# Examples of regression and mixed models

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## Notes

This is the supplementary materials for running regression and mixed models. The code uses the palmer penguin dataset as an example (https://allisonhorst.github.io/palmerpenguins/).

## Basic settings

First, we read the basic packages and set the seed for reproducibility. The most relevant is the tidyverse work environment. See https://www.tidyverse.org/ for more details.

```
# load the package with penguin data
library(palmerpenguins)
# save the data as a named data frame
data <- penguins
# load basic packages
library(readxl)
library(tidyverse)
library(knitr)
# packages for correlation paired plot
library(GGally)
# packages for model performance
library(caret)
library(sjPlot)
library(MuMIn)
# set seed for reproducibility
set.seed(10)
```

```r
# set visual options for numbers
options(scipen=999)
```

## Data visualization

Have a look at the raw data, which has continuous and categorical variables.

```r
glimpse(data)
```

```
## Rows: 344
## Columns: 8
## $ species           <fct> Adelie, Adelie, Adelie, Adelie, Adelie, Adelie, Adel~
## $ island            <fct> Torgersen, Torgersen, Torgersen, Torgersen, Torgerse~
## $ bill_length_mm    <dbl> 39.1, 39.5, 40.3, NA, 36.7, 39.3, 38.9, 39.2, 34.1, ~
## $ bill_depth_mm     <dbl> 18.7, 17.4, 18.0, NA, 19.3, 20.6, 17.8, 19.6, 18.1, ~
## $ flipper_length_mm <int> 181, 186, 195, NA, 193, 190, 181, 195, 193, 190, 186~
## $ body_mass_g       <int> 3750, 3800, 3250, NA, 3450, 3650, 3625, 4675, 3475, ~
## $ sex               <fct> male, female, female, NA, female, male, female, male~
## $ year              <int> 2007, 2007, 2007, 2007, 2007, 2007, 2007, 2007, 2007~
```

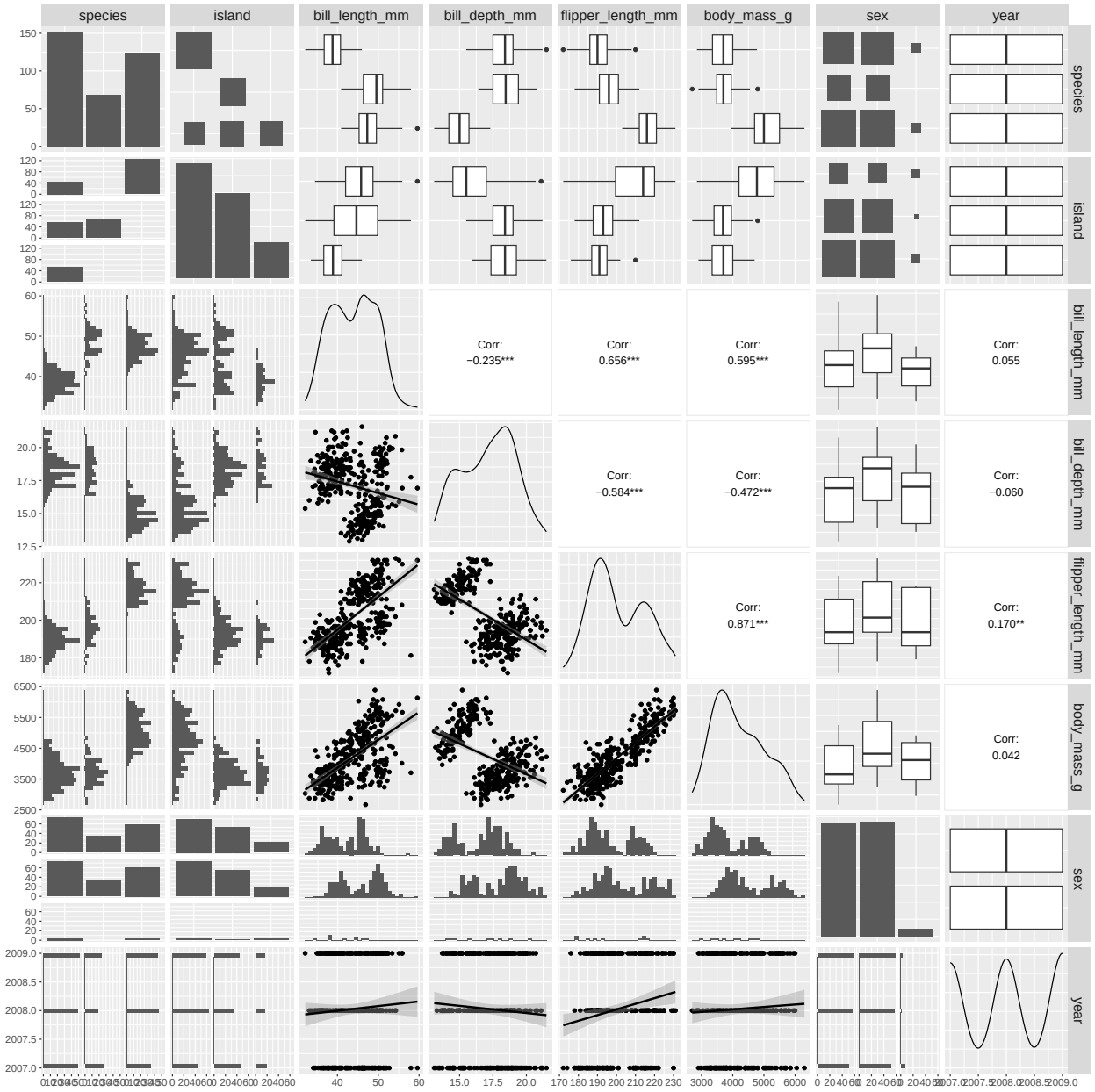
Make a correlation plot of all the variables we are looking at. The correlation coefficient $r$ can be interpreted as follows:

