The presence of sprouted or diseased kernels in wheat can reduce the value of a wheat producers entire crop. It is important to identify these kernels after being harvested, prior to sale.
To this end, a study was conducted examining physical properties of a kernel: density, hardness, size, weight, and moisture content. Two different classes of wheat were considered, hard red winter (hrw) and soft red winter (srw). By visual inspection each kernel condition was classified as `Healthy, Sprout`, or `Scab`. The data is available in file `wheat.csv` on blackboard.

a) Fit a multinomial regression model to identify the properties affecting the kernel condition. Use `Healthy` as the base level for the response.

b) What predictors have a different effect on (all or some) kernel conditions?

c) Find CIs on each estimated coefficient.

d) Predict probabilities for each observed kernel condition.

e) Estimate odds ratios for a one standard deviation change in each predictor.

f) Find a CI on each odds ratio.

g) Fit a multinomial model with `density` as predictor.

h) Plot the probability curves from this multinomial model.

```
wheat = read.csv("wheat.csv",header=T)
str(wheat)
#'data.frame':   275 obs. of  7 variables:
# $ class   : Factor w/ 2 levels "hrw","srw": 1 1 1 1 1 1 1 1 1 1 ...
# $ density : num  1.35 1.29 1.23 1.34 1.26 ...
# $ hardness: num  60.3 56.1 44 53.8 44.4 ...
# $ size    : num  2.3 2.73 2.51 2.27 2.35 ...
# $ weight  : num  24.6 33.3 31.8 32.7 26.1 ...
# $ moisture: num  12 12.2 11.9 12.1 12.1 ...
# $ type    : Factor w/ 3 levels "Healthy","Scab",..: 1 1 1 1 1 1 1 1 1 1 ...

head(wheat)
#  class  density hardness    size  weight moisture    type
#1   hrw 1.349253 60.32952 2.30274 24.6480 12.01538 Healthy
#2   hrw 1.287440 56.08972 2.72573 33.2985 12.17396 Healthy
#3   hrw 1.233985 43.98743 2.51246 31.7580 11.87949 Healthy
#4   hrw 1.336534 53.81704 2.27164 32.7060 12.11407 Healthy
#5   hrw 1.259040 44.39327 2.35478 26.0700 12.06487 Healthy
#6   hrw 1.300258 48.12066 2.49132 33.2985 12.18577 Healthy

summary(wheat)
# class        density          hardness            size            weight          moisture
# hrw:143   Min.   :0.7352   Min.   :-44.080   Min.   :0.5973   Min.   : 8.532   Min.   : 6.486   Hea
# srw:132   1st Qu.:1.1358   1st Qu.:  0.689   1st Qu.:1.8900   1st Qu.:21.982   1st Qu.: 9.540   Sca
#           Median :1.2126   Median : 24.465   Median :2.2303   Median :27.610   Median :11.909   Spr
#           Mean   :1.1885   Mean   : 25.564   Mean   :2.2047   Mean   :27.501   Mean   :11.192
#           3rd Qu.:1.2687   3rd Qu.: 45.606   3rd Qu.:2.5125   3rd Qu.:32.882   3rd Qu.:12.538
#           Max.   :1.6454   Max.   :111.934   Max.   :4.3100   Max.   :46.334   Max.   :14.514

levels(wheat$type)  #Shows the 3 categories
# "Healthy" "Scab"    "Sprout"

# We want to predict type using all other predictors (with class as categorical)

# multinomial regression model
#=============================================================================

library(nnet)
m1 = multinom(type~., wheat)
summary(m1)
# Coefficients:
#       (Intercept)   classsrw   density    hardness      size     weight    moisture
#Scab      30.54650 -0.6481277 -21.59715 -0.01590741 1.0691139 -0.2896482  0.10956505
#Sprout    19.16857 -0.2247384 -15.11667 -0.02102047 0.8756135 -0.0473169 -0.04299695

#Std. Errors:
#       (Intercept)  classsrw  density    hardness      size     weight  moisture
```

```
#Scab      4.289865 0.6630948 3.116174 0.010274587 0.7722862 0.06170252 0.1548407
#Sprout    3.767214 0.5009199 2.764306 0.008105748 0.5409317 0.03697493 0.1127188

#Residual Deviance: 384.2247
#AIC: 412.2247

# fitted equations

# log(pi-scab/pi-healthy) = 30.54650 -0.6481277 class -21.59715 density -0.01590741 hardness +1.06911

# log(pi-sprout/pi-healthy) = 19.17 -0.2247384 class -15.11667 density -0.02102047 hardness  + 0.8756

summary(m1,Wald=T)

