APA-L4

September 6, 2018

1 APA Laboratori 4 - Sistemes lineals (regularitzats)

```
In [1]: # uncomment to install libraries if missing
        #install.packages('car')
        #install.packages('glmnet')
```

```
In [2]: options(repr.plot.width=6, repr.plot.height=6)
```

veiem que les matrius AA^T i A^TA són diferents
definim i

```
In [3]: i <- sqrt(as.complex(-1))
```

i la matriu

```
In [4]: (A <- matrix(c(0,i,0,1),nrow=2,byrow = TRUE))
```

0+0i	0+1i
0+0i	1+0i

$A \cdot A^T$ és la matriu (-1 i; i 1)

```
In [5]: (A %*% t(A))
```

-1+0i	0+1i
0+1i	1+0i

$A^T \cdot A$ és la matriu tot zeros

```
In [6]: (t(A) %*% A)
```

0+0i	0+0i
0+0i	0+0i

1.1 EXEMPLE 1

Resolució d'un problema artificial senzill

Definició del sistema lineal a resoldre

$t = f(x) + \epsilon$

on $f(x) = (1 + 1/9)(x - 1) + 10$ i $\epsilon \sim N(0, 1)$

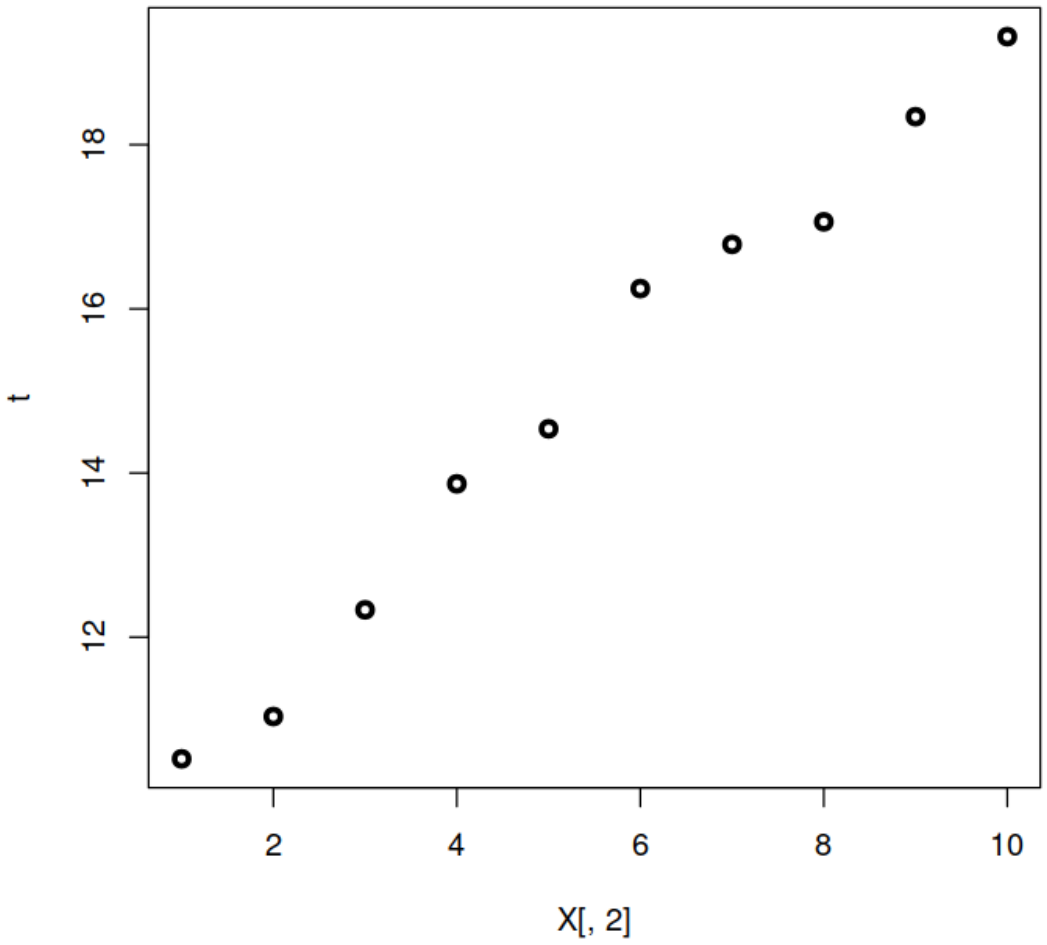
```
In [7]: N <- 10

        X <- matrix(c(rep(1,N), seq(N)),nrow=N)

        X
```

1	1
1	2
1	3
1	4
1	5
1	6
1	7
1	8
1	9
1	10

```
In [8]: t <- seq(10,20,length.out=N) + rnorm(N)

        t
```

