Regression HD sur les données gasoline

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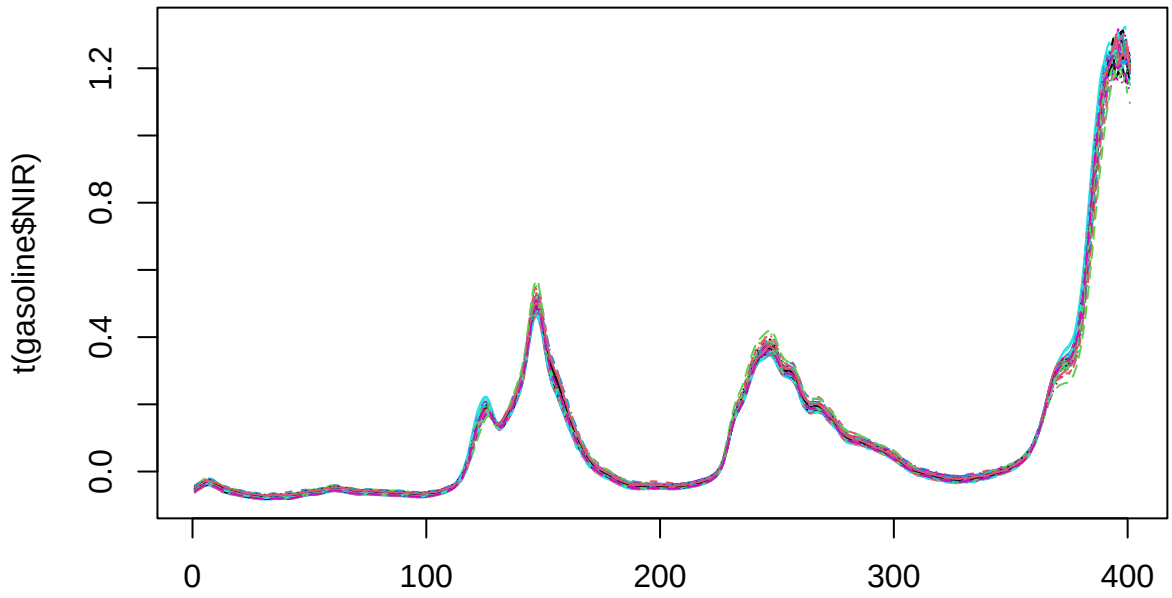
Chargeons les données gasolines (spectres NIR de 60 essences)

```
library(pls)
```

```
library(pls)
data("gasoline")
matplot(t(gasoline$NIR),type='l')
```



Régression linéaire

```
model1=lm(octane~NIR,data=gasoline)
print(anova(model1))
```

```
## Warning in anova.lm(model1): Les tests F d'ANOVA sur un ajustement pratiquement
## parfait ne sont pas fiables
```

```
## Analysis of Variance Table
##
## Response: octane
##           Df Sum Sq Mean Sq F value Pr(>F)
## NIR       59 138.13  2.3411     NaN    NaN
## Residuals  0   0.00     NaN
```

Plus de variables que d'individus, la régression moindres carrés est impossible.

Régression linéaire avec selection forward

C'est un peu technique à mettre en place quand il y a plus de variables que d'individus

```
x=cbind(gasoline$NIR,gasoline$octane)
data=data.frame(octane=x[,402],x[,1:401])
min.model <- lm(octane ~ 1, data=data)
tmp="~"
for (n in seq(900,1700,2)) tmp=paste(tmp,' + X',n,'.nm',sep='')
model1b <- step(min.model, direction = "forward", scope = (tmp),steps=50,trace = F)
summary(model1b)
```

```
##
## Call:
## lm(formula = octane ~ X1208.nm + X1196.nm + X976.nm + X1692.nm +
##     X970.nm + X1206.nm + X1056.nm + X1074.nm + X1098.nm + X1686.nm +
##     X1700.nm + X1544.nm + X1546.nm + X1094.nm + X1552.nm + X1274.nm +
##     X926.nm + X1342.nm + X940.nm + X918.nm + X1026.nm + X1064.nm +
##     X1600.nm + X1280.nm + X1278.nm + X960.nm + X1104.nm + X1320.nm +
##     X1588.nm + X900.nm + X1084.nm + X1080.nm + X1622.nm + X1076.nm +
##     X1318.nm + X1590.nm + X1550.nm + X1680.nm + X1072.nm + X1628.nm +
##     X1570.nm + X932.nm + X1562.nm + X1240.nm + X1328.nm + X1338.nm +
##     X938.nm + X912.nm + X1304.nm + X914.nm, data = data)
##
## Residuals:
##        Min         1Q     Median         3Q        Max
## -2.403e-03 -6.654e-04 -2.852e-05  5.119e-04  2.370e-03
##
## Coefficients:
##               Estimate Std. Error  t value Pr(>|t|)
## (Intercept)   93.95791    0.41417  226.858  < 2e-16 ***
## X1208.nm      58.68357    2.70155   21.722 4.38e-09 ***
## X1196.nm      43.82832    0.70867   61.846 3.81e-13 ***
## X976.nm      282.47025    5.95384   47.443 4.11e-12 ***
## X1692.nm      -6.35868    0.04774 -133.201 3.85e-16 ***
## X970.nm     -145.20891   12.06119  -12.039 7.49e-07 ***
## X1206.nm    -112.98103    2.58944  -43.632 8.72e-12 ***
## X1056.nm    -147.86160    8.71903  -16.958 3.87e-08 ***
## X1074.nm     188.69706    8.22859   22.932 2.71e-09 ***
## X1098.nm     608.35982    9.63038   63.171 3.15e-13 ***
## X1686.nm      -9.57912    0.09472 -101.134 4.58e-15 ***
## X1700.nm       9.54631    0.11672   81.791 3.09e-14 ***
## X1544.nm     -67.11382    5.52940  -12.138 6.99e-07 ***
## X1546.nm     378.07592    5.24191   72.126 9.57e-14 ***
## X1094.nm    -616.08611    8.23124  -74.847 6.86e-14 ***
## X1552.nm    -262.06898    5.00999  -52.309 1.71e-12 ***
## X1274.nm    -282.47975    4.85978  -58.126 6.65e-13 ***
## X926.nm     -187.76911    4.16957  -45.033 6.56e-12 ***
## X1342.nm     273.65088    7.37360   37.112 3.71e-11 ***
## X940.nm      448.88799    8.05103   55.755 9.66e-13 ***
## X918.nm     -278.77900    2.45958 -113.344 1.64e-15 ***
## X1026.nm     195.02443    5.76319   33.840 8.47e-11 ***
## X1064.nm     496.40355    8.11150   61.198 4.19e-13 ***
## X1600.nm    -236.19192    2.87998  -82.012 3.02e-14 ***
## X1280.nm     132.07732    6.18331   21.360 5.08e-09 ***
```

```
## X1278.nm     -58.43611    5.26078  -11.108 1.48e-06 ***
## X960.nm     -262.43222    6.08237  -43.146 9.63e-12 ***
## X1104.nm    -270.86228   10.56058  -25.648 1.00e-09 ***
## X1320.nm    -339.27261    6.40133  -53.000 1.52e-12 ***
## X1588.nm      84.75666    4.49798   18.843 1.53e-08 ***
## X900.nm      -29.28231    1.92112  -15.242 9.81e-08 ***
## X1084.nm    -133.30216   13.11668  -10.163 3.13e-06 ***
## X1080.nm     233.95072    6.78697   34.471 7.19e-11 ***
## X1622.nm      93.24525    1.87888   49.628 2.75e-12 ***
## X1076.nm    -519.53341   14.91602  -34.831 6.55e-11 ***
## X1318.nm     249.64750    7.82555   31.902 1.44e-10 ***
## X1590.nm     105.94648    4.65838   22.743 2.91e-09 ***
## X1550.nm     -87.44534    6.33800  -13.797 2.33e-07 ***
## X1680.nm      -1.27874    0.07273  -17.583 2.82e-08 ***
## X1072.nm     176.73360    6.80680   25.964 8.99e-10 ***
## X1628.nm     -31.18749    0.75996  -41.038 1.51e-11 ***
## X1570.nm     -60.26094    2.22769  -27.051 6.24e-10 ***
## X932.nm      -44.19893    7.69392   -5.745 0.000278 ***
## X1562.nm      63.49092    4.97996   12.749 4.59e-07 ***
## X1240.nm     -32.14533    2.11160  -15.223 9.92e-08 ***
## X1328.nm      86.97972    5.65207   15.389 9.03e-08 ***
## X1338.nm     -65.47727    4.90213  -13.357 3.08e-07 ***
## X938.nm       23.74105    5.77676    4.110 0.002638 **
## X912.nm       33.19357    3.40430    9.750 4.41e-06 ***
## X1304.nm      25.86886    6.14606    4.209 0.002276 **
## X914.nm      -14.72095    4.00124   -3.679 0.005083 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.002377 on 9 degrees of freedom
## Multiple R-squared:      1,  Adjusted R-squared:      1
## F-statistic: 4.891e+05 on 50 and 9 DF,  p-value: < 2.2e-16
```

