# Drug consumption

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### Importació llibreries necessàries per la pràctica

```
library(naivebayes)
                      # Necessària per fer Naive Bayes
## naivebayes 0.9.7 loaded
library(rockchalk)
                      # Necessària per la funció combineLevels
library(MASS)
                      # Utils per funcions estadístiques
## Attaching package: 'MASS'
## The following object is masked from 'package:rockchalk':
##
##
       mvrnorm
library(ca)
                      # Per fer l'anàlisi de correspondències
library(nnet)
                      \# Per a implementar la neural network
library(caret)
                      # Per al trainControl
## Loading required package: lattice
## Loading required package: ggplot2
library(randomForest) # Random forest
## randomForest 4.6-14
## Type rfNews() to see new features/changes/bug fixes.
## Attaching package: 'randomForest'
## The following object is masked from 'package:ggplot2':
##
##
       margin
```

```
library(ggplot2) # Per fer plots
```

Lectura de la base de dades.

#### Binarització de les variable resposta

## The original levels CL3 CL4 CL5 CL6 NON-USER ## have been replaced by NON-USER USER  $\,$ 

Copiem la base de dades en dd2 per poder fer un estudi previ coherent i sense la pèrdua d'interpretabilitat que genera el tractament previ que han tingut les dades i la consegüent transformació de factors a valors reals.

```
dd2$Nscore = as.integer(dd2$Nscore)
dd2$Escore = as.factor(dd2$Escore)
levels(dd2$Escore) = setdiff(16:59, 17)
dd2$Escore = as.integer(dd2$Escore)
dd2$0score = as.factor(dd2$0score)
levels(dd2$0score) = setdiff(24:60, c(25, 27))
dd2$0score = as.integer(dd2$0score)
dd2$Ascore = as.factor(dd2$Ascore)
levels(dd2$Ascore) = setdiff(12:60, c(13, 14, 15, 17, 19, 20, 21, 22))
dd2$Ascore = as.integer(dd2$Ascore)
dd2$Cscore = as.factor(dd2$Cscore)
levels(dd2$Cscore) = setdiff(17:59, c(18, 58))
dd2$Cscore = as.integer(dd2$Cscore)
dd2$Impulsive = as.factor(dd2$Impulsive)
levels(dd2$Impulsive) = 1:10
dd2$Impulsive = as.integer(dd2$Impulsive)
dd2$SS = as.factor(dd2$SS)
levels(dd2$SS) = 1:11
dd2$SS = as.integer(dd2$SS)
```

## 1. Preprocessament de les dades

### 1.1 Estudi de les dades

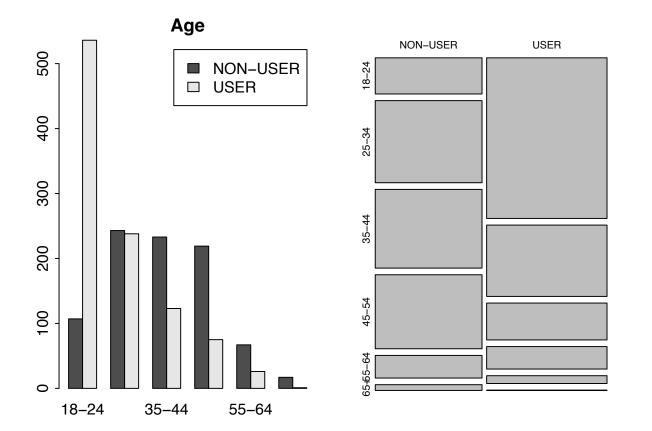
```
summary(dd2[, c(2:13, 29, 18)])
```

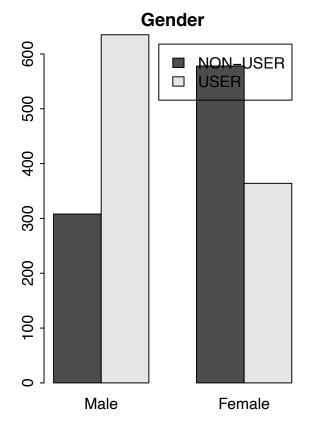
```
Gender
                                           Education
##
      Age
                                                            Country
  18-24:643 Male :943 > 18
##
                                                :506 USA
                                                               : 557
## 25-34:481
             Female:942 University
                                                :480 New Zealand: 5
## 35-44:356
                          Master
                                                :283
                                                      Other
                                                               : 118
## 45-54:294
                          Professional Certificate:270
                                                      Australia : 54
## 55-64: 93
                          18
                                               :100
                                                                : 20
                                                      Ireland
                                                               : 87
## 65+ : 18
                          16
                                               : 99
                                                      Canada
                                               :147
##
                          (Other)
                                                      IJK
                                                                :1044
##
       Nscore
                     Escore
                                    Oscore
                                                  Ascore
## Min. : 1.00
                Min. : 1.00
                               Min. : 1.00
                                             Min. : 1.00
                1st Qu.:19.00
   1st Qu.:18.00
                               1st Qu.:16.00
                                              1st Qu.:20.00
## Median :25.00
                Median :24.00
                               Median :21.00
                                              Median :24.00
        :24.92
                Mean :23.58
                                                    :23.88
## Mean
                                Mean :20.77
                                               Mean
## 3rd Qu.:31.00 3rd Qu.:28.00
                                3rd Qu.:26.00
                                               3rd Qu.:29.00
## Max. :49.00 Max. :42.00
                                Max. :35.00
                                              Max. :41.00
##
##
       Cscore
                    Impulsive
                                      SS
                                                Alcohol
                                                         Nicotine
## Min. : 1.00
                Min. : 1.000
                                      : 1.000 CL0: 34
                                                         CL0:428
                                 Min.
```