#Coefficients:
#       (Intercept)   classsrw   density    hardness      size     weight    moisture
#Scab      30.54650 -0.6481277 -21.59715 -0.01590741 1.0691139 -0.2896482  0.10956505
#Sprout    19.16857 -0.2247384 -15.11667 -0.02102047 0.8756135 -0.0473169 -0.04299695

#Std. Errors:
#       (Intercept)  classsrw  density    hardness      size     weight  moisture
#Scab      4.289865 0.6630948 3.116174 0.010274587 0.7722862 0.06170252 0.1548407
#Sprout    3.767214 0.5009199 2.764306 0.008105748 0.5409317 0.03697493 0.1127188

#Value/SE (Wald statistics):
#       (Intercept)   classsrw   density  hardness     size    weight   moisture
#Scab      7.120620 -0.9774285 -6.930664 -1.548229 1.384349 -4.694269  0.7075983
#Sprout    5.088261 -0.4486513 -5.468523 -2.593279 1.618714 -1.279702 -0.3814532

#Residual Deviance: 384.2247
#AIC: 412.2247

# but no p-values shown, so try this way

# tests
sum.fit  = summary(m1)
test.stat = sum.fit$coefficients/sum.fit$standard.errors
p.value  = 2*(1-pnorm(q = abs(test.stat)))
test.stat
#       (Intercept)   classsrw   density  hardness     size    weight   moisture
#Scab      7.120620 -0.9774285 -6.930664 -1.548229 1.384349 -4.694269  0.7075983
#Sprout    5.088261 -0.4486513 -5.468523 -2.593279 1.618714 -1.279702 -0.3814532

p.value
#        (Intercept)  classsrw      density    hardness      size       weight  moisture
#Scab   1.074474e-12 0.3283570 4.188649e-12 0.121567269 0.1662515 2.675618e-06 0.4791947
#Sprout 3.613623e-07 0.6536832 4.538002e-08 0.009506554 0.1055089 2.006500e-01 0.7028670
```

```
round(p.value,3)
#       (Intercept) classsrw density hardness   size weight moisture
#Scab             0   0.3284       0   0.1216 0.1663 0.0000   0.4792
#Sprout           0   0.6537       0   0.0095 0.1055 0.2006   0.7029

# There is no evidence that wheat class, size, and moisture have different effects on kernel conditio
# There is evidence that hardness has some effect on kernel Sprout only
# There is evidence that weight has some effect on kernel Scab only

# Effects across all kernel conditions

library(car)
Anova(m1)

#Analysis of Deviance Table (Type II tests)
#Response: type
#         LR Chisq Df Pr(>Chisq)
#class       0.964  2     0.6175
#density    90.555  2  < 2.2e-16 ***
#hardness    7.074  2     0.0291 *
#size        3.211  2     0.2008
#weight     28.230  2  7.411e-07 ***
#moisture    1.193  2     0.5506

# density, hardness and weight have some effect on wheat kernel condition

# CIs on betas
conf.beta<-confint(m1)
# , , Scab
#                   2.5 %        97.5 %
#(Intercept)  22.13851497  38.954475222
#classsrw     -1.94776958   0.651514098
#density     -27.70474380 -15.489565975
#hardness     -0.03604523   0.004230411
#size         -0.44453927   2.582767006
#weight       -0.41058295  -0.168713512
#moisture     -0.19391723   0.413047326

#, , Sprout
#                   2.5 %       97.5 %
#(Intercept)  11.78496433 26.552173165
#classsrw     -1.20652328  0.757046542
#density     -20.53461137 -9.698731394
#hardness     -0.03690744 -0.005133494
#size         -0.18459306  1.935820104
#weight       -0.11978643  0.025152642
#moisture     -0.26392179  0.177927888
```

```
# predict probabilities

pi.hat = predict(m1, newdata = wheat, type = "probs")
head(pi.hat)
#     Healthy        Scab     Sprout
#1 0.8552110 0.046396827 0.09839221
#2 0.7492553 0.021572158 0.22917255
#3 0.5172800 0.068979903 0.41374011
#4 0.8982064 0.006740716 0.09505287
#5 0.5103245 0.176260796 0.31341473
#6 0.7924907 0.015304122 0.19220522

# Odds ratios for a c=1 unit sdev increase in each predictor
#==============================================================================

summary(wheat)