- measure of *linear* relationship
- between *-1.0* (perfectly *negative*) and *+1.0* (perfectly *positive*)
- *0* means *no* (linear) relationship

**correlation is not regression**

- correlation = the extent to which x and y move together
- regression = the impact of a change of unit on x in y

```r
data %>%
  ggpairs(lower=list(continuous=wrap("smooth", colour="black")),
          upper = list(continuous = wrap("cor", size=4, colour = "black"))) +
  # plot settings
  theme(strip.text = element_text(size = 14),
        axis.text = element_text(size = 10))
```




# Linear regression

First, let's have a look at simple linear regression.

**The Estimates** can be manually read as follows. If in a hypothetical model, we are trying to predict the variable X based on the variables A, B, and sex, which have an estimate of 1,3, and -1 (for male). And the intercept is 0.5. If a data point has the following values for the hypothetical variables encoded in the data.

- X (the predicted variable) = 370
- A = 364
- B = 3
- sex = male

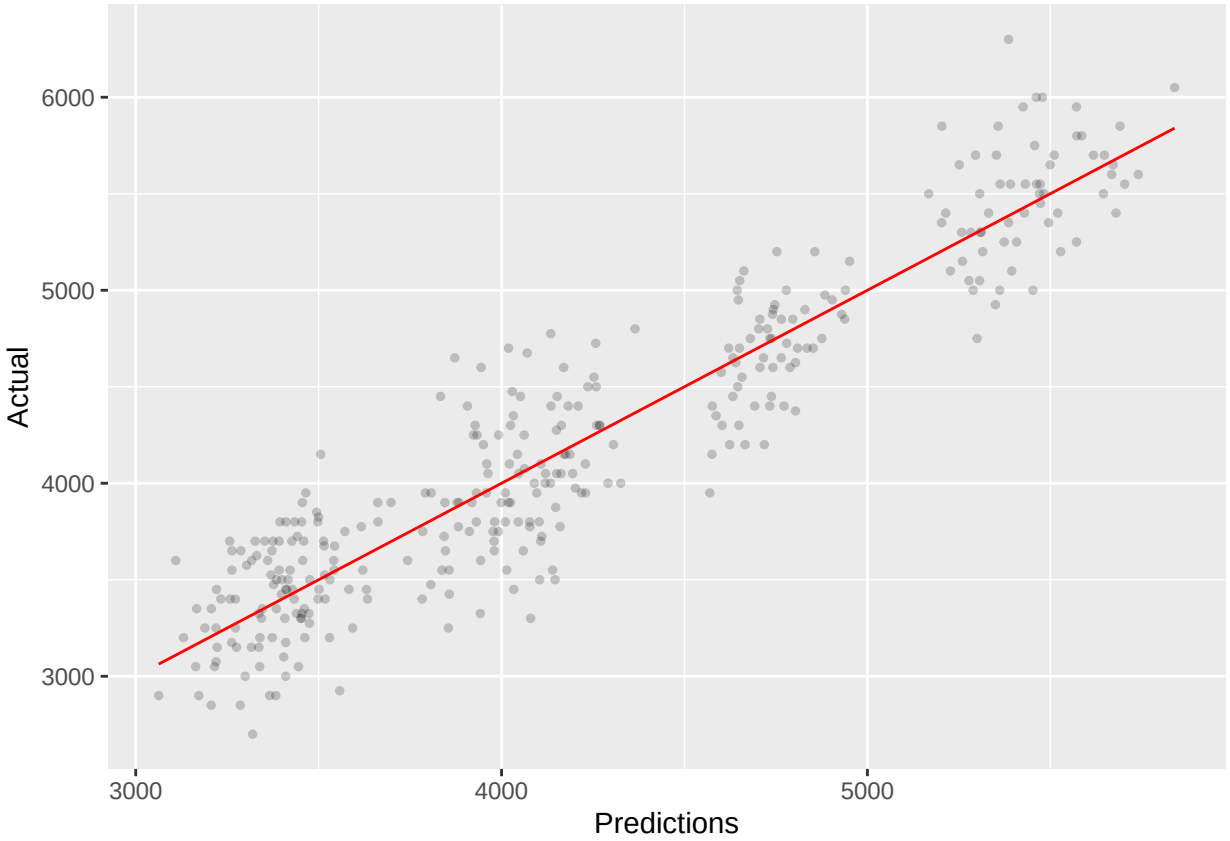
Then, the predicted X would be = the intercept 0.5 + (1 * 364) + (3 * 3) + (-1 * 1) = 372.5.

```
# arrange the data a bit
tmp <- data %>%
  # change the coding to numerical values if needed
  mutate(body_mass_g = as.numeric(body_mass_g)) %>%
  # rename the variables to be predicted
  rename(To_Predict = body_mass_g) %>%
  # remove the rows with NA values
  drop_na()

# creating the model
model <- lm(To_Predict ~ species + bill_length_mm + bill_depth_mm +
              flipper_length_mm + sex,
            data = tmp)

# visualizing the model
summary(model)
```

```
