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Solutions for Exam in

Applied Statistical Methods

in Animal Sciences

Spring Semester 2024

Date: 2024-05-27

Name:

Legi-Nr:

Problem	Maximum Number of Points	Number of Points Reached
1	22	
2	18	
3	12	
4	16	
5	40	
Total	108	

Questions in German are in italics

Problem 1: Linear Regression

According to Figure 1 of (Chen et al. 2023) the concentration of citrate in milk between days in milk (DIM) 20 and 50 can be modeled by a linear regression. The dataset shown below contains measurements of 20 cows with their respective days in milk.

Gemäss Abbildung 1 von (Chen et al. 2023) kann die Zitratkonzentration in der Milch zwischen DIM 20 und 50 mit einer linearen Regression modelliert werden. Der nachfolgend gezeigte Datensatz enthält Beobachtungen von 20 Kühen.

Cow	DIM	Citrate
1	22	9.10
2	22	9.23
3	22	9.10
4	24	8.68
5	24	9.10
6	24	9.14
7	25	8.69
8	26	8.85
9	27	8.93
10	29	8.67
11	29	8.54
12	30	9.34
13	31	8.63
14	33	8.66
15	35	8.78
16	36	8.29
17	42	8.86
18	44	8.34
19	44	8.72
20	46	8.26

The dataset is available from

https://charlotte-ngs.github.io/asmasss2024/data/asm_exam_2024_p01.csv

- a) Write down the linear regression model in matrix-vector notation. List the meaning of all vectors and matrices used in the model. Furthermore, insert all information known from the dataset into the known components of the dataset.

Geben Sie das lineare Regressionsmodell als Gleichung in Matrix-Vektor-Notation an. Spezifizieren Sie alle verwendeten Vektoren und Matrizen im Modell. Die bekannten Größen aus dem Datensatz soll in die bekannten Komponenten des Modells eingesetzt werden.

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Solution

The regression model is given as

$$y = Xb + e$$

where vectors

- y : vector of length $n = 20$ with known observations of the response variable
- b : vector of length $p = 2$ with unknown effects (intercept and slope)
- e : vector of length $n = 20$ with unknown random residuals

and Matrix X of dimension $n \times p$ contains a column of all ones and the column with DIM values.

The known components are y and X and they can be specified by the information from the dataset

$$y = \begin{bmatrix} 9.1 \\ 9.23 \\ 9.1 \\ 8.68 \\ 9.1 \\ 9.14 \\ 8.69 \\ 8.85 \\ 8.93 \\ 8.67 \\ 8.54 \\ 9.34 \\ 8.63 \\ 8.66 \\ 8.78 \\ 8.29 \\ 8.86 \\ 8.34 \\ 8.72 \\ 8.26 \end{bmatrix}, X = \begin{bmatrix} 1 & 22 \\ 1 & 22 \\ 1 & 22 \\ 1 & 24 \\ 1 & 24 \\ 1 & 24 \\ 1 & 25 \\ 1 & 26 \\ 1 & 27 \\ 1 & 29 \\ 1 & 29 \\ 1 & 30 \\ 1 & 31 \\ 1 & 33 \\ 1 & 35 \\ 1 & 36 \\ 1 & 42 \\ 1 & 44 \\ 1 & 44 \\ 1 & 46 \end{bmatrix}$$

b) Fit a linear regression model with Citrate as response variable using the 'lm()' function in R. Specify the estimates obtained by the model fit for the following components

- slope
- intercept
- residual variance

Passen Sie ein lineares Regressionsmodell mit Zitratkonzentration als Zielgrösse an. Verwenden Sie dazu die Funktion 'lm()' in R. Geben Sie die erhaltenen Schätzwerte für die folgenden Komponenten an

- die Steigung,
- der Achsenabschnitt und
- die Varianz der Residuen

6

Solution

The linear regression model fit is given by

```
lm_cit_dim <- lm(Citrate ~ DIM, data = tbl_p01)
smry_lm_cit_dim <- summary(lm_cit_dim)
smry_lm_cit_dim
```

```
##
## Call:
## lm(formula = Citrate ~ DIM, data = tbl_p01)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.37391 -0.16177 -0.01203  0.14531  0.52570
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  9.566262   0.221608  43.168  < 2e-16 ***
## DIM         -0.025065   0.006988  -3.587  0.00211 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2424 on 18 degrees of freedom
## Multiple R-squared:  0.4168, Adjusted R-squared:  0.3845
## F-statistic: 12.87 on 1 and 18 DF,  p-value: 0.002107
```

The estimates for the quantities asked in the problem are listed in the following table

Quantity	Estimate
Slope	-0.0250654
Intercept	9.5662617
Variance of Residuals	0.0587783

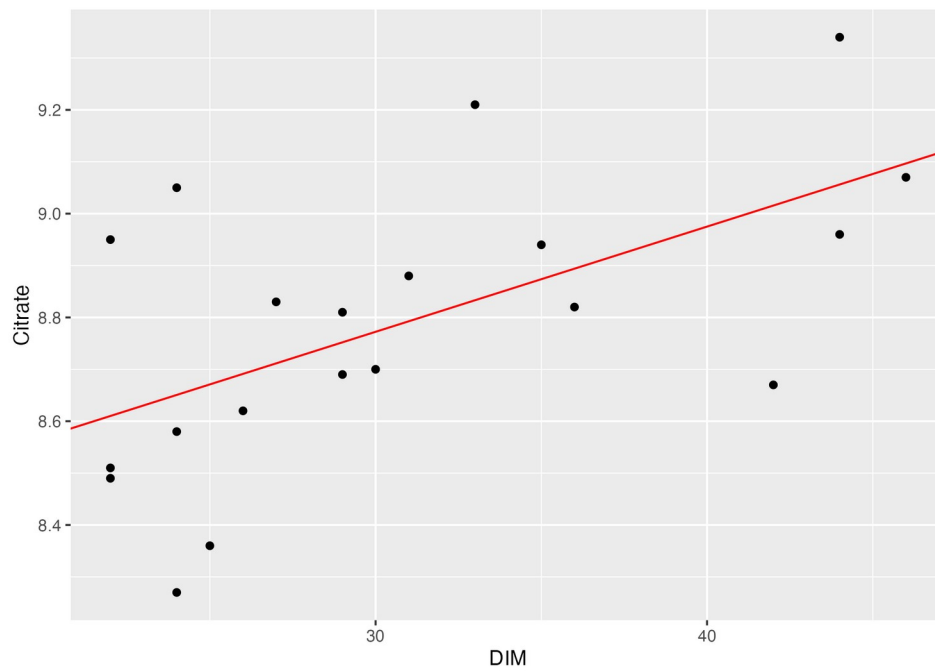
c) Which of the two plots reflects the modelling results found under Problem 1b)? If possible insert the following components into the correct plot below

