CompStat/R - Paper 3

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Part I: Linear regression

In this first part of the paper, we will program a function which estimates the unknown parameters β and σ of a (ordinary) linear regression model

$$y = X\beta + \varepsilon, \qquad \varepsilon \sim N(0, \sigma^2 I)$$

by the ordinary least squares (OLS) method. For a given design matrix X and response vector y the OLS estimator is given by

$$\hat{\beta} = (X'X)^{-1}X'y \tag{1}$$

with covariance matrix

$$Var(\hat{\beta}) = \sigma^2 (X'X)^{-1} \tag{2}$$

where σ^2 has to be estimated via the sum of squared residuals (SSR):

$$\hat{\sigma}^2 = \frac{SSR}{df} = \frac{\sum_i (y_i - x_i'\hat{\beta})^2}{n - k}.$$
(3)

The term df refers to the degrees of freedom, i.e. the difference between the number of observations n and the number of coefficients k.

Raw implementation

The function linModEst is a raw implementation of the OLS estimator. The function takes the response vector y(y) and design matrix X(x) as arguments and returns a list with the following named elements:

- coefficients: the estimated coefficients $\hat{\beta}$
- vcov: the estimated covariance matrix $\operatorname{Var}(\hat{\beta})$
- sigma: the square root of the estimated scale parameter $\hat{\sigma}^2$
- df: the degrees of freedom df

We use equations (1), (2), and (3) for the implementation and compute the inverse of X'X using the solve function, which numerically solves the equation

$$(X'X) A = I$$

for the matrix $A = (X'X)^{-1}$. To efficiently compute X'X and X'y, we use the crossprod function.

```
linModEst <- function(x, y) {</pre>
  # Computes the OLS estimator and sample variance assuming a (ordinary) linear
  # regression model.
  # Args:
    x: design matrix x
     y: response vector y
  # Returns:
  #
     A list with the following named elements:
        $coefficients: the estimated coefficients
  #
  #
        $vcov: the estimated covariance matrix
        $sigma: the square root of the estimated variance
  #
        $df: the degrees of freedom in the model, i.e. the difference between
             the number of rows and columns of x
  # Compute the inverse of (x'x) using the solve- and crossprod-function
  inv <- solve(crossprod(x), diag(nrow = ncol(x)))</pre>
  # Compute beta hat, i.e. the estimated coefficients
  coefficients <- inv %*% crossprod(x, y)</pre>
  # Compute the degrees of freedom
  df \leftarrow nrow(x) - ncol(x)
  # Compute the sample variance via the sum of squared residuals (SSR)
  SSR <- sum((y - x %*% coefficients)^2)
  sigmaSquared <- SSR / df
  # Compute the covariance matrix
  vcov <- sigmaSquared * inv
  # Create named results list to be returned
  results <- list(coefficients, vcov, sqrt(sigmaSquared), df)
  names(results) <- c("coefficients", "vcov", "sigma", "df")</pre>
  # Return results
  results
}
```

We test our implementation by computing the linear relationship between heart weight, body weight, and sex for the cats dataset contained in the package MASS. In the following piece of code, cbind combines its arguments by columns into a matrix with the number of columns given by the number of arguments and the number of rows given by the greatest length of the given arguments. Shorter arguments are repeated, as long as the matrix number of rows is a multiple of the shorter vector lengths.

Hence, cbind(1, cats\$Bwt, as.numeric(cats\$Sex) - 1) creates a design matrix with an intercept column out of a vector of ones, the variable body weight (bwt), and the variable sex (Sex), which is converted from a factor into a dummy variable using as.numeric. We subtract 1 to receive dummy variable values of 0 and 1, rather than 1 and 2 from the original data. Thus, cbind is used to build a proper design matrix of object type matrix with an intercept and dummy variable, such that our implementation of linModEst works correctly.

```
# Load cats dataset
data(cats, package = "MASS")
# Compute OLS using our implementation
linModEst(
 x = cbind(1, cats$Bwt, as.numeric(cats$Sex) - 1),
 y = cats$Hwt
## $coefficients
               [,1]
## [1,] -0.41495263
## [2,] 4.07576892
## [3,] -0.08209684
##
## $vcov
##
                           [,2]
                                        [,3]
               [,1]
## [1,] 0.52900070 -0.20504763 0.06563743
## [2,] -0.20504763  0.08690026 -0.04696312
## [3,] 0.06563743 -0.04696312 0.09244480
##
## $sigma
## [1] 1.457138
##
## $df
## [1] 141
```

