Module 3: Recommended Exercises - Solution

TMA4268 Statistical Learning V2024

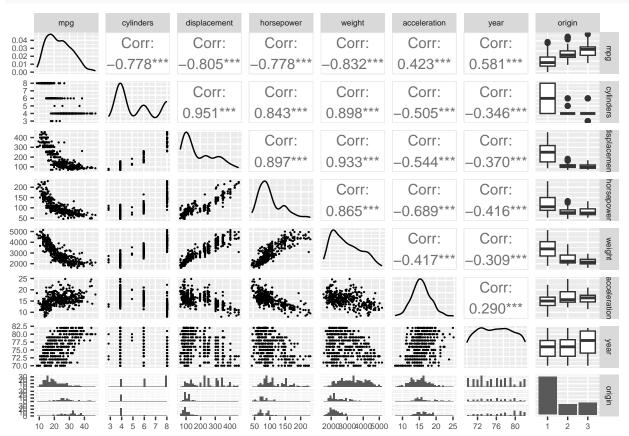
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January 25, 2024

Problem 1

a)

```
library(ISLR)
Auto <- subset(Auto, select = -name)
# Auto$origin = factor(Auto$origin)
summary(Auto)
##
                      cylinders
                                     displacement
                                                      horsepower
                                                                        weight
         mpg
##
   Min. : 9.00
                    Min.
                         :3.000
                                    Min.
                                         : 68.0
                                                    Min.
                                                           : 46.0
                                                                    Min.
                                                                           :1613
   1st Qu.:17.00
                    1st Qu.:4.000
                                    1st Qu.:105.0
                                                    1st Qu.: 75.0
                                                                    1st Qu.:2225
  Median :22.75
                    Median :4.000
                                    Median :151.0
                                                    Median: 93.5
                                                                    Median:2804
          :23.45
## Mean
                   Mean
                           :5.472
                                    Mean
                                           :194.4
                                                    Mean
                                                           :104.5
                                                                    Mean
                                                                           :2978
##
   3rd Qu.:29.00
                    3rd Qu.:8.000
                                    3rd Qu.:275.8
                                                    3rd Qu.:126.0
                                                                    3rd Qu.:3615
           :46.60
##
  Max.
                           :8.000
                                           :455.0
                                                           :230.0
                                                                           :5140
                   Max.
                                    Max.
                                                    Max.
                                                                    Max.
    acceleration
                         year
                                        origin
## Min.
          : 8.00
                           :70.00
                                    Min.
                                           :1.000
                   Min.
  1st Qu.:13.78
                    1st Qu.:73.00
                                    1st Qu.:1.000
##
## Median :15.50
                   Median :76.00
                                    Median :1.000
## Mean
          :15.54
                   Mean
                          :75.98
                                    Mean
                                          :1.577
##
   3rd Qu.:17.02
                    3rd Qu.:79.00
                                    3rd Qu.:2.000
## Max.
           :24.80
                   Max.
                           :82.00
                                    Max.
                                           :3.000
str(Auto)
##
  'data.frame':
                    392 obs. of 8 variables:
   $ mpg
                 : num 18 15 18 16 17 15 14 14 14 15 ...
## $ cylinders
                 : num
                         888888888...
## $ displacement: num
                         307 350 318 304 302 429 454 440 455 390 ...
## $ horsepower : num
                         130 165 150 150 140 198 220 215 225 190 ...
## $ weight
                 : num
                         3504 3693 3436 3433 3449 ...
##
   $ acceleration: num
                         12 11.5 11 12 10.5 10 9 8.5 10 8.5 ...
                 : num 70 70 70 70 70 70 70 70 70 70 ...
##
   $ year
   $ origin
                  : num 1 1 1 1 1 1 1 1 1 1 ...
Auto$origin <- factor(Auto$origin)</pre>
```



b)