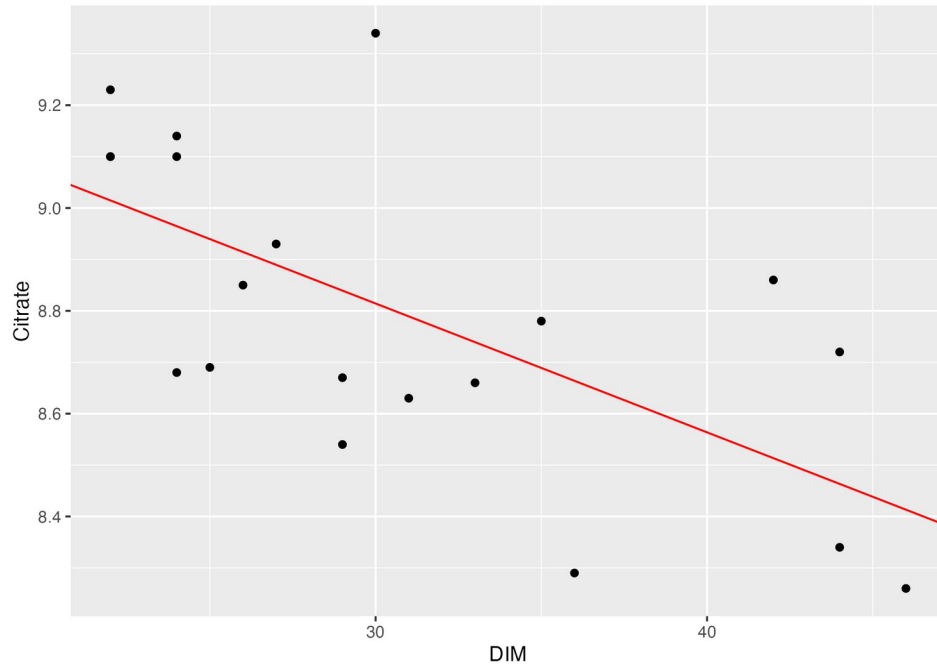
- slope
- intercept
- residual of the data point the the highest citrate concentration

Welcher der beiden nachfolgend gezeigten Plots spiegelt die unter 1b) gefundenen Modellresultate wieder?

- Steigung
- Achsenabschnitt
- Residuum des Datenpunktes mit der höchsten Zitratkonzentration

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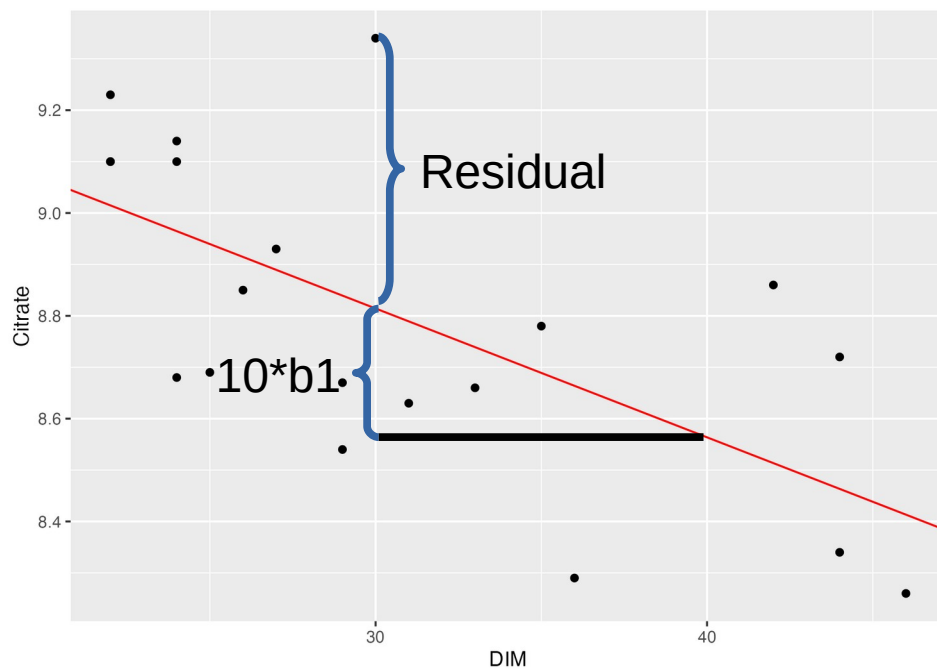




Solution

The second plot is correct. The following components could be inserted into the plot

- slope: inserted as $10 * b_1$
- intercept: not shown in plot
- residual of the data point the the highest citrate concentration: shown as "Residual"



- d) Citrate can be used as biomarker for a negative energy balance (NEB). NEB can be problematic in very early stages of the lactation. Hence there is a certain demand in predicting citrate concentration in milk for days in milk between 1 and 10. Is it possible to use the modelling results found in 1b) to predict citrate concentration for the time span of DIM between 1 and 10. If yes, how are those citrate concentrations predicted? If no, what is the reason that this is not possible?