##
## Call:
## lm(formula = To_Predict ~ species + bill_length_mm + bill_depth_mm +
##     flipper_length_mm + sex, data = tmp)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -779.65 -173.18   -9.05  186.61  914.11
##
## Coefficients:
##                    Estimate Std. Error t value            Pr(>|t|)
## (Intercept)       -1460.995    571.308  -2.557            0.011002 *
## speciesChinstrap   -251.477     81.079  -3.102            0.002093 **
## speciesGentoo      1014.627    129.561   7.831 0.00000000000006852 ***
## bill_length_mm       18.204      7.106   2.562            0.010864 *
## bill_depth_mm        67.218     19.742   3.405            0.000745 ***
## flipper_length_mm    15.950      2.910   5.482 0.00000008440786478 ***
## sexmale             389.892     47.848   8.148 0.00000000000000797 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 287.3 on 326 degrees of freedom
## Multiple R-squared:  0.875,  Adjusted R-squared:  0.8727
## F-statistic: 380.2 on 6 and 326 DF,  p-value: < 0.00000000000000022
```

We can visualize how the predictions align with the actual values.

```
# combine predictions and actual values
cbind(predict(model), tmp$To_Predict) %>%
  as.data.frame() %>%
  rename(Predictions = 1, Actual = 2) %>%
  # make a plot
  ggplot(aes(x = Predictions, y = Actual)) +
  geom_point(size=1, alpha = 0.2) +
  geom_line(aes(y = predict(model)), color = "red")
```




The R-square (R2), which represents the correlation between the actual values and the predicted values. The higher the R2, the better the model (can interpret it as a correlation coefficient).

```
caret::R2(predict(model), tmp$To_Predict) %>% round(digits = 2)
```

```
## [1] 0.87
```

