Practical session - Modèles de régression régularisée

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IV. Medical data

```
tab <- read.table("diabetes.txt", header=TRUE, sep="\t")
head(tab)
```

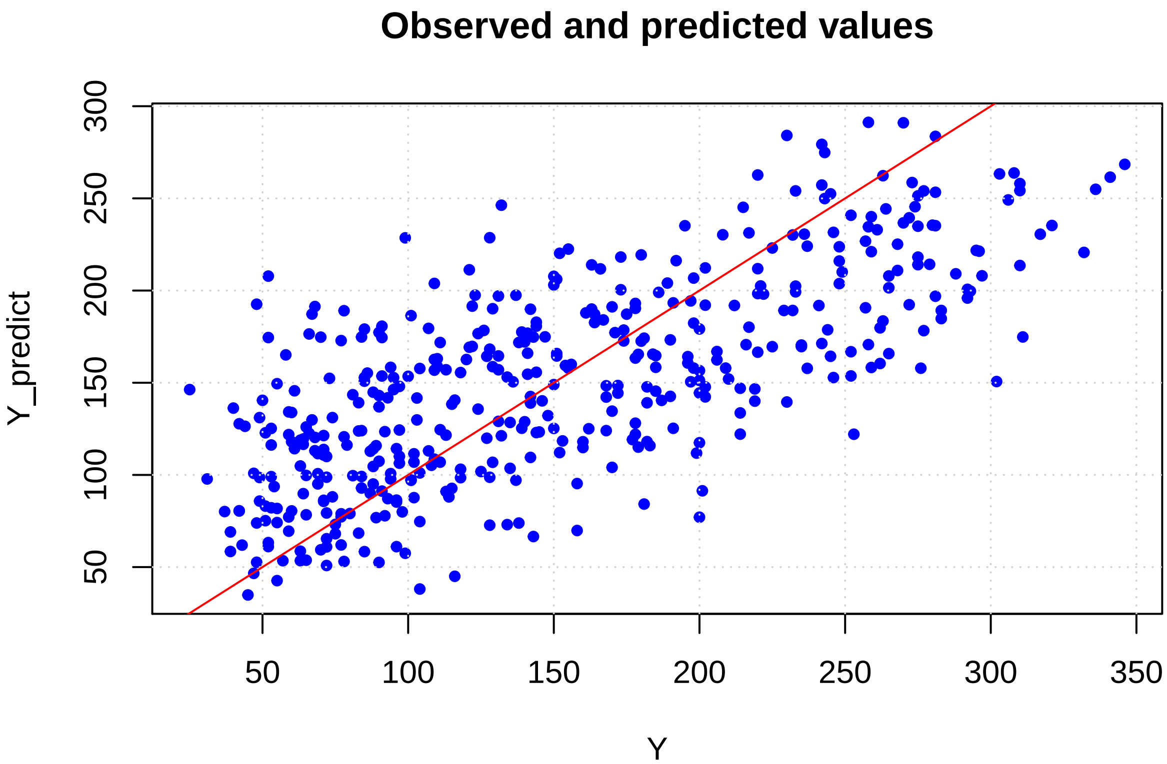
```
##   AGE SEX  BMI  BP  S1    S2 S3 S4     S5 S6   Y
## 1  59   2 32.1 101 157  93.2 38  4 4.8598 87 151
## 2  48   1 21.6  87 183 103.2 70  3 3.8918 69  75
## 3  72   2 30.5  93 156  93.6 41  4 4.6728 85 141
## 4  24   1 25.3  84 198 131.4 40  5 4.8903 89 206
## 5  50   1 23.0 101 192 125.4 52  4 4.2905 80 135
## 6  23   1 22.6  89 139  64.8 61  2 4.1897 68  97
```

```
reg <- lm(Y~., data=tab)
summary(reg)
```

```
##
## Call:
## lm(formula = Y ~ ., data = tab)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -155.827  -38.536   -0.228   37.806  151.353
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -334.56714   67.45462  -4.960 1.02e-06 ***
## AGE           -0.03636    0.21704  -0.168 0.867031
## SEX          -22.85965    5.83582  -3.917 0.000104 ***
## BMI            5.60296    0.71711   7.813 4.30e-14 ***
## BP             1.11681    0.22524   4.958 1.02e-06 ***
## S1            -1.09000    0.57333  -1.901 0.057948 .
## S2             0.74645    0.53083   1.406 0.160390
## S3             0.37200    0.78246   0.475 0.634723
## S4             6.53383    5.95864   1.097 0.273459
## S5            68.48312   15.66972   4.370 1.56e-05 ***
## S6             0.28012    0.27331   1.025 0.305990
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 54.15 on 431 degrees of freedom
## Multiple R-squared:  0.5177, Adjusted R-squared:  0.5066
## F-statistic: 46.27 on 10 and 431 DF,  p-value: < 2.2e-16
```

```r
Y <- tab$Y
Y_predict <- predict(reg, tab)

plot(Y, Y_predict, col="blue", pch=20,
     main="Observed and predicted values")
grid()
abline(a=0, b=1, col="red")
```



1. Model selection

A. Backward regression

```r
regbackward <- step(reg, direction="backward")
```

```
## Start:  AIC=3539.64
## Y ~ AGE + SEX + BMI + BP + S1 + S2 + S3 + S4 + S5 + S6
##
##          Df Sum of Sq     RSS    AIC
## - AGE     1        82 1264068 3537.7
## - S3      1       663 1264649 3537.9
## - S6      1      3080 1267066 3538.7
## - S4      1      3526 1267512 3538.9
## <none>                1263986 3539.6
## - S2      1      5799 1269785 3539.7
## - S1      1     10600 1274586 3541.3
## - SEX     1     44999 1308984 3553.1
## - S5      1     56016 1320001 3556.8
## - BP      1     72100 1336086 3562.2
## - BMI     1    179033 1443019 3596.2
```

