The values in the column 'Num_ID' are NOT unique.\n")
}</pre>
```

The values in the column 'Num_ID' are unique.

```
hawks_select <- subset(hawks_select, select = -BandNumber)
```

Point 2. We are going to correct the variable Wing that had a record with no value:

```
# El atributo tiene un valor NA, vamos a calcular una media condicional:

media_alas_especie_edad <- aggregate(Wing ~ Species + Age, data = hawks_select, FUN = function(x) mean(x)
# Calculamos las medias de la columna 'Wing' para cada especie y edad, excluyendo los valores NA
# Imputamos el valor faltante en la columna 'Wing' segun la especie y la edad
# iteramos sobre cada registro usdando un bucle for empezando por 1 hasta el valor del numero de filas
# usando 'nrow'

for (i in 1:nrow(hawks_select)) {
    # Si el valor de 'Wing' que estamos buscando es NA, buscamos la media que corresponde a la especie y
    if (is.na(hawks_select$Wing[i])) {
        # Filtramos el 'data.frame' según la especie y edad
        media_especie_edad <- media_alas_especie_edad$Wing[media_alas_especie_edad$Species == hawks_select$
        # imputamos la media que corresponda
        hawks_select$Wing[i] <- media_especie_edad
    }
}
# Verificamos que no haya valores NA en la columna
if (!any(is.na(hawks_select$Wing))) {</pre>
```

```
cat("Todos los valores NA en la columna 'Wing' han sido correctamente imputados")
} else {
  cat("Aun quedan valores NA en la columna 'Wing'. \n")
}
```

Todos los valores NA en la columna 'Wing' han sido correctamente imputados

Point 3. We go on to correct the NA values in the 'Weight' table using the same method as above. That is, we impute the mean according to age and species:

```
# El atributo tiene diez registros con NA, vamos a calcular una media condicional:

media_peso_especie_edad <- aggregate(Weight ~ Species + Age, data = hawks_select, FUN = fuaction(x) mea

# Calculamos las medias de la columna 'Weight' para cada especie y edad, excluyendo los valores NA

# Imputamos el valor faltante en la columna 'Weight' según la especie-edad

# iteramos sobre cada registro usando un bucle 'for' empezando por 1 hasta el valor del numero de filas

# empleando 'nrow'

for (i in 1:nrow(hawks_select)) {

# Si el valor de 'Weight' que estamos buscando es NA, buscamos la media que corresponde a la especie

if (is.na(hawks_select$Weight[i])) {

# Filtramos el 'data.frame' según la especie y edad

media_especie_edad <- media_peso_especie_edad$Weight[media_peso_especie_edad$Species == hawks_select

# imputamos la media que corresponda al registro NA

hawks_select$Weight[i] <- media_especie_edad

}

# Verificamos que no haya valores NA en la columna

if (!any(is.na(hawks_select$Weight))) {

cat("Aun quedan valores NA en la columna 'Weight' han sido correctamente imputados")

} else {

cat("Aun quedan valores NA en la columna 'Weight'. \n")
}
```

Todos los valores NA en la columna 'Weight' han sido correctamente imputados

Point 4. The variable 'Culmen' contains 7 NA records which we will correct using the same procedure as above, i.e. calculating the mean of the beak dimensions according to age > and species.

```
# El atributo tiene 7 registros NAs, vamos a calcular una media condicional:

media_pico_especie_edad <- aggregate(Culmen ~ Species + Age, data = hawks_select, FUN = function(x) mean

# Calculamos las medias de la columna 'Culmen' para cada especie y edad, excluyendo los valores NA

# Imputamos el valor faltante en la columna 'Culmen' según la especie-edad

# iteramos sobre cada registro usando un bucle 'for' empezando por 1 hasta el valor del numero de filas

# empleando 'nrow'
```

```
for (i in 1:nrow(hawks_select)) {
    # Si el valor de 'Culmen' que estamos buscando es NA, buscamos la media que corresponde a la especie ;
    if (is.na(hawks_select$Culmen[i])) {
        # Filtramos el 'data.frame' según la especie y edad
        media_especie_edad <- media_pico_especie_edad$Culmen[media_pico_especie_edad$Species == hawks_select
        # imputamos la media que corresponda al registro NA
        hawks_select$Culmen[i] <- media_especie_edad
    }
}

# Verificamos que no haya valores NA en la columna
if (!any(is.na(hawks_select$Culmen))) {
    cat("Todos los valores NA en la columna 'Culmen' han sido correctamente imputados")
} else {
    cat("Aun quedan valores NA en la columna 'Culmen'. \n")
}</pre>
```

Todos los valores NA en la columna 'Culmen' han sido correctamente imputados

Point 5. The variable 'Hallux' contains another suitable number of NA records. We apply the corrective policies previously implemented:

Todos los valores NA en la columna 'Hallux' han sido correctamente imputados

Before going on to check the tables and variables created and modified, let's round to one decimal place.

```
# Copia de seguridad

hawks_select_copy <- hawks_select

# Redondeamos a un decimal en la tabla 'hawks_select':

hawks_select$Weight <- round(hawks_select$Weight, 1)

hawks_select$Wing <- round(hawks_select$Wing, 1)

hawks_select$Culmen <- round(hawks_select$Culmen, 1)

hawks_select$Hallux <- round(hawks_select$Hallux, 1)

# Redondeamos a dos decimales en la tabla 'media_alas_especie_X'(alas, espolon, peso, pico)

media_alas_especie_edad$Wing <- round(media_alas_especie_edad$Wing, 1)

media_espolon_especie_edad$Hallux <- round(media_espolon_especie_edad$Hallux, 1)

media_peso_especie_edad$Weight <- round(media_peso_especie_edad$Weight, 1)

media_pico_especie_edad$Culmen <- round(media_pico_especie_edad$Culmen, 1)
```

Based on the summary() performed at the beginning, there seem to be outliers in the records, aside from the issues with infinite or 'NA' values. At first, we may be tempted to impute these apparent outliers or attribute the variability to age differences. Age is the trap in this database. It can greatly influence physiological measurements and may be, as we maintain, the main cause of variability.

However, clearly from the results of the summary() function, we can see extreme values in the 'Hallux' variable. A minimum of 9.50 and a maximum of 341.40, unless some of the analyzed specimens are prehistoric birds, doesn't seem very normal. And as for the 'Wing' variable, we can make the same assertion, although the values are less extreme.

Therefore, we will need to identify outliers beyond the normal range using the interquartile range or IQR. It is a statistical dispersion measure that represents the difference between the third quartile (Q3) and the first quartile (Q1). Quartiles divide a data distribution into four equal parts.

The first quartile is the value below which 25% of the data lies, the third quartile is the value below which 75% of the data lies, and the IQR represents the range where half of the data lies. Outliers are therefore those that are above or below Q1 or Q3 in that distribution.

In our case, we need to expand the margins, meaning extend the range beyond Q1 and Q3, so multiply by +- 1.5. The lower limit will be negative, so unless it's a typographical error, we doubt that the claw or spur has a negative length. However, we don't know what the minimum is because we are talking about birds in a developmental period.

This allow us to observe the lower and upper limits of each variable of interest or those we suspected to have issues. Also include the other variables to ensure that there are no problems. In theory, there should be no infinite values, so the use of the na.rm() function to remove them will not be necessary. Subsequently, proceding to represent them in box plots.

print("Aplicando IQR")

[1] "Aplicando IQR"

```
hallux_iqr <- IQR(hawks_select$Hallux)</pre>
weight_iqr <- IQR(hawks_select$Weight)</pre>
culmen_iqr <- IQR(hawks_select$Culmen)</pre>
# Establecemos los limites #
# Nota: El limite inferior queda en negativo, asi que salvo error tipográfico, dudamos que la garra o e
# Variable 'wing'
wing_limite_bajo <- quantile(hawks_select$Wing, 0.25) -1.5 * wing_iqr</pre>
wing_limite_alto <- quantile(hawks_select$Wing, 0.75) + 1.5 * wing_iqr</pre>
hallux_limite_bajo <- quantile(hawks_select$Hallux, 0.25) -1.5 * hallux_iqr
hallux_limite_alto <- quantile(hawks_select$Hallux, 0.75) +1.5 * hallux_iqr
weight_limite_bajo <- quantile(hawks_select$Weight, 0.25) -1.5 * weight_iqr
weight_limite_alto <- quantile(hawks_select$Weight, 0.75) +1.5 * weight_iqr
culmen_limite_bajo <- quantile(hawks_select$Culmen, 0.25) -1.5 * culmen_iqr
culmen_limite_alto <- quantile(hawks_select$Culmen, 0.75) +1.5 * culmen_iqr</pre>
# identificamos los valores atipicos en cada una de las variables:
wing_outliers <- hawks_select$Wing[hawks_select$Wing < wing_limite_bajo | hawks_select$Wing > wi
hallux_outliers <- hawks_select$Hallux[hawks_select$Hallux < hallux_limite_bajo | hawks_select$Hallux >
weight_outliers <- hawks_select$Weight[hawks_select$Weight < weight_limite_bajo | hawks_select$Weight >
culmen_outliers <- hawks_select$Culmen[hawks_select$Culmen < culmen_limite_bajo | hawks_select$Culmen >
print("Visualizamos los valores fuera de rango")
```

[1] "Visualizamos los valores fuera de rango"

```
# Convertimos los vectores en 'data.frames'#
hallux_outliers_df <- data.frame(hallux_outliers)
weight_outliers_df <- data.frame(weight_outliers)
wing_outliers_df <- data.frame(wing_outliers)
culmen_outliers_df <- data.frame(culmen_outliers)

# Imprimimos tablas en el documento
kable(hallux_outliers_df, caption = "Outliers en 'Hallux'")</pre>
```

Table 1: Outliers en 'Hallux'

 $\frac{\text{hallux_outliers}}{101.0}$

$hallux_{_}$	_outliers
	308.0
	341.4
	143.0
	82.8
	121.0
	130.0

kable(weight_outliers_df, caption = "Outliers en 'Weight'")

Table 2: Outliers en 'Weight'

 $\underline{\underline{\text{weight}}\underline{-\text{outliers}}}$

kable(wing_outliers_df, caption = "Outliers en 'Wing'")

Table 3: Outliers en 'Wing'

 $\underline{\underline{\text{wing_outliers}}}$

kable(culmen_outliers_df, caption = "Outliers en 'Culmen'")

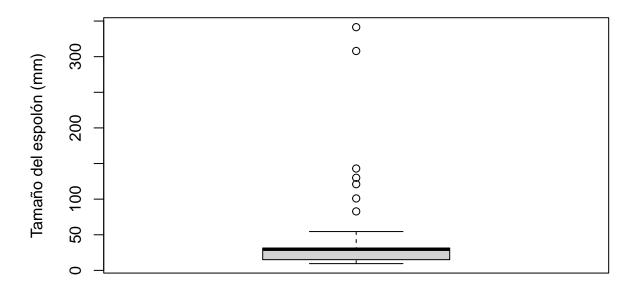
Table 4: Outliers en 'Culmen'

 $\underline{\underline{\text{culmen}_\text{outliers}}}$

We proceed to the graphical representation, but considering that the only outliers are in the variable 'hallux':

Representación de la variable 'Hallux' boxplot(hawks_select\$Hallux, main = "Hallux", ylab = "Tamaño del espolón (mm)", outline = TRUE)

Hallux



The graphical representation shows us that, indeed, we have 7 values outside the dispersion ranges. At this point, we must decide what to do with these values and we choose to impute the species- and age-dependent mean to them:

```
print("imputamos las medias en 'Hallux' a outliers segun especie y edad")
```

[1] "imputamos las medias en 'Hallux' a outliers segun especie y edad"