Zitratkonzentration wird als Biomarker für eine negative Energiebilanz (NEB) verwendet. Eine NEB kann zu Beginn einer Laktation zu Problemen führen. Somit besteht ein Bedürfnis die Zitratkonzentration in der Milch für die Zeitperiode von DIM zwischen 1 und 10 vorherzusagen. Ist es möglich die Zitratkonzentration für die Zeitperiode von DIM zwischen 1 und 10 mit den Ergebnissen aus 1b) vorherzusagen? Falls ja, wie würde eine solche Vorhersage gemacht werden? Falls nein, was ist der Grund weshalb eine Vorhersage nicht möglich ist?

2

Solution

It is not possible, because DIM between 1 and 10 are outside of the DIM range of the dataset. Figure 1 in (Chen et al. 2023) shows that before DIM 20 the relationship is different from what was modelled in 1b). Hence a prediction of the citrate concentration would be **extrapolation** which is not allowed here.

Problem 2: Fixed Linear Effects Model

In the dataset below, the influence of the breed on the citrate concentration in milk is investigated.

Im nachfolgenden Datensatz soll der Einfluss der Rasse auf die Zitratkonzentration in der Milch untersucht werden.

Cow	DIM	Breed	Citrate
1	22	BS	8.71
2	22	HO	9.99
3	22	BS	8.84
4	24	BS	8.87
5	24	BS	9.03
6	24	BS	8.57
7	25	BS	9.25
8	26	HO	9.22
9	27	HO	9.57
10	29	BS	8.66
11	29	BS	8.80
12	30	BS	8.80
13	31	HO	9.67
14	33	HO	9.21
15	35	HO	9.63
16	36	HO	8.83
17	42	HO	8.76
18	44	HO	8.95
19	44	BS	8.67
20	46	BS	8.56

The dataset is available from

https://charlotte-ngs.github.io/asmasss2024/data/asm_exam_2024_p02.csv

- a) Fit a linear fixed effects model to the dataset shown above. Use 'Citrate' as response variable, 'DIM' as regression predictor and 'Breed' as fixed effect.

Passen Sie ein lineares Modell mit fixen Effekten an den oben gezeigten Datensatz an. Verwenden Sie Citrate als Zielgrösse, DIM als Regressionsvariable und Breed als fixen Effekt.

6

Solution

The fixed linear effects model is fitted as follows

```
lm_cit_dim_br <- lm(Citrate ~ DIM + Breed, data = tbl_p02)
smry_lm_cit_dim_br <- summary(lm_cit_dim_br)
smry_lm_cit_dim_br
```

```
##
## Call:
## lm(formula = Citrate ~ DIM + Breed, data = tbl_p02)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.41096 -0.16520 -0.02042  0.18088  0.41835
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  9.481374   0.245866  38.563  < 2e-16 ***
## DIM         -0.023621   0.008004  -2.951  0.008936 **
## BreedH0      0.609940   0.124814   4.887  0.000139 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2689 on 17 degrees of freedom
## Multiple R-squared:  0.6144, Adjusted R-squared:  0.569
## F-statistic: 13.54 on 2 and 17 DF,  p-value: 0.0003038
```

b) What are the estimates for the following parameters based on the modelling results of 2a)

- regression slope
- group mean of Citrate for animals of breed BS
- group mean of Citrate for animals of breed HO

Wie lauten die Schätzwerte für die folgenden Parameter aufgrund der Modellresultate

- *Steigung der Regressionsgeraden*
- *Gruppenmittel der Tiere der Rasse BS*
- *Gruppenmittel der Tiere der Rasse HO*

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Solution

Estimates for the regression slope is: -0.0236211

Group means are determined based on the dataset as check

```
library(dplyr)
tbl_gr_means_p02 <- tbl_p02 %>%
  group_by(Breed) %>%
  summarise(GrM_Cit = mean(Citrate),
            GrM_DIM = mean(DIM))
tbl_gr_means_p02
```

```
## # A tibble: 2 x 3
##   Breed GrM_Cit GrM_DIM
##   <chr>   <dbl>   <dbl>
## 1 BS      8.80     29
## 2 HO      9.31    32.9
```

Group means based on modelling results for breed BS

```
smry_lm_cit_dim_br$coefficients["(Intercept)", "Estimate"] +
  tbl_gr_means_p02$GrM_DIM[tbl_gr_means_p02$Breed == cur_breed] *
  smry_lm_cit_dim_br$coefficients["DIM", "Estimate"]
```

```
## [1] 8.796364
```

Group means based on modelling results for breed HO

```
smry_lm_cit_dim_br$coefficients["(Intercept)", "Estimate"] +
  tbl_gr_means_p02$GrM_DIM[tbl_gr_means_p02$Breed == cur_breed] *
  smry_lm_cit_dim_br$coefficients["DIM", "Estimate"] +
  smry_lm_cit_dim_br$coefficients["BreedHO", "Estimate"]
```

```
## [1] 9.314444
```

- c) What are the expected value for citrate concentration for animals of breed BS and HO at DIM 30?
Wie gross sind die erwarteten Zitratkonzentrationen für Tiere der Rasse BS und HO bei DIM 30?

6

Solution

Expected value of citrate concentration for animals of breed BS

```
smry_lm_cit_dim_br$coefficients["(Intercept)", "Estimate"] +  
  n_dim_pred * smry_lm_cit_dim_br$coefficients["DIM", "Estimate"]
```

```
## [1] 8.772743
```

Expected value of citrate concentration for animals of breed HO

```
smry_lm_cit_dim_br$coefficients["(Intercept)", "Estimate"] +  
  n_dim_pred * smry_lm_cit_dim_br$coefficients["DIM", "Estimate"] +  
  smry_lm_cit_dim_br$coefficients["BreedHO", "Estimate"]
```

```
## [1] 9.382683
```

Problem 3: Interactions

Use the following dataset to fit a fixed linear model assuming that the regression of **Citrate** on **DIM** shows an interaction with the **Breed** factor.