# class        density          hardness            size            weight          moisture
# hrw:143   Min.   :0.7352   Min.   :-44.080   Min.   :0.5973   Min.   : 8.532   Min.   : 6.486   Hea
# srw:132   1st Qu.:1.1358   1st Qu.:  0.689   1st Qu.:1.8900   1st Qu.:21.982   1st Qu.: 9.540   Sca
#           Median :1.2126   Median : 24.465   Median :2.2303   Median :27.610   Median :11.909   Spr
#           Mean   :1.1885   Mean   : 25.564   Mean   :2.2047   Mean   :27.501   Mean   :11.192
#           3rd Qu.:1.2687   3rd Qu.: 45.606   3rd Qu.:2.5125   3rd Qu.:32.882   3rd Qu.:12.538
#           Max.   :1.6454   Max.   :111.934   Max.   :4.3100   Max.   :46.334   Max.   :14.514

sd.wheat = apply(wheat[,-c(1,7)],2,sd)
sd.wheat
#   density   hardness       size     weight   moisture
# 0.1313021 27.3561563  0.4906125  7.9154398  2.0332132

# coeffs
beta.hat2<-coefficients(m1)[1,2:7]
beta.hat2
#    classsrw      density     hardness         size       weight     moisture
# -0.64812774 -21.59715489  -0.01590741   1.06911387  -0.28964823   0.10956505

beta.hat3<-coefficients(m1)[2,2:7]
beta.hat3
#    classsrw      density     hardness         size       weight     moisture
# -0.22473837 -15.11667138  -0.02102047   0.87561352  -0.04731690  -0.04299695

# add column class
c.value = c(class=1,sd.wheat)
round(c.value,3)
#   class  density hardness     size   weight moisture
#   1.000    0.131   27.356    0.491    7.915    2.033
```

```
# Odds ratios (scab vs. healthy)
round(exp(c.value*beta.hat2),3)
#   class  density hardness     size   weight moisture
#   0.523    0.059    0.647    1.690    0.101    1.250
round(1/exp(c.value*beta.hat2),3)
#   class  density hardness     size   weight moisture
#   1.912   17.043    1.545    0.592    9.902    0.800

# scab vs. healthy
# Odds change by 0.059 for a 0.13 increase in density, holding other vars constant
# Odds change by 17.04 for a 0.13 decrease in density, holding other vars constant
# Odds change by  9.90 for a 7.92 decrease in weight, holding other vars constant

# Odds ratios (sprout vs. healthy)
round(exp(c.value*beta.hat3),3)
#   class  density hardness     size   weight moisture
#   0.799    0.137    0.563    1.537    0.688    0.916
round(1/exp(c.value*beta.hat3),3)
#   class  density hardness     size   weight moisture
#   1.252    7.278    1.777    0.651    1.454    1.091

# sprout vs. healthy
# Odds change by  7.28 for a 0.13 decrease in density, holding other vars constant
# Odds change by  1.45 for a 7.92 decrease in weight, holding other vars constant

# For larger density, weight, more likely a kernel is healthy ????????

# CIs for OR
ci.OR2<-exp(c.value*conf.beta[2:7,1:2,1])
round(ci.OR2,4)
#          2.5 % 97.5 %
#classsrw 0.1426 1.9184
#density  0.0263 0.1308
#hardness 0.3730 1.1227
#size     0.8040 3.5507
#weight   0.0388 0.2630
#moisture 0.6742 2.3159

ci.OR3<-exp(c.value*conf.beta[2:7,1:2,2])
round(ci.OR3,4)
#          2.5 % 97.5 %
#classsrw 0.2992 2.1320
#density  0.0675 0.2799
#hardness 0.3643 0.8690
#size     0.9134 2.5850
#weight   0.3875 1.2203
#moisture 0.5847 1.4359
```

```
# model with density
#==============================================================================

m2 = multinom(type ~ density,wheat)
summary(m2)
# Coefficients:
#       (Intercept)   density
#Scab      29.37827 -24.56215
#Sprout    19.12165 -15.47633

#Std. Errors:
#       (Intercept)  density
#Scab      3.676892 3.017842
#Sprout    3.337092 2.691429

#Residual Deviance: 459.4246
#AIC: 467.4246

beta.hat = coefficients(m2)
beta.hat
#       (Intercept)   density
#Scab      29.37827 -24.56215
#Sprout    19.12165 -15.47633

# predict probabilities

pi.hat = predict(m2, newdata = wheat, type = "probs")
head(pi.hat)
#     Healthy       Scab    Sprout
#1 0.8366072 0.01943493 0.1439578
#2 0.6435285 0.06823514 0.2882363
#3 0.4134757 0.16296658 0.4235578
#4 0.8056325 0.02557888 0.1687886
#5 0.5240738 0.11162920 0.3642970
#6 0.6921854 0.05357109 0.2542435

# predict types
pi.hat = data.frame(pi.hat)
aux = apply(pi.hat,1,which.max)
head(aux)
# 1 2 3 4 5 6
# 1 1 3 1 1 1
names(pi.hat)
# "Healthy" "Scab"    "Sprout"
yhat = names(pi.hat)[aux]
head(yhat)
```