We verify our results by comparing them to the output of R's lm function:

```
summary(lm(Hwt ~ Bwt + Sex, data = cats))
```

```
##
## Call:
## lm(formula = Hwt ~ Bwt + Sex, data = cats)
##
## Residuals:
      Min
               1Q Median
                               3Q
                                      Max
## -3.5833 -0.9700 -0.0948 1.0432 5.1016
## Coefficients:
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) -0.4149
                          0.7273 -0.571
                                             0.569
                4.0758
## Bwt
                           0.2948 13.826
                                            <2e-16 ***
               -0.0821
## SexM
                           0.3040 -0.270
                                             0.788
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 1.457 on 141 degrees of freedom
## Multiple R-squared: 0.6468, Adjusted R-squared: 0.6418
## F-statistic: 129.1 on 2 and 141 DF, p-value: < 2.2e-16
```

As we can see, our implementation is correct.

Extend implementation

In this section, we write a new function linMod(formula, data), which estimates a linear regression model specified by formula and uses our linModEst function defined above to estimate the model parameters again by the OLS method. linMod returns a list with the following named elements:

• coefficients: named vector of the estimated coefficients $\hat{\beta}$ • vcov: named estimated covariance matrix $\widehat{\mathrm{Var}}(\hat{\beta})$ • sigma: the square root of the estimated scale parameter $\hat{\sigma}^2$ • df: the degrees of freedom df• formula: the formula that represents the model equation
• call: the arguments with which linMod was called

Below, we use the model.frame, model.extract, and model.matrix functions, which are very convenient for working with objects of the class formula. model.frame returns a data.frame containing only the variables from its passed data argument, which are used in the formula expression given. The returned data.frame from the model.frame function has additional attributes, but these are not needed in our application. With model.extract, we are able to extract the response variable from the data.frame created by model.frame. Moreover, using model.matrix, we can create the design matrix (of object class matrix) again only from formula and data arguments. By default, the matrix returned by model.matrix includes an intercept and converts factor variables into proper dummy variables (i.e. a factor variable with L levels results in L-1 dummy variables). More precisely, the default intercept is taken over from the formula object, which then by default adds an intercept term to the model equation, if not specified otherwise. Finally, we use match.call to return the call of our function with all the specified arguments by their full names.

```
linMod <- function(formula, data) {</pre>
  # Computes the OLS estimator and sample variance assuming a (ordinary) linear
  # regression model with model equation specified by the formula-argument.
  #
  # Args:
      formula: a formula specifying the linear model equation
  #
      data: a data.frame, list or environment, containing the variables used in
            formula
  #
  # Returns:
     A list with the following named elements:
        $coefficients: named vector of the estimated coefficients
  #
        $vcov: named estimated covariance matrix
  #
        $sigma: the square root of the estimated variance
        $df: the degrees of freedom in the model
        $formula: the formula that represents the model equation
        $call: the arguments with which the function was called
  # Extract the response variable using the model.extract function on the
  # data.frame returned by model.frame
  y <- model.extract(model.frame(formula, data = data), "response")
  # Create the design matrix using model.matrix, which overtakes an intercept
  # specified in the formula argument by default and converts factor variables into proper
  # dummy variables
  x <- model.matrix(formula, data = data)
  # Use previously defined linModEst for estimation
```

```
tmp <- linModEst(x, y)

# Prepare the output
rownames(tmp$coefficients) <- colnames(x)
colnames(tmp$vcov) <- colnames(x)
rownames(tmp$vcov) <- colnames(x)

# Create results list to be returned
results <- c(tmp, formula, match.call())
names(results) <- c("coefficients", "vcov", "sigma", "df", "formula", "call")

# Return results
results
}</pre>
```