Verwenden Sie den folgenden Datensatz für die Anpassung eines fixen linearen Modells unter der Annahme, dass die Regression von Citrate auf DIM eine Interaktion mit dem Faktor Breed zeigt.

Cow	DIM	Breed	Citrate
1	22	BS	8.21
2	22	HO	9.51
3	22	BS	8.34
4	24	BS	8.37
5	24	BS	8.53
6	24	BS	8.07
7	25	BS	8.75
8	26	HO	8.74
9	27	HO	9.10
10	29	BS	8.16
11	29	BS	8.30
12	30	BS	8.30
13	31	HO	9.20
14	33	HO	8.75
15	35	HO	9.16
16	36	HO	8.36
17	42	HO	8.30
18	44	HO	8.49
19	44	BS	8.17
20	46	BS	8.06

The dataset is available from

https://charlotte-ngs.github.io/asmasss2024/data/asm_exam_2024_p03.csv

- a) Fit a fixed linear effects model including an interaction term between 'DIM' and 'Breed'.

Passen Sie ein fixes lineares Modell an unter Berücksichtigung der Interaktion zwischen DIM und Breed.

6

Solution

The fixed linear effects model including an interaction term between DIM and Breed is fitted to the data by

```
lm_cit_dim_br_inta <- lm(Citrate ~ DIM * Breed, data = tbl_p03)
smry_lm_cit_dim_br_inta <- summary(lm_cit_dim_br_inta)
smry_lm_cit_dim_br_inta
```

```
##
## Call:
## lm(formula = Citrate ~ DIM * Breed, data = tbl_p03)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.40476 -0.13973  0.00115  0.13979  0.40915
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  8.618906   0.274677  31.378 8.45e-16 ***
## DIM          -0.011122   0.009131  -1.218  0.24084
## BreedHO       1.655131   0.481022   3.441  0.00336 **
## DIM:BreedHO  -0.032311   0.014883  -2.171  0.04531 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.2423 on 16 degrees of freedom
## Multiple R-squared:  0.7172, Adjusted R-squared:  0.6642
## F-statistic: 13.53 on 3 and 16 DF,  p-value: 0.0001181
```

- b) What is the expected difference in citrate concentration in the milk for animals of both breeds ('BS' and 'HO') between DIM 30 and 40?

Was beträgt der erwartete Unterschied in der Zitratkonzentration in der Milch für Tiere der beiden Rassen BS und HO zwischen DIM 30 und 40?

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Solution

The expected difference in citrate concentration in the milk for animals of breed

- BS corresponds to the regression coefficient times the difference in DIM

```
n_delta_dim <- n_dim_end_intac - n_dim_start_intac
n_delta_citr_bs <- smry_lm_cit_dim_br_inta$coefficients["DIM", "Estimate"] * n_delta_dim
n_delta_citr_bs
```

```
## [1] -0.1112216
```

- HO corresponds to the regression coefficient plus the interaction term times the difference in DIM

```
n_delta_dim <- n_dim_end_intac - n_dim_start_intac
n_delta_citr_ho <- (smry_lm_cit_dim_br_inta$coefficients["DIM", "Estimate"] +
  smry_lm_cit_dim_br_inta$coefficients["DIM:BreedHO", "Estimate"]) * n_delta_dim
n_delta_citr_ho
```

```
## [1] -0.4343358
```

Problem 4: Contrasts

The dataset below is used to fit a fixed linear effects model with **Citrate** as response and **Breed** as fixed effect.

Der nachfolgende Datensatz wird für die Anpassung eines fixen linearen Modells mit Citrate als Zielgrösse und Breed als fixen Effekt verwendet

Cow	Breed	Citrate
1	BS	8.71
2	HO	9.99
3	BS	8.84
4	BS	8.87
5	BS	9.03
6	BS	8.57
7	BS	9.25
8	HO	9.22
9	HO	9.57
10	BS	8.66
11	BS	8.80
12	BS	8.80
13	HO	9.67
14	HO	9.21
15	HO	9.63
16	HO	8.83
17	HO	8.76
18	HO	8.95
19	BS	8.67
20	BS	8.56

The dataset is available from

https://charlotte-ngs.github.io/asmasss2024/data/asm_exam_2024_p04.csv

- a) Use 'treatment' contrasts to fit a fixed linear model with 'Citrate' as response and 'Breed' as fixed effect. Verify the obtained 'Breed'-effect estimates using appropriate group means of 'Citrate' and solutions of the least-squares normal equations.

Verwenden Sie 'treatment' Kontraste für die Anpassung des fixen linearen Modells mit 'Citrate' als Zielgrösse und 'Breed' als fixen Effekt. Verifizieren Sie die erhaltenen Schätzungen der 'Breed'-Effekte anhand der passenden Gruppen-Mittel und anhand von Lösungen der Least-Squares Normalgleichungen.

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Solution

Treatment contrasts are used by default by `lm()` when fitting a FLEM. Hence the fit is obtained by

```
lm_cit_br <- lm(Citrate ~ Breed, data = tbl_p04)
smry_lm_cit_br <- summary(lm_cit_br)
smry_lm_cit_br

##
## Call:
## lm(formula = Citrate ~ Breed, data = tbl_p04)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.55444 -0.15886 -0.04136  0.23912  0.67556
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)   8.7964      0.0969  90.774 < 2e-16 ***
## BreedH0       0.5181      0.1445   3.586  0.00211 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3214 on 18 degrees of freedom
## Multiple R-squared:  0.4168, Adjusted R-squared:  0.3844
## F-statistic: 12.86 on 1 and 18 DF,  p-value: 0.00211
```

Assuming treatment contrasts, verification via group means is done as follows

- Intercept estimate corresponds to the mean of all BS animals

```
mean(tbl_p04$Citrate[tbl_p04$Breed == "BS"])
```

```
## [1] 8.796364
```