```
for (i in 1:nrow(hawks_select)) {
    # Si el valor de 'Hallux' que estamos buscando es superior a 55.9, buscamos la media que correspon
    if (hawks_select$Hallux[i] > hallux_limite_alto) {
        # Filtramos el 'data.frame' según la especie y edad
        media_especie_edad <- media_espolon_especie_edad$Hallux[media_espolon_especie_edad$Species == hawks
        # imputamos la media que corresponda al registro NA
        hawks_select$Hallux[i] <- media_especie_edad
    }
}

# Verificamos que no haya valores NA en la columna
if (!any(hawks_select$Hallux[i] > hallux_limite_alto)) {
    cat("Todos los valores Outliers en la columna 'Hallux' han sido correctamente imputados")
} else {
    cat("Aun quedan valores Outliers en la columna 'Hallux'. \n")
}
```

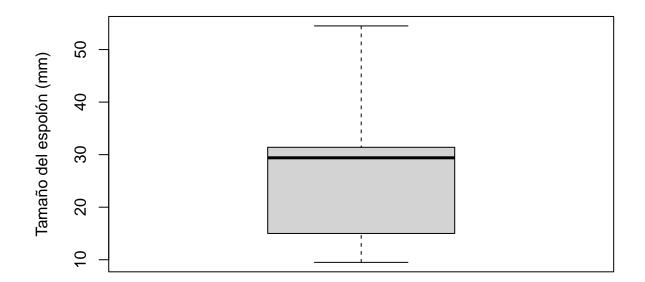
Todos los valores Outliers en la columna 'Hallux' han sido correctamente imputados

The operation appears to have been successful, we repeat with the box chart:

```
# Representación de la variable 'Hallux' en busca de confirmar que no quedan outliers:

boxplot(hawks_select$Hallux, main = "Hallux", ylab = "Tamaño del espolón (mm)", outline = TRUE)
```

Hallux



Indeed, no out-of-range values left in the variable.

Table Integrity revision

summary(hawks_select)

```
##
         Year
                        Month
                                           Day
                                                       Species
                                                                 Age
                                             : 1.00
##
    Min.
           :1992
                           : 8.000
                                                       CH: 70
                                                                 A:224
                    Min.
                                      Min.
##
    1st Qu.:1995
                    1st Qu.: 9.000
                                      1st Qu.: 9.00
                                                       RT:577
                                                                 I:684
    Median:1999
                    Median :10.000
                                      Median :16.00
                                                       SS:261
##
##
    Mean
           :1998
                    Mean
                           : 9.843
                                      Mean
                                             :15.74
    3rd Qu.:2001
                    3rd Qu.:10.000
                                      3rd Qu.:23.00
##
##
    Max.
           :2003
                    Max.
                           :11.000
                                              :31.00
                                      Max.
##
         Wing
                         Weight
                                           Culmen
                                                            Hallux
##
           : 37.2
                            : 56.0
                                       Min.
                                               : 8.60
                                                                : 9.50
    Min.
                     Min.
                                                        Min.
    1st Qu.:202.0
##
                     1st Qu.: 185.0
                                       1st Qu.:12.78
                                                        1st Qu.:15.00
   Median :370.0
                     Median : 970.0
                                       Median :25.50
                                                        Median :29.40
##
           :315.6
                            : 770.5
                                               :21.79
##
   Mean
                     Mean
                                       Mean
                                                        Mean
                                                                :25.21
```

```
3rd Qu.:390.0
                     3rd Qu.:1120.0
                                       3rd Qu.:27.30
                                                        3rd Qu.:31.40
            :480.0
                             :2030.0
                                                                :54.50
##
    Max.
                     Max.
                                       Max.
                                               :39.20
                                                        Max.
        Num id
##
   Min.
##
           :
              1.0
##
    1st Qu.:227.8
   Median :454.5
##
   Mean
            :454.5
##
    3rd Qu.:681.2
##
    Max.
            :908.0
```

No infinite values, and the means, although quite disparate as in the case of 'wing' - considering that it does not discriminate developing birds - do not contain extreme values.

Continue examining the table, now analyzing the variables using the name() function.

```
names(hawks_select)
     [1] "Year"
                    "Month"
                               "Day"
                                          "Species" "Age"
                                                                "Wing"
                                                                           "Weight"
     [8] "Culmen"
                    "Hallux"
                               "Num_id"
head(hawks_select, 3)
     Year Month Day Species Age Wing Weight Culmen Hallux Num_id
## 1 1992
               9
                   19
                           RT
                                 Ι
                                    385
                                            920
                                                  25.7
                                                          30.1
                                                                     1
## 2 1992
               9
                   22
                           RT
                                 Ι
                                    376
                                            930
                                                  26.8
                                                          32.2
                                                                     2
## 3 1992
               9
                   23
                           RT
                                 Ι
                                    381
                                            990
                                                  26.7
                                                          31.3
                                                                     3
```

Next we will analyse the structure with the str() function which gives us a more complete overview of the table structure:

```
# Realizamos un resumen estadistico de todas la variables:
str(hawks_select)
```

```
908 obs. of 10 variables:
  'data.frame':
##
                  : int
   $ Month : int
                  9 9 9 9 9 9 9 9 9 ...
                  19 22 23 23 27 28 28 29 29 30 ...
           : int
   $ Species: Factor w/ 3 levels "CH", "RT", "SS": 2 2 2 1 3 2 2 2 2 2 ...
##
           : Factor w/ 2 levels "A", "I": 2 2 2 2 2 2 1 1 2 ...
   $ Age
##
   $ Wing
           : num
                  385 376 381 265 205 412 370 375 412 405 ...
                  920 930 990 470 170 1090 960 855 1210 1120 ...
##
   $ Weight : num
##
  $ Culmen : num
                 25.7 26.8 26.7 18.7 12.5 28.5 25.3 27.2 29.3 26 ...
                  30.1 32.2 31.3 23.5 14.3 32.2 30.1 30 31.3 30.2 ...
  $ Hallux : num
   $ Num_id : int 1 2 3 4 5 6 7 8 9 10 ...
```

We observe that we have 908 records in 10 variables. At this point, we do not consider changing the measurement scale to kilograms for the 'Weight' variable, which seems more appropriate, especially for the

juvenile bird population. We also do not consider any changes necessary in the types of variables present in the table.

Regarding the "additional tables" that contain the means of different physiological measurements for different species based on their age, we do not believe it is necessary to analyze them using any R function, as they are highly summarized tables with 6 records and 3 variables.

Inventory

At this point, our dataset consists of:

Table 'hawks_select' with all the relevant variables for the analysis and with the cleaning process applied.

Additional tables with means of wing length, hallux size, weight, and culmen length in relation to species and age. These tables contain 6 records and 3 variables each.

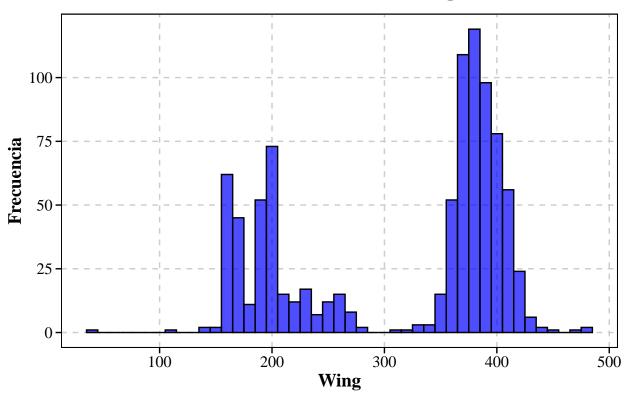
Distribution of variables in the 'hawks_select' table.

• Histograms.

[1] "Distribucion del tamaño de las alas"

```
ggplot(hawks_select, aes(x= Wing)) +
  geom_histogram(binwidth = 10, color = "black", fill= "blue", alpha= 0.7) +
  mi_tema() +
  labs(title = "Distribucion 'Wing'", x = "Wing", y = "Frecuencia")
```

Distribucion 'Wing'

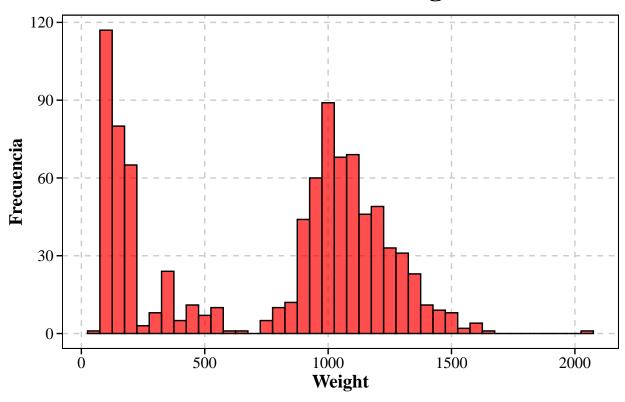


```
# Histograma paea 'Weight'
print("Distribucion del tamaño del peso")
```

[1] "Distribucion del tamaño del peso"

```
ggplot(hawks_select, aes(x = Weight)) +
  geom_histogram(binwidth = 50, color= "black", fill= "red", alpha = 0.7) +
  mi_tema() +
  labs(title = "Distribucion 'Weight'", x = "Weight", y = "Frecuencia")
```

Distribucion 'Weight'

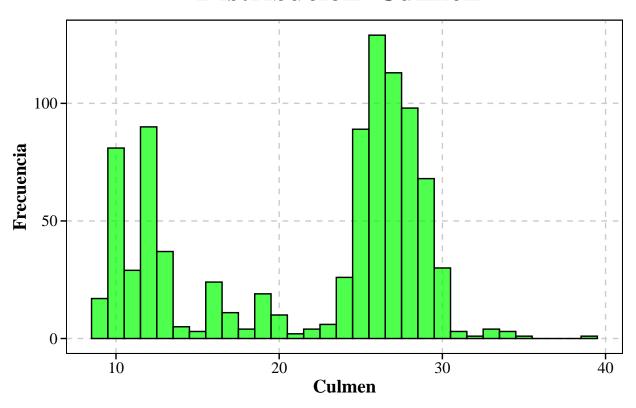


```
# Histograma para 'Culmen'
print("Distribucion del tamaño del pico")
```

[1] "Distribucion del tamaño del pico"

```
ggplot(hawks_select, aes(x = Culmen)) +
  geom_histogram(binwidth = 1, color = "black", fill = "green", alpha = 0.7) +
  mi_tema() +
  labs(title = "Distribucion 'Culmen'", x = "Culmen", y = "Frecuencia")
```

Distribucion 'Culmen'

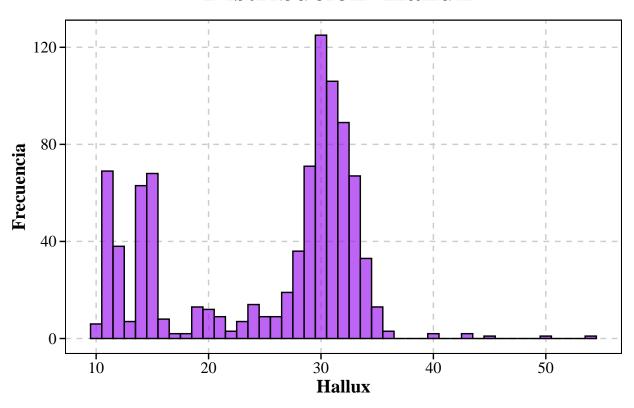


```
# Histograma para 'Hallux'
print("Distribucion del tamaño de los espolones")
```

[1] "Distribucion del tamaño de los espolones"