We can also extract the effect size of each variable by calculating how much the variance explained by the model drops when a given variable is removed.

```
# open an empty table to store the output
effect.table <-NULL %>% as.data.frame()

# extract a list with all the predictors, removing those we don't use
valid.names <- names(tmp)[!names(tmp) %in% c("To_Predict",
                                             "year",
                                             "island")]


# for each predictor
for(i in 0:length(valid.names)) {

  if(i == 0){
    # write the formula
    frm <- as.formula(paste("To_Predict ~ ",
                            paste(valid.names, collapse = "+")))
```

```
    # feed it to the model
    model.tmp <- lm(frm, data = tmp)

    #Determine R2:
    effect.table <- rbind(effect.table,
                          c("all factors",
                            caret::R2(predict(model.tmp), tmp$To_Predict)))
  }else{

    # write the formula
    frm <- as.formula(paste("To_Predict ~ ",
                            paste(valid.names[-i], collapse = "+")))
    # feed it to the model
    model.tmp <- lm(frm, data = tmp)

    #Determine R2:
    effect.table <- rbind(effect.table,
                          c(valid.names[i],
                            caret::R2(predict(model.tmp), tmp$To_Predict)))
  }}

# adjust column names
colnames(effect.table) <- c("Factor", "Var.exp")

# add a column for effect size
 effect.table <- effect.table %>%
  # make the column numeric
  mutate(Var.exp = as.numeric(Var.exp),
         # effect size = gap of variance explained with the main model
         Effect.size = as.numeric(effect.table$Var.exp[1]) - Var.exp) %>%
  filter(Factor != "all factors") %>%
  mutate(Effect.size = round(Effect.size, digits = 4))

# visual check
effect.table %>% arrange(desc(Effect.size))
```

```
##              Factor   Var.exp Effect.size
## 1           species 0.8230078      0.0520
## 2               sex 0.8494949      0.0255
## 3 flipper_length_mm 0.8634357      0.0115
## 4     bill_depth_mm 0.8705155      0.0044
## 5    bill_length_mm 0.8724449      0.0025
```

## Linear mixed models

These models are similar to regression models. However, they include the distinction between fixed and random effects. Fixed effects are the variables that have a fixed type of interaction with the response variable while the random effects are the variables that do not. In short, mixed models consider that the **intercept and the slope can vary** across members of a group.

First, we compare which model is better. Typically, we look at the AIC (Akaike) score. The calculation of AIC not only regards the goodness of fit of a model, but also takes into account the simplicity of the model.

In this way, AIC deals with the trade-off between goodness of fit and complexity of the model, and as a result, disencourages overfitting. A smaller AIC is preferred.

