Lab04

Amanda Mentesana

2025-03-21

Firstly, set up libraries and read dataset.

```
knitr::opts_chunk$set(echo = FALSE)

#install libraries
library(readr)
```

```
## Warning: package 'readr' was built under R version 4.4.2
```

```
library(EnvStats)
```

```
## Warning: package 'EnvStats' was built under R version 4.4.2

##
## Attaching package: 'EnvStats'

## The following objects are masked from 'package:stats':
##
##     predict, predict.lm
```

```
library(ggplot2)
```

```
## Warning: package 'ggplot2' was built under R version 4.4.2
```

```
library(ggfortify)
```

```
## Warning: package 'ggfortify' was built under R version 4.4.3
```

```
library(class)
```

```
## Warning: package 'class' was built under R version 4.4.2
```

```
#read the wine data set
wine <- read_csv("C:/Users/amanda/Downloads/wine/wine.data")
```

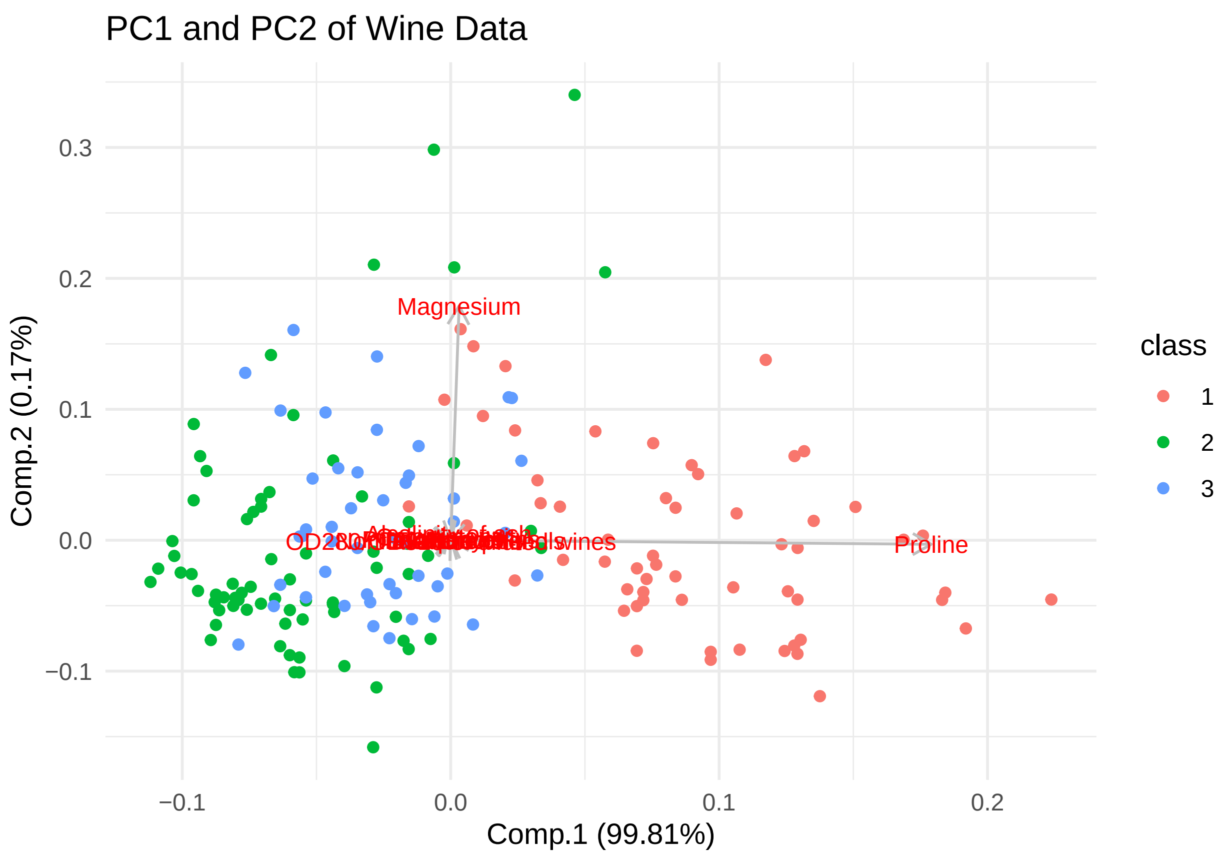
```
## Rows: 177 Columns: 14
```

```
## -- Column specification --------------------------------------------------------
## Delimiter: ","
## dbl (14): 1, 14.23, 1.71, 2.43, 15.6, 127, 2.8, 3.06, .28, 2.29, 5.64, 1.04,...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this message.
```

```r
colnames(wine) <- c("class","Alcohol","Malic acid","Ash","Alcalinity of ash","Magnesium","Total phenols
```