```
ggplot(hawks_select, aes(x = Hallux)) +
    mi_tema() +
    # scale_y_log10() + # aplicamos escala logaritmica para poder representar los datos de frecuencia (y)
    # scale_x_log10() + # aplicamos escala logaritmica para poder representar las medidas adecuadamente
    geom_histogram(binwidth = 1, color = "black", fill = "purple", alpha = 0.7) +
    labs(title = "Distribucion 'Hallux'", x = "Hallux", y = "Frecuencia")
```

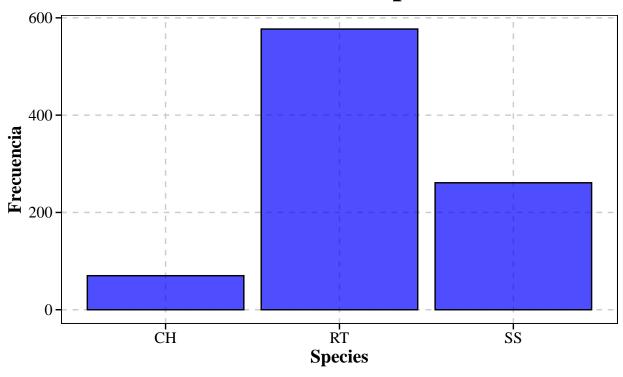
Distribucion 'Hallux'



```
# labs(caption = "Escalas logatimica en base 10 en los ejes X-Y")
```

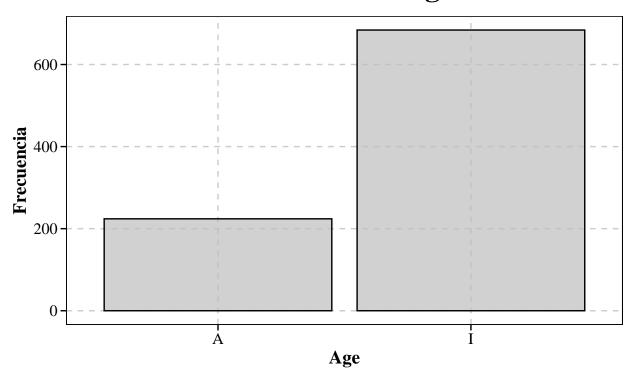
• Bar charts for categorical variables in 'hawks_select'.

Distribucion 'Species'



Cooper's Hawk (CH), Red-Tailed Hawk (RT) o Sharp-Shinned Hawk (SS)

Distribucion 'Age'



A = Adulto I = Infantes

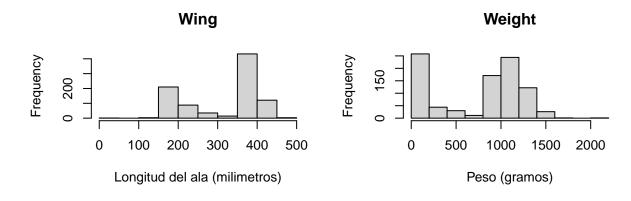
On the one hand, we observed an over-representation of the RT species and an under-representation of CH. On the other hand, the child population of the sample is higher than the adult population.

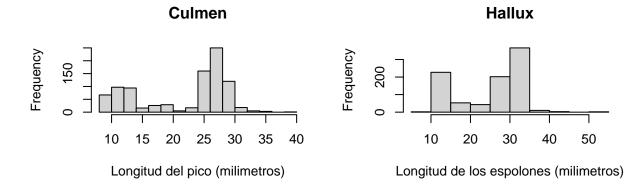
• Other visualisations of the variable distributions:

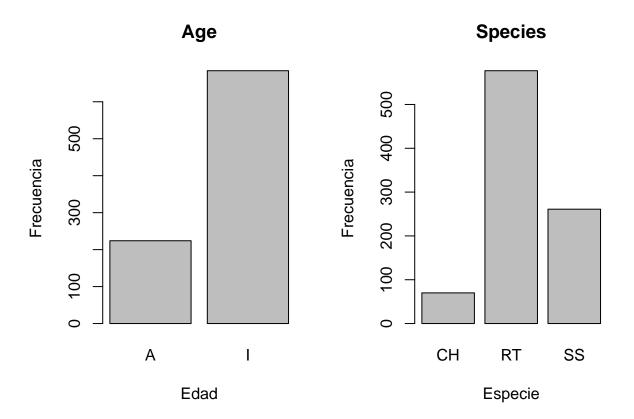
[1] "Distribuciones de variables en la tabla 'hawks_select' \n"

```
# Establecemos las opciones gráficas con `par()` y con `mfrow()`configuramos la matriz de
par(mfrow = c(2,2))

hist(hawks_select$Wing, main= "Wing", xlab = "Longitud del ala (milimetros)")
hist(hawks_select$Weight, main = "Weight", xlab = "Peso (gramos)")
hist(hawks_select$Culmen, main = "Culmen", xlab = "Longitud del pico (milimetros)")
hist(hawks_select$Hallux, main = "Hallux", xlab = "Longitud de los espolones (milimetros)")
```

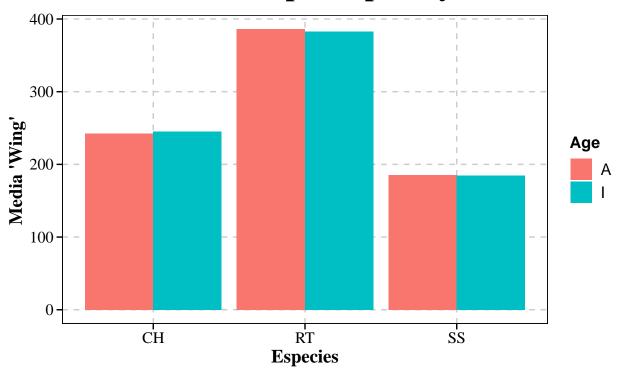






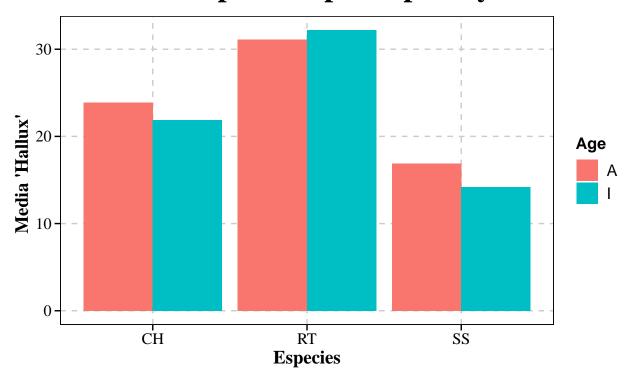
Distribution of variables in annexed tables - averages according to age and species

Medias de alas por especie y edad



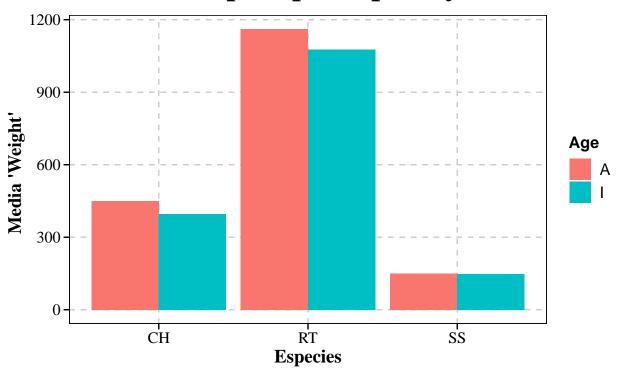
Cooper's Hawk (CH), Red-Tailed Hawk (RT) o Sharp-Shinned Hawk (SS)

Medias de espolones por especie y edad



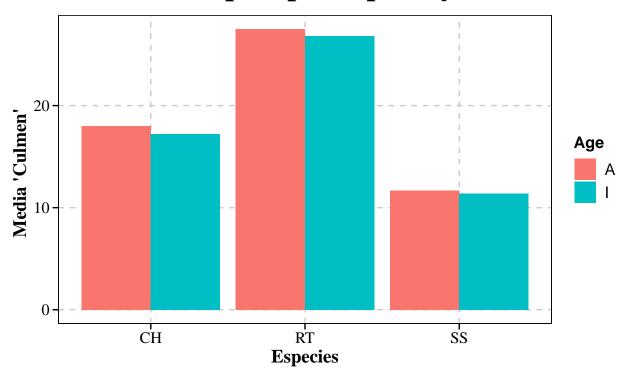
Cooper's Hawk (CH), Red-Tailed Hawk (RT) o Sharp-Shinned Hawk (SS)

Medias de peso por especie y edad



Cooper's Hawk (CH), Red-Tailed Hawk (RT) o Sharp-Shinned Hawk (SS)

Medias de pico por especie y edad



Cooper's Hawk (CH), Red-Tailed Hawk (RT) o Sharp-Shinned Hawk (SS)

Study using k-means aggregation method

Using the 'hawks_select' table, where we have selected the relevant variables for our study, we will employ the k-means clustering method. This method will group observations into 'k' clusters based on the nearest mean. It is an unsupervised clustering method used when there are no pre-defined labels for the data (James et al. 2013; Gareth et al. 2013; Cannon et al. 2013b).

By "no pre-defined labels," we mean that the data does not have a predetermined category or class assigned to it. In other words, we do not know which group each data point belongs to, as there are no right or wrong answers in the variable(s) Gironés Roig (2017).

The most common uses of this technique are in segmentation - e.g., customers, to understand their needs -, dimensionality reduction - or to group into smaller clusters -, data understanding - to improve data representation -, defect or problem detection - e.g., outliers or when there are values far from the mean and logic -, and classification - after applying the algorithm, labels can be assigned.

The main objectives, but not exclusive, for applying this algorithm in this case would be:

- 1. Segmentation: Although we already know the labels CH, RT, SS -, we can explore if these species have notable differences in their characteristics and if coherent data groups are formed. It will also allow us to gain a better understanding of the data and identify potential subgroups.
- 2. Analysis of physical characteristics and age: Clustering will reveal differences between adults and immature individuals.
- 3. Problem detection: By applying the summary() function earlier, we suspected the presence of possible outliers or extreme values. With this algorithm, we can confirm or dismiss this hypothesis.

Application of the k-means method to the numerical variables in the 'hawks_select' dataset When applying the algorithm, we will use the normalized variables 'Wing', 'Weight', 'Culmen', and 'Hallux'. This ensures that all features have equal weighting in the formation of clusters or groups [@montoliucolásraúl]. We will carry this out using the scale() function in R, which performs normalization by default and follows the formula: z = (x-m)/d

Here, x is the original value, m is the mean of the variable, d is the standard deviation, and z is the standardized or z-score value [@scalefu]. We aim to find 3 clusters, one for each hawk species, but it is also possible to have 6 clusters considering the age groups. Therefore, we will apply the k-means algorithm twice, with 3 and 6 clusters respectively.