If you see the warning "boundary (singular) fit: see help('isSingular')", it means that the model can make too accurate predictions and it considers statistically irrealist, i.e., the model overfits. If that happens, you can try removing some variables to avoid the warning. You can also report the model but highlighting that there is the possibility of overfitting.

```
# arrange the data a bit
tmp <- data %>%
  # change the coding to numerical values if needed
  mutate(body_mass_g = as.numeric(body_mass_g)) %>%
  # rename the variables to be predicted
  rename(To_Predict = body_mass_g) %>%
  # remove the rows with NA values
  drop_na()

# for random slope, e.g., (1+flipper_length_mm|island), data=base)
# This model, in addition to a random intercept for island, also contains a random slope in flipper leng

# model with all factors, using year and island as random effects
model1 <- lmerTest::lmer(To_Predict ~ (1|year) + (1|island) +
                          species + bill_length_mm + bill_depth_mm +
                          flipper_length_mm + sex,
                         # if you want to suppress the singularity warning
                         #control=lmerControl(check.conv.singular =
                         #.makeCC(action = "ignore",  tol = 1e-4)),
                         data = tmp)
```

```
## boundary (singular) fit: see help('isSingular')
```

```
# model with only measurements
model2 <- lmerTest::lmer(To_Predict ~ (1|year) + (1|island) +
                          bill_length_mm + bill_depth_mm +
                          flipper_length_mm,
                         # if you want to suppress the singularity warning
                         #control=lmerControl(check.conv.singular =
                         #.makeCC(action = "ignore",  tol = 1e-4)),
                         data = tmp)

# model with only categorical variables
model3 <- lmerTest::lmer(To_Predict ~ (1|year) + (1|island) +
                          species + sex,
                         # if you want to suppress the singularity warning
                         #control=lmerControl(check.conv.singular =
                         #.makeCC(action = "ignore",  tol = 1e-4)),
                         data = tmp)
```

```
## boundary (singular) fit: see help('isSingular')
```

```
# null model
model4 <- lmerTest::lmer(To_Predict ~ (1|year) + (1|island),
                         # if you want to suppress the singularity warning
```

```
                        #control=lmerControl(check.conv.singular =
                        #.makeCC(action = "ignore",  tol = 1e-4)),
                        data = tmp)
```

```
## boundary (singular) fit: see help('isSingular')
```

```
# comparing all the models
anova(model1, model2, model3, model4,
      # avoid that anova refits the models to ML
      refit = FALSE)
```

```
## Data: tmp
## Models:
## model4: To_Predict ~ (1 | year) + (1 | island)
## model2: To_Predict ~ (1 | year) + (1 | island) + bill_length_mm + bill_depth_mm + flipper_length_mm
## model3: To_Predict ~ (1 | year) + (1 | island) + species + sex
## model1: To_Predict ~ (1 | year) + (1 | island) + species + bill_length_mm + bill_depth_mm + flipper_
##        npar    AIC    BIC  logLik deviance   Chisq Df            Pr(>Chisq)
## model4    4 5246.0 5261.3 -2619.0   5238.0
## model2    7 4864.1 4890.7 -2425.0   4850.1 387.965  3 < 0.00000000000000022 ***
## model3    7 4754.6 4781.3 -2370.3   4740.6 109.456  0
## model1   10 4675.9 4713.9 -2327.9   4655.9  84.745  3 < 0.00000000000000022 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We can also test what happens when we remove one factor at a time.

```
drop1(model1,test="Chisq")
```

```
## Single term deletions using Satterthwaite's method:
##
## Model:
## To_Predict ~ (1 | year) + (1 | island) + species + bill_length_mm + bill_depth_mm + flipper_length_m
##                     Sum Sq Mean Sq NumDF  DenDF F value                Pr(>F)
## species           10318128 5159064     2 272.53 62.8403 < 0.00000000000000022
## bill_length_mm      555365  555365     1 324.66  6.7647              0.009723
## bill_depth_mm       854382  854382     1 316.55 10.4068              0.001387
## flipper_length_mm  2600439 2600439     1 159.41 31.6748   0.00000008017057969
## sex                5356973 5356973     1 325.92 65.2509   0.00000000000001294
##
## species           ***
## bill_length_mm    **
## bill_depth_mm     **
## flipper_length_mm ***
## sex               ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We visualize the output of the best model.

**The scaled residuals** should ideally be centered around 0, which would mean that the predictions are quite close to the real data points.

**The Estimates** can be manually read as follows. If in a hypothetical model, we are trying to predict the variable X based on the variables A, B, and sex, which have an estimate of 1,3, and -1 (for male). And the intercept is 0.5. If a data point has the following values for the hypothetical variables encoded in the data.

- X (the predicted variable) = 370
- A = 364
- B = 3
- sex = male

Then, the predicted X would be = the intercept 0.5 + (1 * 364) + (3 * 3) + (-1 * 1) = 372.5.

**The random effect** part tells you how much variance you find among levels of your grouping factors, plus the residual variance. If the variance is high, it means that the factors explain a lot of variation, e.g., we divide the variance of a factor by the total variance: $1/(1 + 3) = 0.25$. So the random effects explain 25% of the variance that is left over after the variance explained by the fixed effects.

**Correlation of fixed effects** is about the expected correlation of the regression coefficients. It is telling you that if you did the experiment again and it so happened that the coefficient for X got smaller, it is likely that the coefficient of Y would go up (or down).