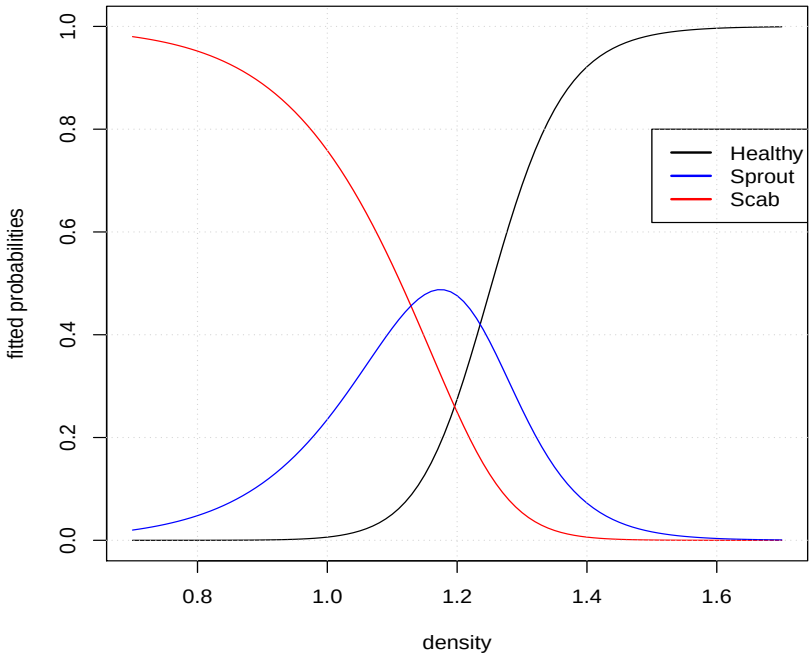
```
# "Healthy" "Healthy" "Sprout"  "Healthy" "Healthy" "Healthy"

d3 = data.frame(pi.hat,yhat,y=wheat$type)
head(d3)
#    Healthy       Scab    Sprout    yhat       y
#1 0.8366072 0.01943493 0.1439578 Healthy Healthy
#2 0.6435285 0.06823514 0.2882363 Healthy Healthy
#3 0.4134757 0.16296658 0.4235578  Sprout Healthy
#4 0.8056325 0.02557888 0.1687886 Healthy Healthy
#5 0.5240738 0.11162920 0.3642970 Healthy Healthy
#6 0.6921854 0.05357109 0.2542435 Healthy Healthy
tail(d3)
#         Healthy       Scab     Sprout    yhat    y
#270 0.5015487050 0.12111876 0.37733253 Healthy Scab
#271 0.3473956428 0.20032065 0.45228370  Sprout Scab
#272 0.5603059980 0.09728167 0.34241233 Healthy Scab
#273 0.0001847703 0.92679846 0.07301677    Scab Scab
#274 0.1972207464 0.31494160 0.48783765  Sprout Scab
#275 0.0120237501 0.70101699 0.28695926    Scab Scab

table(d3$yhat,d3$y)
#          Healthy Scab Sprout
#  Healthy      74    9     27
#  Scab          0   48     16
#  Sprout       22   26     53

aux = prop.table(table(d3$yhat,d3$y))
aux
#             Healthy       Scab     Sprout
#  Healthy 0.26909091 0.03272727 0.09818182
#  Scab    0.00000000 0.17454545 0.05818182
#  Sprout  0.08000000 0.09454545 0.19272727

# error rate
1 - sum(diag(aux))
# 0.3636364
```