```
print("Aplicando k-means")
```

[1] "Aplicando k-means"

[1] "para tres grupos"

```
set.seed(131)

tres_grupos <- 3
kmeans3_result <- kmeans(hawks_z, centers = tres_grupos)
print("para seis grupos")</pre>
```

[1] "para seis grupos"

```
set.seed(131)
seis_grupos <- 6
kmeans6_result <- kmeans(hawks_z, centers = seis_grupos)

# Agregamos la información de los clusteres a los datos de la tabla original:
hawks_select$Cluster3 <- as.factor(kmeans3_result$cluster)
hawks_select$Cluster6 <- as.factor(kmeans6_result$cluster)</pre>
```

At this point, it is necessary to clarify that by using set.seed(), we are ensuring randomness. Seeds are numbers used to initialize the random number generator (RNG). Regardless of the chosen number, it guarantees that any procedure involving random numbers is replicable. This is particularly important in algorithms like k-means, which are sensitive to random initialization and can produce different results in each execution (MacQueen 1967; Kaufman and Rousseeuw 2009)

Next, we will visualize each combination of variables and the corresponding results for analysis:

• Graphs for 3 groups:

```
print("Graficando k-means para tres grupos")
```

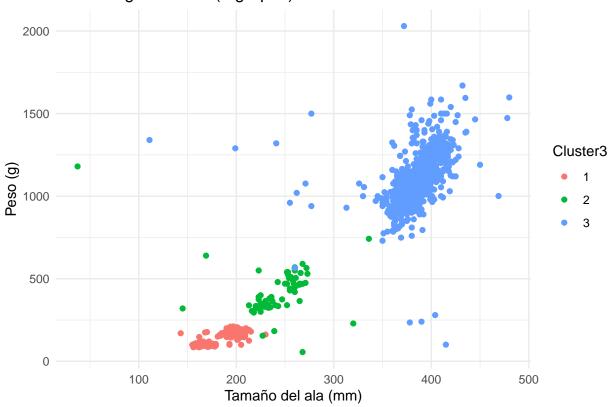
[1] "Graficando k-means para tres grupos"

```
# Tres grupos #
###############
# Wing vs Weight
print("Tres grupos: Wing vs Weight")
```

[1] "Tres grupos: Wing vs Weight"

```
ggplot(hawks_select, aes(x = Wing, y = Weight, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Tamaño del ala (mm)", y = "Peso (g)") +
  theme_minimal()
```

Clustering k-means (3 grupos)

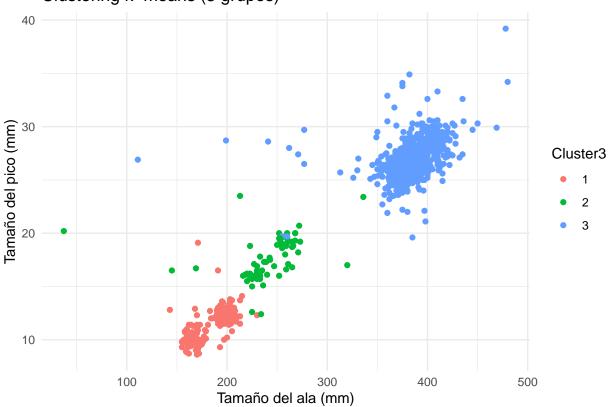


```
# Wing vs Culmen
print("Tres grupos: Wing vs Culmen")
```

[1] "Tres grupos: Wing vs Culmen"

```
ggplot(hawks_select, aes(x = Wing, y = Culmen, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Tamaño del ala (mm)", y = "Tamaño del pico (mm)")
  theme_minimal()
```

Clustering k-means (3 grupos)

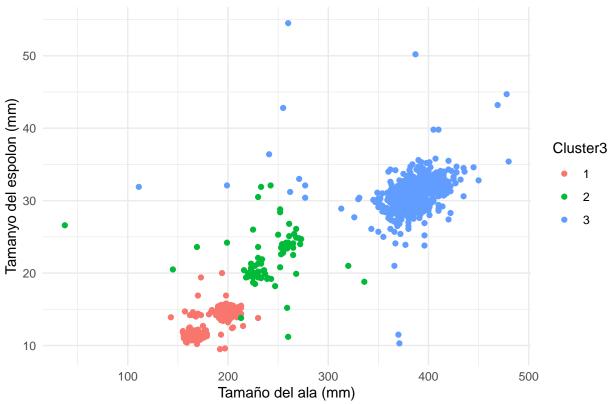


```
# Wing vs Hallux print("Tres grupos: Wing vs Hallux")
```

[1] "Tres grupos: Wing vs Hallux"

```
ggplot(hawks_select, aes(x = Wing, y = Hallux, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Tamaño del ala (mm)", y = "Tamanyo del espolon (mm
  theme_minimal()
```

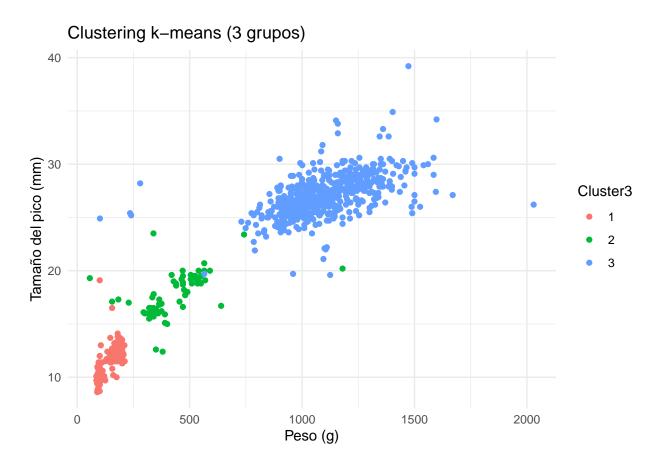




```
# Weight vs Culmen
print("Tres grupos: Weight vs Culmen")
```

[1] "Tres grupos: Weight vs Culmen"

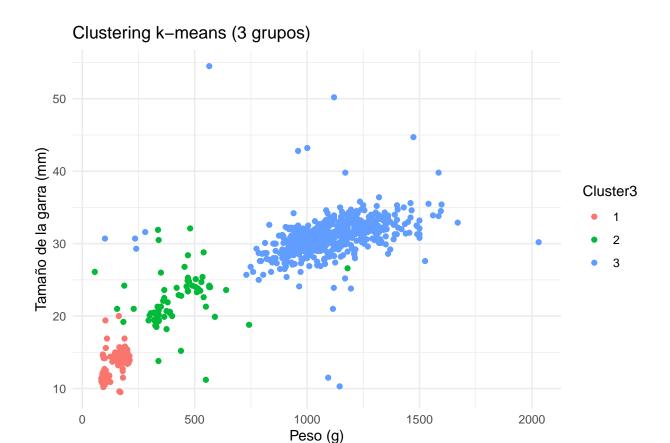
```
ggplot(hawks_select, aes(x = Weight, y = Culmen, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Peso (g)", y = "Tamaño del pico (mm)") +
  theme_minimal()
```



```
# Weight vs Hallux print("Tres grupos: Weight vs Hallux")
```

[1] "Tres grupos: Weight vs Hallux"

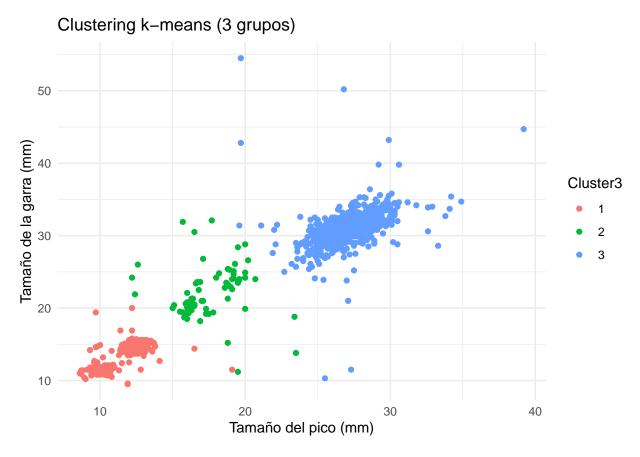
```
ggplot(hawks_select, aes(x = Weight, y = Hallux, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Peso (g)", y = "Tamaño de la garra (mm)") +
  theme_minimal()
```



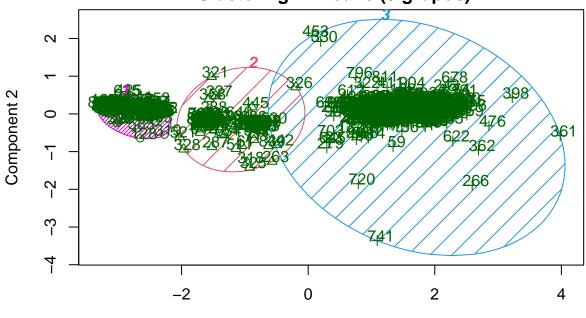
```
# Culmen vs Hallux print("Tres grupos: Culmen vs Hallux")
```

[1] "Tres grupos: Culmen vs Hallux"

```
ggplot(hawks_select, aes(x = Culmen, y = Hallux, color = Cluster3)) +
  geom_point() +
  labs(title = "Clustering k-means (3 grupos)", x = "Tamaño del pico (mm)", y = "Tamaño de la garra (mm
  theme_minimal()
```



CLUSPLOT(hawks_z) Clustering k-means (3 grupos)



Component 1
These two components explain 97.53 % of the point variability.

The measurements of 'wing' and 'Culmen', that is, beak and wings, appear to tend to separate the three bird species. Weight also does not seem to be the most consistent grouping measure, as there is a lot of overlap. In general, it tends to mix observations. We assume that the problem is the mixing of juvenile and adult populations.

Charts for 6 groups:

```
print("Graficando k-means para seis grupos")
```

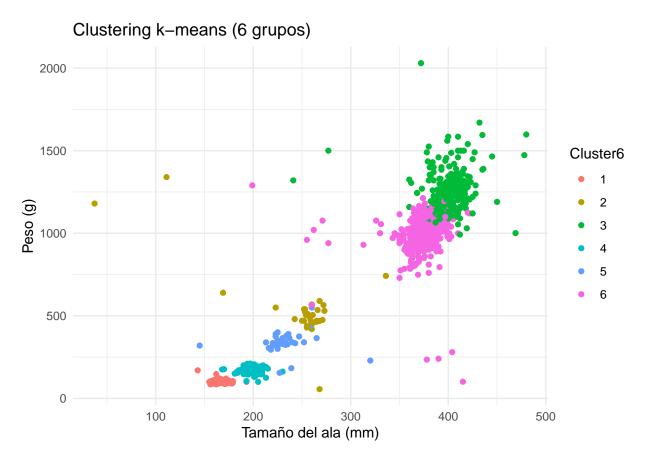
[1] "Graficando k-means para seis grupos"

```
# Seis grupos#
###############

# Wing vs Weight
print("Seis grupos: Wing vs Weight")
```

[1] "Seis grupos: Wing vs Weight"

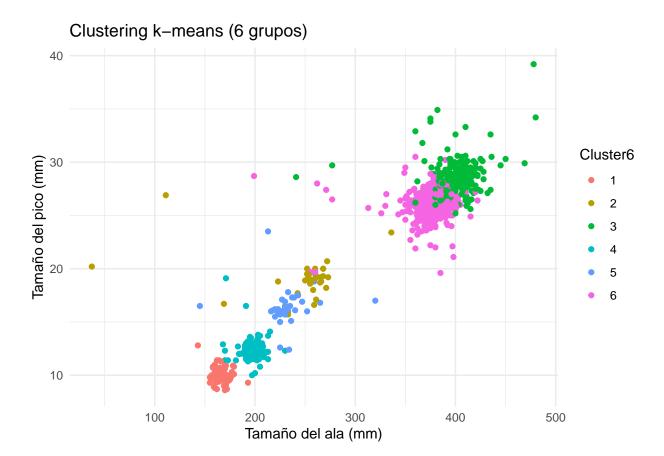
```
ggplot(hawks_select, aes(x = Wing, y = Weight, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Tamaño del ala (mm)", y = "Peso (g)") +
  theme_minimal()
```



```
# Wing vs Culmen
print("Seis grupos: Wing vs Culmen")
```

[1] "Seis grupos: Wing vs Culmen"

```
ggplot(hawks_select, aes(x = Wing, y = Culmen, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Tamaño del ala (mm)", y = "Tamaño del pico (mm)")
  theme_minimal()
```

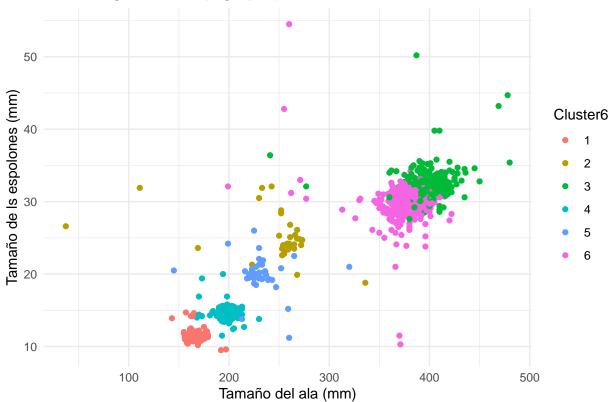