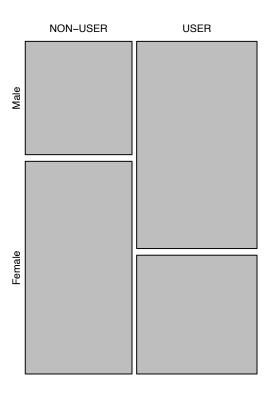
```
1st Qu.:20.00
                   1st Qu.: 3.000
                                    1st Qu.: 5.000
                                                     CL1: 34
                                                               CL1:193
##
   Median :25.00
                   Median : 4.000
                                    Median : 7.000
                                                     CL2: 68
##
                                                               CL2:204
##
                   Mean : 4.801
   Mean
         :24.44
                                    Mean : 6.561
                                                     CL3:198
                                                               CL3:185
   3rd Qu.:29.00
                   3rd Qu.: 6.000
                                    3rd Qu.: 9.000
                                                     CL4:287
                                                               CL4:108
##
                   Max. :10.000
##
   Max. :41.00
                                    Max. :11.000
                                                     CL5:759
                                                               CL5:157
                                                     CL6:505
                                                               CL6:610
##
##
       Cannabis
##
   NON-USER:886
   USER
           :999
##
##
##
##
##
##
```

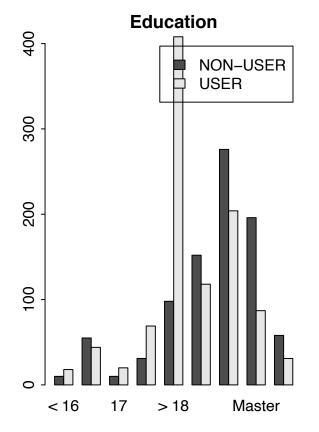
### 1.2 Barplots i graficació de taules de contingència

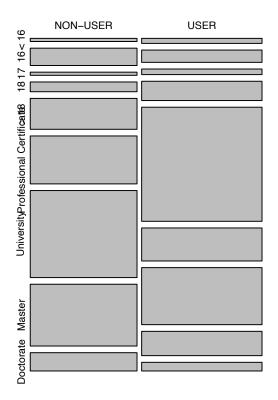
```
par(mfrow = c(1, 2), mex = 0.4)
for(i in c(2:5, 13, 29)) {
   tab = table(dd2$Cannabis, dd2[,i])
   barplot(tab, beside = TRUE, legend = levels(dd$Cannabis), main = colnames(dd2)[i])
   plot(tab, main = "")
}
```