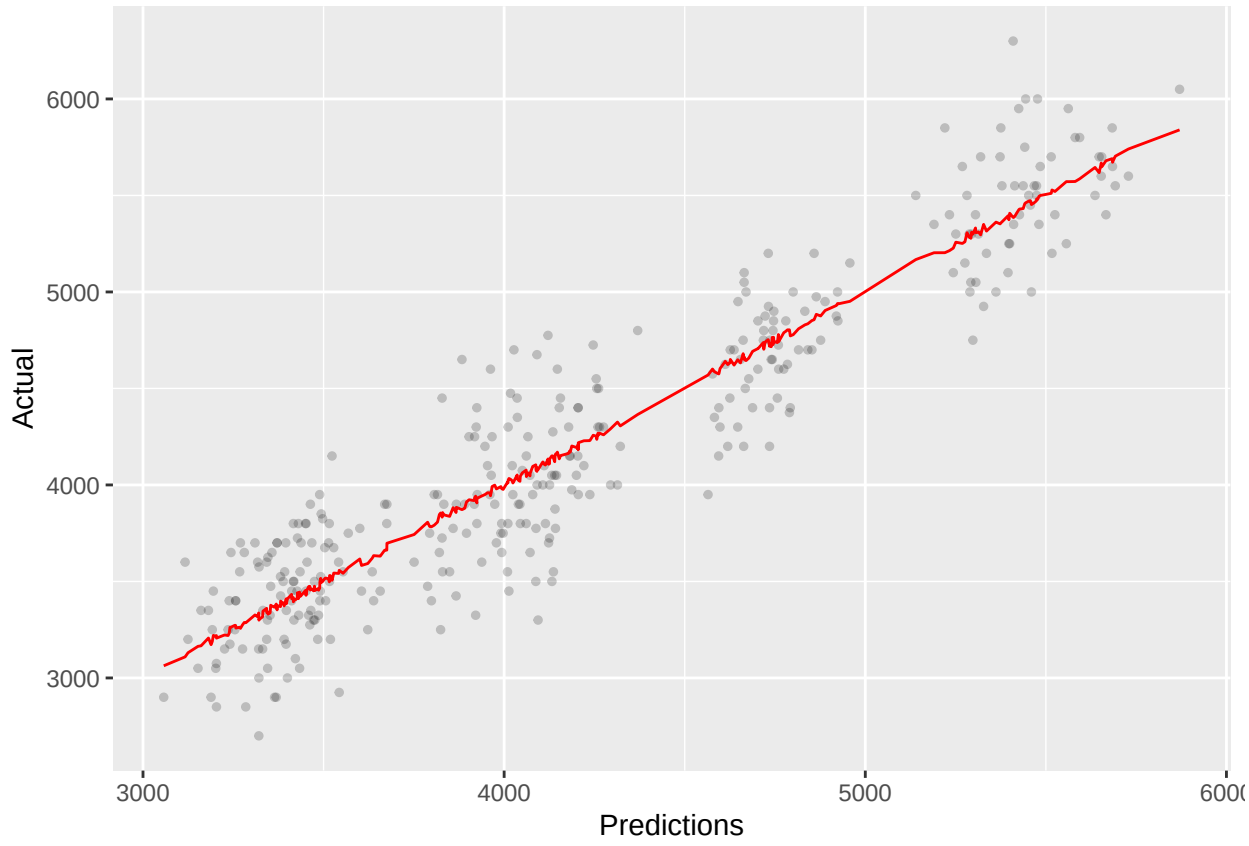
```
summary(model1)
```

```
## Linear mixed model fit by REML. t-tests use Satterthwaite's method [
## lmerModLmerTest]
## Formula: To_Predict ~ (1 | year) + (1 | island) + species + bill_length_mm +
##     bill_depth_mm + flipper_length_mm + sex
##    Data: tmp
##
## REML criterion at convergence: 4655.9
##
## Scaled residuals:
##      Min       1Q   Median       3Q      Max
## -2.77114 -0.60182 -0.01518  0.64234  3.10817
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  year     (Intercept)   784.8   28.01
##  island   (Intercept)     0.0    0.00
##  Residual             82098.0  286.53
## Number of obs: 333, groups:  year, 3; island, 3
##
## Fixed effects:
##                    Estimate Std. Error        df t value            Pr(>|t|)
## (Intercept)       -1608.292    580.323   269.712  -2.771             0.00597 **
## speciesChinstrap   -262.185     81.304   324.311  -3.225             0.00139 **
## speciesGentoo       973.655    132.800   218.510   7.332 0.0000000000043681 ***
## bill_length_mm       18.533      7.126   324.662   2.601             0.00972 **
## bill_depth_mm        64.062     19.858   316.552   3.226             0.00139 **
## flipper_length_mm    16.978      3.017   159.406   5.628 0.0000000801705797 ***
## sexmale             386.365     47.830   325.917   8.078 0.0000000000000129 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Correlation of Fixed Effects:
```

```
##             (Intr) spcsCh spcsGn bll_l_ bll_d_ flpp__
## spcsChnstrp  0.305
## speciesGent  0.364  0.536
## bll_lngth_m -0.170 -0.829 -0.409
## bll_dpth_mm -0.328  0.152  0.702 -0.138
## flppr_lngt_ -0.744 -0.033 -0.627 -0.207 -0.218
## sexmale      0.602  0.375  0.056 -0.375 -0.455 -0.182
## optimizer (nloptwrap) convergence code: 0 (OK)
## boundary (singular) fit: see help('isSingular')
```