This is expected to be the same as

```
smry_lm_cit_br$coefficients["(Intercept)", "Estimate"]
```

```
## [1] 8.796364
```


- The difference between the group means of HO animals minus the group mean of the BS animals corresponds to the reported breed effect, hence

```
mean(tbl_p04$Citrate[tbl_p04$Breed == "HO"]) - mean(tbl_p04$Citrate[tbl_p04$Breed == "BS"])
```

```
## [1] 0.5180808
```

is expected to be the same as

```
smry_lm_cit_br$coefficients["BreedHO", "Estimate"]
```

```
## [1] 0.5180808
```

- The breed effect estimated can also be verified via solutions of the least squares normal equations

```
mat_X <- model.matrix(Citrate ~ 0 + Breed, tbl_p04)
attr(mat_X, "assign") <- NULL
attr(mat_X, "contrasts") <- NULL
colnames(mat_X) <- NULL
mat_X <- cbind(matrix(rep(1,nrow(mat_X))), ncol = 1), mat_X)
mat_xtx <- crossprod(mat_X)
mat_xtx_ginv <- MASS::ginv(mat_xtx)
mat_xty <- crossprod(mat_X, tbl_p04$Citrate)
mat_b_sol <- crossprod(mat_xtx_ginv, mat_xty)
mat_b_sol
```

```
##           [,1]
## [1,] 6.036936
## [2,] 2.759428
## [3,] 3.277508
```

Contrasts matrix for treatment contrasts

```
fac_breed <- as.factor(tbl_p04$Breed)
contr_mat_breed_treat <- contrasts(fac_breed)
contr_mat_breed_treat <- cbind(matrix(rep(1,nrow(contr_mat_breed_treat))), ncol = 1),
                             contr_mat_breed_treat)
est_mat_breed_treat <- solve(contr_mat_breed_treat)
est_mat_breed_treat
```

```
##      BS HO
##      1  0
## HO -1  1
```

For the effects estimates, we are looking at the second and the third row of the matrix `est_mat_breed_treat`. We are prepending a column of zeroes to the second and the third row of `est_mat_breed_treat`.

```
n_nrow_est_mat <- nrow(est_mat_breed_treat)
mat_q_efun <- cbind(matrix(0, nrow = (nrow(est_mat_breed_treat)-1), ncol = 1),
                    matrix(est_mat_breed_treat[2:n_nrow_est_mat,],
                            nrow = (nrow(est_mat_breed_treat)-1)))
crossprod(t(mat_q_efun), mat_b_sol)
```

```
##          [,1]  
## [1,] 0.5180808
```

- b) Use 'sum' contrasts to fit a fixed linear model with 'Citrate' as response and 'Breed' as fixed effect. Verify the obtained 'Breed'-effect estimates using appropriate group means of 'Citrate' and solutions of the least-squares normal equations.

Verwenden Sie 'sum' Kontraste für die Anpassung des fixen linearen Modells mit 'Citrate' als Zielgrösse und 'Breed' als fixen Effekt. Verifizieren Sie die erhaltenen Schätzungen der 'Breed'-Effekte anhand der passenden Gruppen-Mittel und anhand von Lösungen der Least-Squares Normalgleichungen.

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Solution

The fixed linear effects model using sum contrasts is fitted as shown below

```
lm_cit_br_csum <- lm(Citrate ~ Breed, data = tbl_p04, contrasts = list(Breed = "contr.sum"))
smry_lm_cit_br_csum <- summary(lm_cit_br_csum)
smry_lm_cit_br_csum
```

```
##
## Call:
## lm(formula = Citrate ~ Breed, data = tbl_p04, contrasts = list(Breed = "contr.sum"))
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -0.55444 -0.15886 -0.04136  0.23912  0.67556
##
## Coefficients:
##              Estimate Std. Error t value Pr(>|t|)
## (Intercept)  9.05540     0.07223 125.373  < 2e-16 ***
## Breed1      -0.25904     0.07223  -3.586  0.00211 **
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 0.3214 on 18 degrees of freedom
## Multiple R-squared:  0.4168, Adjusted R-squared:  0.3844
## F-statistic: 12.86 on 1 and 18 DF,  p-value: 0.00211
```

- Contrasts Matrix for Sum Contrasts From the contrasts matrix, we get the matrix of estimable functions.

```
fac_breed <- as.factor(tbl_p04$Breed)
contr_mat_breed_sum <- contrasts(C(fac_breed, sum))
contr_mat_breed_sum <- cbind(matrix(rep(1,nrow(contr_mat_breed_sum)), ncol = 1), contr_mat_breed_sum)
est_mat_breed_sum <- solve(contr_mat_breed_sum)
est_mat_breed_sum
```

```
##      BS   HO
## [1,] 0.5  0.5
## [2,] 0.5 -0.5
```

The matrix `est_mat_breed_sum` tells us that the estimate for the intercept (first row) is computed as the mean of the group means for the two breeds and the estimate for the breed effect (second row) is computed as half of the difference between group means for the first breed minus the group mean of the second breed.

Hence the estimate of the intercept is

```
mean(c(mean(tbl_p04$Citrate[tbl_p04$Breed == "BS"]),
       mean(tbl_p04$Citrate[tbl_p04$Breed == "HO"])))
```

```
## [1] 9.055404
```

and has to be equal to

```
smry_lm_cit_br_csum$coefficients["(Intercept)", "Estimate"]
```

```
## [1] 9.055404
```

The estimate for the breed-effect is obtained by

```
0.5 * (mean(tbl_p04$Citrate[tbl_p04$Breed == "BS"]) - mean(tbl_p04$Citrate[tbl_p04$Breed == "HO"])))
```

```
## [1] -0.2590404
```

which is the same as

```
smry_lm_cit_br_csum$coefficients["Breed1", "Estimate"]
```

```
## [1] -0.2590404
```

The verification with the solution of the least squares normal equation is done with

```
n_nrow_est_mat <- nrow(est_mat_breed_sum)
mat_q_efun <- cbind(matrix(0, nrow = (nrow(est_mat_breed_sum)-1), ncol = 1),
                   matrix(est_mat_breed_sum[2:n_nrow_est_mat,],
                           nrow = (nrow(est_mat_breed_sum)-1)))
crossprod(t(mat_q_efun), mat_b_sol)
```

```
##           [,1]
## [1,] -0.2590404
```

Problem 5: Linear Mixed Effects Models

Use the dataset below to fit a linear mixed effects model. In this model **Citrate** is the response and **DIM** and **Breed** are regression variables and fixed effects, respectively. You do not have to include any interaction effects.