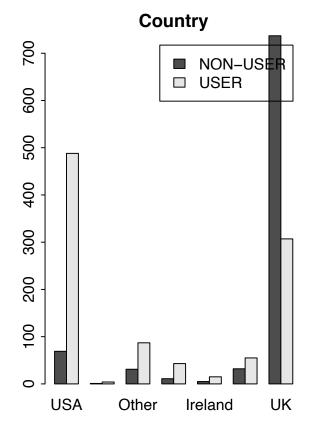


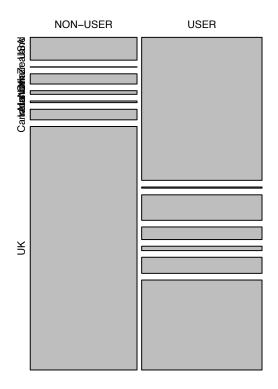


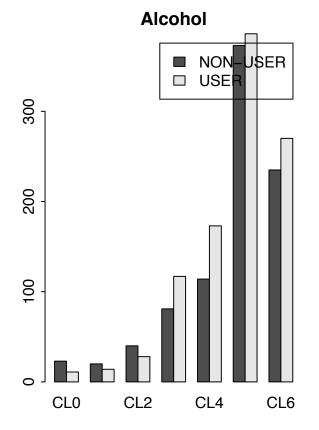


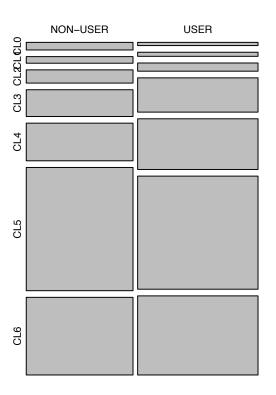


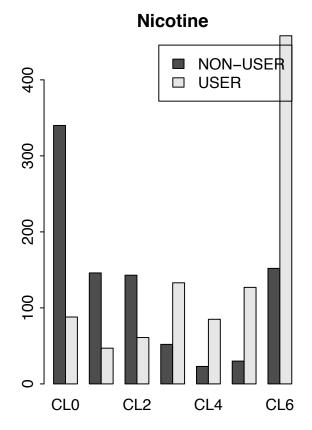


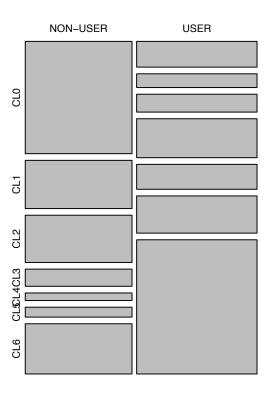




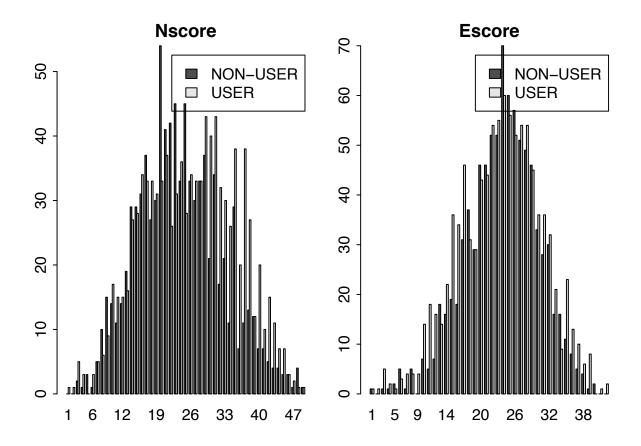


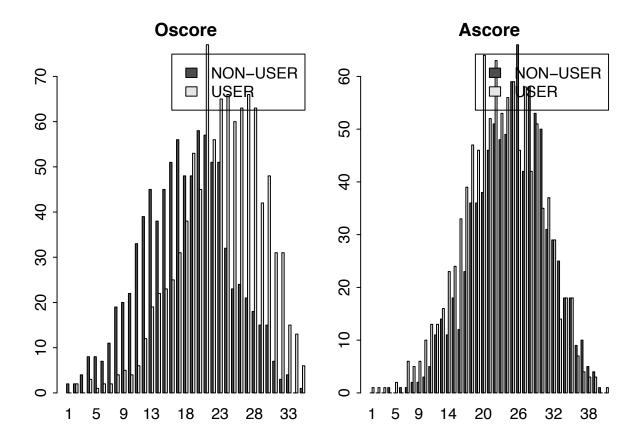


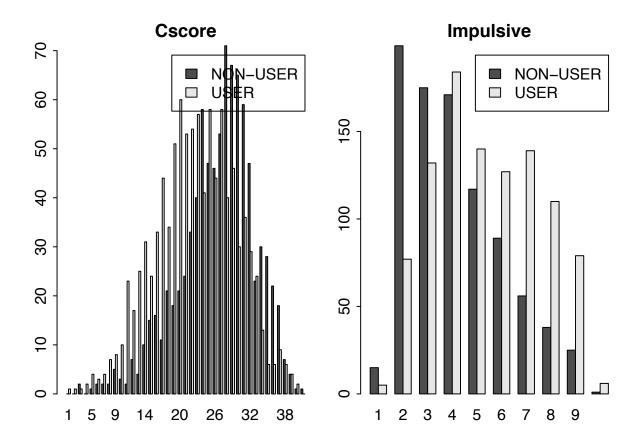


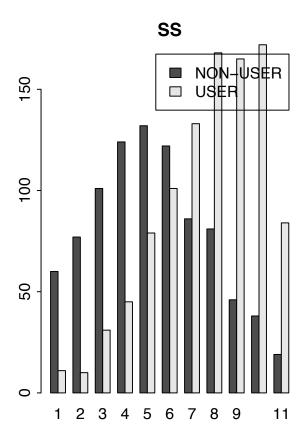


```
for(i in 6:12) {
   tab = table(dd2$Cannabis, dd2[,i])
   barplot(tab, beside = TRUE, legend = levels(dd$Cannabis), main = colnames(dd2)[i])
}
```