1. 10.5172099974777 2. 11.0330281219168 3. 12.3327878698062 4. 13.8678111799862 5. 14.537991447224 6. 16.2463202458024 7. 16.7851313168272 8. 17.0597219689461 9. 18.3404934580554 10. 19.3159355759765

```
In [9]: options(repr.plot.width=6, repr.plot.height=6)
        plot(X[,2],t,lwd=3)
```



1.1.1 Solució de problemes de mínims quadrats de l'estil

$\min_w ||t - Xw||^2$

1) Resolució mitjançant la pseudo-inversa

$X^T \cdot X$

```
In [10]: (C <- t(X) %*% X)
```

$$\begin{matrix} 10 & 55 \\ 55 & 385 \end{matrix}$$

$(X^T \cdot X)^{-1} \cdot X^T$

```
In [11]: (X.pseudo <- solve(C) %*% t(X))
```

```
0.40000000  0.33333333  0.26666667  0.20000000  0.133333333  0.066666667  0.00000000  -0.06666
-0.05454545  -0.04242424  -0.03030303  -0.01818182  -0.006060606  0.006060606  0.01818182  0.030303
```

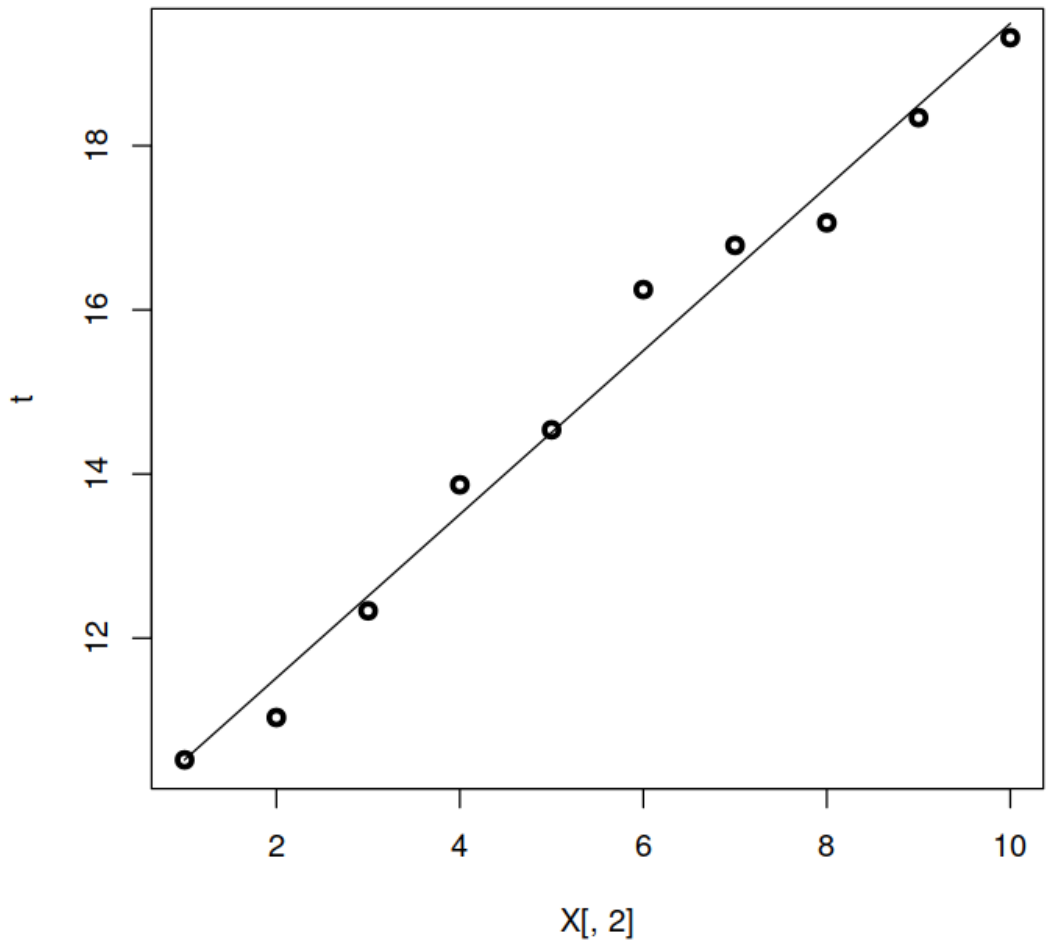
```
In [12]: (X.pseudo %*% X) # és pseudo-inversa esquerra d'X
```

```
1.000000e+00  8.881784e-16
1.387779e-17  1.000000e+00
```

```
In [13]: (w <- X.pseudo %*% t) # solució del problema
```

```
9.5224515
0.9965803
```

```
In [14]: plot(X[,2],t,lwd=3)
         lines (X[,2], w[2,1]*X[,2]+w[1,1], type="l")
```