Correlation matrix for the Auto data set where we omit the column origin:

cor(subset(Auto, select = -origin))

```
##
                           cylinders displacement horsepower
                                                                   weight
## mpg
                 1.0000000 -0.7776175
                                         -0.8051269 -0.7784268 -0.8322442
                            1.0000000
## cylinders
                -0.7776175
                                          0.9508233
                                                    0.8429834
                                                                0.8975273
## displacement -0.8051269
                            0.9508233
                                          1.0000000
                                                     0.8972570
                                                                0.9329944
## horsepower
                -0.7784268
                            0.8429834
                                          0.8972570
                                                     1.0000000
                                                                0.8645377
                -0.8322442
                            0.8975273
                                          0.9329944
                                                     0.8645377
## weight
                                                                1.0000000
## acceleration 0.4233285 -0.5046834
                                         -0.5438005 -0.6891955 -0.4168392
                 0.5805410 -0.3456474
                                         -0.3698552 -0.4163615 -0.3091199
##
  year
##
                acceleration
## mpg
                   0.4233285 0.5805410
                  -0.5046834 -0.3456474
## cylinders
## displacement
                  -0.5438005 -0.3698552
                  -0.6891955 -0.4163615
## horsepower
## weight
                  -0.4168392 -0.3091199
## acceleration
                   1.0000000 0.2903161
## year
                   0.2903161 1.0000000
```

c)

```
fit.lm <- lm(mpg ~ ., data = Auto)
summary(fit.lm)
##
## Call:
  lm(formula = mpg ~ ., data = Auto)
##
## Residuals:
##
       Min
                1Q Median
                                3Q
                                       Max
##
  -9.0095 -2.0785 -0.0982
                            1.9856 13.3608
##
##
  Coefficients:
##
                  Estimate Std. Error t value Pr(>|t|)
## (Intercept)
                -1.795e+01
                           4.677e+00
                                      -3.839 0.000145 ***
## cylinders
                -4.897e-01
                            3.212e-01
                                       -1.524 0.128215
## displacement
                2.398e-02
                            7.653e-03
                                        3.133 0.001863 **
## horsepower
                -1.818e-02
                            1.371e-02
                                       -1.326 0.185488
## weight
                -6.710e-03
                            6.551e-04 -10.243
                                               < 2e-16
## acceleration
                7.910e-02
                            9.822e-02
                                        0.805 0.421101
## year
                 7.770e-01
                            5.178e-02
                                       15.005
                                               < 2e-16 ***
## origin2
                 2.630e+00
                            5.664e-01
                                        4.643 4.72e-06 ***
## origin3
                 2.853e+00
                            5.527e-01
                                        5.162 3.93e-07 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 3.307 on 383 degrees of freedom
## Multiple R-squared: 0.8242, Adjusted R-squared: 0.8205
## F-statistic: 224.5 on 8 and 383 DF, p-value: < 2.2e-16
# kable(broom::tidy(fit.lm))
```

- i. The F-statistic in the very last line of the summary output shows that it is extremely unlikely that we would see such a result if none of the variables had any explanatory power the p-value is < 2.2e 16! So we can be sure that the set of predictors is explaining the response to a quite large degree. This is also confirmed by both a quite high R^2 and R^2_{adjust} (both around 0.82).
- ii. Yes, there is very strong evidence for a relationship between the weight of a car and the response. The p-value is extremely small. The interpretation is that, if a car weights 1000 kg more, we have a decrease of $1000 \cdot (-6.710 \cdot 10^{-3}) = -6.71$ miles per gallon (mpg), that is, the car can drive 6.71 miles less far per gallon of fuel.
- iii. The estimated coefficient $\hat{\beta}_{year} = 0.77$ suggests that a newer car model has higher mpg compared to an older one. A one year newer model should thus, in average, be able to drive 0.77 miles longer per gallon fuel compared to the older car.

d)

Remember that if we want to test whether a factor variable with more than two levels should be removed from the model, we actually have to test whether all slope coefficients that are associated with the respective binary dummy variables are zero simultaneously. Look again at equation (3.30) in the course book (p.85).