On autorise au maximum 50 étapes (donc 50 variables dans le modèle) étant donné qu'on n'a que 60 individus.

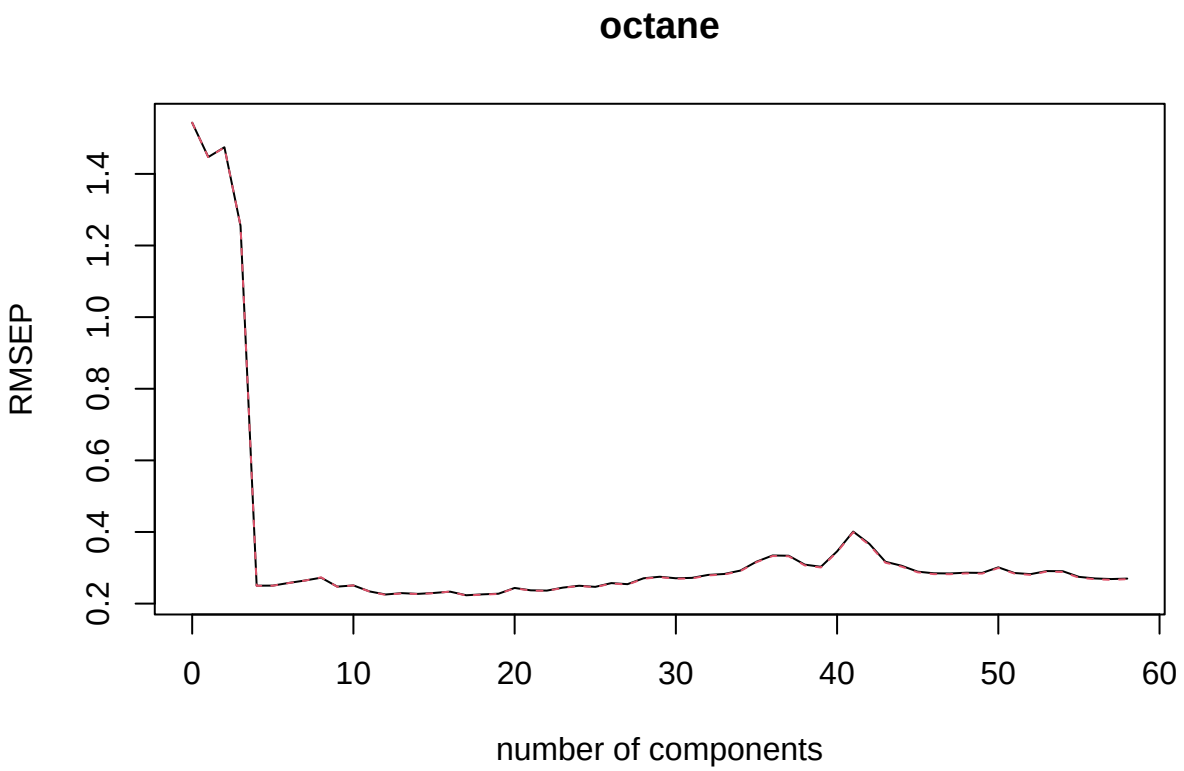
Régression PCR

```
library(pls)
model2=pcr(octane~NIR,data=gasoline,validation='LOO')
summary(model2)
```

```
## Data:    X dimension: 60 401
##  Y dimension: 60 1
## Fit method: svdpc
## Number of components considered: 58
##
## VALIDATION: RMSEP
## Cross-validated using 60 leave-one-out segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV           1.543    1.447    1.474    1.255   0.2501   0.2503   0.2578
## adjCV        1.543    1.446    1.474    1.255   0.2496   0.2500   0.2575
##        7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
## CV      0.2646   0.2724   0.2474    0.2508    0.2340    0.2255    0.2293
## adjCV   0.2643   0.2733   0.2471    0.2508    0.2336    0.2244    0.2286
```

```
##        14 comps  15 comps  16 comps  17 comps  18 comps  19 comps  20 comps
## CV       0.2272    0.2298    0.2334    0.2233    0.2259    0.2276    0.2437
## adjCV    0.2266    0.2292    0.2337    0.2225    0.2252    0.2270    0.2430
##        21 comps  22 comps  23 comps  24 comps  25 comps  26 comps  27 comps
## CV       0.2371    0.2364    0.2447    0.2499    0.2468    0.2573    0.2543
## adjCV    0.2363    0.2356    0.2439    0.2495    0.2457    0.2565    0.2531
##        28 comps  29 comps  30 comps  31 comps  32 comps  33 comps  34 comps
## CV       0.2707    0.2750    0.2707    0.2719    0.2802    0.2828    0.2922
## adjCV    0.2696    0.2738    0.2693    0.2704    0.2787    0.2813    0.2908
##        35 comps  36 comps  37 comps  38 comps  39 comps  40 comps  41 comps
## CV       0.3171    0.3345    0.3337    0.3088    0.3029    0.3459    0.4011
## adjCV    0.3157    0.3329    0.3322    0.3066    0.3009    0.3441    0.3994
##        42 comps  43 comps  44 comps  45 comps  46 comps  47 comps  48 comps
## CV       0.3670    0.3169    0.3058    0.2892    0.2847    0.2842    0.2863
## adjCV    0.3639    0.3143    0.3033    0.2873    0.2824    0.2822    0.2844
##        49 comps  50 comps  51 comps  52 comps  53 comps  54 comps  55 comps
## CV       0.2858    0.3013    0.2855    0.2823    0.2908    0.2904    0.2747
## adjCV    0.2839    0.2995    0.2840    0.2801    0.2896    