2) Resolució mitjançant la SVD

```
In [15]: (s <- svd(X))
```

$d 1. 19.8217110839779 2. 1.44905821253278

$u

0.0571102	0.58497262
0.1070474	0.48685286
0.1569846	0.38873309
0.2069218	0.29061332
0.2568590	0.19249355
0.3067962	0.09437379
0.3567334	-0.00374598
0.4066706	-0.10186575
0.4566078	-0.19998551
0.5065449	-0.29810528

$v

0.1421813	0.9898406
0.9898406	-0.1421813

Les dues columnes d'X són linealment independents, i per tant els dos valors singulars són diferents de 0; en altres paraules, $rang(X) = 2 = min(10, 2)$, per tant X és "full rank"

ara comprovem que $X = UDV^T$

```
In [16]: D <- diag(s$d)
         s$u %*% D %*% t(s$v)
```

1	1
1	2
1	3
1	4
1	5
1	6
1	7
1	8
1	9
1	10

Ara ho apliquem a la solució del problema de mínims quadrats

$\min_w ||t - Xw||^2$

```
In [17]: D <- diag(1/s$d)
         (w <- s$v %*% D %*% t(s$u) %*% t)
```

9.5224515
0.9965803

noteu que obtenim la mateixa solució

La rutina `glm()` implementa regressió lineal per mínims quadrats si li demanem mitjançant el paràmetre `family = gaussian`

```
In [18]: (mostra <- data.frame(x=X,t=t))
```

x.1	x.2	t
1	1	10.51721
1	2	11.03303
1	3	12.33279
1	4	13.86781
1	5	14.53799
1	6	16.24632
1	7	16.78513
1	8	17.05972
1	9	18.34049
1	10	19.31594

Noteu que glm sempre afegeix un terme *intercept* o *offset* (un regressor constant 1) per defecte, així que tenim dues opcions:

1) desactivar-lo (el "-1" a la fòrmula següent) i usar la nostra pròpia columna de 1's

```
In [19]: model1 <- glm (t ~ x.2 + x.1 - 1, data=mostra, family = gaussian)
```

2) usar la que glm ja posa (recomanat) i desactivar la nostra pròpia columna de 1's

```
In [20]: model2 <- glm (t ~ x.2, data=mostra, family = gaussian)
```

Els coefficients (el vector w)

```
In [21]: model1$coefficients
         model2$coefficients
```

x.2 0.996580286450059 **x.1** 9.52245154272654
(Intercept) 9.52245154272653 **x.2** 0.99658028645006
** Per què la SVD?**

a. En formar la matriu $X^T X$ es pot perdre informació

```
In [22]: eps <- 1e-3
         (X.eps <- matrix(c(1,eps,0,1,0,eps),nrow=3))
```

1.000	1.000
0.001	0.000
0.000	0.001

```
In [23]: ((C.eps <- t(X.eps) %*% X.eps))
```

1.000001	1.000000
1.000000	1.000001

```
In [24]: solve(C.eps) # comencem a tenir problemes ...
```

500000.3	-499999.8
-499999.8	500000.3

```
In [25]: eps <- 1e-10
         (X.eps <- matrix(c(1,eps,0,1,0,eps),nrow=3))
```

1e+00	1e+00
1e-10	0e+00
0e+00	1e-10

```
In [26]: (C.eps <- t(X.eps) %*% X.eps)
```

1	1
1	1

```
In [27]: solve(C.eps) # dóna error (la matriu 2x2 "tot uns" és singular)
```

```
    Error in solve.default(C.eps): Lapack routine dgesv: system is exactly singular: U[2,2]
Traceback:


    1. solve(C.eps)

    2. solve.default(C.eps)
```

(el determinant és 1ů1 - 1ů1 = 0)
però no ho hauria de ser ... aquesta no és la nostra matriu ... el problema és que l'operacio X^T X fa perdre molta precissió numèrica (hem perdut epsilon)

b. El número de condició d'una matriu

El número de condició d'una matriu és el producte entre la norma de la matriu i la norma de la seva inversa Dóna una indicació de l'exactitud dels resultats de la inversió d'una matriu Valors prop d'1 indiquen una matriu ben condicionada

El número de condició de la matriu $X^T X$ és el quadrat del de la matriu X

Incidentalment, el número de condició corresponent a usar la norma-2 equival al quocient entre el valor singular més gran i el més petit (no nul) de la matriu

La rutina `kappa()` calcula el número de condició

```
In [28]: kappa(X, exact=TRUE)

         kappa(t(X) %*% X, exact=TRUE)
```

13.6790302229004
187.115867839024
veiem-ho amb un exemple:

```
In [29]: (X <- matrix(c(rep(1,N), 100+seq(N)),nrow=N))
```

1	101
1	102
1	103
1	104
1	105
1	106
1	107
1	108
1	109
1	110

```
In [30]: kappa(X, exact=TRUE)

         kappa(t(X) %*% X, exact=TRUE)
```