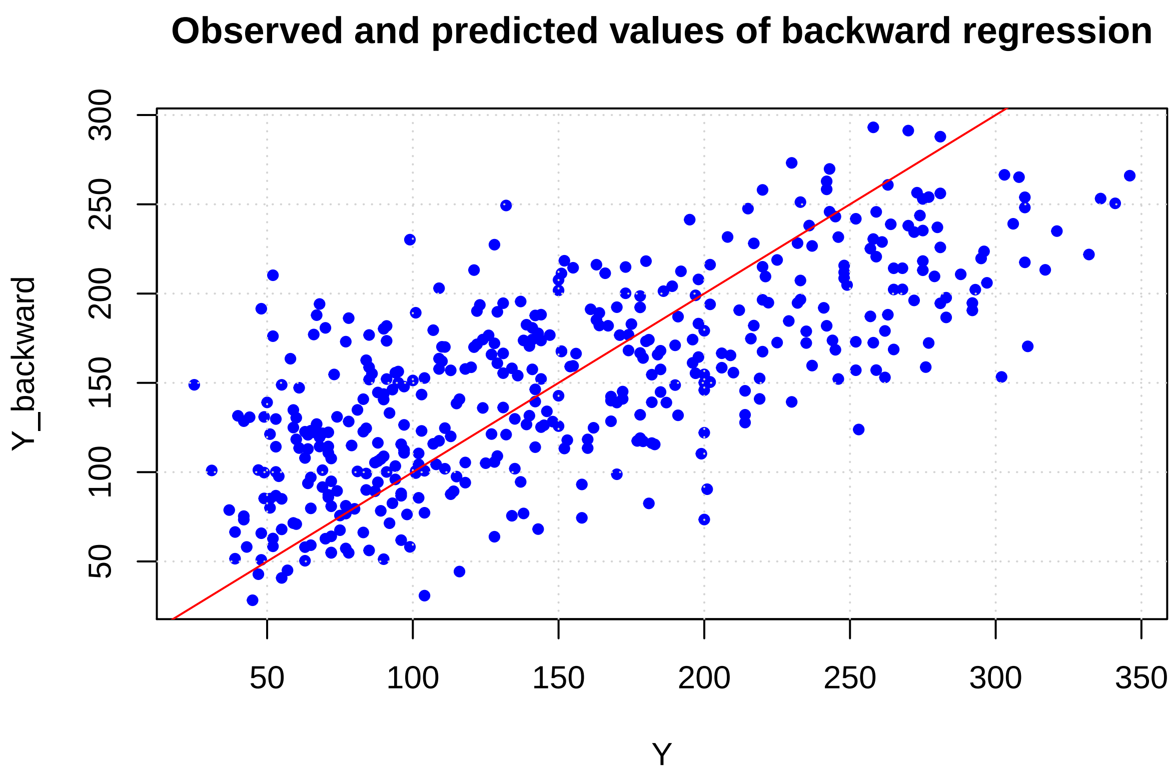
```
##
## Step:  AIC=3537.67
## Y ~ SEX + BMI + BP + S1 + S2 + S3 + S4 + S5 + S6
##
##         Df Sum of Sq     RSS    AIC
## - S3    1       646 1264715 3535.9
## - S6    1      3001 1267069 3536.7
## - S4    1      3543 1267611 3536.9
## <none>              1264068 3537.7
## - S2    1      5751 1269820 3537.7
## - S1    1     10569 1274637 3539.4
## - SEX   1     45830 1309898 3551.4
## - S5    1     55964 1320032 3554.8
## - BP    1     73847 1337915 3560.8
## - BMI   1    179084 1443152 3594.2
##
## Step:  AIC=3535.9
## Y ~ SEX + BMI + BP + S1 + S2 + S4 + S5 + S6
##
##         Df Sum of Sq     RSS    AIC
## - S6    1      3093 1267808 3535.0
## - S4    1      3247 1267961 3535.0
## <none>              1264715 3535.9
## - S2    1      7505 1272219 3536.5
## - S1    1     26839 1291554 3543.2
## - SEX   1     46381 1311096 3549.8
## - BP    1     73533 1338248 3558.9
## - S5    1     97508 1362223 3566.7
## - BMI   1    178542 1443256 3592.3
##
## Step:  AIC=3534.98
## Y ~ SEX + BMI + BP + S1 + S2 + S4 + S5
##
##         Df Sum of Sq     RSS    AIC
## - S4    1      3686 1271494 3534.3
## <none>              1267808 3535.0
## - S2    1      7472 1275280 3535.6
## - S1    1     26378 1294186 3542.1
## - SEX   1     44684 1312492 3548.3
## - BP    1     82152 1349960 3560.7
## - S5    1    102520 1370328 3567.3
## - BMI   1    189976 1457784 3594.7
##
## Step:  AIC=3534.26
## Y ~ SEX + BMI + BP + S1 + S2 + S5
##
##         Df Sum of Sq     RSS    AIC
## <none>              1271494 3534.3
## - S2    1     39377 1310871 3545.7
## - SEX   1     41856 1313350 3546.6
## - S1    1     65236 1336730 3554.4
## - BP    1     79625 1351119 3559.1
## - BMI   1    190592 1462086 3594.0
## - S5    1    294092 1565586 3624.2
```

```r
summary(regbackward)
```

```
##
## Call:
## lm(formula = Y ~ SEX + BMI + BP + S1 + S2 + S5, data = tab)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -158.275  -39.476   -2.065   37.219  148.690
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -313.7666    25.3848 -12.360  < 2e-16 ***
## SEX          -21.5910     5.7056  -3.784 0.000176 ***
## BMI            5.7111     0.7073   8.075 6.69e-15 ***
## BP             1.1266     0.2158   5.219 2.79e-07 ***
## S1            -1.0429     0.2208  -4.724 3.12e-06 ***
## S2             0.8433     0.2298   3.670 0.000272 ***
## S5            73.3065     7.3083  10.031  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 54.06 on 435 degrees of freedom
## Multiple R-squared:  0.5149, Adjusted R-squared:  0.5082
## F-statistic: 76.95 on 6 and 435 DF,  p-value: < 2.2e-16
```

```r
Y_backward <- predict(regbackward, tab)

plot(Y, Y_backward, col="blue", pch=20,
     main="Observed and predicted values of backward regression")
grid()
abline(a=0, b=1, col="red")
```