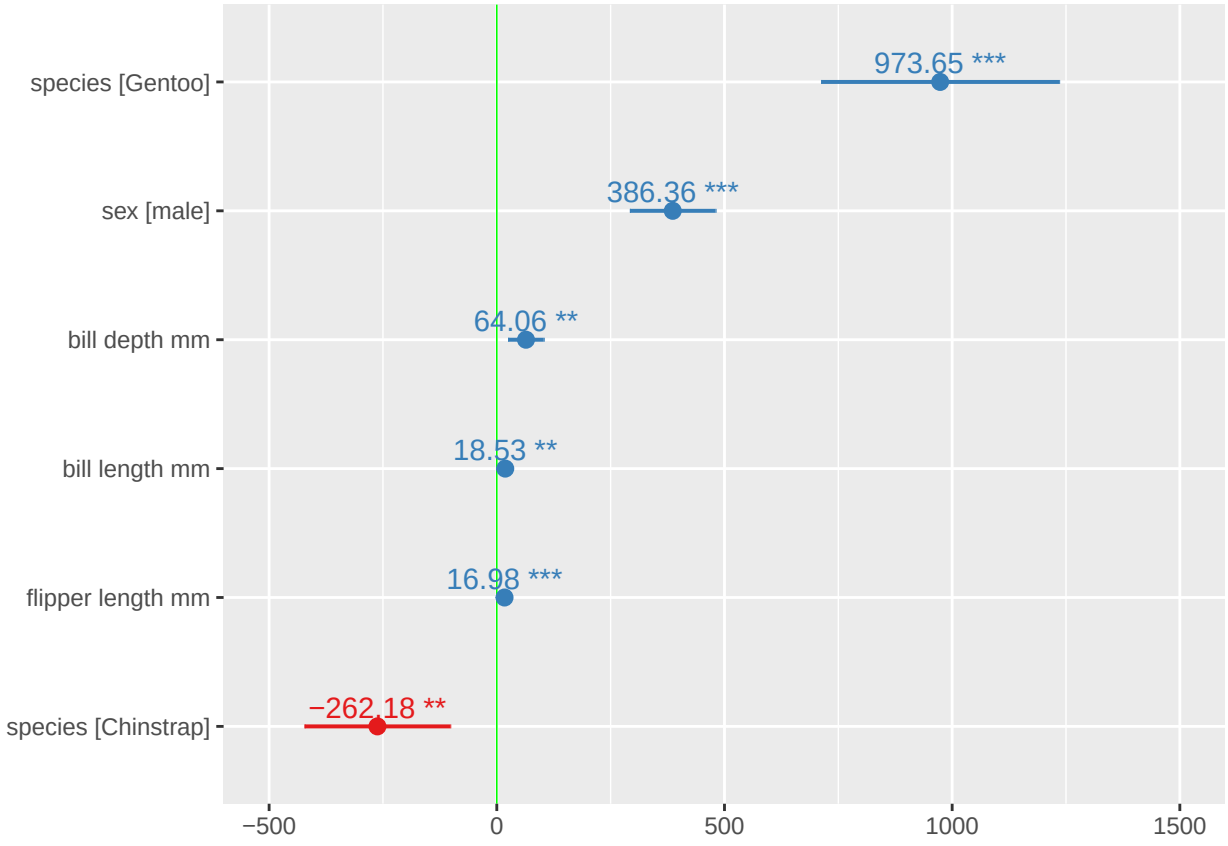
We can visualize how the predictions align with the actual values.

```
# combine predictions and actual values
cbind(predict(model1), tmp$To_Predict) %>%
  as.data.frame() %>%
  rename(Predictions = 1, Actual = 2) %>%
  # make a plot
  ggplot(aes(x = Predictions, y = Actual)) +
  geom_point(size=1, alpha = 0.2) +
  geom_line(aes(y = predict(model)), color = "red")
```