3878.27583919044
15041023.4842573

Una solució molt senzilla és centrar la segona columna:

```
In [31]: X <- matrix(c(rep(1,N), 100+seq(N)),nrow=N)

         X[,2] <- X[,2] - mean(X[,2])

         X
```

1	-4.5
1	-3.5
1	-2.5
1	-1.5
1	-0.5
1	0.5
1	1.5
1	2.5
1	3.5
1	4.5

```
In [32]: kappa(X, exact=TRUE)

         kappa(t(X) %*% X, exact=TRUE)
```

2.87228132326901
8.25

Hi ha una relació senzilla entre els dos sistems lineals; en altres paraules, podem "post-processar els coeficients de sortida perquè corresponguin a la matriu inicial

Nota: hi ha una rutina que calcula directament la pseudo-inversa (ho fa via la SVD):

```
In [33]: library(MASS)

         ginv(X)
```

0.10000000	0.10000000	0.10000000	0.10000000	0.100000000	0.100000000	0.10000000	0.100000
-0.05454545	-0.04242424	-0.03030303	-0.01818182	-0.006060606	0.006060606	0.01818182	0.030303

1.2 EXEMPLE 2

Anem a analitzar dades de greix corporal mitjançant regressió normal i ridge (regularitzada)

```
In [34]: bodyfat.data <- read.table(file = "bodyfatdata.txt", header=FALSE, col.names = c('trice

         summary(bodyfat.data)

         attach(bodyfat.data)

         N <- nrow(bodyfat.data)
```

```
    triceps          thigh           midarm         bodyfat
 Min.   :14.60   Min.   :42.20   Min.   :21.30   Min.   :11.70
 1st Qu.:21.50   1st Qu.:47.77   1st Qu.:24.75   1st Qu.:17.05
 Median :25.55   Median :52.00   Median :27.90   Median :21.20
 Mean   :25.30   Mean   :51.17   Mean   :27.62   Mean   :20.20
 3rd Qu.:29.90   3rd Qu.:54.62   3rd Qu.:30.02   3rd Qu.:24.27
 Max.   :31.40   Max.   :58.60   Max.   :37.00   Max.   :27.20
```

let us start with standard linear regression this time we directly use the method `lm()`; `lm()` is actually called by glm() for gaussian noise and is the workhorse for least squares

```
In [35]: (model <- lm(bodyfat ~ ., data = bodyfat.data))
         summary(model)
```

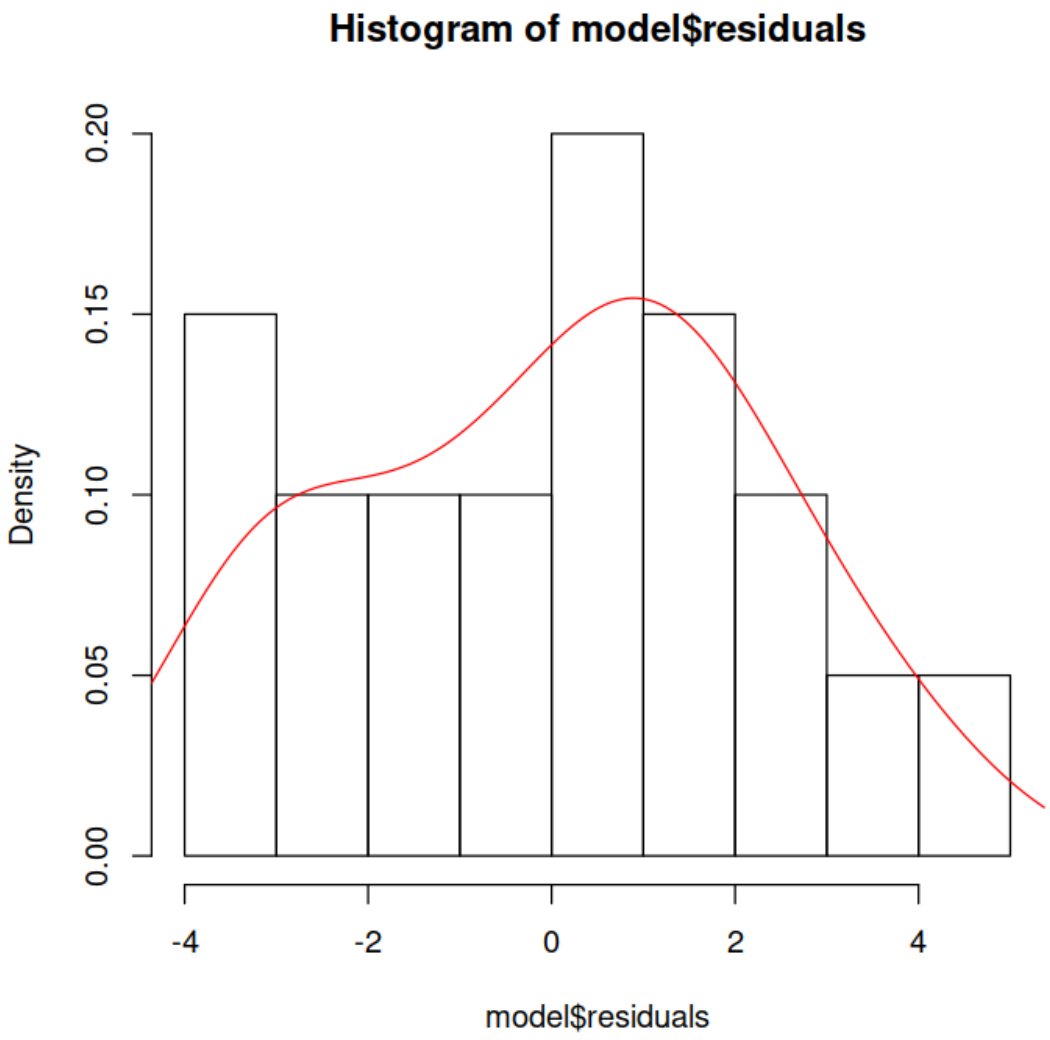
```
Call:
lm(formula = bodyfat ~ ., data = bodyfat.data)

Coefficients:
(Intercept)      triceps        thigh       midarm
    117.085        4.334       -2.857       -2.186
```

```
Call:
lm(formula = bodyfat ~ ., data = bodyfat.data)

Residuals:
    Min      1Q  Median      3Q     Max
-3.7263 -1.6111  0.3923  1.4656  4.1277

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  117.085     99.782   1.173    0.258
triceps        4.334      3.016   1.437    0.170
```

```
thigh          -2.857      2.582  -1.106    0.285
midarm         -2.186      1.595  -1.370    0.190

Residual standard error: 2.48 on 16 degrees of freedom
Multiple R-squared:  0.8014,Adjusted R-squared:  0.7641
F-statistic: 21.52 on 3 and 16 DF,  p-value: 7.343e-06
```