B. Forward regression

```
regforward <- step(lm(Y~1, data=tab), list(upper=reg), direction="forward")
```

```
## Start:  AIC=3841.99
## Y ~ 1
##
##         Df Sum of Sq     RSS    AIC
## + BMI    1    901427 1719582 3657.7
## + S5     1    839308 1781701 3673.4
## + BP     1    510851 2110158 3748.2
## + S4     1    485646 2135363 3753.4
## + S3     1    408507 2212502 3769.1
## + S6     1    383437 2237572 3774.1
## + S1     1    117824 2503186 3823.7
## + AGE    1     92527 2528482 3828.1
## + S2     1     79403 2541607 3830.4
## <none>               2621009 3842.0
## + SEX    1      4860 2616149 3843.2
##
## Step:  AIC=3657.7
## Y ~ BMI
##
##         Df Sum of Sq     RSS    AIC
## + S5     1    302888 1416694 3574.1
## + BP     1    136477 1583105 3623.1
## + S4     1    111511 1608071 3630.1
## + S3     1     97767 1621815 3633.8
## + S6     1     73738 1645844 3640.3
```

```
## + AGE    1     17087 1702495 3655.3
## + S1     1     12008 1707574 3656.6
## <none>                1719582 3657.7
## + S2     1      1228 1718354 3659.4
## + SEX    1       197 1719385 3659.6
##
## Step:  AIC=3574.06
## Y ~ BMI + S5
##
##        Df Sum of Sq     RSS    AIC
## + BP    1     53985 1362709 3558.9
## + S1    1     27624 1389070 3567.4
## + S3    1     26914 1389781 3567.6
## + S2    1      9256 1407438 3573.2
## + SEX   1      6881 1409813 3573.9
## + S6    1      6801 1409893 3573.9
## <none>                1416694 3574.1
## + S4    1      2376 1414318 3575.3
## + AGE   1       176 1416518 3576.0
##
## Step:  AIC=3558.88
## Y ~ BMI + S5 + BP
##
##        Df Sum of Sq     RSS    AIC
## + S1    1   31277.3 1331431 3550.6
## + S3    1   29921.2 1332787 3551.1
## + SEX   1   17532.1 1345177 3555.2
## + S2    1   10809.8 1351899 3557.4
## <none>                1362709 3558.9
## + S4    1    3218.7 1359490 3559.8
## + AGE   1    2106.4 1360602 3560.2
## + S6    1    1240.1 1361469 3560.5
##
## Step:  AIC=3550.62
## Y ~ BMI + S5 + BP + S1
##
##        Df Sum of Sq     RSS    AIC
## + SEX   1   20560.5 1310871 3545.7
## + S2    1   18080.9 1313350 3546.6
## + S4    1   15188.0 1316243 3547.6
## + S3    1   14360.4 1317071 3547.8
## <none>                1331431 3550.6
## + S6    1    2898.8 1328533 3551.7
## + AGE   1     472.0 1330959 3552.5
##
## Step:  AIC=3545.74
## Y ~ BMI + S5 + BP + S1 + SEX
##
##        Df Sum of Sq     RSS    AIC
## + S2    1     39377 1271494 3534.3
## + S4    1     35591 1275280 3535.6
## + S3    1     35001 1275870 3535.8
## <none>                1310871 3545.7
## + S6    1      5288 1305583 3546.0
```