Let's again test our implementation:

```
linMod(Hwt ~ Bwt + Sex, data = cats)
```

```
## $coefficients
                    [,1]
## (Intercept) -0.41495263
## Bwt
             4.07576892
             -0.08209684
## SexM
##
## $vcov
##
             (Intercept)
                                Bwt
                                          SexM
## (Intercept) 0.52900070 -0.20504763 0.06563743
             ## SexM
              0.06563743 -0.04696312 0.09244480
##
## $sigma
## [1] 1.457138
##
## $df
## [1] 141
##
## $formula
## Hwt ~ Bwt + Sex
##
## $call
## linMod(formula = Hwt ~ Bwt + Sex, data = cats)
```

As we can see, the output has the desired format and the correct results.

Part II: S3 for linear models

In this section we will expand upon our linear model function using R's S3 class system. Our goal is to improve the function by returning a more concise output and ultimately replicating the results of the 1m function. We'll start by redefining the function 1inMod from Part I and assigning its return a class attribute named 1inMod. This means that the 1inMod function now is a constructor function. As the name implies, this function "constructs" instances of class 1inMod. There is no formal definition of the "class" in R. Instead, a list is of a certain class, which is assigned by a class attribute. Hence, the output of 1inMod is a list of class 1inMod. The assigned class can now be used to call class-specific methods of generic functions such as print or summary.

1. Define the class

First we implement the constructor linMod (modified function from Part I). For some additional calculations later (in the summary method section), we also return the data x and the response y.

```
linMod <- function(formula, data) {</pre>
  # Extract the response variable and create the design matrix
  y <- model.extract(model.frame(formula, data = data), "response")
  x <- model.matrix(formula, data = data)
  # Calulcate model using linModEst from Part I
  tmp <- linModEst(x, y)</pre>
  # Prepare the output
  rownames(tmp$coefficients) <- colnames(x)</pre>
  colnames(tmp$vcov) <- colnames(x)</pre>
  rownames(tmp$vcov) <- colnames(x)</pre>
  # Create results list to be returned and additionally add x and y as list
  results <- c(tmp, formula, match.call(), list(x, y))
  names(results) <- c("coefficients", "vcov", "sigma", "df",</pre>
                       "formula", "call", "x", "y")
  # Redefine the results list class attribute as "linMod"
  # This makes linMod a constructor for instances of class "linMod"
  class(results) <- "linMod"</pre>
  # Return instance of class "linMod"
  results
}
```

Now we would like to have a look at the structure of our list, which is an instance of the linMod class:

```
# Call constructur function which constructs an instance of class "linMod"
# Internally it still uses the model calculations from Part I (linModEst)
modelFit <- linMod(Hwt ~ Bwt + Sex, data = cats)

# Verify the structure of modelFit
str(modelFit)

## List of 8
## $ coefficients: num [1:3, 1] -0.415 4.0758 -0.0821</pre>
```

```
##
     ..- attr(*, "dimnames")=List of 2
##
     ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
     .. ..$ : NULL
##
##
  $ vcov
                  : num [1:3, 1:3] 0.529 -0.205 0.0656 -0.205 0.0869 ...
##
     ..- attr(*, "dimnames")=List of 2
     ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
##
     ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
##
   $ sigma
                  : num 1.46
##
   $ df
                  : int 141
                  :Class 'formula' length 3 Hwt ~ Bwt + Sex
## $ formula
     ....- attr(*, ".Environment")=<environment: R_GlobalEnv>
## $ call
                  : language linMod(formula = Hwt ~ Bwt + Sex, data = cats)
## $ x
                  : num [1:144, 1:3] 1 1 1 1 1 1 1 1 1 1 ...
    ..- attr(*, "dimnames")=List of 2
##
     ....$ : chr [1:144] "1" "2" "3" "4" ...
##
##
     ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
##
     ..- attr(*, "assign")= int [1:3] 0 1 2
##
     ..- attr(*, "contrasts")=List of 1
##
     .. .. $ Sex: chr "contr.treatment"
## $ y
                  : Named num [1:144] 7 7.4 9.5 7.2 7.3 7.6 8.1 8.2 8.3 8.5 ...
##
    ..- attr(*, "names")= chr [1:144] "1" "2" "3" "4" ...
## - attr(*, "class")= chr "linMod"
```

As we can see, we successfully redefined linMod such that the returned list is of class linMod.