Consequently, we have to test here whether $\beta_{\text{origin2}} = \beta_{\text{origin3}} = 0$ at the same time, and for this we need the F-test, which is implemented in the anova() function in R:

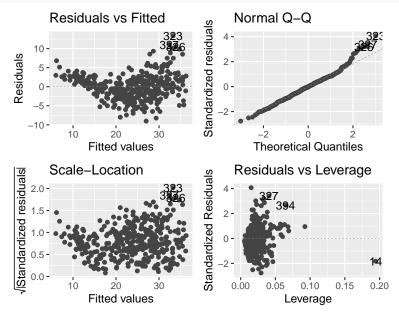
```
anova(fit.lm)
```

```
## Analysis of Variance Table
##
## Response: mpg
##
                     Sum Sq Mean Sq
                 Df
                                      F value
                                                 Pr(>F)
## cylinders
                  1 14403.1 14403.1 1317.3788 < 2.2e-16 ***
## displacement
                     1073.3 1073.3
                                      98.1735 < 2.2e-16 ***
## horsepower
                      403.4
                              403.4
                                      36.8977 3.004e-09 ***
                  1
## weight
                  1
                      975.7
                              975.7
                                      89.2447 < 2.2e-16 ***
## acceleration
                  1
                        1.0
                                1.0
                                       0.0884
                                                  0.7664
                                     221.2650 < 2.2e-16 ***
## year
                  1
                     2419.1
                             2419.1
## origin
                  2
                      356.0
                              178.0
                                      16.2787 1.639e-07 ***
## Residuals
                383
                     4187.4
                               10.9
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

The p-value associated with origin is now the one we can look at. Clearly, p is very small, thus the origin of the car has an influence on the response mpg.

e)

```
library(ggfortify)
autoplot(fit.lm, smooth.colour = NA)
```



- In the residual vs fitted plot (the so-called Tukey-Anscombe plot) there is evidence of non-linearity.
- Observation 14 has an unusually high leverage. This does not necessarily need to be a problem, but it would be wise to double-check that this observation is not an outlier.

f)

```
set.seed(2332)
n <- 100

par(mfrow = c(2, 3))
for (i in 1:6) {
    sim <- rnorm(n)</pre>
```

```
qqnorm(sim, pch = 1, frame = FALSE)
    qqline(sim, col = "blue", lwd = 1)
}
          Normal Q-Q Plot
                                            Normal Q-Q Plot
                                                                               Normal Q-Q Plot
                                       က
Sample Quantiles
                                  Sample Quantiles
                                                                     Sample Quantiles
                                       2
    0
                                                                         0
                                       0
    ī
                                                                         7
                                       7
    ကု
                  0
                                                     0
          -2
              _1
                                                -1
                                                                               -2
                                                                                   -1
                                                                                       0
          Theoretical Quantiles
                                                                               Theoretical Quantiles
                                             Theoretical Quantiles
          Normal Q-Q Plot
                                            Normal Q-Q Plot
                                                                               Normal Q-Q Plot
                                  Sample Quantiles
                                                                     Sample Quantiles
Sample Quantiles
    0
                                       0
                                                                         0
                                       7
    ^{2}
                                                                         7
                  0
                                                    0
          Theoretical Quantiles
                                             Theoretical Quantiles
                                                                               Theoretical Quantiles
\mathbf{g}
fit.lm1 <- lm(mpg ~ displacement + weight + year * origin, data = Auto)
summary(fit.lm1)
##
## Call:
## lm(formula = mpg ~ displacement + weight + year * origin, data = Auto)
## Residuals:
##
                  1Q Median
        Min
                                     3Q
                                             Max
   -8.7710 -2.0204 -0.0207 1.7045 13.0017
##
## Coefficients:
                    Estimate Std. Error t value Pr(>|t|)
##
## (Intercept)
                 -5.117e+00 5.259e+00
                                             -0.973 0.331220
## displacement 4.803e-03 5.032e-03
                                              0.955 0.340420
## weight
                  -6.685e-03 5.543e-04 -12.060
                                                     < 2e-16 ***
## year
                   6.152e-01 6.614e-02
                                              9.302 < 2e-16 ***
## origin2
                  -3.735e+01 1.026e+01
                                             -3.642 0.000307 ***
                  -2.532e+01 9.441e+00
                                             -2.682 0.007631 **
## origin3
                                              3.865 0.000130 ***
## year:origin2 5.187e-01 1.342e-01
## year:origin3 3.564e-01 1.213e-01
                                              2.937 0.003514 **
## ---
```