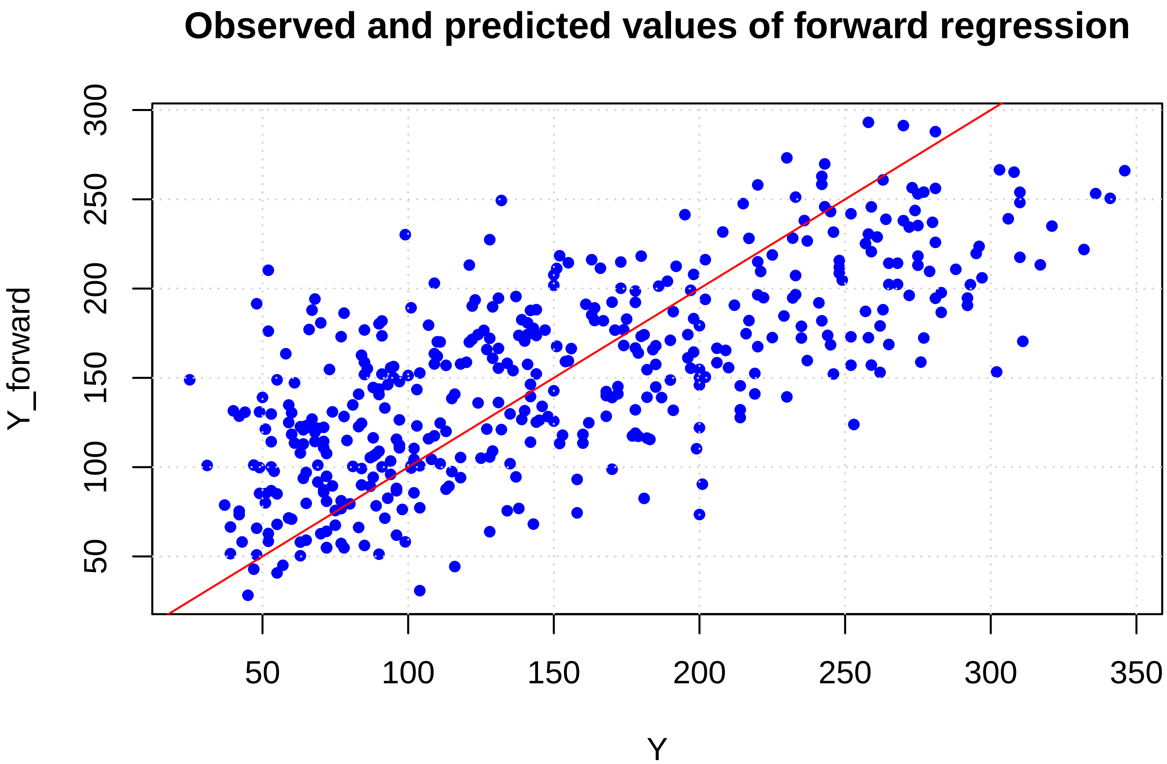
```
## + AGE    1        49 1310822 3547.7
##
## Step:  AIC=3534.26
## Y ~ BMI + S5 + BP + S1 + SEX + S2
##
##        Df Sum of Sq     RSS    AIC
## <none>               1271494 3534.3
## + S4    1    3686.2 1267808 3535.0
## + S6    1    3532.6 1267961 3535.0
## + S3    1     394.8 1271099 3536.1
## + AGE   1      10.9 1271483 3536.3
```

```
summary(regforward)
```

```
##
## Call:
## lm(formula = Y ~ BMI + S5 + BP + S1 + SEX + S2, data = tab)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -158.275  -39.476   -2.065   37.219  148.690
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -313.7666    25.3848 -12.360  < 2e-16 ***
## BMI            5.7111     0.7073   8.075 6.69e-15 ***
## S5            73.3065     7.3083  10.031  < 2e-16 ***
## BP             1.1266     0.2158   5.219 2.79e-07 ***
## S1            -1.0429     0.2208  -4.724 3.12e-06 ***
## SEX          -21.5910     5.7056  -3.784 0.000176 ***
## S2             0.8433     0.2298   3.670 0.000272 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 54.06 on 435 degrees of freedom
## Multiple R-squared:  0.5149, Adjusted R-squared:  0.5082
## F-statistic: 76.95 on 6 and 435 DF,  p-value: < 2.2e-16
```

```
Y_forward <- predict(regforward, tab)

plot(Y, Y_forward, col="blue", pch=20,
     main="Observed and predicted values of forward regression")
grid()
abline(a=0, b=1, col="red")
```



C. Stepwise regression

```r
regboth <- step(reg, direction="both")
```

```
## Start:  AIC=3539.64
## Y ~ AGE + SEX + BMI + BP + S1 + S2 + S3 + S4 + S5 + S6
##
##          Df Sum of Sq     RSS    AIC
## - AGE     1        82 1264068 3537.7
## - S3      1       663 1264649 3537.9
## - S6      1      3080 1267066 3538.7
## - S4      1      3526 1267512 3538.9
## <none>                1263986 3539.6
## - S2      1      5799 1269785 3539.7
## - S1      1     10600 1274586 3541.3
## - SEX     1     44999 1308984 3553.1
## - S5      1     56016 1320001 3556.8
## - BP      1     72100 1336086 3562.2
## - BMI     1    179033 1443019 3596.2
##
## Step:  AIC=3537.67
## Y ~ SEX + BMI + BP + S1 + S2 + S3 + S4 + S5 + S6
##
##          Df Sum of Sq     RSS    AIC
## - S3      1       646 1264715 3535.9
## - S6      1      3001 1267069 3536.7
## - S4      1      3543 1267611 3536.9
## <none>                1264068 3537.7
## - S2      1      5751 1269820 3537.7
```