```
# Wing vs Hallux
print("Seis grupos: Wing vs Hallux")
```

[1] "Seis grupos: Wing vs Hallux"

```
ggplot(hawks_select, aes(x = Wing, y = Hallux, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Tamaño del ala (mm)", y = "Tamaño de ls espolones
  theme_minimal()
```

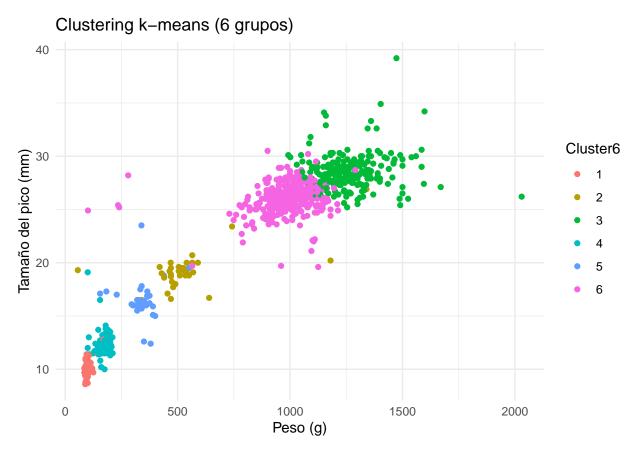




```
# Weight vs Culmen
print("Seis grupos: Weight vs Culmen")
```

[1] "Seis grupos: Weight vs Culmen"

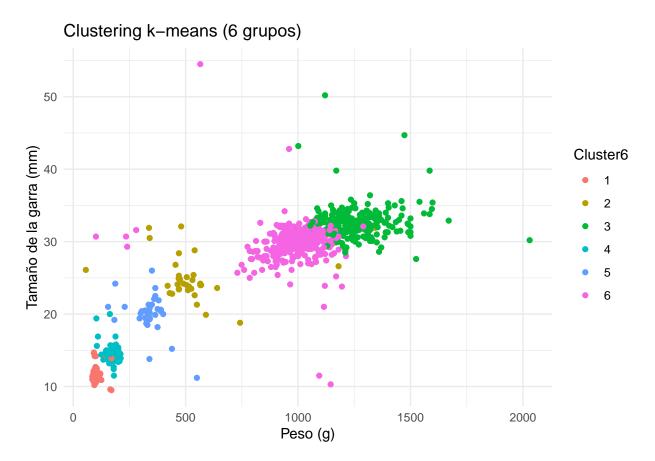
```
ggplot(hawks_select, aes(x = Weight, y = Culmen, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Peso (g)", y = "Tamaño del pico (mm)") +
  theme_minimal()
```



```
# Weight vs Hallux
print("Seis grupos: Weight vs Hallux")
```

[1] "Seis grupos: Weight vs Hallux"

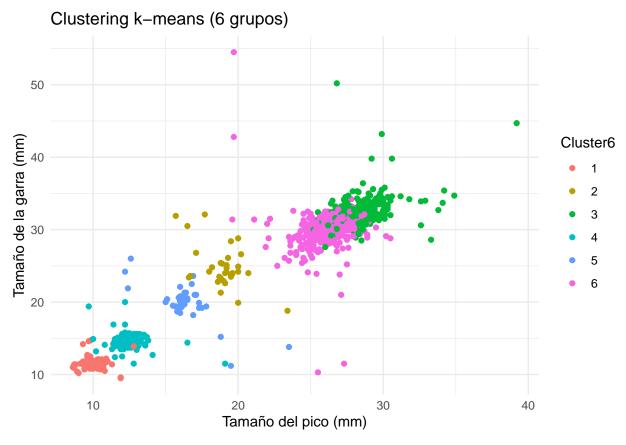
```
ggplot(hawks_select, aes(x = Weight, y = Hallux, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Peso (g)", y = "Tamaño de la garra (mm)") +
  theme_minimal()
```

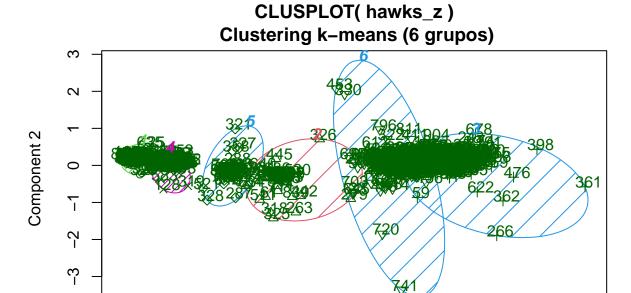


```
# Culmen vs Hallux
print("Seis grupos: Culmen vs Hallux")
```

[1] "Seis grupos: Culmen vs Hallux"

```
ggplot(hawks_select, aes(x = Culmen, y = Hallux, color = Cluster6)) +
  geom_point() +
  labs(title = "Clustering k-means (6 grupos)", x = "Tamaño del pico (mm)", y = "Tamaño de la garra (mm
  theme_minimal()
```





Component 1
These two components explain 97.53 % of the point variability.

0

2

4

-2

We observe that forcing the creation of 6 groups does not result in convincing outcomes. In general, everything suggests that there are 3 groups, although not very homogeneous, which tend to mix and confuse the algorithm when trying to group them.

Analysis of the results At this point, as we have observed throughout, the graphs of the different variables suggest the existence of 3 groups, although not very homogeneous. Ideally, we would have been able to make the clusters comparable across different age groups and species by including age as an analytical variable. However, the k-means algorithm is designed to work with continuous variables, and both species and age are categorical.

One possible solution that was not addressed at the beginning of this exercise would have been to create indicator variables (dummy variables) with values of 1 and 0. However, this approach would have also brought problems, as k-means assigns equal importance to all variables, and the indicator variables would have played an inappropriate role in the analysis. Additionally, the analysis seemed much more complex with dummy variables.

Since we still do not have a clear idea of how many groups we can label the data with, we will try to perform hierarchical clustering. Given the nature of the dataset, we made the mistake of assuming that we could guess the number of clusters based on the nature of the data. Therefore, we will attempt to use hierarchical clustering based on the Euclidean method.

print("clustering jerarquico")

[1] "clustering jerarquico"

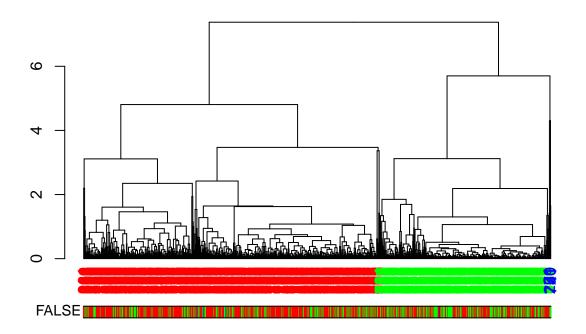
```
# Calculamos la matriz de distancias
distancias <- dist(hawks_z, method = "euclidean")

# Realizamos el clustering jerárquico
clustering_jerarquico <- hclust(distancias, method = "complete")

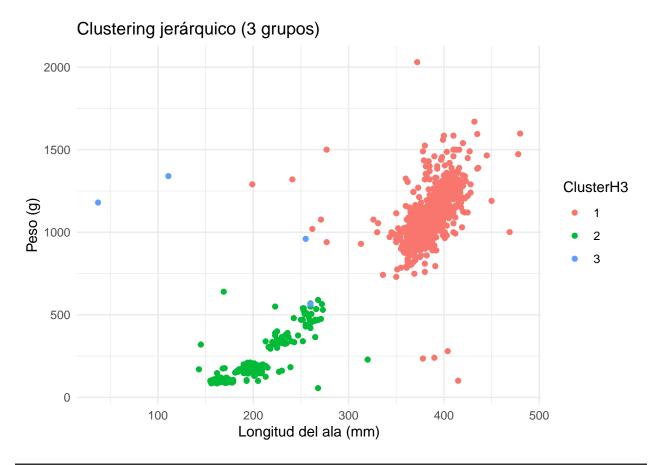
# Cortamos el árbol para obtener 3 clusters
clusters_jerarquico3 <- cutree(clustering_jerarquico, k = 3)

# Añadimos la información de los clusters al data frame original
hawks_select$ClusterH3 <- as.factor(clusters_jerarquico3)

# Visualizamos el dendrograma
dend <- as.dendrogram(clustering_jerarquico)
# Coloreamos las ramas del dendrograma según los grupos
colors <- rainbow(3)[clusters_jerarquico3]
labels_colors(dend) <- colors[order.dendrogram(dend)]
plot(dend)
colored_bars(colors[order.dendrogram(dend)], dend, rowLabels = FALSE)</pre>
```



```
# Graficamos un ejemplo de dispersión para los clusters jerárquicos
ggplot(hawks_select, aes(x = Wing, y = Weight, color = ClusterH3)) +
  geom_point() +
  labs(title = "Clustering jerárquico (3 grupos)", x = "Longitud del ala (mm)", y = "Peso (g)") +
  theme_minimal()
```



visualizamos la tabla con la agrupacion de los resultados:
table(clusters_jerarquico3)

```
## clusters_jerarquico3
## 1 2 3
## 576 328 4
```

We observe that it has created two groups. In general, we can conclude that the dataset was not particularly well-suited for the k-means method due to the aforementioned aspects. With limitations, we can affirm that the data, when applying the algorithm, seems to fall into 3 heterogeneous groups, which would not allow us to confidently assign an observation to a specific group or label these observations.

Example 2

Analysis applying DBSCAN and OPTICS methods.

Based on the same dataset that has been created, including the normalized scores, we will proceed to perform an analysis using DBSCAN and OPTICS.

We will use the 'DBSCAN' library, which focuses on efficiently implementing DBSCAN and OPTICS. Additionally, we will complement it with the use of the 'fpc' library, which includes a 'cluster.stats' function that can evaluate the results of an OPTICS clustering.

OPTICS (Ordering Points to Identify the Clustering Structure), introduced by Ankerst et al. in 1999, is an extension of the DBSCAN algorithm that can help us better handle the problem of variable density among

clusters, which was evident when applying k-means. OPTICS does not directly assign clusters but orders the points to highlight their density, facilitating visualization with a reachability plot that shows the distance between each point. While theoretically, we do not have outliers in the dataset, if present, OPTICS does not exclude outliers but identifies them by assigning them a higher reachability value.

Let's proceed with OPTICS:

```
print("aplicamos optics al dataset que ya tenemos")
```

[1] "aplicamos optics al dataset que ya tenemos"

```
# Configuramos eps= x o la distancia máxima entre dos puntos:
# El grupo debe tener como mínimo 'minPts'= x observaciones para ser agrupado

optics_result <- dbscan::optics(hawks_z, minPts = 10)
optics_result

## OPTICS ordering/clustering for 908 objects.
## Parameters: minPts = 10, eps = 3.07716556342231, eps_cl = NA, xi = NA
## Available fields: order, reachdist, coredist, predecessor, minPts, eps,
## eps_cl, xi