0.2883    0.2724
##        56 comps  57 comps  58 comps
## CV       0.2702    0.2686    0.2699
## adjCV    0.2681    0.2664    0.2682
##
## TRAINING: % variance explained
##         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps  8 comps
## X         72.57    83.90    90.86    95.46    96.70    97.66    98.16    98.52
## octane    18.99    19.62    46.50    97.69    97.78    97.79    97.79    97.79
##         9 comps  10 comps  11 comps  12 comps  13 comps  14 comps  15 comps
## X         98.85     99.09     99.29     99.40     99.51     99.60     99.68
## octane    98.33     98.38     98.72     98.86     98.87     98.89     98.93
##         16 comps  17 comps  18 comps  19 comps  20 comps  21 comps  22 comps
## X          99.73     99.79     99.84     99.86     99.89     99.90     99.92
## octane     98.93     99.03     99.03     99.03     99.05     99.08     99.10
##         23 comps  24 comps  25 comps  26 comps  27 comps  28 comps  29 comps
## X          99.93     99.94     99.95     99.96     99.96     99.97     99.97
## octane     99.12     99.13     99.22     99.24     99.31     99.31     99.34
##         30 comps  31 comps  32 comps  33 comps  34 comps  35 comps  36 comps
## X          99.98     99.98     99.98     99.98     99.99     99.99     99.99
## octane     99.40     99.41     99.41     99.42     99.42     99.43     99.47
##         37 comps  38 comps  39 comps  40 comps  41 comps  42 comps  43 comps
## X          99.99     99.99     99.99     99.99     99.99     99.99    100.00
## octane     99.53     99.61     99.63     99.63     99.66     99.81     99.83
##         44 comps  45 comps  46 comps  47 comps  48 comps  49 comps  50 comps
## X         100.00    100.00    100.00    100.00    100.00    100.00    100.00
## octane     99.84     99.85     99.87     99.87     99.87     99.88     99.88
##         51 comps  52 comps  53 comps  54 comps  55 comps  56 comps  57 comps
## X         100.00    100.00    100.00    100.00    100.00    100.00    100.00
## octane     99.91     99.93     99.94     99.97     99.98     99.98     99.99
##         58 comps
## X         100.00
## octane     99.99
```

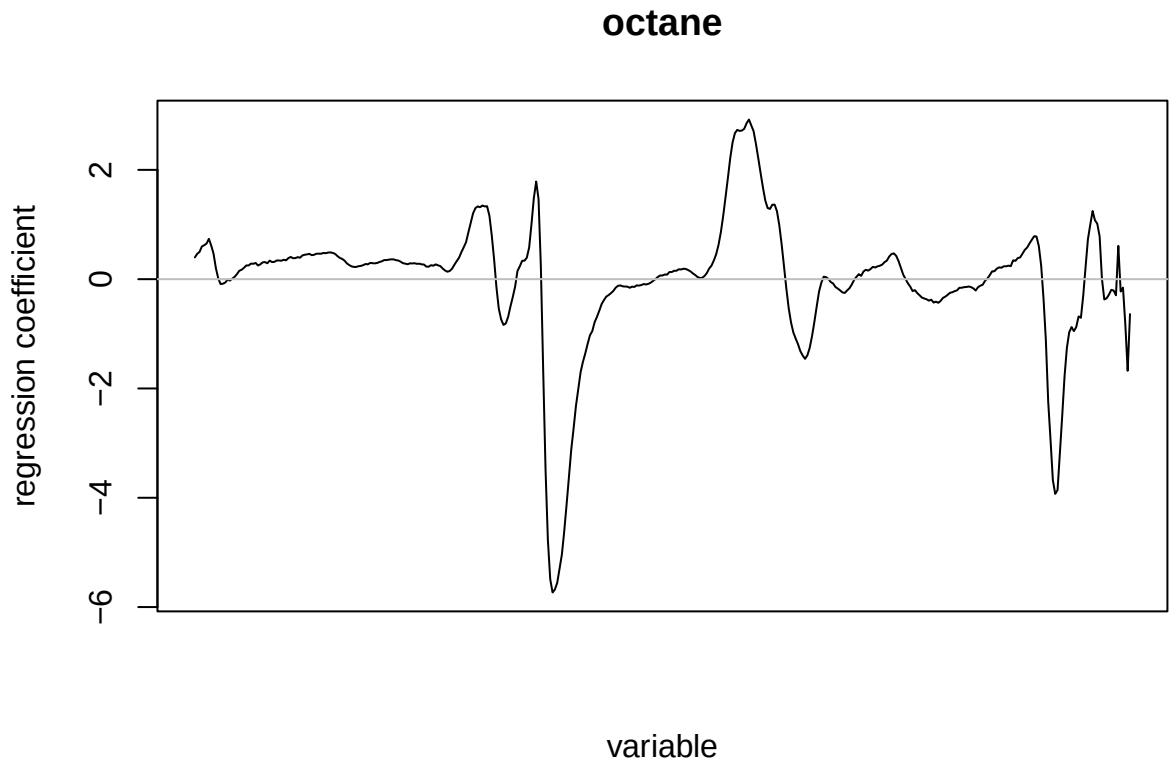
```
plot(RMSEP(model2))
```



4 composantes semblent le plus efficaces.