How to read this output:
$x = (1, triceps, thigh, midarm)^T$
$w = (117.085, 4.334, -2.857, -2.186)^T$
the model is $y(x; w) = w^T x = 117.085 + 4.334 * triceps - 2.857 * thigh - 2.186 * midarm$
The residuals are the differences $(t_n - y(x_n; w)), n = 1, \ldots N$
let's inspect `model$residuals`

```
In [36]: dens <- density(model$residuals)
         hist(model$residuals, prob=T)
         lines(dens,col="red")
```



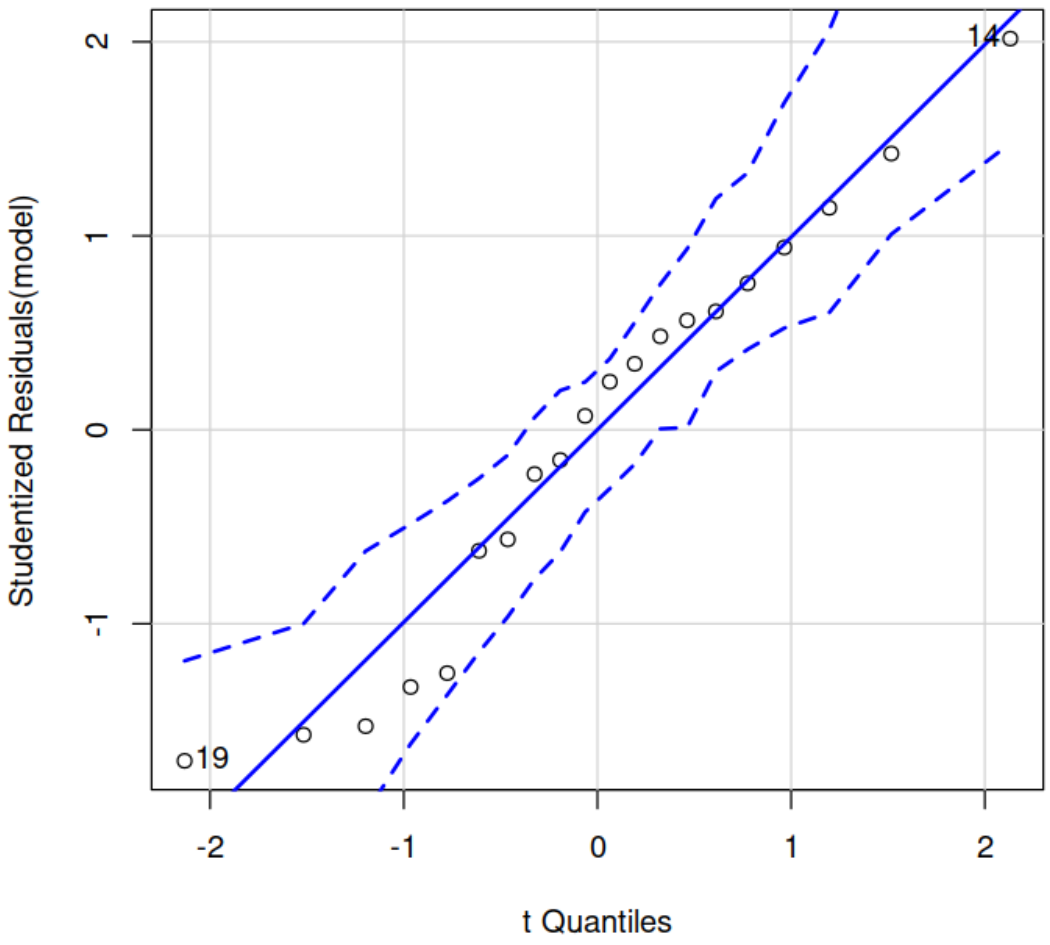
Do the residuals look Gaussian? this is direct indication of model validity (since it was our departing assumption)