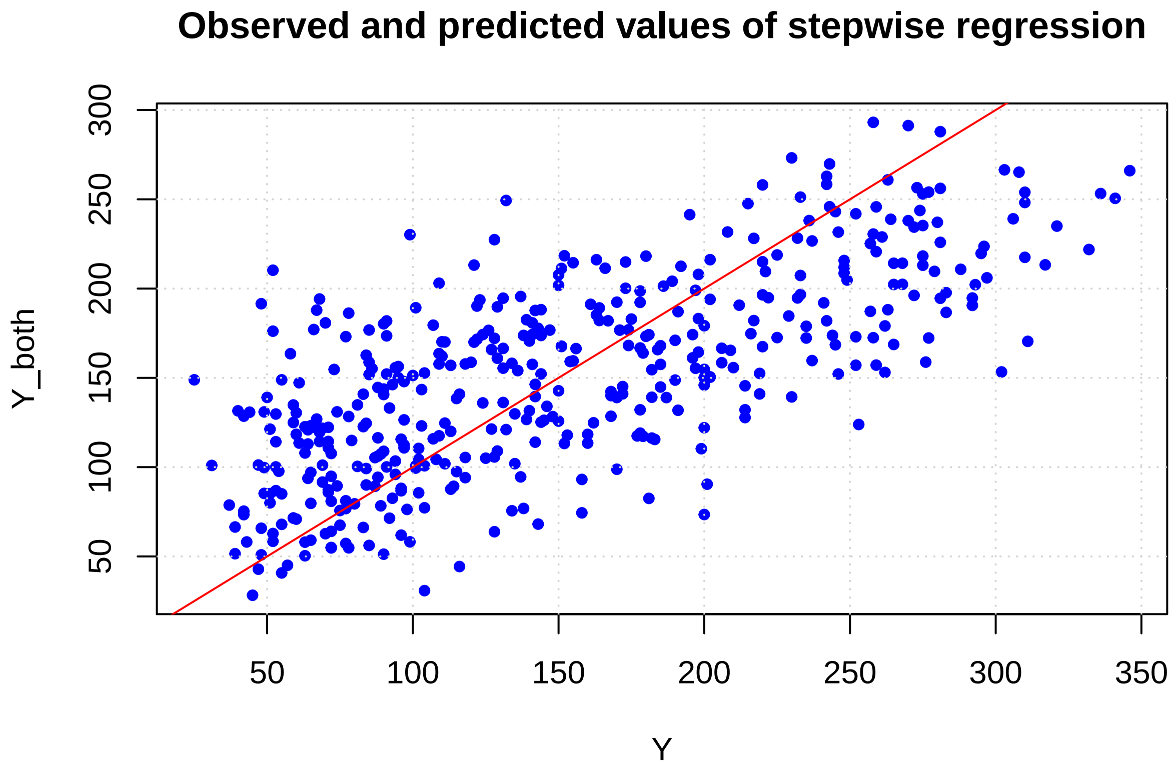
```
## - S1     1     10569 1274637 3539.4
## + AGE    1        82 1263986 3539.6
## - SEX    1     45830 1309898 3551.4
## - S5     1     55964 1320032 3554.8
## - BP     1     73847 1337915 3560.8
## - BMI    1    179084 1443152 3594.2
##
## Step:  AIC=3535.9
## Y ~ SEX + BMI + BP + S1 + S2 + S4 + S5 + S6
##
##        Df Sum of Sq     RSS    AIC
## - S6    1      3093 1267808 3535.0
## - S4    1      3247 1267961 3535.0
## <none>              1264715 3535.9
## - S2    1      7505 1272219 3536.5
## + S3    1       646 1264068 3537.7
## + AGE   1        66 1264649 3537.9
## - S1    1     26839 1291554 3543.2
## - SEX   1     46381 1311096 3549.8
## - BP    1     73533 1338248 3558.9
## - S5    1     97508 1362223 3566.7
## - BMI   1    178542 1443256 3592.3
##
## Step:  AIC=3534.98
## Y ~ SEX + BMI + BP + S1 + S2 + S4 + S5
##
##        Df Sum of Sq     RSS    AIC
## - S4    1      3686 1271494 3534.3
## <none>              1267808 3535.0
## - S2    1      7472 1275280 3535.6
## + S6    1      3093 1264715 3535.9
## + S3    1       738 1267069 3536.7
## + AGE   1         0 1267807 3537.0
## - S1    1     26378 1294186 3542.1
## - SEX   1     44684 1312492 3548.3
## - BP    1     82152 1349960 3560.7
## - S5    1    102520 1370328 3567.3
## - BMI   1    189976 1457784 3594.7
##
## Step:  AIC=3534.26
## Y ~ SEX + BMI + BP + S1 + S2 + S5
##
##        Df Sum of Sq     RSS    AIC
## <none>              1271494 3534.3
## + S4    1      3686 1267808 3535.0
## + S6    1      3533 1267961 3535.0
## + S3    1       395 1271099 3536.1
## + AGE   1        11 1271483 3536.3
## - S2    1     39377 1310871 3545.7
## - SEX   1     41856 1313350 3546.6
## - S1    1     65236 1336730 3554.4
## - BP    1     79625 1351119 3559.1
## - BMI   1    190592 1462086 3594.0
## - S5    1    294092 1565586 3624.2
```

```r
summary(regboth)
```

```
##
## Call:
## lm(formula = Y ~ SEX + BMI + BP + S1 + S2 + S5, data = tab)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -158.275  -39.476   -2.065   37.219  148.690
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -313.7666    25.3848 -12.360  < 2e-16 ***
## SEX          -21.5910     5.7056  -3.784 0.000176 ***
## BMI            5.7111     0.7073   8.075 6.69e-15 ***
## BP             1.1266     0.2158   5.219 2.79e-07 ***
## S1            -1.0429     0.2208  -4.724 3.12e-06 ***
## S2             0.8433     0.2298   3.670 0.000272 ***
## S5            73.3065     7.3083  10.031  < 2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 54.06 on 435 degrees of freedom
## Multiple R-squared:  0.5149, Adjusted R-squared:  0.5082
## F-statistic: 76.95 on 6 and 435 DF,  p-value: < 2.2e-16
```

```r
Y_both <- predict(regboth, tab)

plot(Y, Y_both, col="blue", pch=20,
     main="Observed and predicted values of stepwise regression")
grid()
abline(a=0, b=1, col="red")
```