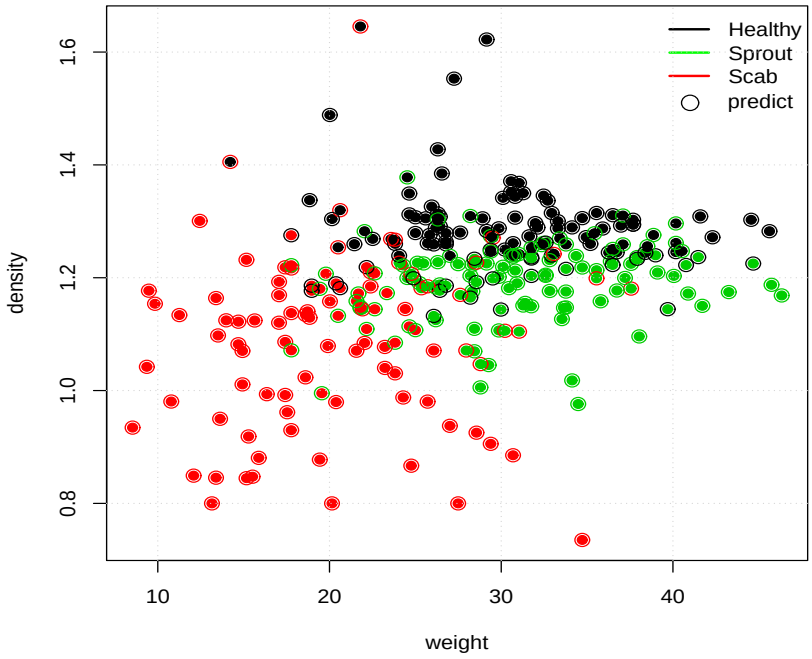
```
# plot
#=============================================================================
b11 = beta.hat[1,1]
b12 = beta.hat[1,2]
b21 = beta.hat[2,1]
b22 = beta.hat[2,2]

f1=function(x){1/(1 + exp(b11 + b12*x) + exp(b21 + b22*x))}
f2=function(x){exp(b11 + b12*x)/(1 + exp(b11 + b12*x) + exp(b21 + b22*x))}
f3=function(x){exp(b21 + b22*x)/(1 + exp(b11 + b12*x) + exp(b21 + b22*x))}
curve(f1,0.7,1.7,ylab="fitted probabilities",xlab="density")
curve(f2,0.7,1.7,col="red",add=T)
curve(f3,0.7,1.7,col="blue",add=T)
colors = c("black","blue","red")
labels = c("Healthy", "Sprout", "Scab")
legend(x=1.5,y=0.8,legend=labels,col=colors,lwd = c(2,2,2))
grid()


# model with 2 continuous predictors:  density and weight
#=============================================================================

m3 = multinom(type ~ density+weight,wheat)
summary(m3)

# predict probabilities
pi.hat = predict(m3, newdata = wheat, type = "probs")
head(pi.hat)
#    Healthy        Scab    Sprout
#1 0.8246586 0.037971920 0.1373694
#2 0.6684405 0.018277788 0.3132817
#3 0.4608537 0.056144549 0.4830018
#4 0.8129651 0.008687927 0.1783470
#5 0.5221491 0.125759109 0.3520918
#6 0.7113905 0.014721635 0.2738879

# predict types
pi.hat = data.frame(pi.hat)
aux = apply(pi.hat,1,which.max)
head(aux)
# 1 2 3 4 5 6
# 1 1 3 1 1 1
names(pi.hat)
# "Healthy" "Scab"    "Sprout"
yhat = names(pi.hat)[aux]
head(yhat)
# "Healthy" "Healthy" "Sprout"  "Healthy" "Healthy" "Healthy"
```

```
d4 = data.frame(pi.hat,yhat,y=wheat$type)
head(d4)
#    Healthy        Scab    Sprout    yhat       y
#1 0.8246586 0.037971920 0.1373694 Healthy Healthy
#2 0.6684405 0.018277788 0.3132817 Healthy Healthy
#3 0.4608537 0.056144549 0.4830018  Sprout Healthy
#4 0.8129651 0.008687927 0.1783470 Healthy Healthy
#5 0.5221491 0.125759109 0.3520918 Healthy Healthy
#6 0.7113905 0.014721635 0.2738879 Healthy Healthy

table(d4$yhat,d4$y)
#          Healthy Scab Sprout
#  Healthy      70    8     25
#  Scab          6   63     17
#  Sprout       20   12     54
aux = prop.table(table(d4$yhat,d4$y))
aux