# Obtenemos el orden de las observaciones o puntos
print("Obtenemos la odenacion de los puntos")</pre>
```

[1] "Obtenemos la odenacion de los puntos"

optics_result\$order

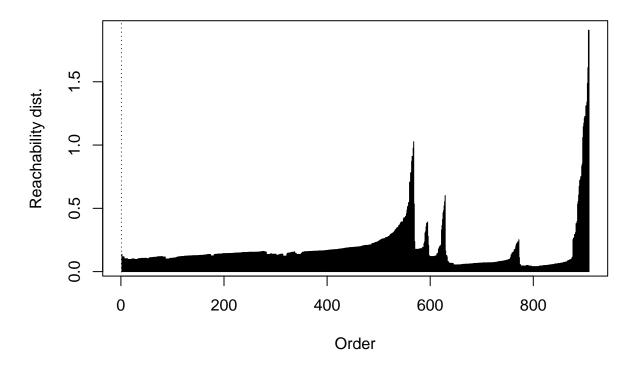
```
1 571 390 267 260 245 620 185 184 150 149 137
                                                          93 824 764 650 408 233
##
    [19] 193
              25 236 487 481 426 378 317 787 771 594 467 281
                                                               12
                                                                   87 134 119 278
    [37] 203 765 334 861 844 701 471 223 283 116 648 891 832 707 681 547 508 337
                               7 165 555 365 532 131
##
   [55] 762 579 139 251
                          80
                                                       11 402 784 295 364 206 515
##
    [73] 457 876 561 550 391
                              33 222 774 717 552 292 403 372 250 823 506 460 179
                  43 758 589 871 848 671 450
##
   [91] 154
              48
                                              79 898 760 473
                                                                3 113 715 423 483
## [109] 438 427 270 647 135
                              90
                                  31 696 782 740 590 182 323 190 157 342 800 465
## [127] 338 180 178 679 181 354 556 778 726 528 437 526
                                                          45 355 544 743 649 582
## [145] 336 155 855 309 615 854 893 169 433 274 585 240 110
                                                               21 572 183 692 862
## [163]
             51 286 789 733 324 719 846 560 505 478 867 878 576 466 434 380 230
## [181]
          19 194 853 489 504 114 617 136 138
                                              71 709 258 770 290 205 237 596 780
## [199] 775 602 600 601 581 397 745 117 907 868 674 676 537
                                                               32 553 412 177
## [217]
         49 200 672 151 559 605 606 593 881 769 496 531 888 197 159 123 385 497
## [235] 883 882 614 540 901 744 558 369 209 208 204 455 694 275 514 367
                                                                          609 608
## [253] 892 812 631 566 501 405 300 224 785 199
                                                      72 691 207
                                                  47
                                                                   10
                                                                      294
                                                                           46 153
## [271] 118 430 147
                      55
                          27 163 241 816 591 444 377 124 551 485 428 384 351
                                                                           66 262
## [289]
          14 798 847 658 872 548 289 254 186 174 120
                                                      91
                                                          82 777 246 229
              50 335 732 529 522 226 421 875 866 833 817 705 632 517 269 641 752
## [307]
## [325] 388 492 804 573 225 716 502 389 564 541 350
                                                       13 441 869 856 759 728 683
## [343] 578 252
                  95
                      60 567 480 164 291 293 597 127
                                                      81
                                                          73 126 409 718 482 257
## [361]
          22
               9
                  97 536 271 860 669 468 187 616
                                                  92 792 827 723 463 217 158 344
                               8 525 543 220 885 462 115 106 280 666 102 786 256
## [379] 238 768 446 145 472
                             89 499 387 264 773 44 58 886 261 189 470 704 247
## [397] 586
               6 435 592 452
```

```
## [415] 63 879 845 538 273 731 392 534 469 298 440 18 96 105 607 242 598 790
## [433] 303 17 750 133 192 75 494 366 682 902 418 140 652 339 382 146 77 613
## [451] 109 407 510 94 706 235 843 838 265 664 401 610 651 858 259 406 491 539
## [469] 248 512 34 894 76 410 793
                                    24 767 584
                                               37
                                                   36 507 332 285
                                                                  15 474 484
## [487] 297 373 665 376 863 156
                               20 333 436 721
                                               70 255 629
                                                           16 343 396 232 900
## [505] 39 52 399 348 903 549 498
                                   30 331 612 797 906
                                                       62 695
                                                               35 272 244
## [523] 346 880 175 554 162 282 381 296 479 766 148 714
                                                       38 456
                                                               64 210 345 667
## [541] 700 411 322 795 166 88 904 359 356 349 347 191 132
                                                           74 811 796 622 476
## [559] 243 414 603 398 326 362 908
                                    59 699 445 819 809 788 686 680 673 459 400
  [577] 310
              4 588 353 239 108
                               67 415 702 577 542 249 530 711 111 234 839 634
## [595] 877 842 851 889 850 830 826 772 643 424 371
                                                   57
                                                       42 708 533 599 821 808
## [613] 524 757 443 299 221 393 288 56
                                       86 188 642 742 442 327 263 287 662 735
## [631] 841 685 899 897 884 896 763 836 807 794 779 738 727 725 697 887 688 639
## [649] 623 416 316 284 219 621 104 840 746 475 313 595 523 500 630 214 822 730
## [667] 619 776 751 687 370 170 803 828 799 202 801 749 722 516 783 458 374  69
## [685] 84
            29 276 301 228 461 171
                                     5 624 176 160 905 448 375 172 644 802 306
## [703] 835 734 684 660 625 519 439 447 404 143  83 895 747 486 454 431 689 557
## [721] 312 857 395 488 413 340 98 513 477 464 167 129 611 198 218 675 546 814
## [739] 168
            99 693 518 227 568 195 201 161 420 653 569 677 383 53 781 216 825
## [775] 724 874 791 663 580 570 562 852 657 587 451 495 737 575 565 308 646 659
## [793] 655 654 626 503 859 831 761 736 712 527 422 849 805 748 636 520 307 304
## [811] 656 314 311 627 449 535 429 419 870 834 638 417 125 810 729 628 302 633
## [829] 829 386 268 815 690 101 670 394 41 604 806 368 755 196 756 144
                                                                      85 668
## [847] 379 432 574 710 68 637 493 873 509 142 753 100 212 122 112 813 563 698
## [865] 661 865 713 130 65 231 141 818 107 363 121 213 329 864 320 635 425 583
## [883] 319 128 305 328 152 318 640 754 321 521 325 511 358 678 330 703 645 490
## [901] 23 453 266 361 279 720 61 741
```

Creating a reachability diagram:

```
# Diagrama o gráfica de alcance
plot(optics_result, main= "Diagrama de alcanzabilidad de OPTICS")
```

Diagrama de alcanzabilidad de OPTICS



We have identified one large cluster, two small clusters, and two medium-sized clusters. This conclusion was reached after experimenting with different parameter values for eps (maximum distance between two points) and minPts (minimum number of points in a neighborhood) in the clustering of observations. There is a reachability order of approximately 600 points that marks the valley of a large cluster. Valleys represent high reachability distances, indicating clusters, while peaks represent the separation between clusters. We observe that the clusters are not uniform, and the reachability plot reveals a total of 5 clusters. To further analyze the clusters, we can create a reachability plot that shows the distances between nearby points within the same cluster and between different clusters.

```
## Dibujo de trazas variables alas-peso

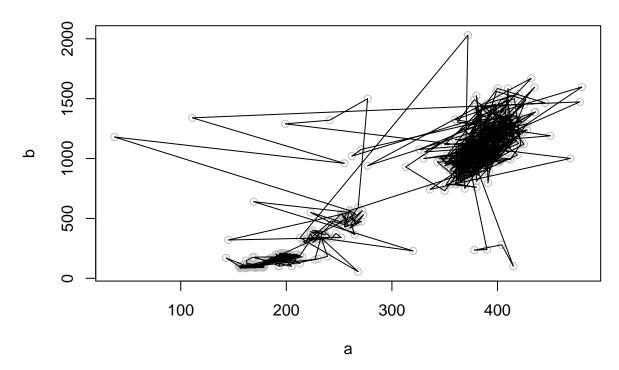
# Selección de columnas

a <- hawks_select$Wing
b <- hawks_select$Weight
c <- hawks_select$Culmen
d <- hawks_select$Hallux

# Creación de la grafica
plot(a, b, col="grey")

# agregamos trazos al par 'Alas-Peso'
title("Trazas Alas-peso")
polygon(a[optics_result$order], b[optics_result$order])</pre>
```

Trazas Alas-peso



And now the graph for the traces:

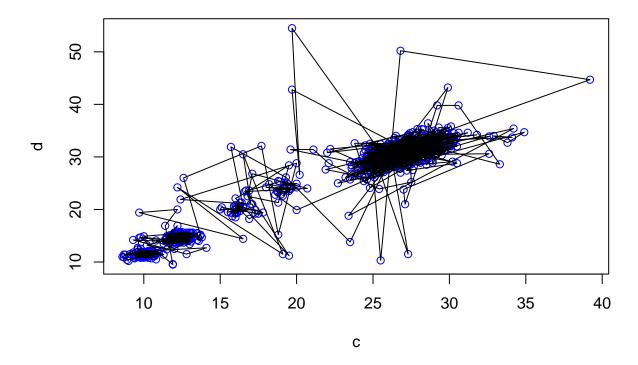
```
# Dibujo de trazas pico-espolon

c <- hawks_select$Culmen
d <- hawks_select$Hallux

# Creación de la grafica
plot(c, d, col="blue")

# agregamos trazos al par 'Alas-Peso'
title("Trazas pico-espolón")
polygon(c[optics_result$order], d[optics_result$order])</pre>
```

Trazas pico-espolón



At this point, the graphs show a large number of points and it is still difficult to understand. We decided to apply the knowledge learned in the previous PEC and use Principal Component Analysis (PCA) to reduce the dimensionality and gain better insights into the variables [@minería2023b]. We will use the devtools package and the ggbiplot library.

Devtools is an R package designed to facilitate development. It provides useful functions for development tasks, especially related to package installation from the repository and version control on GitHub. It also includes features for building, loading packages, and running tests ("Tools to Make Developing R Packages Easier," n.d.; "Function Reference," n.d.; Devtools 2023).

On the other hand, ggbiplot is an R package that provides a ggplot2-based implementation of biplot graphs for prcomp(). It is particularly useful for visualizing high-dimensional data. In a biplot, both observations and variables are represented in the same two-dimensional space. However, it should be noted that ggbiplot is no longer actively maintained (Vu 2023; MYaseen208 2014).

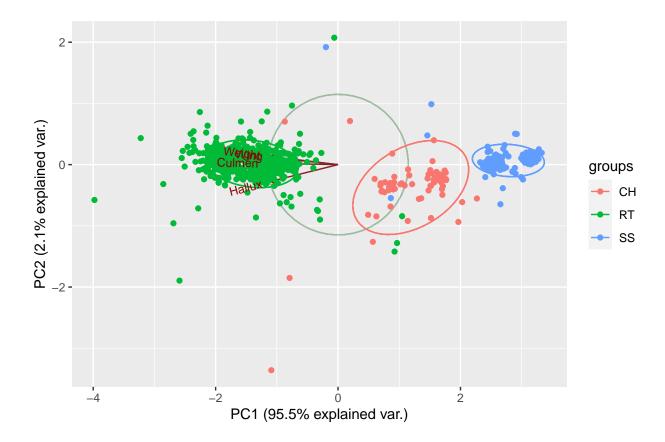
Based on the above, it is important to note that ggbiplot is not available in the official CRAN repository and needs to be installed from GitHub using an intermediary tool like devtools.

We proceed with PCA and the plot using ggbiplot.