Verwenden Sie den nachfolgenden Datensatz um ein lineares gemischtes Modell anzupassen. In diesem Modell sei 'Citrate' die Zielgrösse und 'DIM' die Regressionvariable und 'Breed' ein fixer Effekt. Interaktionseffekte müssen nicht berücksichtigt werden.

ID	Sire	Dam	DIM	Breed	Citrate
5	1	NA	22	BS	9.30
6	1	NA	22	HO	9.26
7	1	5	22	BS	8.92
8	1	5	24	BS	9.30
9	1	6	24	BS	9.03
10	1	6	24	BS	8.82
11	2	7	25	BS	9.09
12	2	7	26	HO	9.04
13	2	8	27	HO	9.71
14	2	8	29	BS	8.52
15	2	9	29	BS	9.18
16	3	9	30	BS	8.85
17	3	10	31	HO	9.04
18	3	10	33	HO	9.04
19	3	11	35	HO	9.44
20	3	11	36	HO	9.18
21	3	12	42	HO	8.88
22	4	12	44	HO	8.96
23	4	13	44	BS	8.74
24	4	13	46	BS	8.52

The dataset is available from

https://charlotte-ngs.github.io/asmasss2024/data/asm_exam_2024_p05.csv

- a) Use a sire model to predict breeding values for all sires. Please specify the model in the form of an equation in matrix-vector notation and explain the meaning of all model components. Write down the expected values and the variance-covariance matrices for all random effects in the model. Put all the information from the data into the model components consisting of response variable, regression and fixed effects, random effects, and their associated design matrices. Construct the mixed model equations and provide solutions to these equations. Extract predicted breeding values for all sires and estimates for the regression and fixed effects from these solutions.

The following assumptions can be made

- the ratio λ_s between residual variance and sire variance is given by $\lambda_s = \sigma_e^2/\sigma_s^2 = 7.11$
- the sires are assumed to be unrelated

Verwenden Sie ein Vatermodell zur Schätzung der Zuchtwerte aller männlichen Tiere. Bitte geben Sie die Modellgleichung in Matrix-Vektor-Schreibweise an und erläutern Sie die Bedeutung aller Modellkomponenten. Schreiben Sie die Erwartungswerte und die Varianz-Kovarianzmatrizen aller zufälligen Effekte im Modell auf. Verwenden Sie alle Informationen aus den Daten für die genaue Spezifikation der Modellkomponenten, wie zum Beispiel Zielgrösse, Regressionseffekte, fixe Effekte, zufällige Effekte und die zugehörigen Designmatrizen. Stellen Sie die Mixed-Model-Gleichungen auf und lösen Sie diese Gleichungen. Extrahieren Sie die geschätzten Zuchtwerte aller männlichen Tiere und die Schätzungen für die Regressionseffekte und für die fixen Effekte aus den Lösungen.

Die folgenden Annahmen können getroffen werden:

- das Verhältnis (λ_s) zwischen der Residuenvarianz und der Vätervarianz beträgt $\lambda_s = \sigma_e^2/\sigma_s^2 = 7.11$
- die Väter sind untereinander nicht verwandt

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Solution

- Model as equation:

$$y = Xb + Zs + e$$

where

y	vector of observations
b	vector of intercept, regression coefficient and fixed effects
s	vector of random sire breeding values
e	vector of random residuals
X	design matrix linking observations to fixed effects
Z	design matrix linking observations to sire breeding values

- Expected values and the variance-covariance matrices:

Random effects are y , s and e . Their expected values correspond to

$$E \begin{bmatrix} y \\ s \\ e \end{bmatrix} = \begin{bmatrix} Xb \\ 0 \\ 0 \end{bmatrix}$$

The variance-covariance matrices

$$var \begin{bmatrix} y \\ s \\ e \end{bmatrix} = \begin{bmatrix} V & ZS & R \\ SZ^T & S & 0 \\ R & 0 & R \end{bmatrix}$$

where $var(s) = S = I * \sigma_s^2$, $var(e) = R = I * \sigma_e^2$ and $var(y) = V = ZSZ^T + R = ZZ^T \sigma_s^2 + R$ with given sire-variance component σ_s^2 and given residual variance component σ_e^2 .

- Information from data to model components

$$y = \begin{bmatrix} 9.3 \\ 9.26 \\ 8.92 \\ 9.3 \\ 9.03 \\ 8.82 \\ 9.09 \\ 9.04 \\ 9.71 \\ 8.52 \\ 9.18 \\ 8.85 \\ 9.04 \\ 9.04 \\ 9.44 \\ 9.18 \\ 8.88 \\ 8.96 \\ 8.74 \\ 8.52 \end{bmatrix}, b = \begin{bmatrix} b_0 \\ b_{DIM} \\ b_{BreedHO} \end{bmatrix}, s = \begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \end{bmatrix}, e = \begin{bmatrix} e_5 \\ e_6 \\ e_7 \\ e_8 \\ e_9 \\ e_{10} \\ e_{11} \\ e_{12} \\ e_{13} \\ e_{14} \\ e_{15} \\ e_{16} \\ e_{17} \\ e_{18} \\ e_{19} \\ e_{20} \\ e_{21} \\ e_{22} \\ e_{23} \\ e_{24} \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 22 & 0 \\ 1 & 22 & 1 \\ 1 & 22 & 0 \\ 1 & 24 & 0 \\ 1 & 24 & 0 \\ 1 & 24 & 0 \\ 1 & 24 & 0 \\ 1 & 25 & 0 \\ 1 & 26 & 1 \\ 1 & 27 & 1 \\ 1 & 29 & 0 \\ 1 & 29 & 0 \\ 1 & 30 & 0 \\ 1 & 31 & 1 \\ 1 & 33 & 1 \\ 1 & 35 & 1 \\ 1 & 36 & 1 \\ 1 & 42 & 1 \\ 1 & 44 & 1 \\ 1 & 44 & 0 \\ 1 & 46 & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