#             Healthy       Scab     Sprout
#  Healthy 0.25454545 0.02909091 0.09090909
#  Scab    0.02181818 0.22909091 0.06181818
#  Sprout  0.07272727 0.04363636 0.19636364

# error rate
1 - sum(diag(aux))
# 0.32

# plot observed types
colors = c("black","green","red")
labels = c("Healthy", "Sprout", "Scab")
linewidth = rep(2,3)

plot(density~weight,wheat,col=d4$y,pch=19)
legend("topright",legend=labels,col=colors,lwd = linewidth,bty="n")
grid()

# 2-in-1 plot
par(mfrow=c(1,2))
plot(density~weight,wheat,col=d4$y,pch=19,main="observed")
grid()
plot(density~weight,wheat,col=ypred,pch=19,main="predicted",ylab="")
legend("topright",legend=labels,bty="n",text.col=colors,cex=0.7)
grid()
par(mfrow=c(1,1))
```

```
# plot observed and predicted in one plot

# observed types
plot(density~weight,wheat,col=d4$y,pch=19)
colors = c("black","green","red")
labels = c("Healthy", "Sprout", "Scab")
linewidth = rep(2,3)
legend("topright",legend=labels,col=colors,lwd = linewidth,bty="n")
grid()
# predictions (circles)
points(density~weight,wheat,col=ypred,pch=21,cex=1.5)
symbols(41,1.51,circles=0.5,inches=F,add=T)
text(45.1,1.51,"predict")



# knn
#=============================================================================

library(class)
y = wheat$type
x = wheat[,c(2,5)]
head(x)
x = scale(x)

set.seed(1)
ypred = knn(x,x,y,3)

table(ypred,y)
#                     y
#  ypred     Healthy Scab Sprout
#  Healthy       79    7     16
#  Scab           4   67      9
#  Sprout        13    9     71

aux = prop.table(table(ypred,y))
aux
#         y
#ypred        Healthy       Scab     Sprout
#  Healthy 0.28727273 0.02545455 0.05818182
#  Scab    0.01454545 0.24363636 0.03272727
#  Sprout  0.04727273 0.03272727 0.25818182

# error rate
1-sum(diag(aux))
# 0.2109091
```

```
# plot predicted types
colors = c("black","green","red")
labels = c("Healthy", "Sprout", "Scab")
linewidth = rep(2,3)

plot(density~weight,wheat,col=ypred,pch=19,main="knn predictions")
legend("topright",legend=labels,col=colors,lwd = linewidth,bty="n")
grid()

# 2-in-1 plot
par(mfrow=c(1,2))
plot(density~weight,wheat,col=d4$y,pch=19,main="observed")
grid()
plot(density~weight,wheat,col=ypred,pch=19,main="knn predicted",ylab="")
legend("topright",legend=labels,bty="n",text.col=colors,cex=0.7)
grid()
```