On peut tracer les coefficients obtenus avec 4 composantes

```
plot(model2, plottype = "coef", ncomp=4,xaxt='n')
```



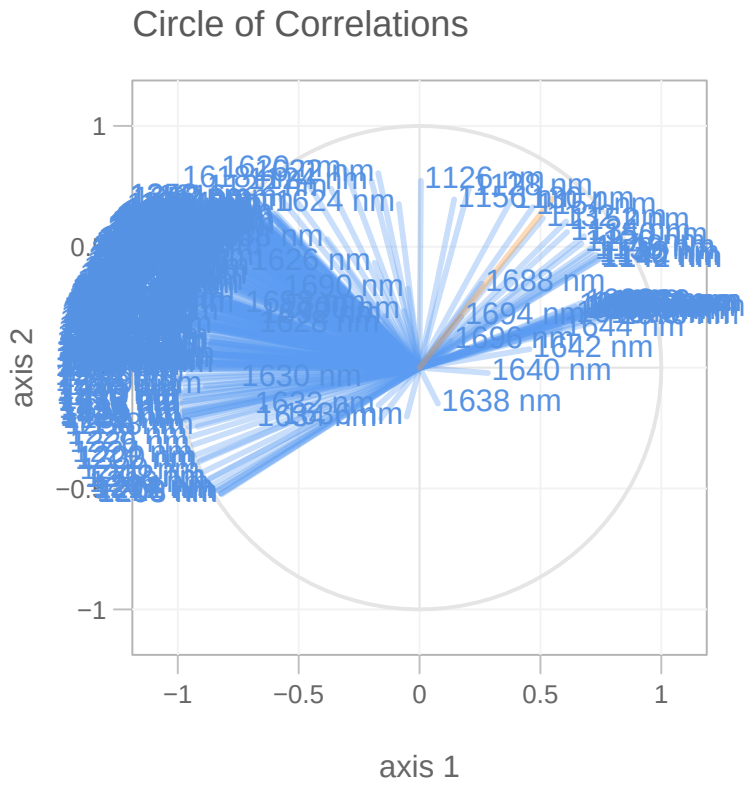
Régression PLS

```
library(plsdepot)
x=cbind(gasoline$NIR,gasoline$octane)
tmp=plsreg1(x[,1:401],x[,402,drop=F],comps=10,crosval=T)
print(tmp$Q2)
```

```
##          PRESS        RSS           Q2  LimQ2     Q2cum
## 1  43.6845776 59.0000000  0.259583431 0.0975 0.2595834
## 2  14.0556907 40.9797905  0.657009211 0.0975 0.7460439
## 3   1.4245598 11.9217690  0.880507682 0.0975 0.9696542
## 4   1.1169883  1.3381513  0.165275072 0.0975 0.9746696
## 5   0.8289363  1.0226792  0.189446399 0.0975 0.9794684
## 6   0.7875466  0.7828962 -0.005940009 0.0975 0.9793464
## 7   0.7013576  0.6485442 -0.081433822 0.0975 0.9776645
## 8   0.6702106  0.5629184 -0.190599933 0.0975 0.9734074
## 9   0.4687944  0.4180883 -0.121280670 0.0975 0.9701822
## 10  0.3497069  0.3327009 -0.051114710 0.0975 0.9686580
```

On va conserver 5 composantes PLS, ré-estimons le modèle

```
model2=plsreg1(x[,1:401],x[,402,drop=F],comps=5,crosval=T)
plot(model2,what='variables',comps=c(1,2))
```



On ne voit pas grand chose vu le grand nombre de variables, néanmoins certaines sont corrélées positivement et d'autres négativement avec la première composante PLS

calcul des VIP

Les VIPs ne sont pas implémentés dans ce package, on peut les calculer à la main

```
VIP=matrix(0,401,5)
for (j in 1:401){
  for (h in 1:5){
    VIP[j,h]=sqrt(401/sum(model2$R2[1:h])*sum(model2$R2[1:h]*(model2$raw.wgs[j,1:h]^2)))
  }
}
rownames(VIP)=colnames(x)[1:401]
```

Un VIP>.8 est généralement signe que la variable a une importance sur la prediction