```
# vamos a necesitar el paquete 'devtools':
if (!require('devtools')) install.packages('devtools'); library(devtools)

# usamos la función 'install_github' para la instalación de 'ggbiplot':
install_github("vqv/ggbiplot"); library(ggbiplot)

pca_result <- prcomp(hawks_select[,c("Wing", "Weight", "Culmen", "Hallux")], scale = TRUE)</pre>
```



```
# Obtener los resultados del PCA
pca_variances <- pca_result$sdev^2
pca_proportions <- pca_variances / sum(pca_variances)
pca_loadings <- pca_result$rotation

# Imprimir los resultados
cat("Varianzas explicadas por cada componente principal:\n")</pre>
```

Varianzas explicadas por cada componente principal:

```
cat(pca_variances, "\n")
```

3.818186 0.08320639 0.06543398 0.03317334

```
cat("\nProporciones de varianzas explicadas por cada componente principal:\n")
```

##

Proporciones de varianzas explicadas por cada componente principal:

```
cat(pca_proportions, "\n")
```

0.9545466 0.0208016 0.01635849 0.008293336

```
cat("\nLoadings de cada variable en cada componente principal:\n")
```

##

Loadings de cada variable en cada componente principal:

print(pca_loadings)

```
PC1
                             PC2
                                          PC3
                                                     PC4
## Wing
                      0.35899878 -0.69365839
          -0.4996307
                                               0.3746026
## Weight -0.4988718
                      0.40751286
                                  0.71581475
                                               0.2695727
## Culmen -0.5053149
                      0.06469731 -0.06588903 -0.8579800
## Hallux -0.4961381 -0.83717824 0.04589029
                                               0.2255520
```

Principal Component Analysis (PCA) is a dimensionality reduction technique that allows us to visualize and understand the structure of a multidimensional dataset. In this case, we applied PCA to a dataset of hawks with four variables of interest: wing size, culmen size, hallux size, and weight.

In this analysis, PC1 explains approximately 95% of the total variance in the data. It appears that PC1 is strongly influenced by all the variables, as the loading coefficients of the variables in PC1 are relatively similar in magnitude. This suggests that the four variables are correlated, as they increase or decrease together. Hypothetically, this could be interpreted as larger hawks tending to have longer wings, higher weight, larger culmen size, and bigger hallux, which seems logical.

The remaining principal components (PC2, PC3, and PC4) explain only a small fraction of the total variance (around 4.55%). However, they can still be useful for identifying subtle patterns in the data. For example, the loading coefficient of the Hallux variable in PC2 is negative and of large magnitude, indicating that hallux length varies in the opposite direction to the other variables in this dimension. This could suggest the existence of different adaptation strategies among hawk species.

Although this is a hypothesis and beyond the scope of this work, it is an exciting discovery. By observing a large negative loading value (-0.84) for the hallux size, we find that hawks with larger hallux have smaller culmen size, shorter wings, and lower weight. Could this indicate an evolutionary advantage for birds of this species? Could it be an adaptation strategy because the smaller bird is more agile and more effective in attacking?

As PCA is an exploratory rather than inferential technique, these hypotheses should be treated with caution. However, there is no doubt that extracting such insights from this unintelligible amalgamation of information is highly exciting. The patterns identified in this analysis need to be confirmed with further studies. Other data analysis techniques, such as clustering analysis, could be applied to identify groups of hawks with similar characteristics or to study hunting behavior. In any case, the results open up new questions that should be confirmed with other types of inferential studies.

At this point, we consider that there is "noise" in the dataset, variables that tend to confuse the model. We cannot consider these outliers, as we have mathematically shown - we believe. Before continuing with the analysis, an interesting option would be to use DBSCAN, as the groups are neither "spherical" nor have similar shapes, and it is clear that centroid-based methods like k-means present problems.

Therefore, we will analyze the dataset using DBSCAN:

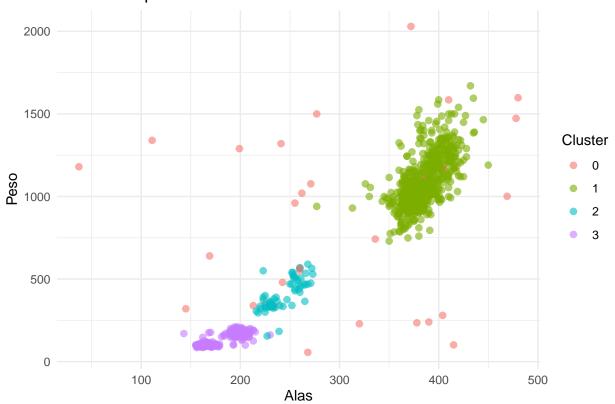
```
# Aplicando DBSCAN en terminos parecidos a la aplicación de OPTICS de partida, pero vamos
dbscan_result <- dbscan(hawks_z, eps= 0.5, minPts = 5)

# Agregamos el resultado al DF principal. Aprovechamos para agregar OPTICS tambien e integrar resultado
# Agregamos a los datos el resultado de DBSCAN
hawks_select$Dbscan_cluster <- as.factor(dbscan_result$cluster)

# agregamos a los datos el resultado de OPTICS
hawks_select$Optics_order <- as.factor(optics_result$order)

# Graficamos los clusteres en un 'scatter plot' utilizando 'Wing' y 'Weight'
ggplot(hawks_select, aes(x = Wing, y= Weight, color = Dbscan_cluster)) +
    theme_minimal() +
    geom_point(alpha = 0.6, size = 2) +
    labs(title = "Clusteres aplicando DBSCAN", x= "Alas", y = "Peso", color= "Cluster")</pre>
```

Clusteres aplicando DBSCAN



We observe more clearly that there are 3 distinguishable groups, where some observations have not been grouped according to the 'minPts' parameters.

The fpc package provides us with the ability to obtain different statistics, such as the number of clusters, their sizes, radii, etc., which could be relevant at this stage of the analysis. We have different data that lend themselves to this, so we proceed to apply different cluster stats. On one hand, we will apply it to the results of both k-means algorithms, and on the other hand, we will apply it to the results of OPTICS.

```
hawks_select$Cluster3i <- as.integer(as.character(hawks_select$Cluster3))
hawks_select$Cluster6i <- as.integer(as.character(hawks_select$Cluster6))
dist_matrix <- dist(hawks_select[, c("Wing", "Weight", "Culmen", "Hallux")])</pre>
# Sacamos las estadísticas del cluster3
clust3_stats <- cluster.stats(dist_matrix, hawks_select$Cluster3i)</pre>
clust6_stats <- cluster.stats(dist_matrix, hawks_select$Cluster6i)</pre>
print(clust3_stats)
## $n
## [1] 908
## $cluster.number
## [1] 3
## $cluster.size
## [1] 258 72 578
## $min.cluster.size
## [1] 72
##
## $noisen
## [1] 0
```

\$diameter

##

##

[1,]

\$average.distance

\$median.distance

\$average.toother

\$separation.matrix

\$separation

[1] 132.5468 1147.4518 1929.4797

[1] 50.30685 153.64087 201.17756

[1] 7.435725 7.435725 19.724350

[1] 49.7358 128.8547 160.0241

[1] 901.5759 576.2512 918.5395

[,1]

[2,] 7.435725 0.000000 19.72435

[,2]

0.000000 7.435725 166.40379

```
## [3,] 166.403786 19.724350 0.00000
##
## $ave.between.matrix
           [,1] [,2]
                              [,3]
## [1,] 0.0000 287.4075 978.0813
## [2,] 287.4075  0.0000 705.1815
## [3,] 978.0813 705.1815 0.0000
## $average.between
## [1] 862.5289
## $average.within
## [1] 154.5396
##
## $n.between
## [1] 209316
##
## $n.within
## [1] 202462
## $max.diameter
## [1] 1929.48
##
## $min.separation
## [1] 7.435725
## $within.cluster.ss
## [1] 22171518
## $clus.avg.silwidths
##
         1
## 0.8212357 0.4079904 0.7032361
##
## $avg.silwidth
## [1] 0.713353
##
## $g2
## NULL
##
## $g3
## NULL
## $pearsongamma
## [1] 0.8297008
## $dunn
## [1] 0.003853746
##
## $dunn2
## [1] 1.428626
##
## $entropy
## [1] 0.8460272
```

##

```
## $wb.ratio
## [1] 0.1791703
##
## $ch
## [1] 3682.096
##
## $cwidegap
## [1] 25.49549 530.27966 364.97685
##
## $widestgap
## [1] 530.2797
##
## $sindex
## [1] 14.56867
##
## $corrected.rand
## NULL
##
## $vi
## NULL
```

Imprimimos las estadísticas del cluster 6 print(clust6_stats)

```
## $n
## [1] 908
##
## $cluster.number
## [1] 6
##
## $cluster.size
## [1] 113 34 220 145 39 357
##
## $min.cluster.size
## [1] 34
## $noisen
## [1] 0
##
## $diameter
        92.34766 1293.59824 1038.77856 114.28263 396.50448 1208.46738
## [1]
##
## $average.distance
## [1] 15.98279 189.98254 147.29935 26.58533 74.05301 121.20192
##
## $median.distance
## [1] 11.27231 87.73374 116.79790 21.12061 46.35645 90.35535
## $separation
## [1] 3.238827 8.648699 2.469818 3.238827 7.435725 2.469818
##
## $average.toother
## [1] 785.6934 534.4848 667.0840 751.9300 586.3602 600.9891
##
```

```
## $separation.matrix
##
                       [,2]
                                  [,3]
                                            [,4]
                                                      [,5]
                                                                 [.6]
             [,1]
       0.000000 88.332384 851.410148 3.238827 23.541028 195.674372
## [2,] 88.332384 0.000000 131.617400 78.378887
                                                 8.648699 19.724350
2.469818
## [4,]
       3.238827 78.378887 810.457723
                                        0.000000
                                                  7.435725 166.403786
## [5,] 23.541028 8.648699 467.966292
                                        7.435725
                                                  0.000000 45.824993
## [6,] 195.674372 19.724350 2.469818 166.403786 45.824993
                                                             0.000000
##
## $ave.between.matrix
             [,1]
                     [,2]
                               [,3]
                                         [, 4]
                                                  [,5]
                                     78.67764 246.4084 915.7699
## [1,]
          0.00000 448.5850 1188.3015
## [2,] 448.58495 0.0000 764.9961 377.26015 225.1303 517.2763
## [3,] 1188.30153 764.9961
                            0.0000 1113.69641 945.4998 280.9675
## [4,]
        78.67764 377.2601 1113.6964
                                      0.00000 173.2561 840.9943
## [5,] 246.40843 225.1303 945.4998 173.25612
                                               0.0000 674.8356
## [6,] 915.76989 517.2763 280.9675 840.99427 674.8356
                                                        0.0000
##
## $average.between
## [1] 667.6799
##
## $average.within
## [1] 99.87152
## $n.between
## [1] 306072
##
## $n.within
## [1] 105706
##
## $max.diameter
## [1] 1293.598
##
## $min.separation
## [1] 2.469818
##
## $within.cluster.ss
## [1] 11461700
##
## $clus.avg.silwidths
   1
## 0.77725969 0.08270163 0.41214301 0.62646887 0.48767732 0.51277985
## $avg.silwidth
## [1] 0.5222836
##
## $g2
## NULL
##
## $g3
## NULL
##
## $pearsongamma
## [1] 0.5871572
```

```
##
## $dunn
##
   [1] 0.001909262
##
## $dunn2
   [1] 0.4141309
##
##
## $entropy
##
   [1] 1.520995
##
## $wb.ratio
   [1] 0.1495799
##
##
## $ch
## [1] 3008.181
##
## $cwidegap
        38.03617 530.27966 364.97685 26.30836 111.07876 320.24625
##
## $widestgap
##
   [1] 530.2797
##
## $sindex
   [1] 5.367926
##
##
## $corrected.rand
## NULL
##
## $vi
## NULL
```

We can draw several conclusions from the results:

- 1. Clusters: The first clustering method produces 3 clusters, while the second one produces 6 clusters, as we specified in the k-means algorithm. A higher number of clusters can result in a higher resolution of the data but may lead to over-segmentation, which seems to be the case here.
- 2. Minimum cluster size: The first method has a minimum cluster size of 72, while the second method has a minimum cluster size of 34. The second method identifies smaller clusters in the data. Mini-clusters can be both advantageous and disadvantageous, but in this context, it seems to be a disadvantage.
- 3. Cluster diameters: The second method identifies more compact clusters with a diameter of 1929.5, compared to 1293.6 in the first method. This seems to favor the second method, i.e., 6 clusters.
- 4. Average silhouette: The average silhouette value for the first method is 0.71, which is better than the value of 0.52 for the second method. This indicates that the first method assigns objects to clusters more effectively, making it better in this regard.
- 5. Dunn indices: The values are 0.004 and 0.002 for the first and second methods, respectively. The Dunn index is used as a metric to evaluate the quality of clustering. Values close to zero indicate poor clustering quality. Both methods seem to poorly group the objects, but the first method performs slightly better.

It appears that the first method produces clusters with a higher silhouette, while the second method identifies smaller and more compact groups. However, both methods offer subpar results overall.

We will now proceed with our analysis by applying cluster.stats to the results of DBSCAN. Unlike OPTICS, DBSCAN groups points that are close in data space and within areas of density above a threshold. It may leave some points unassigned, as we observed in the previous graph. These unassigned groups are considered noise or outliers.

Unlike OPTICS, however, DBSCAN directly provides a point-to-cluster assignment. This means that we can use cluster stats with the results of DBSCAN to obtain various clustering metrics. However, as with OPTICS, some of the metrics provided by cluster stats may be less relevant for a density-based clustering method like DBSCAN than for k-means. Nevertheless, it can be interesting to apply it and see the results.