Let's do a more informative plot (a QQ-plot), which plots actual quantiles against theoretical quantiles of a comparison distribution (Gaussian in this case)

```
In [37]: library(car)
         qqPlot(model)
```

```
Loading required package: carData
```

1. 14 2. 19



The solid line corresponds to the theoretical quantiles therefore in this case the residuals are not even close (the tails are heavier, the central part is flatter)

This is how we can compute the mean square error

```
In [38]: prediction <- predict(model)
         (mean.square.error <- sum((bodyfat - prediction)^2)/N)
```

4.92024440837828

Is this number large or small? it depends on the magnitude of the targets! a very good practice is to normalise it, by dividing by the variance of the target:

```
In [39]: (norm.mse <- sum((bodyfat - prediction)^2) / ((N-1)*var(bodyfat)))
```

0.198641449137629

If we divide the mean square error by the variance of the targets t, we get the proportion of the variability of the target that is NOT explained by the model

A model with 'norm.mse' equal to 1 is as good as the best constant model (namely, the model that always outputs the average of the target)

models with 'norm.mse' above 0.5 are so so, beyond 0.7 they begin to be quite bad

models with 'norm.mse' below 0.2 are quite good

The Multiple R-squared (usually used by statisticians) is obtained by subtracting this quantity form one; that is, the proportion of the target variability that is explained by the model; in this case it reaches 80%

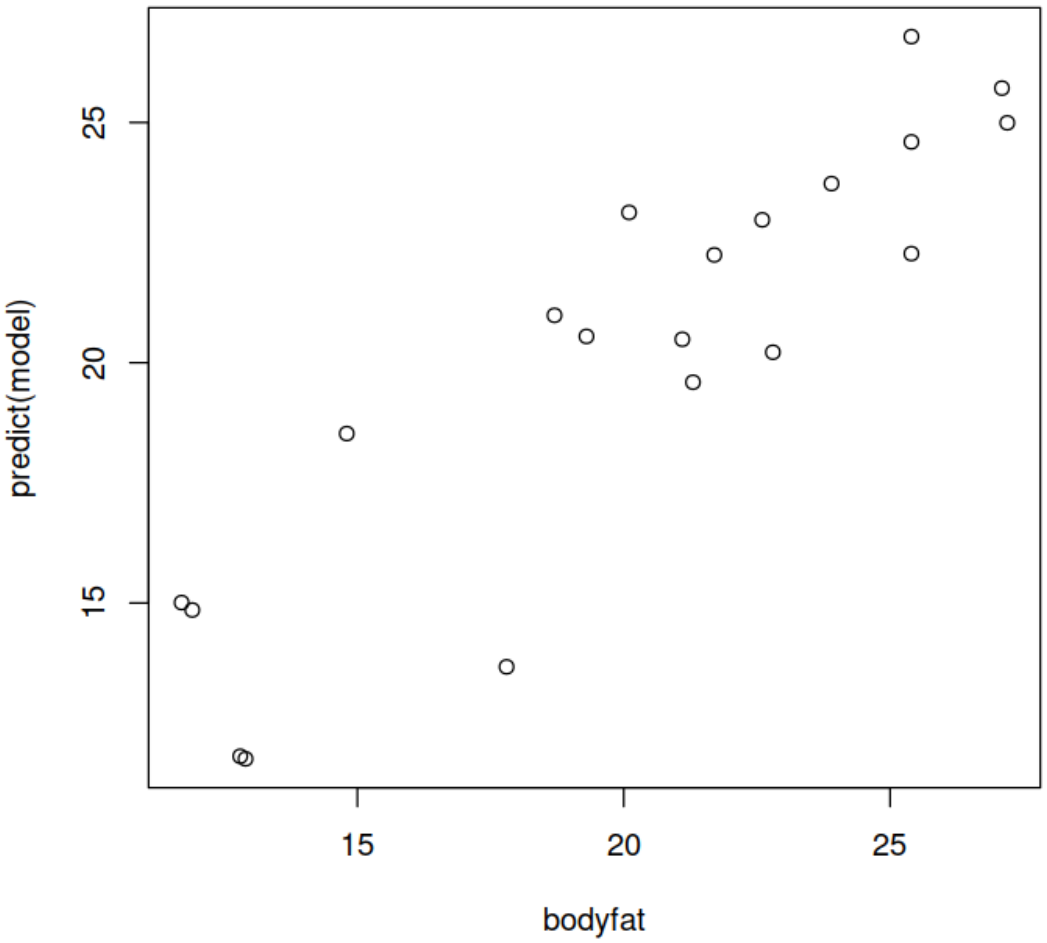
```
In [40]: (R.squared <- (1 - norm.mse)*100)
```