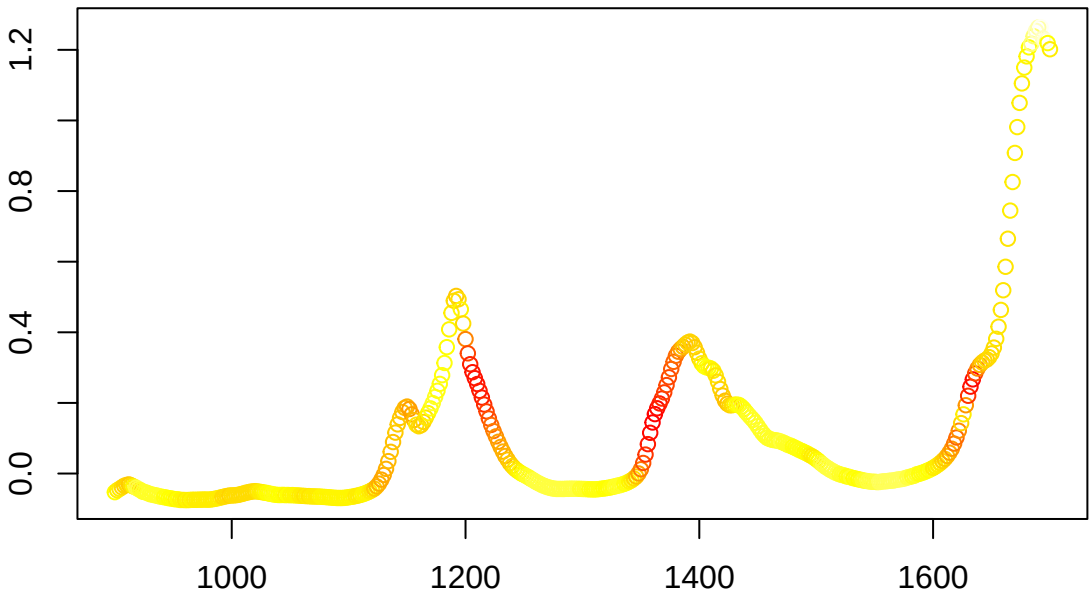
```
vip5=VIP[,5]
print(sort(vip5,decreasing = T)[1:50])
```

```
##  1634 nm  1636 nm  1362 nm  1360 nm  1358 nm  1364 nm  1638 nm  1208 nm
## 1.983240 1.977585 1.932420 1.928871 1.900198 1.894388 1.881106 1.865221
##  1632 nm  1206 nm  1210 nm  1212 nm  1356 nm  1366 nm  1214 nm  1204 nm
## 1.863573 1.858243 1.852577 1.812422 1.804902 1.803425 1.796586 1.791321
##  1216 nm  1368 nm  1354 nm  1630 nm  1218 nm  1370 nm  1202 nm  1372 nm
## 1.736321 1.723010 1.721043 1.699718 1.670232 1.662528 1.639609 1.631660
##  1640 nm  1374 nm  1220 nm  1352 nm  1376 nm  1378 nm  1222 nm  1620 nm
## 1.622554 1.613363 1.587454 1.576908 1.566747 1.522408 1.488407 1.473901
##  1380 nm  1350 nm  1224 nm  1618 nm  1642 nm  1200 nm  1382 nm  1226 nm
## 1.462477 1.421538 1.419367 1.393152 1.363824 1.355776 1.355456 1.326368
##  1622 nm  1616 nm  1628 nm  1228 nm  1384 nm  1154 nm  1348 nm  1152 nm
## 1.324735 1.291240 1.272816 1.270583 1.251501 1.242518 1.239138 1.236150
##  1128 nm  1130 nm
## 1.223943 1.216564
```

Beaucoup de variables ont des VIP importants.

Pour ce type de donées spectrales, on peut par exemple représenter graphiquement la courbe moyenne en mettant en couleur plus ou moins chaude suivant si le VIP est important (rouge = variables importantes)

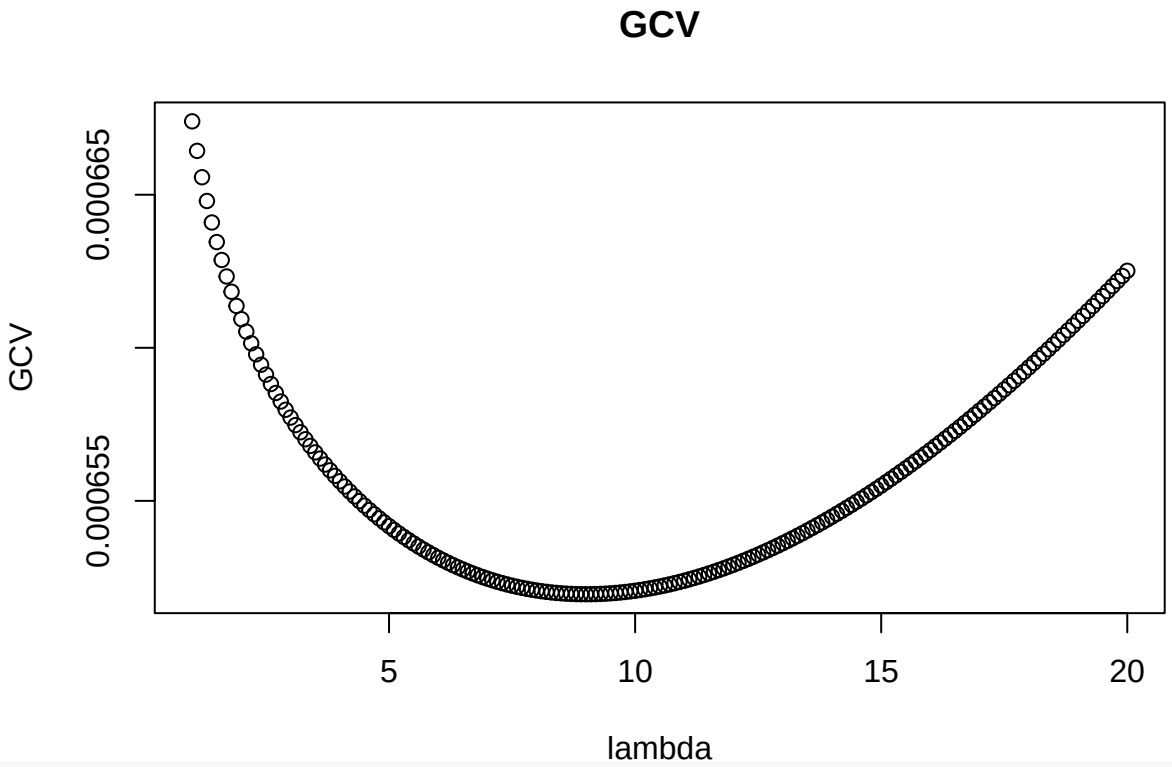
```
vip5_normalises=(vip5-min(vip5))/(max(vip5)-min(vip5))
plot(seq(900,1700,2),colMeans(gasoline$NIR),col=heat.colors(40)[40*(1-vip5_normalises)],xlab="",ylab="")
```



Régression ridge

Effectuons la régression ridge et cherchons le meilleur lambda.

```
model_ridge <- lm.ridge(octane~NIR,data=gasoline,lambda=seq(1,20,0.1))
plot(seq(1,20,0.1),model_ridge$GCV,xlab='lambda',ylab='GCV',main='GCV')
```




```
print(model_ridge$lambda[which.min(model_ridge$GCV)])
```

```
## [1] 9
```

```
print(min(model_ridge$GCV))
```