```
## Convertimos el resultado de DBSCAN a factor
clusters_dbscan <- dbscan_result$cluster
#Eliminamos los puntos de ruido que son ceros
no_noise_idx <- which(clusters_dbscan != 0)
# Conviertimos el objeto "distancias" en una matriz completa
distancias_matrix <- as.matrix(distancias)

# Aplicamos la funcion cluster.stats
dbscan_stats <- cluster.stats(distancias_matrix[no_noise_idx, no_noise_idx], clusters_dbscan[no_noise_idx]
# Impresion de los resultados
print(dbscan_stats)</pre>
```

```
## $n
## [1] 873
## $cluster.number
## [1] 3
##
## $cluster.size
## [1] 557 59 257
## $min.cluster.size
## [1] 59
##
## $noisen
## [1] 0
##
## $diameter
## [1] 2.454986 1.660387 1.302045
## $average.distance
## [1] 0.6726576 0.6010459 0.4207059
##
## $median.distance
## [1] 0.6129363 0.6098050 0.4548728
##
## $separation
## [1] 1.0368159 0.6010496 0.6010496
##
## $average.toother
## [1] 3.955004 2.377565 3.985860
##
## $separation.matrix
```

```
[,1]
                 [,2]
## [1,] 0.000000 1.0368159 2.6057370
## [2,] 1.036816 0.0000000 0.6010496
## [3,] 2.605737 0.6010496 0.0000000
## $ave.between.matrix
            [,1]
                     [,2]
## [1,] 0.000000 2.728048 4.236678
## [2,] 2.728048 0.000000 1.617959
## [3,] 4.236678 1.617959 0.000000
## $average.between
## [1] 3.769642
##
## $average.within
## [1] 0.5936465
##
## $n.between
## [1] 191175
## $n.within
## [1] 189453
##
## $max.diameter
## [1] 2.454986
## $min.separation
## [1] 0.6010496
##
## $within.cluster.ss
## [1] 202.6517
##
## $clus.avg.silwidths
      1
                    2
## 0.7489718 0.6097164 0.7318734
## $avg.silwidth
## [1] 0.7345269
##
## $g2
## NULL
## $g3
## NULL
## $pearsongamma
## [1] 0.9029
##
## $dunn
## [1] 0.2448281
##
## $dunn2
## [1] 2.405323
##
```

```
## $entropy
## [1] 0.8288014
##
## $wb.ratio
##
   [1] 0.1574809
##
## $ch
## [1] 6951.856
##
## $cwidegap
  [1] 0.4580172 0.4829025 0.3966234
##
## $widestgap
## [1] 0.4829025
##
## $sindex
## [1] 0.7371039
##
## $corrected.rand
## NULL
##
## $vi
## NULL
```

The results obtained from the DBSCAN clustering using the cluster stats function can be summarized as follows:

• Number of clusters: Three clusters were formed.

\$cluster.number [1] 3

- Noise points were effectively removed according to the provided code.
- Cluster sizes: The cluster sizes range from 557.59 to 257 points, indicating significant variation in point density across different regions.
- Cluster diameters: The maximum distance between any pair of points within a cluster is 2.45, 1.66, and 1.30, respectively. This suggests that the dispersion within clusters varies.
- Average and median distances: These values vary in line with what has been observed so far regarding the clusters.
- Separation between clusters: The minimum separation between clusters ranges from 1.03 to 2.61. Clusters 2 and 3 are closer to each other compared to cluster 1, suggesting a possible similarity in the nature of the data grouped in these two clusters.
- Average silhouette width: The average silhouette width is relatively high at 0.73. This indicates that most points are well grouped. The silhouette width ranges from -1 to 1, with higher values indicating better assignment to clusters.
- Dunn index: A value of 0.24 is relatively low. This indicates that the clusters are not well separated or compact, which is also observed in the graphs.
- Entropy: The entropy value of 0.83 can be considered high, suggesting a fairly uniform distribution among points.

Next, we extract an ordered clustering performed by OPTICS using eps_cl = 0.065 to observe the results and see if they differ from the previously generated DBSCAN clustering.

```
## Extraccion de un clustering DBSCAN cortando la alcanzabilidad en el valor eps_cl
optics_result2 <- extractDBSCAN(optics_result, eps_cl = .99)
optics_result2</pre>
```

```
## OPTICS ordering/clustering for 908 objects.
## Parameters: minPts = 10, eps = 3.07716556342231, eps_cl = 0.99, xi = NA
## The clustering contains 2 cluster(s) and 13 noise points.
##
## 0 1 2
## 13 567 328
##
## Available fields: order, reachdist, coredist, predecessor, minPts, eps,
## eps_cl, xi, cluster
```

By manipulating the cutoff value for alkalinity, we obtain two groups with minimal noise. With other cutoff configurations, such as an eps_cl = .055, we obtain three groups with the following configuration, which seems more appropriate:

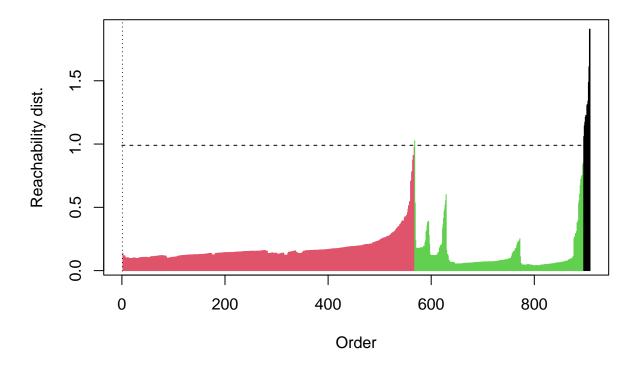
 $0\ 1\ 2\ 3$

31 559 60 258

We plotted the results.

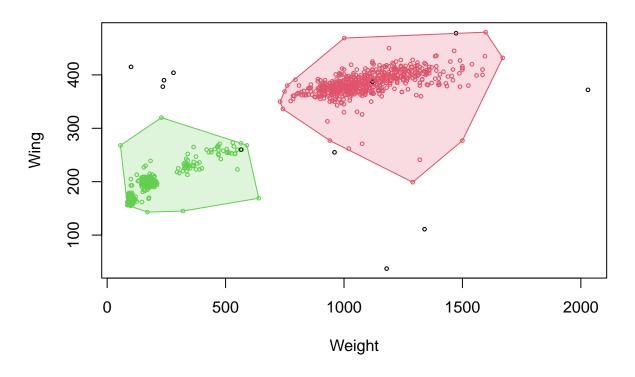
plot optics results
plot(optics_result2)

Reachability Plot

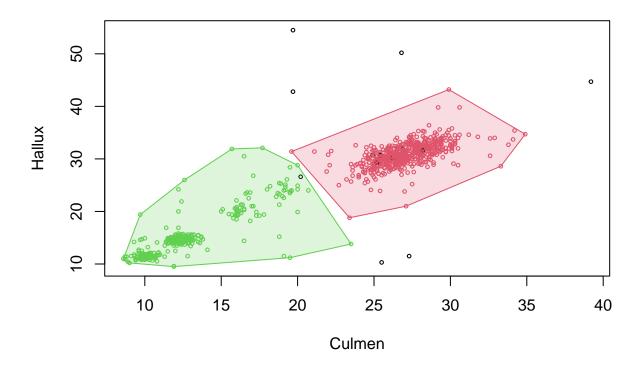


Another visualisation:

Convex Cluster Hulls



Convex Cluster Hulls



Conclusions

And at this point, we conclude the two examples. We could conclude that from the dataset, three heterogeneous clusters can be extracted, and the DBSCAN method with and without OPTICS appears to be superior to k-means for a dataset like the reference one, which has a lot of noise and data variability. However, in neither of the two cases can the results be considered satisfactory.

Comparison of Clustering Methods: K-means and DBSCAN

Clustering is a widely used method in data analysis to identify patterns and underlying structures. Two of the most popular clustering algorithms are K-means and DBSCAN. Each has its own strengths and weaknesses:

K-means

The K-means algorithm is an unsupervised prototype-based clustering method that aims to minimize the total variance within a group. It is simple and effective and has been a reference tool for decades, but with limitations. A predefined number of centroids are randomly selected, and data points are assigned to the nearest centroid or group with the closest mean. Then, the centroids are recalculated, and the process is repeated until a convergence criterion is met. This method has limitations.

It requires the prior specification of the number of clusters, which may be unknown in real-world situations.

Additionally, K-means tends to generate circular clusters and may not work well with clusters of more complex shapes or with noise, as we have seen in our dataset.

DBSCAN

DBSCAN (Density-Based Spatial Clustering of Applications with Noise) is a density-based clustering algorithm. It groups points together that have a sufficiently high number of points in their neighborhood and can discover clusters of non-linear shapes. DBSCAN does not require the prior specification of the number of clusters. On the downside, it is sensitive to the selection of input parameters, such as the maximum distance (eps) and the minimum number of points required to form a dense cluster (minPts). It can be challenging to interpret its results, especially in cases where clusters are close and exhibit density variations. This requires experience and time to fine-tune or refine the model. Additionally, DBSCAN's dependency on the Euclidean distance measure can be a disadvantage in high-dimensional datasets, where the curse of dimensionality can distort distances between points.

We have also explored the OPTICS algorithm, which can be considered an extension of DBSCAN. It addresses the limitations of DBSCAN in terms of identifying clusters with variable density. With OPTICS, it is possible to graphically represent the clustering results and extract clusters from a hierarchy of densities, which is useful in contexts where clustering patterns are not initially evident.

Comparison of Results

In our analysis, we applied both methods (or multiple methods) to a dataset of birds of prey and compared the results. Each of these algorithms has provided valuable insights.

We observed that K-means generated relatively uniform clusters with moderate variation in cluster sizes and good separation between them. However, the clustering produced by DBSCAN showed greater variation in cluster sizes and higher density within the clusters. Additionally, DBSCAN was able to identify clusters with more complex shapes than K-means and handled noise and outliers better. OPTICS provided an intuitive visual representation of the data's structure and density, allowing us to better understand the interrelationships between the identified groups.

Regarding clustering validation, we used various metrics. The average silhouette width, which measures the cohesion and separation of clusters, was high for both techniques, indicating a good assignment of points to clusters. However, the Dunn index, which is based on the relationship between the internal compactness of clusters and the separation between them, was lower for DBSCAN, suggesting that the clusters might not be well-separated or compact.

Both methods can be useful tools for data clustering, but their performance may vary depending on the characteristics of the dataset, especially with real-world data that exhibit high variance and high levels of noise, as in the case developed in this work. The choice between different techniques is part of the data scientist's work. The selection of the clustering algorithm should be guided by the nature of the dataset and the research questions, so it is vital to understand the strengths and weaknesses of each technique or method.

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