fitted probabilities
0.0
0.2
0.4
0.6
0.8
1.0
0.8
1.0
1.2
1.4
1.6
density
Healthy
Sprout
Scab


density
0.8
1.0
1.2
1.4
1.6
10
20
30
40
weight
Healthy
Sprout
Scab
predict

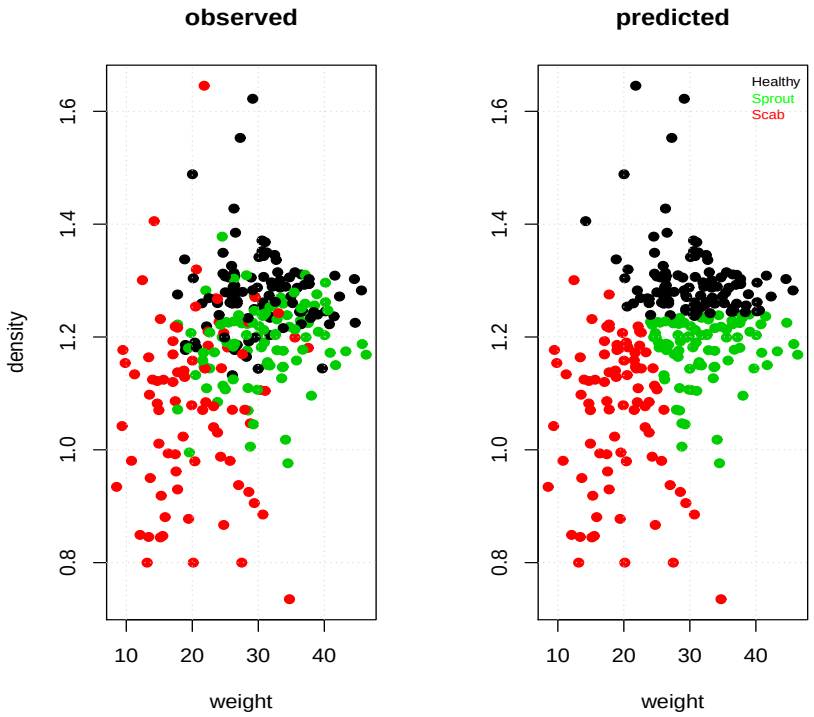


Figure 1: Multinomial model classification

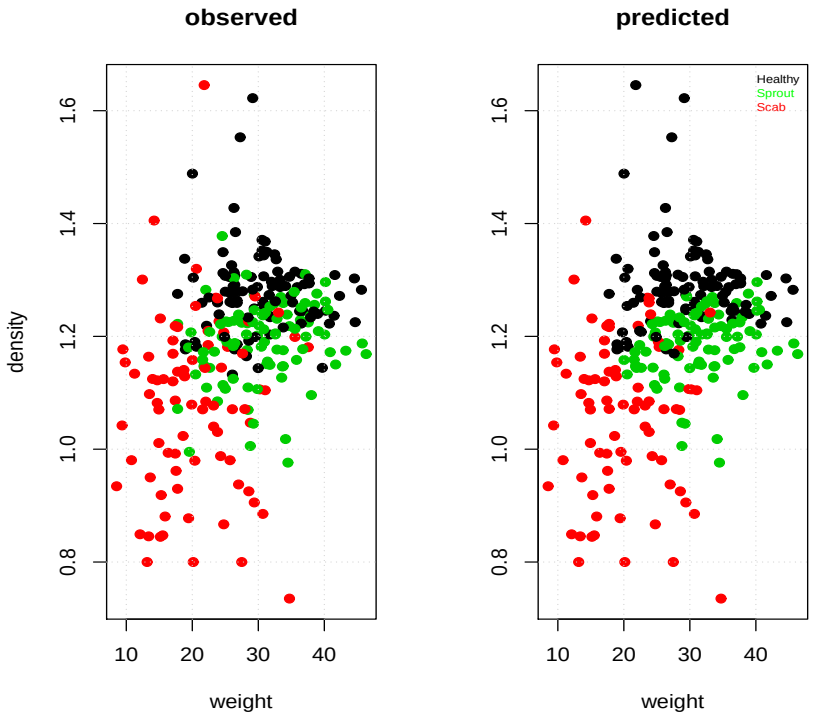


Figure 2: K-nearest neighbor classification