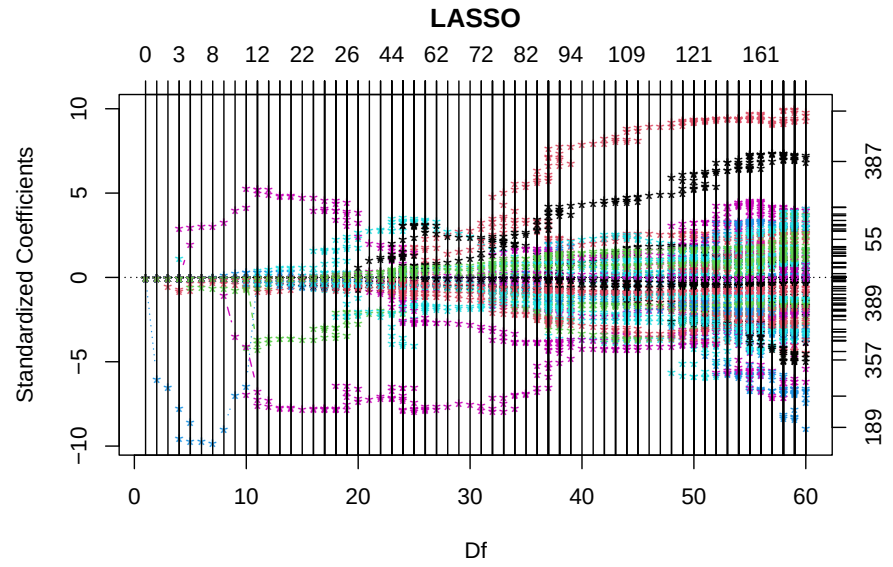
```
## [1] 0.0006519503
```

D'après l'indice de validation croisée généralisée (GCV), le labmbda optimal est 9. Ré-éstimons alors le modèle.

```
model_ridge <- lm.ridge(octane~NIR,data=gasoline,lambda=9)
```

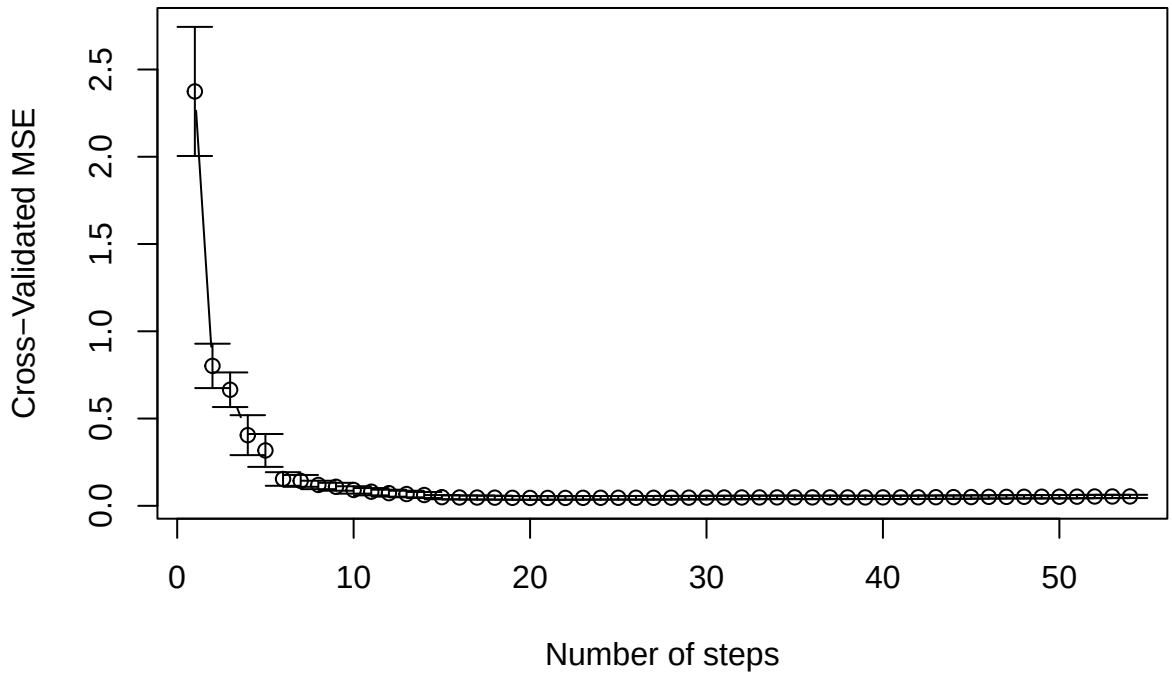
Régression lasso

```
model_lasso <- lars(gasoline$NIR,gasoline$octane,type="lasso",trace=F,normalize=TRUE)
plot(model_lasso,xvar='df', plottype='coeff')
```



Cherchons le lambda optimal

```
cv=cv.lars(gasoline$NIR,gasoline$octane, K = 10,trace = FALSE, plot.it = TRUE, se = TRUE,type = c("lasso"),mode='step')
```



On peut afficher le lambda optimal d'après le CVMSE

```
print(model_lasso$lambda[which.min(cv$cv)])
```

```
## [1] 0.10126
```

où encore prendre le lambda qui conduit à la solution la plus parcimonieuse avec une erreur inférieur à l'erreur minimal + l'erreur d'estimation de cette erreur :

```
tmp=which.min(cv$cv)
tmp2=min(which(cv$cv < cv$cv[tmp]+cv$cv.error[tmp]))
print(model_lasso$lambda[tmp2])
```

```
## [1] 0.1548565
```