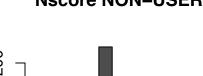




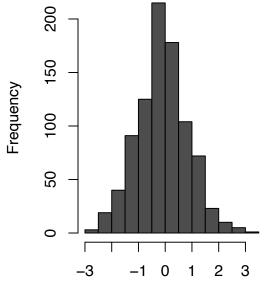




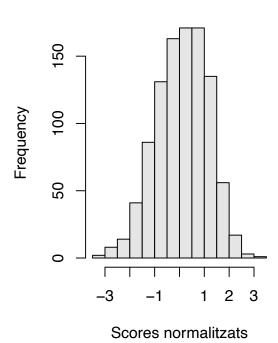
### 1.3 Histogrames scores

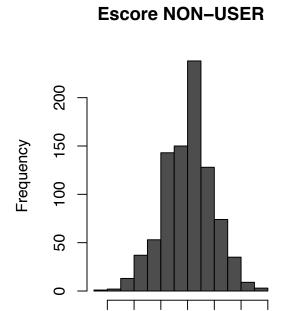


# **Nscore NON-USER**



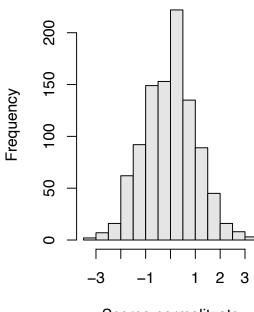
**Nscore USER** 





-3





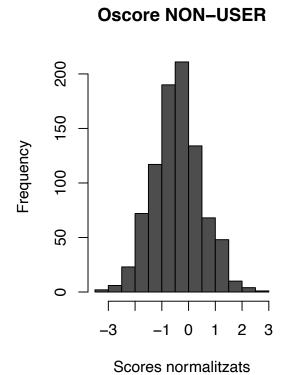
**-1** 0

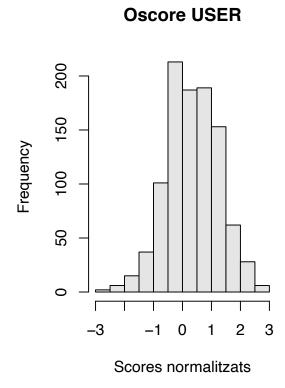
2

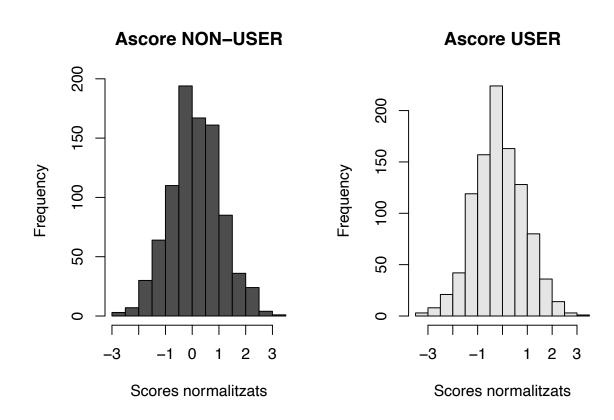
3

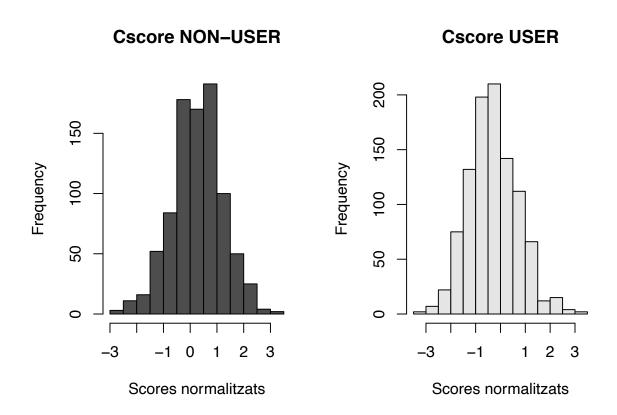
1

Scores normalitzats





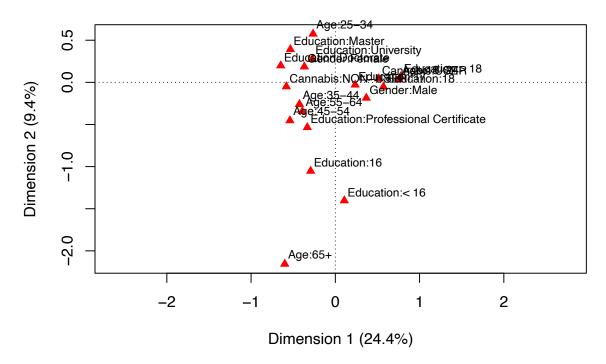




# 1.4 Anàlisi de correspondències

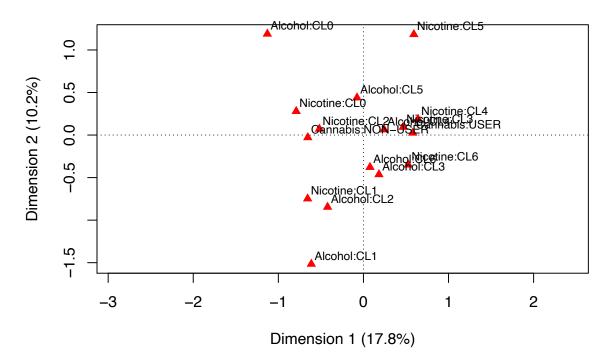
```
ca = mjca(dd2[,c(2:4, 18)], lambda = "Burt")
plot(ca, main = "Edat, educació i gènere")
```

# Edat, educació i gènere



```
ca = mjca(dd2[,c(13, 29, 18)], lambda = "Burt")
plot(ca, main = "Alcohol i nicotina")
```

# Alcohol i nicotina

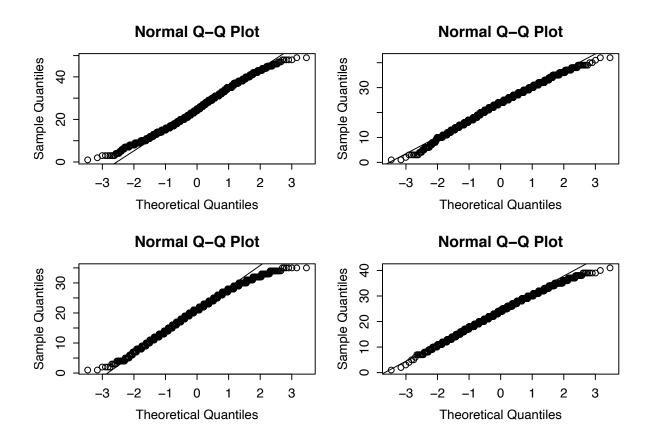


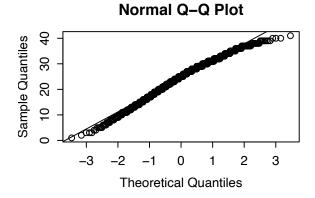
### 1.5 Test de Wilcox per les variables de personalitat

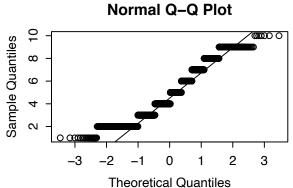
### 1.5.1 Normalitat variables de personalitat

```
par(mfrow = c(2, 2), mex = 0.7)

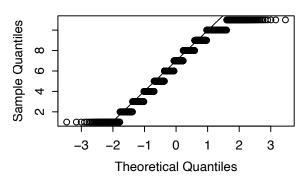
for (i in 6:12) {
    qqnorm(dd2[, i])
    qqline(dd2[, i])
}
```