2. Print method

Now we'd like to define a printing method for all objects of class linMod so that the function returns a more readable and concise output. We want to use a format that resembles the style for printing the lm information. To avoid writing a function with a new name, we define a new method print.linMod for the generic function print, assigned to the class linMod:

```
print.linMod <- function(x, ...) {</pre>
  # Print the function call and coefficients for objects of class "linMod"
  # Args:
  # x: instance of class linMod
      ...: passed arguments from generic function to this method
  # Returns:
     No value gets returned. The function just prints to the console
  # Convert coefficients matrix as named vector, which is more covenient
  coefficients <- as.vector(x$coefficients)</pre>
  names(coefficients) <- rownames(x$coefficients)</pre>
  # Create the output using cat, deparse, and print.default
  cat("\nCall:\n", deparse(x$call), "\n\n", "Coefficients:\n",sep="")
  print.default(format(coefficients, digits = 2),
                print.gap = 2L,
                quote = FALSE)
  cat("\n")
}
```

We simply would like to print the model to see that the output is now clear, easy to read, and similar to 1m. It is not necessary to call the defined method above explicitly. R will recognize the newly defined linMod object and then locate the linMod method that we have written for the generic print function. We just need to call print, which R automatically calls if we just enter the object into the console. Thus, we just need to call:

```
# Print modelFit
```

modelFit

The output is now much clearer and more user-friendly.

3. Summary method

Next we'll define a function to add some more information to the linMod object. We would just like to call the summary function, so we'll again write a new method summary.linMod for our class linMod. Therefore, when calling summary, R again automatically detects the class and calls our new method.

To build the summary we need to calculate the *standard errors*, the *t-values*, the *p-values*, the *residuals* and the *coefficient of determination*. let's first have a look at the calculation of these values.

The standard error $\operatorname{se}(\hat{\beta}_i)$ of the estimated coefficient $\hat{\beta}_i$ is given by its estimated standard deviation. Hence, the standard errors $\operatorname{se}(\hat{\beta})$ are given by the square roots of the elements on the diagonal of the estimated covariance matrix $\widehat{\operatorname{Var}(\hat{\beta})}$:

$$\operatorname{se}(\hat{\beta}) = \sqrt{\operatorname{diag}\left(\widehat{\operatorname{Var}(\hat{\beta})}\right)} \in \mathbb{R}^k,$$
 (4)

where the square root is applied element-wise.

The t-value t_i of each estimated coefficient $\hat{\beta}_i$ is a realization of the following t-distributed test statistic:

$$T_i = \frac{\hat{\beta}_i}{\operatorname{se}(\hat{\beta}_i)} \stackrel{H_0}{\sim} t_{(n-k)},\tag{5}$$

which tests if the true coefficient β_i significantly differs from zero, i.e. we test the hypothesis:

$$H_0: \beta_i = 0 \quad vs. \quad H_1: \beta_i \neq 0.$$
 (6)

For the calculation of the corresponding p-value p_i , we need to calculate the probability that our test statistic T_i is greater than or equal to the realization t_i given by the data. Since the t-distribution is symmetric, we have for a two-sided t-test:

$$p_i = 2 \cdot \mathbb{P}(T_i \ge t_i) \tag{7}$$

We can use the pt function in R to compute the probability for a quantile of a t-distribution.