80.1358550862371

The "adjusted R-squared" is the same thing, but adjusted for the complexity of the model, i.e. the number of parameters (three in our case)

Now let us try to see how are the real predictions by plotting the real predictions against the targets:

```
In [41]: plot(bodyfat, predict(model))
```



It is difficult to see if the model is a good predictor; what we need is a numerical assessment of predictive ability. We compute the exact LOOCV as seen in class:

$LOOCV = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{y_i-\hat{y}_i}{1-h_i}\right)^2$

where $H = X(X^TX)^{-1}X^T$ and $h_i = diag(H)_i$

```
In [42]: (LOOCV <- sum( (model$residuals/(1-ls.diag(model)$hat))^2) / N)
```

8.03682803713587

and the corresponding predictive R-square

```
In [43]: (R2.LOOCV = (1 - LOOCV*N/((N-1)*var(bodyfat)))*100)
```

67.5534986626246

we can see that prediction quality is not as good as it seemed (since CV error is worse than training error)

this last number is the one I recommend to do model selection!!!

Let us continue now with *regularized linear regression* (aka ridge regression) this time we need to use the method lm.ridge()

We must first choose a value for lambda (the regularization constant) there are several criteria to do this, the most used of which is the GCV so we optimize the GCV for several values of lambda in a sequence

```
In [44]: library(MASS)
```

notice we start with a wide logarithmic search

```
In [45]: lambdas <- 10^seq(-6,2,0.1)

         select(lm.ridge(bodyfat ~ triceps + thigh + midarm, lambda = lambdas))
```

```
modified HKB estimator is 0.008505093
modified L-W estimator is 0.3098511
smallest value of GCV  at 0.01995262
```

best value (according to GCV) is 0.01995262

we perform a finer search

```
In [46]: lambdas <- seq(0,1,0.001)

         select(lm.ridge(bodyfat ~ triceps + thigh + midarm, lambda = lambdas))
```

```
modified HKB estimator is 0.008505093
modified L-W estimator is 0.3098511
smallest value of GCV  at 0.019
```

Definitely the best value is 0.019, so we refit the model with this precise value:

```
In [47]: (bodyfat.ridge.reg <- lm.ridge(bodyfat ~ triceps + thigh + midarm, lambda = 0.019))
```

```
              triceps      thigh     midarm
43.8401126  2.1174933 -0.9597309 -1.0180612
```

Now let us compare these results with those obtained by standard regression (without regularization)

Hand calculation of coefficients, since we know the theory:

```
In [48]: X <- cbind(rep(1,length=length(bodyfat)),triceps, thigh, midarm)

         (w <- ginv(X) %*% bodyfat)
```

117.084695
4.334092
-2.856848
-2.186060

call to `lm()`, check they should coincide

```
In [49]: model$coefficients
```

(Intercept) 117.084694775123 **triceps** 4.33409200822048 **thigh** -2.85684793616613 **midarm** -2.18606025161192

Notice that the regularized weights are smaller (in absolute value), one by one

Now we calculate the corresponding prediction errors First by standard regression (without regularization, we already did this)

```
In [50]: R2.LOOCV
```

67.5534986626246

Now those with ridge regression (with regularization):

```
In [51]: (1 - bodyfat.ridge.reg$GCV)*100
```

0.019: 67.0394825362933

The prediction errors are quite close and the model is way simpler: we would probably prefer the regularized one