```
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 3.257 on 384 degrees of freedom
## Multiple R-squared: 0.829, Adjusted R-squared: 0.8259
## F-statistic: 265.9 on 7 and 384 DF, p-value: < 2.2e-16</pre>
```

Again, if we want to find evidence whether the interaction term between year and origin is needed, we are actually testing whether two slope coefficients are zero at the same time ($\beta_{\text{year:origin1}} = \beta_{\text{year:origin2}} = 0$). Consequently, we need the F-test, which is implemented in the anova() function:

```
anova(fit.lm1)
```

```
## Analysis of Variance Table
##
## Response: mpg
##
                    Sum Sq Mean Sq
                                     F value
                                                 Pr(>F)
## displacement
                  1 15440.2 15440.2 1455.6706 < 2.2e-16 ***
                            1208.5 113.9364 < 2.2e-16 ***
## weight
                  1
                    1208.5
## year
                     2601.4
                             2601.4 245.2550 < 2.2e-16 ***
                  1
## origin
                  2
                      296.9
                              148.5
                                      13.9977 1.356e-06 ***
                  2
                      198.9
                               99.5
                                       9.3764 0.0001057 ***
## year:origin
## Residuals
                384 4073.1
                               10.6
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
```

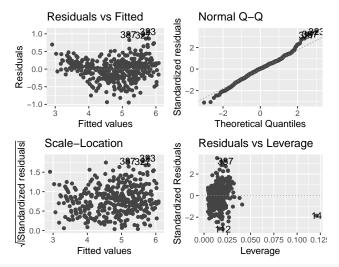
There is very strong evidence that the year-effect depends on the origin of the car, as can be seen by the F-test that is given by the anova table (p = 0.0001057). For European (2) and Japanese (3) cars, it seems that the fuel consumption (mpg) has a steeper slope for year: $\hat{\beta}_{year} = 0.615$ for the reference category 1 (American), whereas $\hat{\beta}_{year} = 0.615 + 0.519$ and $\hat{\beta}_{year} = 0.615 + 0.356$ for category 2 (European) and 3 (Japanese), respectively. This means that the fuel consumption is reduced faster by cars produced outside America (note that mgp is "miles per gallon", thus a higher value means that the car consumes less fuel, as it can drive further per gallon).

Note: For a full understanding of interaction terms, you really do need both the summary() and the anova() tables.

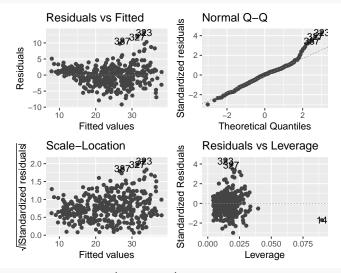
h)

We try three different transformations and look at the residual plots:

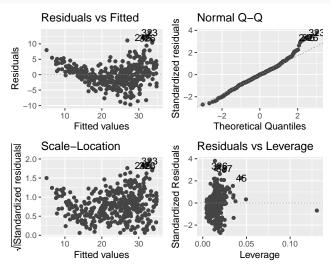
```
# try 3 predictor transformations
Auto$sqrtmpg <- sqrt(Auto$mpg)
fit.lm3 <- lm(sqrtmpg ~ displacement + weight + year + origin, data = Auto)
autoplot(fit.lm3, smooth.colour = NA)</pre>
```



fit.lm4 <- lm(mpg ~ displacement + I(log(weight)) + year + origin, data = Auto)
autoplot(fit.lm4, smooth.colour = NA)</pre>



fit.lm5 <- lm(mpg ~ displacement + I(weight^2) + year + origin, data = Auto)
autoplot(fit.lm5, smooth.colour = NA)</pre>



Problem 2

a)

$$E(\hat{\beta}) = E((X^T X)^{-1} X^T Y) = (X^T X)^{-1} X^T E(Y) = (X^T X)^{-1} X^T E(X\beta + \varepsilon) \tag{1}$$

$$= (X^T X)^{-1} X^T (X \beta + 0) = (X^T X)^{-1} (X^T X) \beta = I \beta = \beta$$
 (2)

$$Cov(\hat{\beta}) = Cov((X^T X)^{-1} X^T Y) = (X^T X)^{-1} X^T Cov(Y) ((X^T X)^{-1} X^T)^T$$
(3)

$$= (X^T X)^{-1} X^T \sigma^2 I((X^T X)^{-1} X^T)^T$$
(4)

$$= \sigma^2 (X^T X)^{-1} \tag{5}$$

(6)

We need to assume that Y is multivariate normal. As $\hat{\beta}$ is a linear transformation of a multivariate normal vector Y, $\hat{\beta}$ is also multivariate normal.

All components of a multivariate normal vector are themselves univariate normal. This means that $\hat{\beta}_j$ is normally distributed with expected value given by the β_j and the variance given by the j'th diagonal element of $\sigma^2(X^TX)^{-1}$.

b)

Fix covariates X and repeat the following procedure many times (nsim = 1000)

- collect Y
- create CI using $\hat{\beta}$ and $\hat{\sigma}$

95 % of the times the CI contains the true β .