1. Compute the PCs and plot the dataset using the 1st and 2nd PC.

```
##      class          Alcohol        Malic acid        Ash
##  Min.   :1.000   Min.   :11.03   Min.   :0.74   Min.   :1.360
##  1st Qu.:1.000   1st Qu.:12.36   1st Qu.:1.60   1st Qu.:2.210
##  Median :2.000   Median :13.05   Median :1.87   Median :2.360
##  Mean   :1.944   Mean   :12.99   Mean   :2.34   Mean   :2.366
##  3rd Qu.:3.000   3rd Qu.:13.67   3rd Qu.:3.10   3rd Qu.:2.560
##  Max.   :3.000   Max.   :14.83   Max.   :5.80   Max.   :3.230
##  Alcalinity of ash   Magnesium      Total phenols     Flavanoids
##  Min.   :10.60     Min.   : 70.00   Min.   :0.980   Min.   :0.340
##  1st Qu.:17.20     1st Qu.: 88.00   1st Qu.:1.740   1st Qu.:1.200
##  Median :19.50     Median : 98.00   Median :2.350   Median :2.130
##  Mean   :19.52     Mean   : 99.59   Mean   :2.292   Mean   :2.023
##  3rd Qu.:21.50     3rd Qu.:107.00   3rd Qu.:2.800   3rd Qu.:2.860
##  Max.   :30.00     Max.   :162.00   Max.   :3.880   Max.   :5.080
##  Nonflavanoid phenols Proanthocyanins Color intensity       Hue
##  Min.   :0.1300       Min.   :0.410   Min.   : 1.280   Min.   :0.480
##  1st Qu.:0.2700       1st Qu.:1.250   1st Qu.: 3.210   1st Qu.:0.780
##  Median :0.3400       Median :1.550   Median : 4.680   Median :0.960
##  Mean   :0.3623       Mean   :1.587   Mean   : 5.055   Mean   :0.957
##  3rd Qu.:0.4400       3rd Qu.:1.950   3rd Qu.: 6.200   3rd Qu.:1.120
##  Max.   :0.6600       Max.   :3.580   Max.   :13.000   Max.   :1.710
##  OD280/OD315 of diluted wines    Proline
##  Min.   :1.270                Min.   : 278.0
##  1st Qu.:1.930                1st Qu.: 500.0
##  Median :2.780                Median : 672.0
##  Mean   :2.604                Mean   : 745.1
##  3rd Qu.:3.170                3rd Qu.: 985.0
##  Max.   :4.000                Max.   :1680.0
```