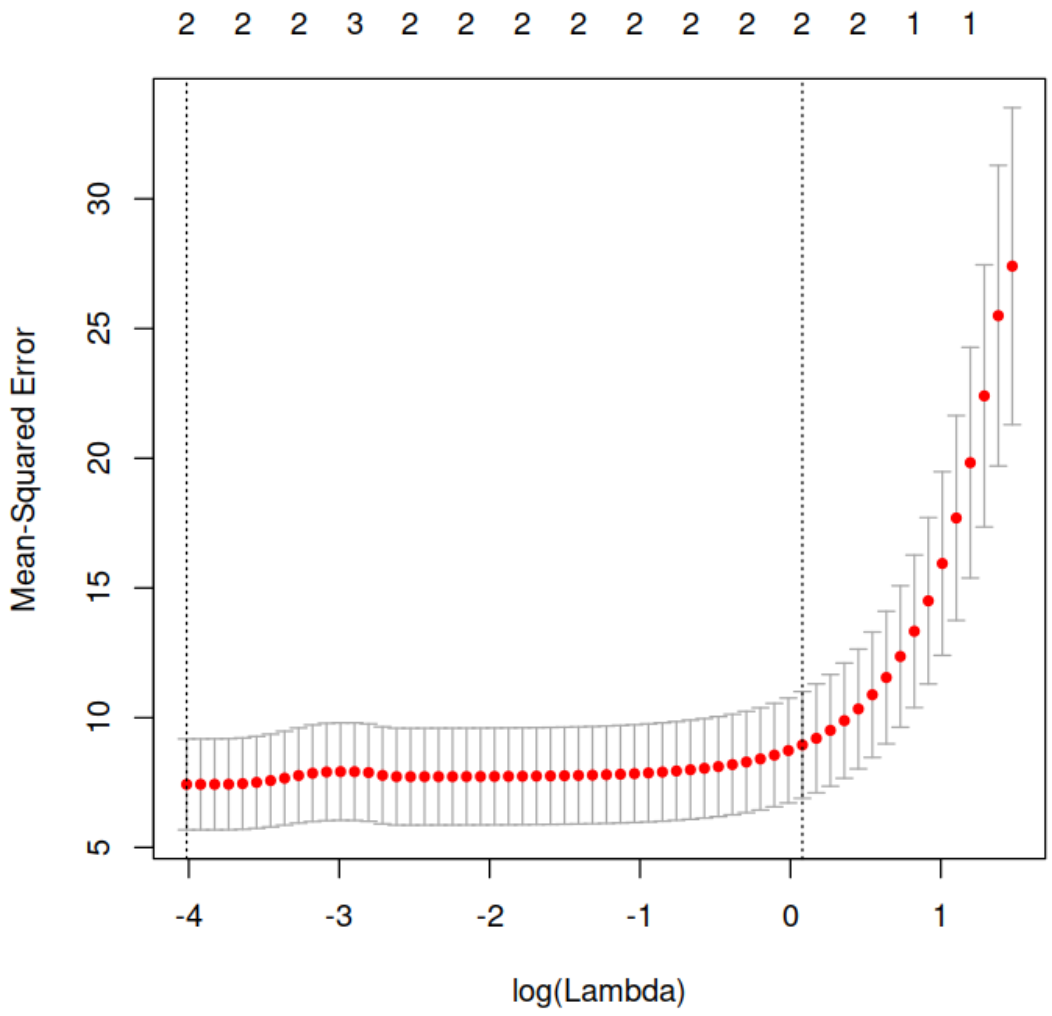
---

Now we use the LASSO: here the coefficients are penalized by the L1 norm. The optimal value for lambda is again chosen by cross-validation

```
In [52]: library(glmnet)

         t <- as.numeric(bodyfat.data[,4])
         x <- as.matrix(bodyfat.data[,1:3])

         model.lasso <- cv.glmnet (x, t, nfolds = length(t))
```

```
Loading required package: Matrix
Loading required package: foreach
Loaded glmnet 2.0-16

Warning message:
Option grouped=FALSE enforced in cv.glmnet, since < 3 observations per fold
```

```
In [53]: plot(model.lasso)
```




```
In [54]: coef(model.lasso)

4 x 1 sparse Matrix of class "dgCMatrix"
                      1
(Intercept) -10.5932144
triceps       0.1088958
thigh         0.5478329
midarm        .
```

lambda.min is the value of lambda that gives minimum mean cross-validated error

```
In [55]: model.lasso$lambda.min
```

0.0180575518391553

Predictions can be made based on the fitted cv.glmnet object; for instance, this would be the TR error with the *optimal* lambda as chosen by LOOCV

```
In [56]: predict (model.lasso, newx = x, s = "lambda.min")
```

1
13.80151
19.34897
21.59742
23.19321
12.64429
22.14266
26.26047
21.51608
18.87550
21.57901
24.94938
24.97125
15.58109
14.21130
12.22415
23.31714
23.38544
26.33414
17.82570
20.14130

And this would be corresponding LOOCV

```
In [57]: (LOOCV <- model.lasso$cvm[model.lasso$lambda == model.lasso$lambda.min])
```

7.42924547792074

and the corresponding predictive R-square

```
In [58]: (R2.LOOCV = (1 - LOOCV*N/((N-1)*var(bodyfat)))*100)
```

70.0064475410934

This LASSO method then seems to deliver a better model