The residuals $\hat{\varepsilon}$ are simply the difference between the response y and the prediction \hat{y} given by the model.

$$\hat{\varepsilon} = y - \hat{y} = y - X\hat{\beta} \tag{8}$$

Lastly, we calculate the *coefficient of determination* R^2 (also known as R-squared), which indicates the proportion of the variance in the dependent variable y that is predictable from the independent variables X. To calculate this coefficient, we need to calculate the sum of squared residuals SSR, and the variation of y, which is usually called SST (total sum of squares):

$$R^2 = 1 - \frac{\text{SSR}}{\text{SST}},\tag{9}$$

with

$$SSR = \sum_{i} \hat{\varepsilon}^{2} \quad and \quad SST = \sum_{i} (y_{i} - \bar{y})^{2}. \tag{10}$$

In the summary.linMod method below, we compute all these values, combine them together, and assign a class attribute to the result that the method returns:

```
summary.linMod <- function(x, ...) {</pre>
  # This summary method for objects of class linMod computes standard errors,
  # t-values, p-values, residuals, and the R-squared of the given model.
  # Args:
     x: instance of class linMod
      ...: passed arguments from generic function to this method
     A list with the following named elements:
  #
        $coefficients: named matrix of the estimated coefficients, their
          standard errors, t values and p values
  #
  #
        $vcov: named estimated covariance matrix
        $sigma: the square root of the estimated variance
        $df: the degrees of freedom in the model
        $formula: the formula that represents the model equation
        $call: the arguments with which the function was called
        $residuals: the residuals of the model
        $rSquared: coefficient of determination of the model
  # Compute extra information for coefficients and combine them
  estimates <- x$coefficients
  stdErrors <- sqrt(diag(x$vcov))</pre>
  tValues <- estimates/stdErrors
  pValues <- 2*pt(-abs(tValues), df=(nrow(x$x)-ncol(x$x)))
  x$coefficients <- cbind(estimates, stdErrors, tValues, pValues)
  colnames(x$coefficients) <- c("Estimate", "Std. Err.", "t value", "P(>|t|)")
  # Compute residuals on basis of estimated response
  residuals <- x$y - (x$x %*% estimates)
  # Compute R-squared of whole model
```

```
# Since the mean of the residuals is zero, we can use the var function
rSquared <- 1-(var(residuals)/var(x$y))

# Combine all results in one list
results <- c(x, list(residuals=as.vector(residuals), rSquared=rSquared))

# Redefine the results to class "summary.linMod"
# This function has now the role of a constructor
class(results) <- "summary.linMod"

# Return results
results
}</pre>
```

After the implementation we can test the structure of our new object:

```
# Call constructur function which constructs an
# instance of class "summary.linMod"
summaryOfModelFit <- summary(modelFit)

# Verify the structure of summaryOfMOdelFit
str(summaryOfModelFit)</pre>
```

```
## List of 10
## $ coefficients: num [1:3, 1:4] -0.415 4.0758 -0.0821 0.7273 0.2948 ...
    ..- attr(*, "dimnames")=List of 2
    ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
    .. ..$ : chr [1:4] "Estimate" "Std. Err." "t value" "P(>|t|)"
##
## $ vcov
                 : num [1:3, 1:3] 0.529 -0.205 0.0656 -0.205 0.0869 ...
    ..- attr(*, "dimnames")=List of 2
##
    ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
    ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
## $ sigma
                : num 1.46
## $ df
                 : int 141
                :Class 'formula' length 3 Hwt ~ Bwt + Sex
## $ formula
   ...- attr(*, ".Environment")=<environment: R GlobalEnv>
## $ call
                 : language linMod(formula = Hwt ~ Bwt + Sex, data = cats)
## $ x
                 : num [1:144, 1:3] 1 1 1 1 1 1 1 1 1 1 ...
    ..- attr(*, "dimnames")=List of 2
    ....$ : chr [1:144] "1" "2" "3" "4" ...
    ....$ : chr [1:3] "(Intercept)" "Bwt" "SexM"
##
    ..- attr(*, "assign")= int [1:3] 0 1 2
##
    ..- attr(*, "contrasts")=List of 1
    .. .. $ Sex: chr "contr.treatment"
                 : Named num [1:144] 7 7.4 9.5 7.2 7.3 7.6 8.1 8.2 8.3 8.5 ...
## $ y
    ..- attr(*, "names")= chr [1:144] "1" "2" "3" "4" ...
##
## $ residuals : num [1:144] -0.737 -0.337 1.763 -0.944 -0.844 ...
## $ rSquared
               : num [1, 1] 0.647
## - attr(*, "class")= chr "summary.linMod"
```

We now have a list of 10 elements in which **\$residuals** and **\$rSquared** are new and the coefficient vector has been extended.