2. Identify the variables that contribute the most to the 1st PC.

```
## Importance of components:
##                             Comp.1      Comp.2       Comp.3       Comp.4
## Standard deviation     314.0465241 13.034437573 3.062882e+00 2.234012e+00
## Proportion of Variance   0.9981074  0.001719388 9.494015e-05 5.050804e-05
## Cumulative Proportion    0.9981074  0.999826814 9.999218e-01 9.999723e-01
##                              Comp.5       Comp.6       Comp.7       Comp.8
## Standard deviation     1.107336e+00 9.160683e-01 5.260813e-01 3.887933e-01
## Proportion of Variance 1.240932e-05 8.492685e-06 2.800883e-06 1.529773e-06
## Cumulative Proportion  9.999847e-01 9.999932e-01 9.999960e-01 9.999975e-01
##                              Comp.9      Comp.10      Comp.11      Comp.12
## Standard deviation     3.303978e-01 2.676655e-01 1.937198e-01 1.451319e-01
## Proportion of Variance 1.104749e-06 7.250605e-07 3.797847e-07 2.131645e-07
## Cumulative Proportion  9.999986e-01 9.999993e-01 9.999997e-01 9.999999e-01
##                             Comp.13
## Standard deviation     9.035657e-02
## Proportion of Variance 8.262448e-08
## Cumulative Proportion  1.000000e+00
```

```
##                      Alcohol                   Malic acid
##                 0.0016464031                -0.0006735032
##                          Ash            Alcalinity of ash
##                 0.0001948773                -0.0046271444
```

```
##                 Magnesium                 Total phenols
##              0.0174715429                  0.0009863499
##               Flavanoids          Nonflavanoid phenols
##              0.0015575348                 -0.0001223031
##          Proanthocyanins               Color intensity
##              0.0005912858                  0.0023300597
##                       Hue OD280/OD315 of diluted wines
##              0.0001708674                  0.0006850453
##                   Proline
##              0.9998302063
```

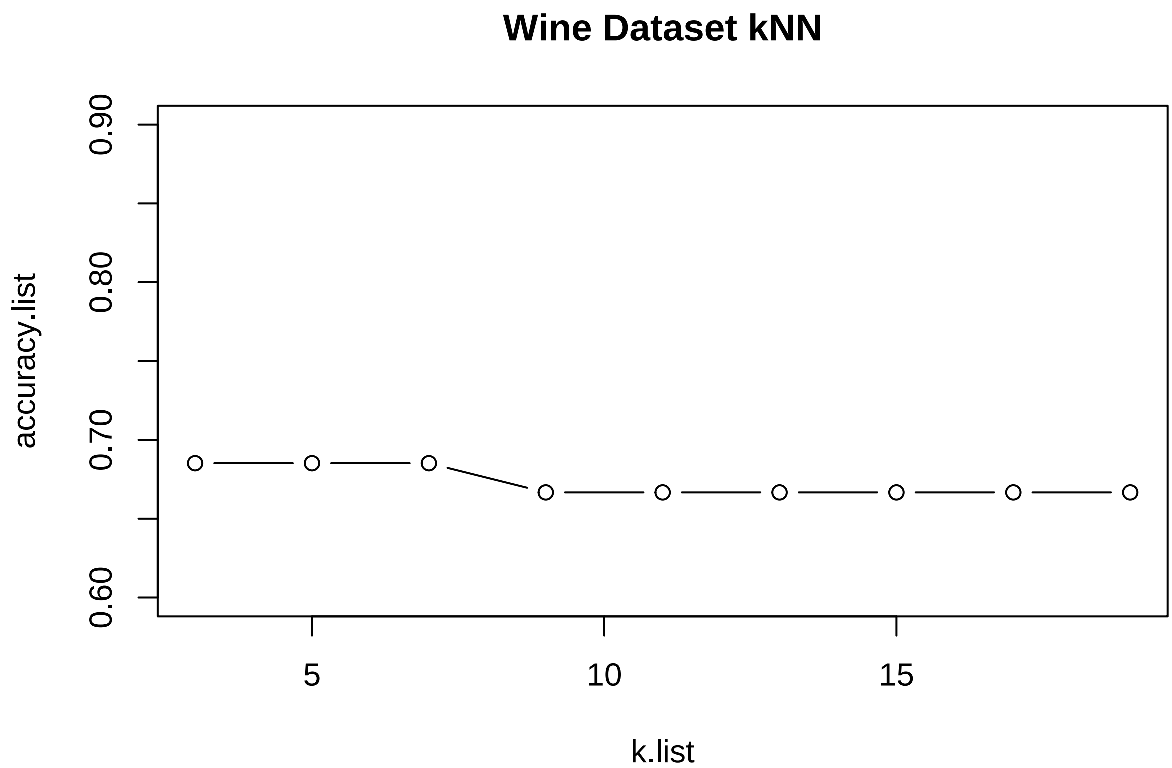
```
##                   Proline                     Magnesium
##              0.9998302063                  0.0174715429
##        Alcalinity of ash               Color intensity
##              0.0046271444                  0.0023300597
##                  Alcohol                    Flavanoids
##              0.0016464031                  0.0015575348
##            Total phenols OD280/OD315 of diluted wines
##              0.0009863499                  0.0006850453
##               Malic acid               Proanthocyanins
##              0.0006735032                  0.0005912858
##                      Ash                           Hue
##              0.0001948773                  0.0001708674
##     Nonflavanoid phenols
##              0.0001223031
```