### Normal Q-Q Plot



```
for (i in 6:12){
   print(wilcox.test(dd[, i] ~ dd$Cannabis))
}
```

```
##
##
   Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 380418, p-value = 1.355e-07
## alternative hypothesis: true location shift is not equal to 0
##
##
##
    Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 455765, p-value = 0.2623
\#\# alternative hypothesis: true location shift is not equal to 0
##
##
##
   Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 240522, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0
##
##
```

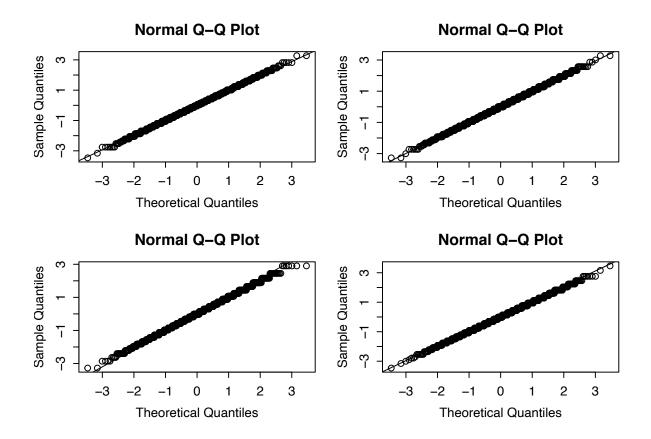
```
##
   Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 507898, p-value = 2.923e-08
## alternative hypothesis: true location shift is not equal to 0
##
##
## Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 593386, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0
##
##
## Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 293817, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0
##
##
##
   Wilcoxon rank sum test with continuity correction
##
## data: dd[, i] by dd$Cannabis
## W = 209760, p-value < 2.2e-16
## alternative hypothesis: true location shift is not equal to 0
```

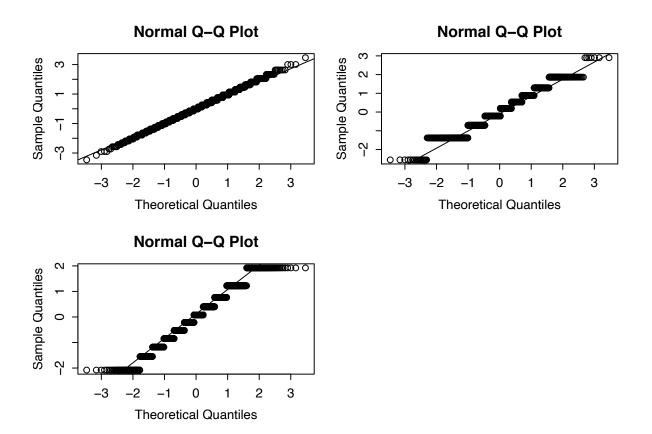
### 1.6 Estudi normalitat per a l'ús de QDA i LDA

Normalitat variable per variable en la base de dades dd que és la base amb les transformacions a valors reals que serà la que s'utilitzarà per a la implementació de QDA i LDA.

```
par(mfrow = c(2, 2), mex = 0.7)

for (i in 6:12) {
    qqnorm(dd[, i])
    qqline(dd[, i])
}
```

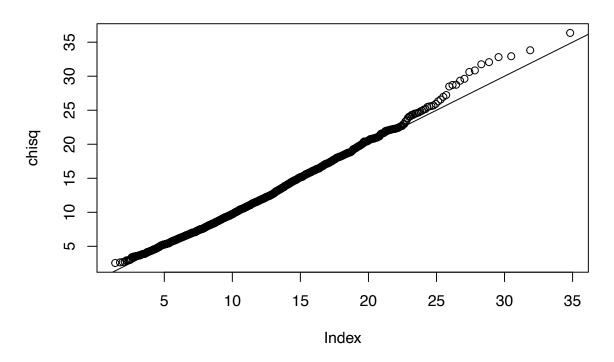




Normalitat multivariada de tot el conjunt de variables explicatives que conformen les dades d'entrenament.

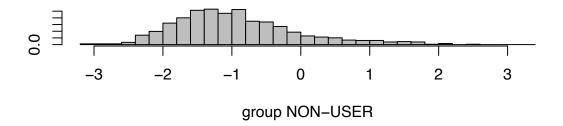
```
db = as.matrix(dd[,2:12])
S = cov(db) # Matriu de covariâncies
d = matrix(0, 1, nrow(db))
m = apply(db,2,mean)
# Mahanalobis
for (i in 1:nrow(db)){
   d[i] = t(db[i,] - m) \%\% solve(S) \%\% (db[i,] - m)
}
# Ordenem pel rank
d = sort(d);
# Correcció de ranks
aux = seq(1, nrow(db))
aux = (aux - 0.5) / nrow(db)
plot(qchisq(aux, ncol(db)), d,xlab = "Index", ylab = "chisq",
     main = "Test normal multivariada")
abline(0, 1)
```