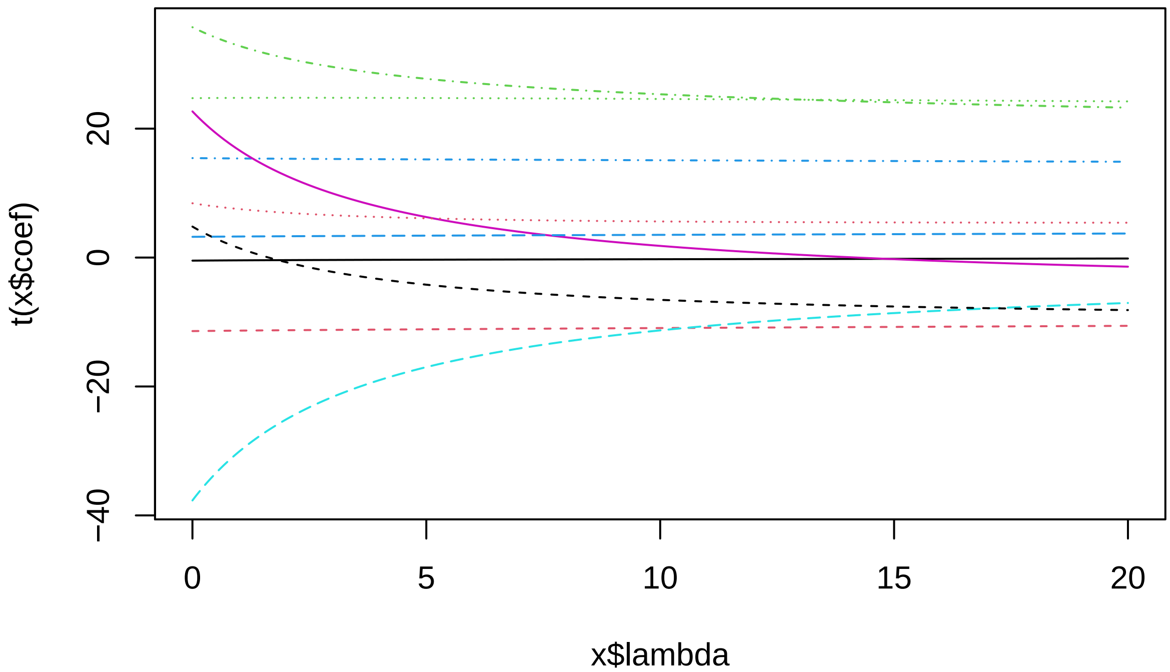
2. Ridge

Ridge regression with λ having a value from 0 to 20 with an increment of 0.01:

```
library(MASS)
resridge <- lm.ridge(Y~., data=tab, lambda=seq(0,20,0.01))
```

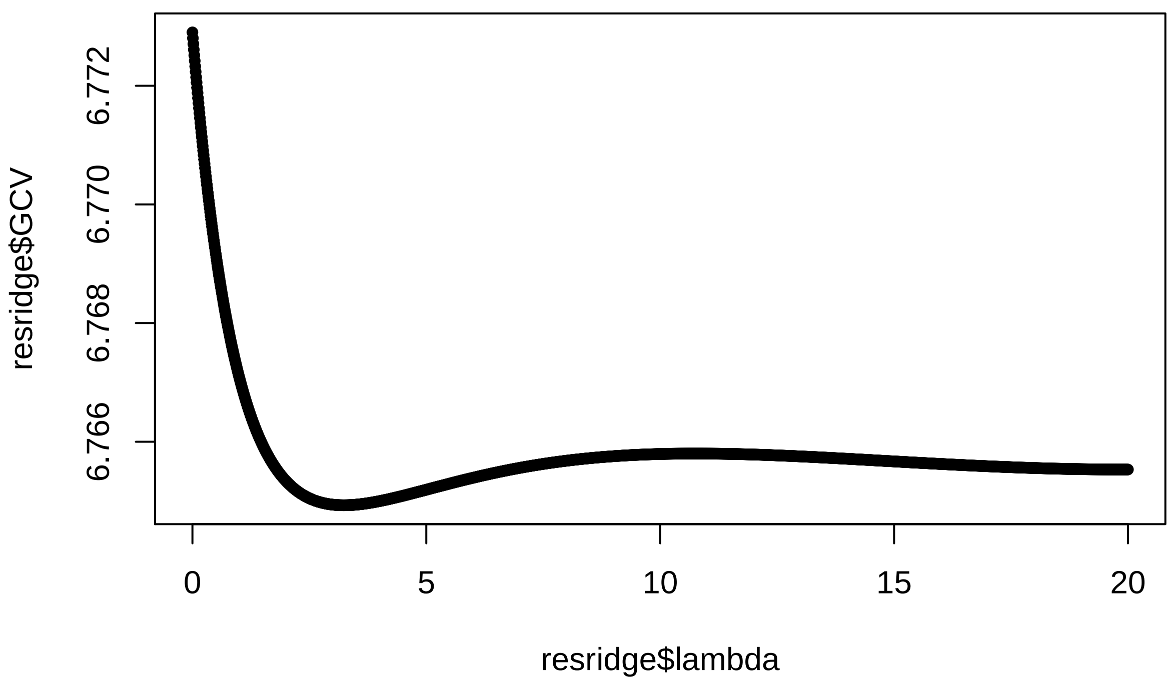
Evolution of the value of the coefficients with respect to λ:

```
plot(resridge)
```



Finding the best λ value:

```
plot(resridge$lambda, resridge$GCV, pch=20)
```




```
best_ridge_lambda <- as.numeric(names(which.min(resridge$GCV)))
print(paste("Best lambda:", best_ridge_lambda))
```

```
## [1] "Best lambda: 3.24"
```

Ridge with the best λ value ($\lambda = 3.24$):

```
best_resridge <- lm.ridge(Y~., data=tab, lambda=best_ridge_lambda)
```

```r
# Values of the coefficients in the "rescaling framework"
best_resridge$coef
```

```
##        AGE         SEX         BMI          BP          S1          S2
##  -0.3668366 -11.2105831  24.7803505  15.2836637 -20.9220865   9.3873897
##          S3          S4          S5          S6
##  -2.5302838   6.4908025  29.2938550   3.3482156
```

```r
# Values of the coefficients in the initial framework
coef(best_resridge)
```

```
##                         AGE          SEX          BMI           BP
## -285.44978529  -0.02801522 -22.46629043   5.61515337   1.10625904
##            S1           S2           S3           S4           S5
##   -0.60522893   0.30901266  -0.19584903   5.03557518  56.14008256
##            S6
##    0.29157202
```