3. Drop the variables least contributing to the 1st PC and rerun PCA.

```
##     Nonflavanoid phenols                           Hue
##              0.0001223031                  0.0001708674
##                      Ash               Proanthocyanins
##              0.0001948773                  0.0005912858
##               Malic acid OD280/OD315 of diluted wines
##              0.0006735032                  0.0006850453
##            Total phenols                    Flavanoids
##              0.0009863499                  0.0015575348
##                  Alcohol               Color intensity
##              0.0016464031                  0.0023300597
##        Alcalinity of ash                     Magnesium
##              0.0046271444                  0.0174715429
##                  Proline
##              0.9998302063
```

4. Train a classifier model (e.g. kNN) to predict wine type using the original dataset.

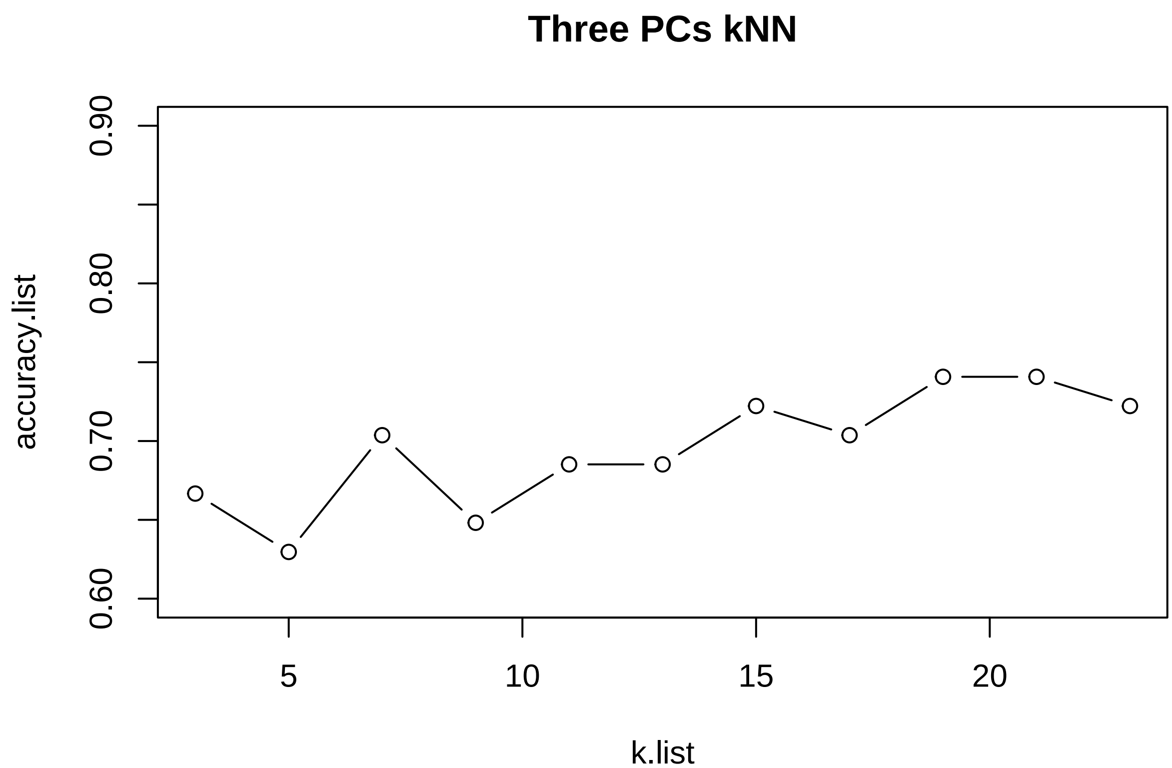
```
## [1] 12
```




```
## [1] 0.6851852 0.6851852 0.6851852 0.6666667 0.6666667 0.6666667 0.6666667
## [8] 0.6666667 0.6666667

## k is maximum at  3

##          actual
## predicted  1  2  3
##         1 15  3  1
##         2  0 14  5
##         3  3  5  8

## [1] 0.6851852

##       Predicted
## Actual  1  2  3
##      1 15  0  3
##      2  3 14  5
##      3  1  5  8

## [1] 0.6851852

##   wine.recall wine.precision   wine.f1
## 1   0.8333333      0.7894737 0.8108108
## 2   0.6363636      0.7368421 0.6829268
## 3   0.5714286      0.5000000 0.5333333
```