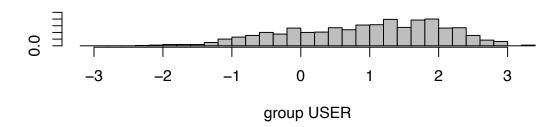
# Test normal multivariada



### 1.6.1 Plot LDA

```
1 = lda(dd[, c(2:12)], grouping = dd[, "Cannabis"])
plot(1, col = "grey")
```





### 2. Entrenament

### 2.1 Separació les dades en training y test

Traiem la variable *Escore* que hem detectat que és no significativa.

```
dd = dd[,-7]

dd2 = dd2[,-7]
```

```
n = nrow(dd)
set.seed(20)
samples = sample(n, round(0.75*n))  # Reservem el 25% de les dades per test
train = dd2[samples, c(2:12, 28, 17)]  # Dades de train amb categories
train.real = dd[samples, c(2:12, 28, 17)]  # Dades de training amb reals
test = dd2[-samples, c(2:12, 28, 17)]  # Dades de test amb categories
test.real = dd[-samples, c(2:12, 28, 17)]  # Dades de test amb reals

ntr = nrow(train)
nte = nrow(test)
```

### **Funcions auxiliars**

### 2.2 Error QDA

Donat un conjunt de dades d'entrenament i de validació i les seves respectives respostes retorna l'error sobre el conjunt de validació havent creat un model amb QDA (suposició de matrius de covariàncies diferents) amb les dades d'entrenament.

```
error_qda = function (X1, y1, Xv, yv, flag) {
  out = qda(y1 ~ ., data = X1)
  pred = predict(out, newdata = Xv)$class
  prediction = table(Truth = yv, Pred = pred)
  if (flag) print(prediction)
  err = 1 - sum(diag(prediction))/length(yv)
}
```

### 2.3 Error LDA

Donat un conjunt de dades d'entrenament i de validació i les seves respectives respostes retorna l'error sobre el conjunt de validació havent creat un model amb LDA (suposició de matrius de covariàncies iguals) amb les dades d'entrenament.

```
error_lda = function (X1, y1, Xv, yv, flag) {
  out = lda(y1 ~ ., data = X1)
  pred = predict(out, newdata = Xv)$class
  prediction = table(Truth = yv, Pred = pred)
  if (flag) print(prediction)
  err = 1 - sum(diag(prediction))/length(yv)
}
```

### 2.4 Error GLM

Aquesta funció genera un model lineal generaltizat binomial amb link inidicat al paràmetre d'entrada *linkage* amb les dades d'entrenament i retorna l'error comés sobre el conjunt de dades de validació. De nou incloem un *flag* que ens indica si volem fer el print de taula de confusió o no.

```
error_glm = function (X1, y1, Xv, yv, linkage, flag) {
    # Generació del model amb les dades de learn
    mod = glm(y1 ~ ., family = binomial(link = linkage), data = as.data.frame(X1))

# Predicció sobre les dades de validació
PI = predict(mod, newdata = as.data.frame(Xv), type = "response")
PI = as.factor(round(PI))
levels(PI) = c("USER", "NON-USER")
prediction = table(Truth = yv, Pred = PI)
if (flag) print(prediction)
err = 1 - sum(diag(prediction))/length(yv)
}
```

### 2.5 Error Naive-Bayes

Retorna l'error de predicció sobre el conjunt de dades de validació entrenant un model Naive-Bayes per classificar amb les dades d'entrenament passades com a entrada.

```
error_naivebayes = function (X1, y1, Xv, yv, flag) {
    # Generació del model amb les dades de learn
    mod = naive_bayes(X1, y1, laplace = 0.1)

# Predicció sobre les dades de validació
PI = predict(mod, newdata = Xv, type = "class")
prediction = table(Truth = yv, Pred = PI)
    if (flag) print(prediction)
    err = 1 - sum(diag(prediction))/length(yv)
}
```

### 2.6 Multilayer perceptron

Donat un conjunt de dades de train i de test retorna l'error sobre el conjunt de test en implementar un *Multilayer perceptron* amb una única capa oculta amb el nombre de neurones i *decay* indicats a l'entrada.

```
error_nnet = function (X1, y1, Xv, yv, size, decay, flag) {
   out = nnet(y1 ~ ., data = X1, size = size, decay = decay, maxit = 10000, trace = F, MaxNWts = 10000)
   pred = predict(out, newdata = Xv, type = "class")
   prediction = table(Truth = yv, Pred = pred)
   if (flag) print(prediction)
   err = 1 - sum(diag(prediction))/length(yv)
}
```