3. Lasso (using glmnet)

Data:

```r
X <- data.matrix(tab[, 1:10])
Y <- tab[, 11]
```

Using glmnet library:

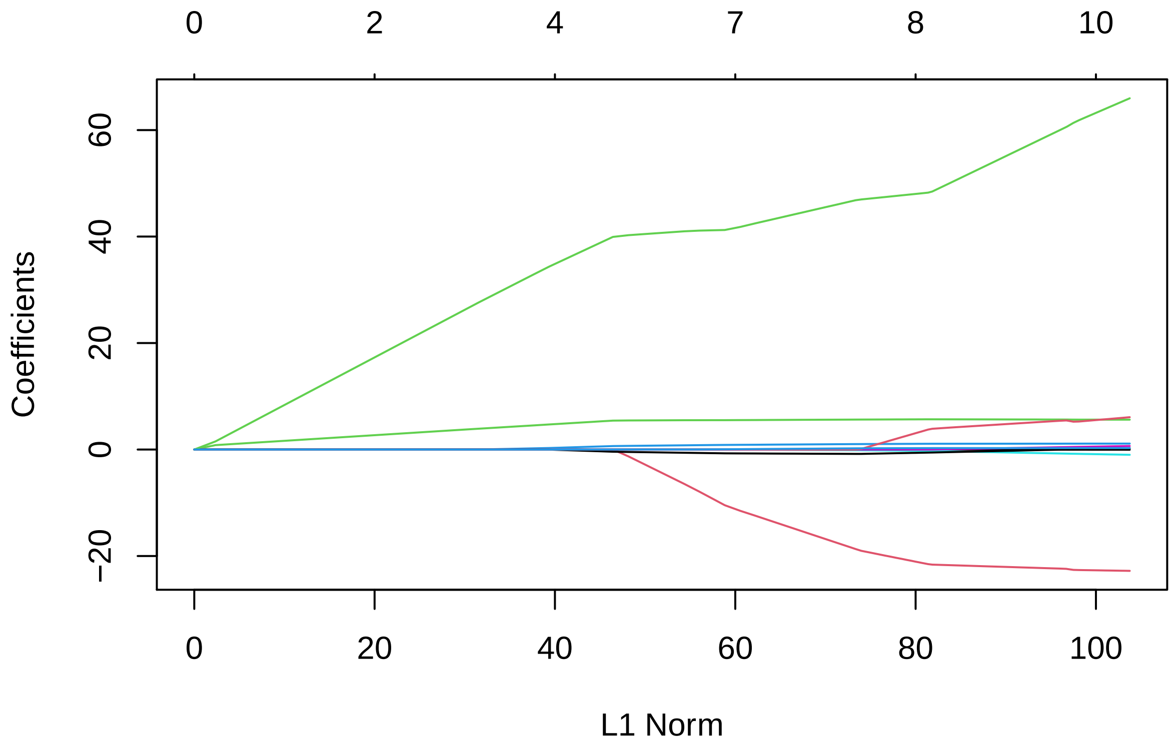
```r
library(glmnet)
```

```
## Loading required package: Matrix
```

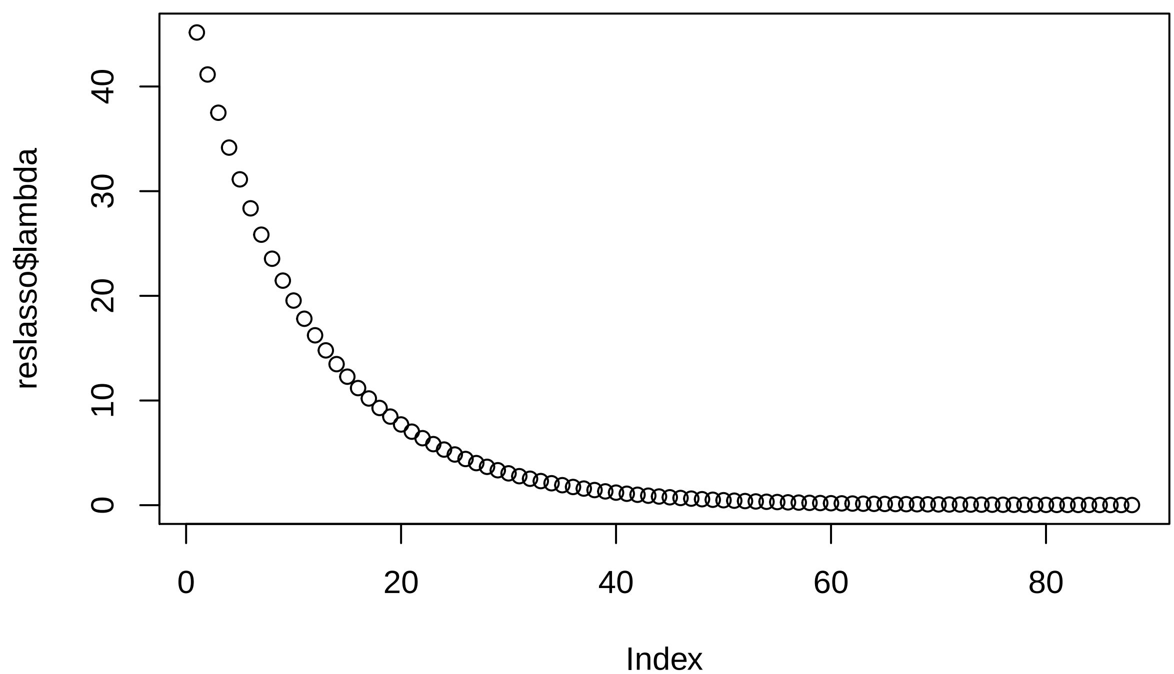
```
## Loaded glmnet 4.1
```

```r
reslasso <- glmnet(X, Y, alpha=1)

plot(reslasso)
```




```
plot(reslasso$lambda)
```