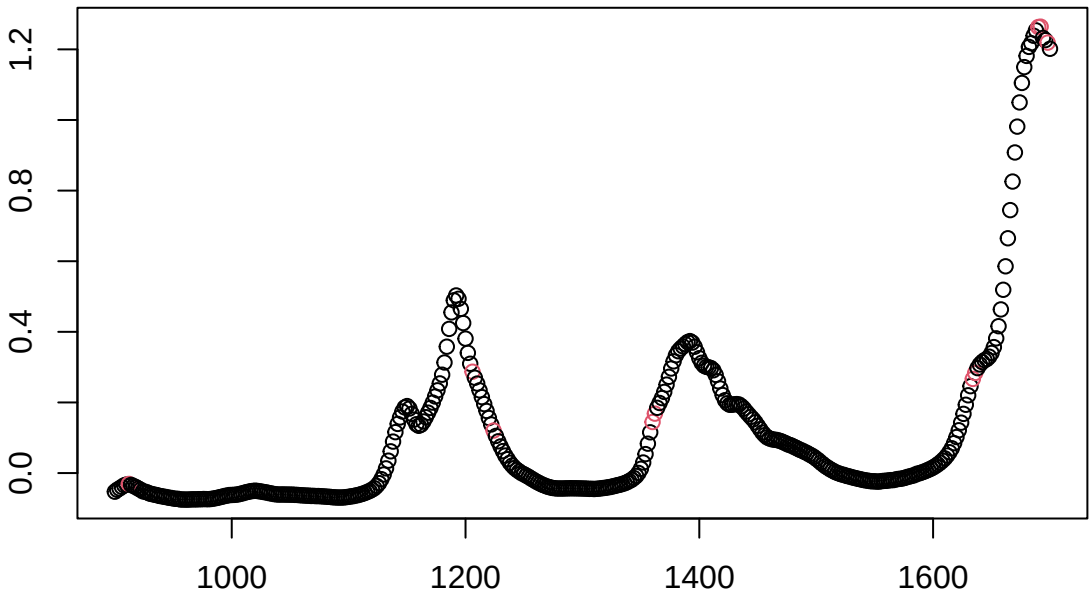
```
lambda_opt=model_lasso$lambda[tmp2]
print(model_lasso$beta[tmp2,])
```

```
##       900 nm       902 nm       904 nm       906 nm       908 nm       910 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       912 nm       914 nm       916 nm       918 nm       920 nm       922 nm
##  10.16650056   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       924 nm       926 nm       928 nm       930 nm       932 nm       934 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       936 nm       938 nm       940 nm       942 nm       944 nm       946 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       948 nm       950 nm       952 nm       954 nm       956 nm       958 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       960 nm       962 nm       964 nm       966 nm       968 nm       970 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       972 nm       974 nm       976 nm       978 nm       980 nm       982 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       984 nm       986 nm       988 nm       990 nm       992 nm       994 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       996 nm       998 nm      1000 nm      1002 nm      1004 nm      1006 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1008 nm      1010 nm      1012 nm      1014 nm      1016 nm      1018 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1020 nm      1022 nm      1024 nm      1026 nm      1028 nm      1030 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1032 nm      1034 nm      1036 nm      1038 nm      1040 nm      1042 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1044 nm      1046 nm      1048 nm      1050 nm      1052 nm      1054 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1056 nm      1058 nm      1060 nm      1062 nm      1064 nm      1066 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1068 nm      1070 nm      1072 nm      1074 nm      1076 nm      1078 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1080 nm      1082 nm      1084 nm      1086 nm      1088 nm      1090 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1092 nm      1094 nm      1096 nm      1098 nm      1100 nm      1102 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1104 nm      1106 nm      1108 nm      1110 nm      1112 nm      1114 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1116 nm      1118 nm      1120 nm      1122 nm      1124 nm      1126 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1128 nm      1130 nm      1132 nm      1134 nm      1136 nm      1138 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1140 nm      1142 nm      1144 nm      1146 nm      1148 nm      1150 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##      1152 nm      1154 nm      1156 nm      1158 nm      1160 nm      1162 nm
```

```
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1164 nm      1166 nm      1168 nm      1170 nm      1172 nm      1174 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1176 nm      1178 nm      1180 nm      1182 nm      1184 nm      1186 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1188 nm      1190 nm      1192 nm      1194 nm      1196 nm      1198 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1200 nm      1202 nm      1204 nm      1206 nm      1208 nm      1210 nm
##   0.00000000   0.00000000   0.00000000 -24.27414293   0.00000000   0.00000000
##       1212 nm      1214 nm      1216 nm      1218 nm      1220 nm      1222 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1224 nm      1226 nm      1228 nm      1230 nm      1232 nm      1234 nm
## -66.45515515   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1236 nm      1238 nm      1240 nm      1242 nm      1244 nm      1246 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1248 nm      1250 nm      1252 nm      1254 nm      1256 nm      1258 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1260 nm      1262 nm      1264 nm      1266 nm      1268 nm      1270 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1272 nm      1274 nm      1276 nm      1278 nm      1280 nm      1282 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1284 nm      1286 nm      1288 nm      1290 nm      1292 nm      1294 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1296 nm      1298 nm      1300 nm      1302 nm      1304 nm      1306 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1308 nm      1310 nm      1312 nm      1314 nm      1316 nm      1318 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1320 nm      1322 nm      1324 nm      1326 nm      1328 nm      1330 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1332 nm      1334 nm      1336 nm      1338 nm      1340 nm      1342 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1344 nm      1346 nm      1348 nm      1350 nm      1352 nm      1354 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1356 nm      1358 nm      1360 nm      1362 nm      1364 nm      1366 nm
##   0.00000000   0.00000000   2.09014186  73.15064889   0.00000000   0.00000000
##       1368 nm      1370 nm      1372 nm      1374 nm      1376 nm      1378 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1380 nm      1382 nm      1384 nm      1386 nm      1388 nm      1390 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1392 nm      1394 nm      1396 nm      1398 nm      1400 nm      1402 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1404 nm      1406 nm      1408 nm      1410 nm      1412 nm      1414 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1416 nm      1418 nm      1420 nm      1422 nm      1424 nm      1426 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1428 nm      1430 nm      1432 nm      1434 nm      1436 nm      1438 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1440 nm      1442 nm      1444 nm      1446 nm      1448 nm      1450 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1452 nm      1454 nm      1456 nm      1458 nm      1460 nm      1462 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1464 nm      1466 nm      1468 nm      1470 nm      1472 nm      1474 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1476 nm      1478 nm      1480 nm      1482 nm      1484 nm      1486 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1488 nm      1490 nm      1492 nm      1494 nm      1496 nm      1498 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1500 nm      1502 nm      1504 nm      1506 nm      1508 nm      1510 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1512 nm      1514 nm      1516 nm      1518 nm      1520 nm      1522 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1524 nm      1526 nm      1528 nm      1530 nm      1532 nm      1534 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1536 nm      1538 nm      1540 nm      1542 nm      1544 nm      1546 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1548 nm      1550 nm      1552 nm      1554 nm      1556 nm      1558 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1560 nm      1562 nm      1564 nm      1566 nm      1568 nm      1570 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1572 nm      1574 nm      1576 nm      1578 nm      1580 nm      1582 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1584 nm      1586 nm      1588 nm      1590 nm      1592 nm      1594 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1596 nm      1598 nm      1600 nm      1602 nm      1604 nm      1606 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1608 nm      1610 nm      1612 nm      1614 nm      1616 nm      1618 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1620 nm      1622 nm      1624 nm      1626 nm      1628 nm      1630 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1632 nm      1634 nm      1636 nm      1638 nm      1640 nm      1642 nm
##   0.00000000  -6.54534233  -5.09717896   0.00000000   0.00000000   0.00000000
##       1644 nm      1646 nm      1648 nm      1650 nm      1652 nm      1654 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1656 nm      1658 nm      1660 nm      1662 nm      1664 nm      1666 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1668 nm      1670 nm      1672 nm      1674 nm      1676 nm      1678 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000
##       1680 nm      1682 nm      1684 nm      1686 nm      1688 nm      1690 nm
##   0.00000000   0.00000000   0.00000000   0.00000000   0.00000000  -1.06749727
##       1692 nm      1694 nm      1696 nm      1698 nm      1700 nm
##  -0.62101996   0.00000000   0.00000000  -0.04092796   0.00000000
```