### 2.6.1 Elecció hiperparàmetres nnet

Fem un plot de l'error de training i de validació en fer un 10-times 10-fold cross validation modificant el número de neurones de la capa oculta de la xarxa.

```
sizes = seq(1, 16, 1)

tr.error = rep(0, 16)
te.error = rep(0, 16)
cont = 1

for (k in sizes) {
    err = c("training" = 0, "test" = 0)
    for (i in 1:10) {
        samples = sample(ntr) # Barrejem aleatôriament les dades de training
        for (j in 1:10) {
            start = round((j - 1)*ntr/10 + 1) # Índex inici
            end = round(j * ntr/10) # Índex final

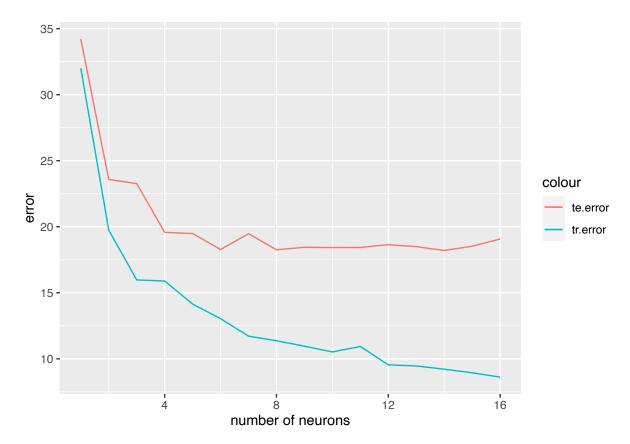
        # Separem en variables explicatives i resposta / learn i validation
        Xl = train[samples[-(start:end)], -13]
        yl = train[samples[start:end], -13]
        Xv = train[samples[start:end], -13]
```

```
yv = train[samples[start:end], 13]

err["test"] = err["test"] + error_nnet(Xl, yl, Xv, yv, k, 0, F)
    err["training"] = err["training"] + error_nnet(Xl, yl, Xl, yl, k, 0, F)
}

tr.error[cont] = err["training"]
te.error[cont] = err["test"]
cont = cont + 1
}

ggplot(as.data.frame(tr.error), aes(sizes)) +
    geom_line(aes(y = tr.error, colour = "tr.error")) +
    geom_line(aes(y = te.error, colour = "te.error")) +
    labs(x = "number of neurons", y = "error")
```



```
best.size = 10
```

Agafem 10 neurones ja que observem que a partir d'aquest punt sobreparametritzem. Fixem ara el nombre de neurones i busquem el decay òptim de nou amb un 10-times 10-fold cross validation.

```
set.seed(41)
decays = seq(1.5, 2.5, by = 0.1)
trc = trainControl(method = "repeatedcv", number = 10, repeats = 10)
model.10x10CV = train(Cannabis ~ ., data = train,
```

```
method = 'nnet', maxit = 1000, trace = FALSE,
                     tuneGrid = expand.grid(.size = best.size, .decay = decays), trControl = trc)
(decay = model.10x10CV$bestTune$decay)
## [1] 2.5
model.10x10CV
## Neural Network
##
## 1414 samples
##
   12 predictor
##
     2 classes: 'NON-USER', 'USER'
##
## No pre-processing
## Resampling: Cross-Validated (10 fold, repeated 10 times)
## Summary of sample sizes: 1272, 1272, 1273, 1272, 1273, 1273, ...
## Resampling results across tuning parameters:
##
    decay Accuracy
##
                      Kappa
##
    1.5
           0.8385296 0.6765912
##
    1.6
           0.8379607 0.6754303
          0.8390196 0.6775250
##
    1.7
    1.8 0.8394521 0.6784082
##
##
    1.9 0.8381795 0.6758508
##
    2.0 0.8381810 0.6758625
##
    2.1 0.8379682 0.6754402
##
    2.2 0.8388153 0.6770783
##
    2.3 0.8386735 0.6768058
##
    2.4 0.8380367 0.6755508
##
    2.5
           0.8395914 0.6786145
##
## Tuning parameter 'size' was held constant at a value of 10
## Accuracy was used to select the optimal model using the largest value.
## The final values used for the model were size = 10 and decay = 2.5.
```

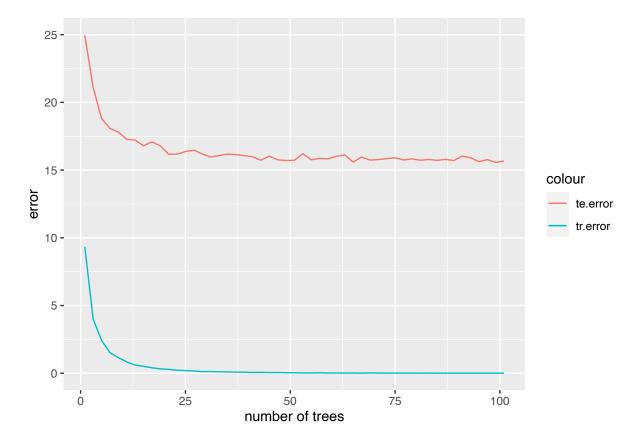
### 2.7 Random forest

Aquest funció retorna l'error en ajustar un model amb un Random Forest de mida k.

```
error_randomforest = function (X1, y1, Xv, yv, k, flag) {
    rf = randomForest (y1 ~ ., data = as.data.frame(X1), ntree = k, proximity = FALSE)
    pred = predict(rf, newdata = Xv, type = "class")
    prediction = table(Truth = yv, Pred = pred)
    if (flag) print(prediction)
    err = 1 - sum(diag(prediction))/length(yv)
}
```

Fem un plot de l'error de training i de validació en fer 10-times 10-fold cross validation en canviar el nombre d'arbres d'un Random Forest.

```
set.seed(12)
ntrees = seq(1, 101, 2)
min_err = 100
tr.error = rep(0, 51)
te.error = rep(0, 51)
cont = 1
for (k in ntrees) {
  err = c("training" = 0, "test" = 0)
  for (i in 1:10) {
      samples = sample(ntr) # Barrejem aleatòriament les dades de training
     for (j in 1:10) {
         start = round((j - 1)*ntr/10 + 1) # Índex inici
         end = round(j * ntr/10) # Índex final
         # Separem en variables explicatives i resposta / learn i validation
         X1 = train[samples[-(start:end)], -13]
         yl = train[samples[-(start:end)], 13]
         Xv = train[samples[start:end], -13]
         yv = train[samples[start:end], 13]
         err["test"] = err["test"] + error_randomforest(X1, y1, Xv, yv, k, F)
         err["training"] = err["training"] + error_randomforest(X1, y1, X1, y1, k, F)
  }
  tr.error[cont] = err["training"]
  te.error[cont] = err["test"]
   cont = cont + 1
}
ggplot(as.data.frame(tr.error), aes(ntrees)) +
 geom_line(aes(y = tr.error, colour = "tr.error")) +
 geom_line(aes(y = te.error, colour = "te.error")) +
 labs(x = "number of trees", y = "error")
```