```
# CI for beta_j
beta0 <- 1
beta1 <- 3
true_beta <- c(beta0, beta1) # vector of model coefficients</pre>
true_sd <- 1 # choosing true sd</pre>
nobs <- 100
X \leftarrow runif(nobs, 0, 1)
Xmat <- model.matrix(~X, data = data.frame(X)) # Design Matrix</pre>
# Count how many times the true value is within the confidence interval
ci_int <- ci_x <- 0
nsim <- 1000
for (i in 1:nsim) {
    y <- rnorm(n = nobs, mean = Xmat %*% true_beta, sd = rep(true_sd, nobs))
    mod \leftarrow lm(y \sim x, data = data.frame(y = y, x = X))
    ci <- confint(mod)</pre>
    ci int[i] <- ifelse(true beta[1] >= ci[1, 1] && true beta[1] <= ci[1, 2], 1,
    ci_x[i] <- ifelse(true_beta[2] >= ci[2, 1] && true_beta[2] <= ci[2, 2], 1, 0)
}
c(mean(ci_int), mean(ci_x))
```

[1] 0.955 0.947

c)

We apply the same idea from b), but now we fix X and x_0 and

- collect Y
- create PI using $\hat{\beta}$ and $\hat{\sigma}$
- simulate Y_0

95 % of the times the PI contains Y_0 .