On peut afficher les longueurs d'ondes séléctionnées

```
plot(seq(900,1700,2),colMeans(gasoline$NIR),col=(abs(model_lasso$beta[tmp2,])>0)+1,xlab="",ylab="")
```



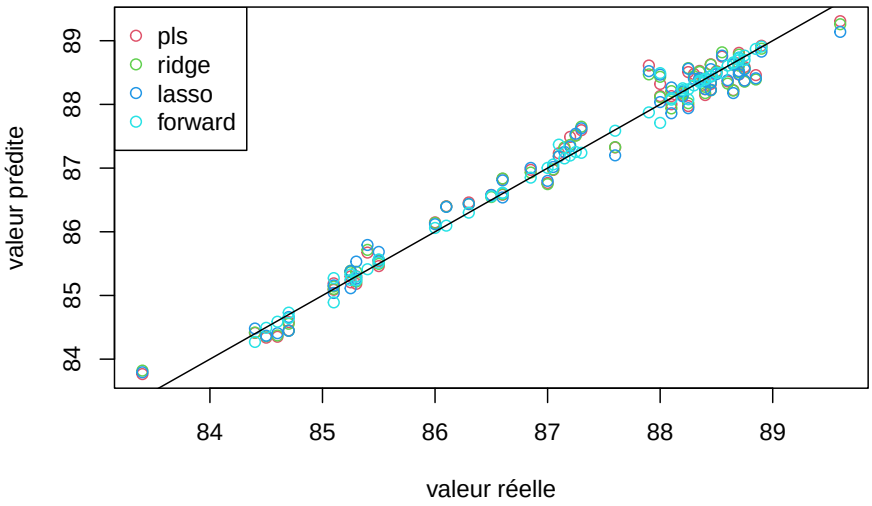
Comparaison des méthodes

Comme les erreurs GCV et CV-MSE ne sont pas comparables directement, on va implémenter à la main une 10-fold CV pour comparer les 3 modèles. Pour la PLS, nous changeons de fonction pour la fonction *plsr* du package *pls* qui comporte une fonction perdict associé contrairement à la fonction que l'on a utilisé jusqu'à maintenant

```
library('pls')
x=cbind(gasoline$NIR,gasoline$octane)
fold=sample(1:10,nrow(gasoline),replace=T)
pred=matrix(0,nrow(gasoline),4)
for (i in 1:10){
  # pls
  model_pls=plsr(octane~NIR,data=data.frame(gasoline[-which(fold==i),]),scale=TRUE,ncomp=5)
  tmp=predict(model_pls,newdata=data.frame(gasoline[which(fold==i),]))
  pred[which(fold==i),1]=tmp[,,5]
  # ridge
  model_ridge <- lm.ridge(octane~NIR,data=data.frame(gasoline[-which(fold==i),]),lambda=9)
  tmp= scale(gasoline$NIR[which(fold==i),], center = model_ridge$xm, scale = model_ridge$scales) %*% model_ridge$coef + model_ridge$ym
  pred[which(fold==i),2]=tmp
  # lasso
  model_lasso=lars(gasoline$NIR[-which(fold==i),],gasoline$octane[-which(fold==i)],type="lasso",trace=F,normalize=TRUE)
  tmp=predict(model_lasso,gasoline$NIR[which(fold==i),],s=lambda_opt,mode="lambda")
  pred[which(fold==i),3]=tmp$fit
  # forward
  x=cbind(gasoline$NIR,gasoline$octane)
  data=data.frame(octane=x[,402],x[,1:401])
  model1b=lm(octane ~ X1208.nm + X1196.nm + X976.nm + X1692.nm +
    X970.nm + X1206.nm + X1056.nm + X1074.nm + X1098.nm + X1686.nm +
    X1700.nm + X1544.nm + X1546.nm + X1094.nm + X1552.nm + X1274.nm +
    X926.nm + X1342.nm + X940.nm + X918.nm + X1026.nm + X1064.nm +
    X1600.nm + X1280.nm + X1278.nm + X960.nm + X1104.nm + X1320.nm +
    X1588.nm + X900.nm + X1084.nm + X1080.nm + X1622.nm + X1076.nm +
    X1318.nm + X1590.nm + X1550.nm + X1680.nm + X1072.nm + X1628.nm +
    X1570.nm + X932.nm + X1562.nm + X1240.nm + X1328.nm + X1338.nm +
    X938.nm + X912.nm + X1304.nm + X914.nm,data=data[-which(fold==i),])
  tmp=predict(model1b,data[which(fold==i),])
  pred[which(fold==i),4]=tmp
}
```

On peut représenter graphiquement les prédictions en fonctions des valeurs réelles, toutes sont très bonnes

```
plot(gasoline$octane,pred[,1],col=2,xlab="valeur réelle",ylab="valeur prédite")
points(gasoline$octane,pred[,2],col=3)
points(gasoline$octane,pred[,3],col=4)
points(gasoline$octane,pred[,4],col=5)
abline(coef = c(0,1))
legend("topleft",legend=c('pls','ridge','lasso','forward'),col=2:5,pch=1)
```



On peut calculer l'erreur quadratique moyenne, mais les trois méthodes sont très proches

```
colnames(pred)=c('pls','ridge','lasso','forward')
colMeans((pred-gasoline$octane)^2)
```

```
##         pls       ridge       lasso     forward
## 0.047159849 0.048763018 0.053218767 0.009582796
```