- Mixed model equations:

$$\begin{bmatrix} X^T X & X^T Z \\ Z^T X & Z^T Z + \lambda_s * I \end{bmatrix} \begin{bmatrix} \hat{b} \\ \hat{s} \end{bmatrix} = \begin{bmatrix} X^T y \\ Z^T y \end{bmatrix}$$

- Solutions of MME

```
mat_xtx <- crossprod(mat_X_p05)
mat_xtz <- crossprod(mat_X_p05, mat_Z_sire)
mat_ztx <- t(mat_xtz)
mat_ztz_lAsinv <- crossprod(mat_Z_sire) + n_lambda_s * diag(1, nrow = n_nr_sire)
mat_coef_sire <- rbind(cbind(mat_xtx, mat_xtz), cbind(mat_ztx, mat_ztz_lAsinv))
mat_rhs_sire <- rbind(crossprod(mat_X_p05, vec_y), crossprod(mat_Z_sire, vec_y))
mat_sol_sire <- solve(mat_coef_sire, mat_rhs_sire)
mat_sol_sire
```

```
##           [,1]
## [1,]  9.5007575600
## [2,] -0.0196080127
## [3,]  0.3196246901
## [4,]  0.0008951716
## [5,]  0.0052561969
## [6,] -0.0086811736
## [7,]  0.0025298051
```

- Estimates of intercept, regression coefficient and fixed effect for BreedHO are given by

```
tbl_sire_result <- tibble::tibble(Effect = c("Intercept",
                                             "Regression Coefficient",
                                             "BreedHO Effect"),
                                Estimate = mat_sol_sire[1:3,])
knitr::kable(tbl_sire_result)
```

Effect	Estimate
Intercept	9.5007576
Regression Coefficient	-0.0196080
BreedHO Effect	0.3196247

- Predicted breeding values for the sires are

```
vec_sire_pbv <- mat_sol_sire[(nrow(mat_sol_sire)-n_nr_sire+1):nrow(mat_sol_sire),]
vec_sire_pbv
```

```
## [1]  0.0008951716  0.0052561969 -0.0086811736  0.0025298051
```

The order of the sires according to the predicted breeding values is given by

```
vec_sire_pbv[order(vec_sire_pbv, decreasing = T)]
```

```
## [1]  0.0052561969  0.0025298051  0.0008951716 -0.0086811736
```


- b) Use an animal model to predict breeding values for all animals in the dataset, including sires and dams. Please specify the model in the form of an equation in matrix-vector notation and explain the meaning of all model components. Write down the expected values and the variance-covariance matrices for all random effects in the model. Put all the information from the data into the model components consisting of response variable, regression and fixed effects, random effects, and their associated design matrices. Construct the mixed model equations and provide solutions to these equations. Extract predicted breeding values for all animals and estimates for the regression and fixed effects from these solutions.

The following assumptions can be made

- the ratio λ_u between residual variance and additive genetic variance is given by $\lambda_u = \sigma_e^2/\sigma_u^2 = 1.78$

Verwenden Sie ein Tiermodell zur Schätzung der Zuchtwerte aller Tiere im Datensatz inklusive von Vätern und Müttern. Bitte geben Sie die Modellgleichung in Matrix-Vektor-Schreibweise an und erläutern Sie die Bedeutung aller Modellkomponenten. Schreiben Sie die Erwartungswerte und die Varianz-Kovarianzmatrizen aller zufälligen Effekte im Modell auf. Verwenden Sie alle Informationen aus den Daten für die genaue Spezifikation der Modellkomponenten, wie zum Beispiel Zielgrösse, Regressionseffekte, fixe Effekte, zufällige Effekte und die zugehörigen Designmatrizen. Stellen Sie die Mixed-Model-Gleichungen auf und lösen Sie diese Gleichungen. Extrahieren Sie die geschätzten Zuchtwerte aller Tiere und die Schätzungen für die Regressionseffekte und für die fixen Effekte aus den Lösungen.

Die folgenden Annahmen können getroffen werden:

- das Verhältnis (λ_u) zwischen der Residuenvarianz und der additiv-genetischen Varianz beträgt $\lambda_u = \sigma_e^2/\sigma_u^2 = 1.78$

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Solution

- Model as equation:

$$y = Xb + Zu + e$$

where

y	vector of observations
b	vector of intercept, regression coefficient and fixed effects
u	vector of random breeding values
e	vector of random residuals
X	design matrix linking observations to fixed effects
Z	design matrix linking observations to sire breeding values

- Expected values and the variance-covariance matrices:

Random effects are y , u and e . Their expected values correspond to

$$E \begin{bmatrix} y \\ u \\ e \end{bmatrix} = \begin{bmatrix} Xb \\ 0 \\ 0 \end{bmatrix}$$

The variance-covariance matrices

$$var \begin{bmatrix} y \\ u \\ e \end{bmatrix} = \begin{bmatrix} V & ZU & R \\ UZ^T & U & 0 \\ R & 0 & R \end{bmatrix}$$

where $var(u) = U = A * \sigma_u^2$, $var(e) = R = I * \sigma_e^2$ and $var(y) = V = ZUZ^T + R$ with given additive genetic variance component σ_u^2 and given residual variance component σ_e^2 .