4. Print method for summary.linMod

Next we would like to have a method to print objects of class summary.linMod in a self-defined way. For this purpose we define a new method print.summary.linMod which, again, is based on the generic function print. The goal is to have an output that is similar to the print.summary.lm method.

```
print.summary.linMod <- function(x, ...) {</pre>
  # Print the function call, the residuals, the extended coefficients,
  # and the R-squared
  #
 # Args:
      x: instance of class summary.linMod
      ...: passed arguments from generic function to this method
  # Returns:
     No value gets returned. The function just prints to the console.
  # Prepare residuals output using the quantile and mean function
  \# Combine the results in the specified order and name it
  resQuant <- quantile(x$residuals)</pre>
  resMean <- mean(x$residuals)</pre>
  residuals <- c(resQuant[1:3], resMean, resQuant[4:5])
  names(residuals) <- c("Min.", "1st Qu.", "Median", "Mean", "3rd Qu.", "Max.")</pre>
  # Print everything using cat, deparse, printCoefmat, and print.default
  cat("\nCall:\n", deparse(x$call),"\n\n", "Residuals:\n", sep = "")
  print.default(format(round(residuals, 5), nsmall = 5, scientific = FALSE),
                print.gap = 2L,
                quote = FALSE)
  cat("\nCoefficients:\n", sep = "")
  printCoefmat(x$coefficients, digits = 4, dig.tst = 2, has.Pvalue = TRUE)
  cat("\nMultiple R-squared: ", x$rSquared,
      "\n",
      "More Stats ...",
      sep = "")
}
```

If we simply print the object summaryOfModelFit of class summary.linMod, R again automatically detects the class and chooses the correct method, defined by us above.

```
# Print summaryOfModelFit
summaryOfModelFit
```

```
##
## Call:
## linMod(formula = Hwt ~ Bwt + Sex, data = cats)
##
## Residuals:
##
       Min.
              1st Qu.
                         Median
                                      Mean
                                             3rd Qu.
                                                           Max.
## -3.58330 -0.97004 -0.09479
                                   0.00000
                                             1.04322
                                                       5.10155
##
## Coefficients:
##
               Estimate Std. Err. t value P(>|t|)
```

```
## (Intercept)
               -0.4149
                           0.7273
                                    -0.57
                                             0.57
## Bwt
                           0.2948
                4.0758
                                    13.83
                                           <2e-16 ***
## SexM
                -0.0821
                           0.3040
                                    -0.27
                                             0.79
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Multiple R-squared: 0.6468035
## More Stats ...
```

As we can see, the result is clear, nicely formatted, and similar to the output of print.summary.lm.

5. Plot method

The final method will be a Q-Q plot, which compares two probability distributions. In our case we would like to compare the distribution of the *residuals* $\hat{\varepsilon}$ with the theoretical quantiles of the standard normal distribution to check the normality assumption of the error terms in our model. For that purpose we can use the qqnorm function. Additionally we can draw a line of the ideal relation, using the qqline function from the R base package.

The method will be written for objects of class linMod. In this case, we have to compute the residuals again, because the residual calculation before was done for objects of class summary.linMod, which is not the input here.

```
plot.linMod <- function(x, ...) {
    # Plot a Q-Q plot
    #
    # Args:
    # x: instance of class linMod
    # ...: passed arguments from generic function to this method
    #
    # Returns:
    # No value gets returned. The function plots a graph.

# Compute the residuals
    residuals <- x$y - (x$x %*% x$coefficients)

# Plot residuals against standard normal quantiles using qqnorm
    qqnorm(residuals, main="Normal QQ-Plot of Model Residuals")

# Additionally draw a line with the ideal relation using qqline
    qqline(residuals)
}</pre>
```

If we call the generic plot function R will find the correct method again, because modelFit is of class linMod.

```
# Plot modelFit
plot(modelFit)
```

Normal QQ-Plot of Model Residuals