5. Train a classifier model to predict wine type using the data projected into the first 3 PCs (scores), from PCA model where lowest PCs are dropped.

```
## [1] 12
```




```
##  [1] 0.6666667 0.6296296 0.7037037 0.6481481 0.6851852 0.6851852 0.7222222
##  [8] 0.7037037 0.7407407 0.7407407 0.7222222
```

```
## k is maximum at  19
```

```
##          actual
## predicted  1  2  3
##         1 16  1  1
##         2  0 14  5
##         3  1  7  9
```

```
## [1] 0.7222222
```

```
##       Predicted
## Actual  1  2  3
##      1 16  0  1
##      2  1 14  7
##      3  1  5  9
```

```
## [1] 0.7222222

##   three.recall three.precision  three.f1
## 1    0.9411765       0.8888889 0.9142857
## 2    0.6363636       0.7368421 0.6829268
## 3    0.6000000       0.5294118 0.5625000
```

6. Compare the 2 classification models using contingency tables and prevision/recall/f1 metrics

We can see from the comparison of recall, precision, f1 and accuracy, that these models perform comparably. For the particular run I did, the accuracies from the contingency table sums showed that the models were equally good at predicting the type of wine. In the case of recall, the wine subset performed better at predicting only one of the categories, for precision three and wine were equally matched, and for f1 score three outperformed on 2/3 classifications. Both models are relatively good at predictions, but potentially using both models to make predictions is the optimal choice.

```
##          actual
## predicted  1  2  3
##         1 15  3  1
##         2  0 14  5
##         3  3  5  8

## [1] 0.6851852

##          actual
## predicted  1  2  3
##         1 16  1  1
##         2  0 14  5
##         3  1  7  9

## [1] 0.7222222

##   wine.recall three.recall wine.precision three.precision   wine.f1  three.f1
## 1   0.8333333    0.9411765      0.7894737       0.8888889 0.8108108 0.9142857
## 2   0.6363636    0.6363636      0.7368421       0.7368421 0.6829268 0.6829268
## 3   0.5714286    0.6000000      0.5000000       0.5294118 0.5333333 0.5625000
```