- Information from data to model components

$$y = \begin{bmatrix} 9.3 \\ 9.26 \\ 8.92 \\ 9.3 \\ 9.03 \\ 8.82 \\ 9.09 \\ 9.04 \\ 9.71 \\ 8.52 \\ 9.18 \\ 8.85 \\ 9.04 \\ 9.04 \\ 9.44 \\ 9.18 \\ 8.88 \\ 8.96 \\ 8.74 \\ 8.52 \end{bmatrix}, b = \begin{bmatrix} b_0 \\ b_{DIM} \\ b_{BreedHO} \end{bmatrix}, u = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \\ u_{13} \\ u_{14} \\ u_{15} \\ u_{16} \\ u_{17} \\ u_{18} \\ u_{19} \\ u_{20} \\ u_{21} \\ u_{22} \\ u_{23} \\ u_{24} \end{bmatrix}, e = \begin{bmatrix} e_5 \\ e_6 \\ e_7 \\ e_8 \\ e_9 \\ e_{10} \\ e_{11} \\ e_{12} \\ e_{13} \\ e_{14} \\ e_{15} \\ e_{16} \\ e_{17} \\ e_{18} \\ e_{19} \\ e_{20} \\ e_{21} \\ e_{22} \\ e_{23} \\ e_{24} \end{bmatrix}$$

$$X = \begin{bmatrix} 1 & 22 & 0 \\ 1 & 22 & 1 \\ 1 & 22 & 0 \\ 1 & 24 & 0 \\ 1 & 24 & 0 \\ 1 & 24 & 0 \\ 1 & 25 & 0 \\ 1 & 26 & 1 \\ 1 & 27 & 1 \\ 1 & 29 & 0 \\ 1 & 29 & 0 \\ 1 & 30 & 0 \\ 1 & 31 & 1 \\ 1 & 33 & 1 \\ 1 & 35 & 1 \\ 1 & 36 & 1 \\ 1 & 42 & 1 \\ 1 & 44 & 1 \\ 1 & 44 & 0 \\ 1 & 46 & 0 \end{bmatrix}$$

$$Z =$$

- Mixed model equations:

$$\begin{bmatrix} X^T X & X^T Z \\ Z^T X & Z^T Z + \lambda_u * A^{-1} \end{bmatrix} \begin{bmatrix} \hat{b} \\ \hat{u} \end{bmatrix} = \begin{bmatrix} X^T y \\ Z^T y \end{bmatrix}$$

```
## Loading required package: lme4
```

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

```
## 'as(<dtMatrix>, "dtCMatrix")' is deprecated.
```

```
## Use 'as(., "CsparseMatrix")' instead.
```

```
## See help("Deprecated") and help("Matrix-deprecated").
```

where $\lambda_u = \frac{\sigma_e^2}{\sigma_u^2} = 1.78$ and A corresponds to the numerator relationship matrix given by

$$A =$$

The inverse A_s^{-1} is

$$A^{-1} =$$

- Solutions of MME

```

mat_xtx <- crossprod(mat_X_p05)
mat_xtz <- crossprod(mat_X_p05, mat_Z_ani)
mat_ztx <- t(mat_xtz)
mat_ztz_lAinv <- crossprod(mat_Z_ani) + n_lambda_u * mat_A_inv
mat_coef_ani <- rbind(cbind(mat_xtx, mat_xtz), cbind(mat_ztx, mat_ztz_lAinv))
mat_rhs_ani <- rbind(crossprod(mat_X_p05, vec_y), crossprod(mat_Z_ani, vec_y))
mat_sol_ani <- solve(mat_coef_ani, mat_rhs_ani)
mat_sol_ani

```

```

##           [,1]
##  9.539690005
## -0.021267432
##  0.349117898
## 1 -0.019522398
## 2  0.015023764
## 3 -0.007240318
## 4  0.004130529
## 5  0.060900627
## 6 -0.069010391
## 7 -0.025382473
## 8  0.066991716
## 9 -0.015315320
## 10 -0.100579302
## 11  0.036875067
## 12 -0.065712408
## 13  0.109473105
## 14 -0.046579510
## 15  0.050600530
## 16 -0.019246384
## 17 -0.080664433
## 18 -0.072272549
## 19  0.076382029
## 20  0.024028396
## 21 -0.053822726
## 22 -0.022512425
## 23  0.074186722
## 24  0.035268929

```

- Estimates of intercept, regression coefficient and fixed effect for BreedHO are given by

```

tbl_ani_result <- tibble::tibble(Effect = c("Intercept",
                                           "Regression Coefficient",
                                           "BreedHO Effect"),
                                Estimate = mat_sol_ani[1:3,])
knitr::kable(tbl_ani_result)

```

Effect	Estimate
Intercept	9.5396900
Regression Coefficient	-0.0212674
BreedHO Effect	0.3491179

- Predicted breeding values for all animals: The first two elements are solutions of fixed effects, the remaining elements are predicted breeding values

Animals	Predicted Breeding Values
1	-0.0195224
2	0.0150238
3	-0.0072403
4	0.0041305
5	0.0609006
6	-0.0690104
7	-0.0253825
8	0.0669917
9	-0.0153153
10	-0.1005793
11	0.0368751
12	-0.0657124
13	0.1094731
14	-0.0465795
15	0.0506005
16	-0.0192464
17	-0.0806644
18	-0.0722725
19	0.0763820
20	0.0240284
21	-0.0538227
22	-0.0225124
23	0.0741867
24	0.0352689

References

- Chen, Yansen, Hongqing Hu, Nicolas Gengler, Clément Grelet, and Katrien Wijnrocx. 2023. “Genetic analysis of milk citrate predicted by milk mid- infrared spectra of Holstein cows in early lactation.” *J. Dairy Sci.* <https://doi.org/10.3168/jds.2023-23903>.