```
# PI for Y_0
beta0 <- 1
beta1 <- 3
true_beta <- c(beta0, beta1) # vector of model coefficients</pre>
true_sd <- 1 # choosing true sd</pre>
X <- runif(100, 0, 1)</pre>
Xmat <- model.matrix(~X, data = data.frame(X)) # Design Matrix</pre>
x0 < -c(1, 0.4)
# simulating and fitting models many times
pi_y0 <- 0
nsim <- 1000
for (i in 1:nsim) {
    y <- rnorm(n = 100, mean = Xmat %*% true_beta, sd = rep(true_sd, 100))
    mod \leftarrow lm(y \sim x, data = data.frame(y = y, x = X))
    y0 <- rnorm(n = 1, mean = x0 %*% true_beta, sd = true_sd)
    pi <- predict(mod, newdata = data.frame(x = x0[2]), interval = "predict")[2:3]</pre>
    pi_y0[i] <- ifelse(y0 >= pi[1] && y0 <= pi[2], 1, 0)
}
mean(pi_y0)
```

[1] 0.945

d)

Confidence Interval for $x_0^T \beta$

This corresponds to a CI for $\mu_0 = E(y_0) = \boldsymbol{x}_0^T \boldsymbol{\beta}$ of an observation y_0 at \boldsymbol{x}_0 .

First, by using a) we have that

$$E(\boldsymbol{x}_0^T\hat{\boldsymbol{\beta}}) = \boldsymbol{x}_0^T E(\hat{\boldsymbol{\beta}}) = \boldsymbol{x}_0^T \boldsymbol{\beta}$$

and

$$\operatorname{Var}(\boldsymbol{x}_0^T \hat{\boldsymbol{\beta}}) = \boldsymbol{x}_0^T \operatorname{Var}(\hat{\boldsymbol{\beta}}) \boldsymbol{x}_0 = \sigma^2 \boldsymbol{x}_0^T (X^T X)^{-1} \boldsymbol{x}_0.$$

Consequently,

$$\boldsymbol{x}_0^T \hat{\boldsymbol{\beta}} \sim N(\boldsymbol{x}_0^T \boldsymbol{\beta}, \sigma^2 \boldsymbol{x}_0^T (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{x}_0)$$

or equivalently

$$\frac{\boldsymbol{x}_0^T \hat{\boldsymbol{\beta}} - \mu_0}{\sigma \sqrt{\boldsymbol{x}_0^T (X^T X)^{-1} \boldsymbol{x}_0}} \sim N(0, 1).$$

By substituting σ^2 with an estimator $\hat{\sigma^2}$, the last expression follows a t-distribution with n-p degrees of freedom. Now we can construct a confidence interval with $1-\alpha$ level (in our case $\alpha=0.05$) as follows

$$P\left(-t_{n-p}(1-\alpha/2) \le \frac{x_0^T \hat{\beta} - \mu_0}{\hat{\sigma} \sqrt{x_0^T (X^T X)^{-1} x_0}} \le t_{n-p}(1-\alpha/2)\right) = 1 - \alpha$$

or

$$P\left(\boldsymbol{x}_{0}^{T}\hat{\boldsymbol{\beta}} - t_{n-p}(1 - \alpha/2)\hat{\sigma}\sqrt{\boldsymbol{x}_{0}^{T}(X^{T}X)^{-1}\boldsymbol{x}_{0}} \leq \mu_{0} \leq \boldsymbol{x}_{0}^{T}\hat{\boldsymbol{\beta}} + t_{n-p}(1 - \alpha/2)\hat{\sigma}\sqrt{\boldsymbol{x}_{0}^{T}(X^{T}X)^{-1}\boldsymbol{x}_{0}}\right) = 1 - \alpha$$

For $\alpha = 0.05$ we have the following 95% CI

$$\left[\boldsymbol{x}_{0}^{T} \hat{\boldsymbol{\beta}} - t_{n-p} (1 - 0.05/2) \hat{\sigma} \sqrt{\boldsymbol{x}_{0}^{T} (X^{T} X)^{-1} \boldsymbol{x}_{0}}, \boldsymbol{x}_{0}^{T} \hat{\boldsymbol{\beta}} + t_{n-p} (1 - 0.05/2) \hat{\sigma} \sqrt{\boldsymbol{x}_{0}^{T} (X^{T} X)^{-1} \boldsymbol{x}_{0}} \right]$$

Prediction interval

To construct the PI we can look at the distribution of the prediction error $\hat{\varepsilon}_0 = y_0 - \hat{y}_0 = y_0 - \boldsymbol{x}_0^T \boldsymbol{\beta}$.

We have that

$$E(\hat{\varepsilon}_0) = y_0 - E(\hat{y}_0) = y_0 - E(\boldsymbol{x}_0^T \hat{\boldsymbol{\beta}}) = y_0 - y_0 = 0$$