best.ntree = 50

### 2.8 Cross-validation

Fem un 10 times 10-fold cross validation per avaluar quin dels models proposats és el millor. En aquest cas hem usat QDA, LDA, GLM link logit, GLM link probit, GLM link loglog, Naive Bayes, MLP i Random Forest.

```
# 2. Raining i validation amb la base de dades amb reals
      Xl.r = train.real[samples[-(start:end)], -(11:13)]
      yl.r = train.real[samples[-(start:end)], 13]
      Xv.r = train.real[samples[start:end], -(11:13)]
      yv.r = train.real[samples[start:end], 13]
      # Actualització errors
      error["QDA"] = error["QDA"] + error_qda(Xl.r, yl.r, Xv.r, yv.r, F)
      error["LDA"] = error["LDA"] + error_lda(X1.r, y1.r, Xv.r, yv.r, F)
      error["GLM-logit"] = error["GLM-logit"] + error_glm(X1, y1, Xv, yv, "logit", F)
      error["GLM-probit"] = error["GLM-probit"] + error_glm(X1, y1, Xv, yv, "probit", F)
      error["GLM-loglog"] = error["GLM-loglog"] + error_glm(X1, y1, Xv, yv, "cloglog", F)
      error["Naive-Bayes"] = error["Naive-Bayes"] + error_naivebayes(X1, y1, Xv, yv, F)
      error["Nnet"] = error["Nnet"] + error_nnet(X1, y1, Xv, yv, best.size, decay, F)
      error["Random Forest"] = error["Random Forest"] + error_randomforest(X1, y1, Xv, yv,
                                                                            best.ntree, F)
   }
}
error
##
             QDA
                           LDA
                                   GLM-logit
                                                GLM-probit
                                                               GLM-loglog
##
        19.57712
                      18.45964
                                    15.95485
                                                   15.96883
                                                                 17.12187
##
     Naive-Bayes
                          Nnet Random Forest
##
        17.30591
                      16.04041
                                    15.91295
2.9 Error sobre les dades de test
set.seed(0415)
droga = "Cannabis"
print("GLM")
## [1] "GLM"
a = cbind("te. error", error_glm(train[, -13], train[, droga], test[, -13],
                                 test[, droga], "logit", T))
             Pred
## Truth
             NON-USER
                        USER
##
     NON-USER 174
                         32
##
     USER.
                        224
a = rbind(a, cbind("tr. error", error_glm(train[, -13], train[, droga], train[, -13],
                                           train[, droga], "logit", T)))
##
             Pred
             NON-USER
                        USER
## Truth
    NON-USER 587
                        93
```

##

USER

104

630

```
##
       [,1]
                  [,2]
## [1,] "te. error" "0.154989384288747"
## [2,] "tr. error" "0.139321074964639"
print("Naive Bayes")
## [1] "Naive Bayes"
a = cbind("te. error", error_naivebayes(train[, -13], train[, droga], test[, -13],
                                      test[, droga], T))
##
            Pred
           NON-USER USER
## Truth
   NON-USER 171 35
                  48 217
    USER
a = rbind(cbind(a, error_naivebayes(train[, -13], train[, droga], train[, -13],
                            train[, droga], T)))
##
            Pred
## Truth
           NON-USER USER
##
    NON-USER 574 106
    USER
                 131 603
       [,1]
                  [,2]
                                      [,3]
## [1,] "te. error" "0.176220806794055" "0.167609618104668"
print("nnet")
## [1] "nnet"
a = cbind("te. error", error_nnet(train[, -13], train[, droga], test[, -13],
                              test[, droga], best.size, decay, T))
##
            Pred
           NON-USER USER
## Truth
    NON-USER
                170 36
##
##
    USER
                  41 224
a = rbind(a, cbind("tr. error", error_nnet(train[, -13], train[, droga], train[, -13],
                                        train[, droga], best.size, decay, T)))
            Pred
##
           NON-USER USER
## Truth
##
    NON-USER 583 97
                 99 635
##
    USER
```

```
##
      [,1] [,2]
## [1,] "te. error" "0.16348195329087"
## [2,] "tr. error" "0.138613861386139"
print("Random Forest")
## [1] "Random Forest"
a = cbind("te. error", error_randomforest(train[, -13], train[, droga], test[, -13],
                                       test[, droga], best.ntree, T))
##
           Pred
## Truth NON-USER USER
## NON-USER 167 39
                 42 223
    USER
a = rbind(a, cbind("tr. error", error_randomforest(train[, -13], train[, droga],
                                                train[, -13], train[, droga],
                                                best.ntree, T)))
##
           Pred
## Truth NON-USER USER
##
    NON-USER 680 0
    USER
                 1 733
##
##
       [,1]
                  [,2]
## [1,] "te. error" "0.171974522292994"
## [2,] "tr. error" "0.000707213578500676"
```