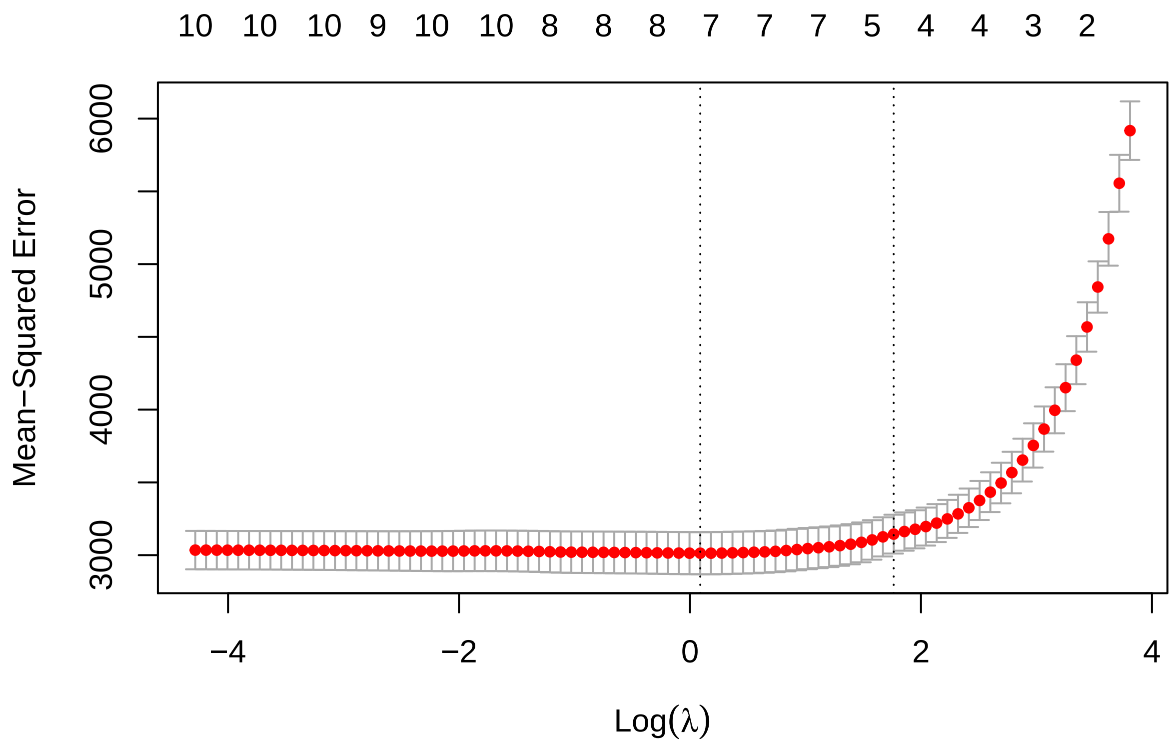

```
reslasso$lambda
```

```
##  [1] 45.16003002 41.14813742 37.49265031 34.16190659 31.12705697 28.36181502
##  [7] 25.84222954 23.54647710 21.45467297 19.54869896 17.81204642 16.22967331
## [13] 14.78787387 13.47415991 12.27715268 11.18648427 10.19270784  9.28721577
## [19]  8.46216512  7.71040969  7.02543815  6.40131759  5.83264218  5.31448632
## [25]  4.84236200  4.41217991  4.02021401  3.66306928  3.33765230  3.04114447
```

```
## [31]  2.77097757  2.52481156  2.30051426  2.09614292  1.90992736  1.74025468
## [37]  1.58565525  1.44479000  1.31643884  1.19949004  1.09293065  0.99583771
## [43]  0.90737023  0.82676196  0.75331471  0.68639230  0.62541510  0.56985495
## [49]  0.51923061  0.47310359  0.43107437  0.39277891  0.35788552  0.32609195
## [55]  0.29712284  0.27072727  0.24667660  0.22476253  0.20479525  0.18660180
## [61]  0.17002461  0.15492010  0.14115742  0.12861739  0.11719137  0.10678041
## [67]  0.09729434  0.08865098  0.08077547  0.07359960  0.06706121  0.06110368
## [73]  0.05567540  0.05072935  0.04622269  0.04211640  0.03837489  0.03496577
## [79]  0.03185951  0.02902920  0.02645032  0.02410055  0.02195952  0.02000870
## [85]  0.01823118  0.01661157  0.01513585  0.01379122
```

K-fold cross-validation to find the best λ value:

```
cv_lasso <- cv.glmnet(X, Y, alpha=1)
plot(cv_lasso)
```




```
best_lasso_lambda <- cv_lasso$lambda.min
print(paste("Best lambda:", best_lasso_lambda))
```

```
## [1] "Best lambda: 1.09293065470271"
```

Lasso with the best lambda:

```
best_lasso <- glmnet(X, Y, alpha=1, lambda=best_lasso_lambda)
coef(best_lasso)
```

```
## 11 x 1 sparse Matrix of class "dgCMatrix"
##                       s0
## (Intercept) -234.8536445
## AGE            .
## SEX          -18.3633828
## BMI            5.6204584
## BP             1.0138099
```

```
## S1              -0.1341321
## S2               .
## S3              -0.8186849
## S4               .
## S5              46.5721608
## S6               0.2161155
```