and by assuming that y_0 and $\hat{y_0}$ are independent and $y_0 \sim N(\boldsymbol{x}_0^T \boldsymbol{\beta}, \sigma^2)$ we have that

$$Var(\hat{\varepsilon}_0) = Var(y_0) + Var(\hat{y}_0) = \sigma^2 + \sigma^2 \boldsymbol{x}_0^T (X^T X)^{-1} \boldsymbol{x}_0 = \sigma^2 (1 + \boldsymbol{x}_0^T (X^T X)^{-1} \boldsymbol{x}_0)$$

and

$$\hat{\varepsilon}_0 = y_0 - \boldsymbol{x}_0^T \hat{\boldsymbol{\beta}} \sim N(0, \sigma^2 (1 + \boldsymbol{x}_0^T (X^T X)^{-1} \boldsymbol{x}_0)).$$

Following the same logic as for the before and by substituting the estimate of variance $\hat{\sigma}^2$ we can construct a prediction interval with $1 - \alpha$ level as follows

$$P\left(-t_{n-p}(1-\alpha/2) \le \frac{y_0 - x_0^T \hat{\beta}}{\hat{\sigma}\sqrt{1+x_0^T(X^TX)^{-1}x_0}} \le t_{n-p}(1-\alpha/2)\right) = 1 - \alpha$$

or

For $\alpha = 0.05$ we have the following 95% PI

$$\left[\boldsymbol{x}_{0}^{T}\hat{\boldsymbol{\beta}}-t_{n-p}(1-0.05/2)\hat{\sigma}\sqrt{1+\boldsymbol{x}_{0}^{T}(X^{T}X)^{-1}\boldsymbol{x}_{0}},\boldsymbol{x}_{0}^{T}\hat{\boldsymbol{\beta}}+t_{n-p}(1-0.05/2)\hat{\sigma}\sqrt{1+\boldsymbol{x}_{0}^{T}(X^{T}X)^{-1}\boldsymbol{x}_{0}}\right]$$

Observe now that the two intervals are similar, but the prediction interval is by construction wider. Specifically, it can be significantly wider in applications where the error variance $\hat{\sigma}^2$ is large.

The connection between CI for β , $\boldsymbol{x}_0^T \beta$ and PI for y at \boldsymbol{x}_0 : The first is CI for a parameter, the second is CI for the expected regression line at the point \boldsymbol{x}_0 (when you only have one covariate, this may be more intuitive), and the last is the PI for the response y_0 . The difference between the two latter is that y are the observations, and $\boldsymbol{x}_0^T \boldsymbol{\beta}$ is the expected value of the observations and hence a function of the model parameters (NOT an observation).

e)

We have a model on the form $Y = X\beta + \varepsilon$ where ε is the error. The error of the model is unknown and unobserved, but we can estimate it by what we call the residuals. The residuals are given by the difference between the true response and the predicted value

$$\hat{\varepsilon} = Y - \hat{Y} = (I - \underbrace{X(X^TX)^{-1}X^\top}_{=H})Y,$$

where H is called the "hat matrix".

Properties of raw residuals: Normally distributed with mean 0 and covariance $Cov(\hat{\varepsilon}) = \sigma^2(I - H)$. This means that the residuals may have different variance (depending on X) and may also be correlated.

In a model check, we want to check that our errors are independent, homoscedastic (same variance for each observation) and not dependent on the covariates. As we don't know the true error, we use the residuals as predictors, but as mentioned, the residuals may have different variances and may be correlated. This is why we don't want to use the raw residuals for model check.

To amend our problem we need to try to fix the residuals so that they at least have equal variances. We do that by working with standardized or studentized residuals.