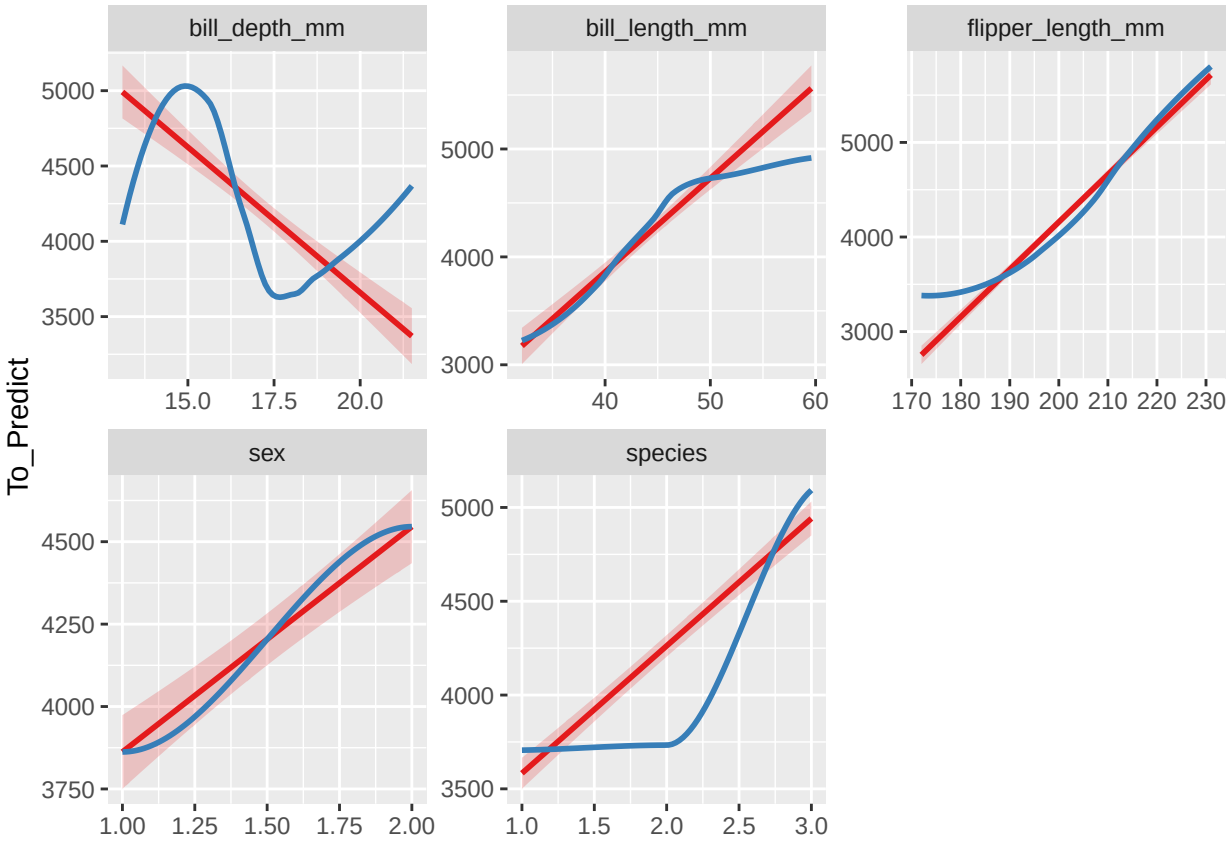

We visualize the fixed effects.

```
#png("plot.png", res=300, height=1100, width=1600)
sjPlot::plot_model(model1, type = "est",  auto.label = FALSE,
                   vline.color = "green", sort.est = TRUE, show.values = TRUE)
```




```
#dev.off()
#sjPlot::plot_model(model1, type = "pred")
sjPlot::plot_model(model1, type = "slope")
```

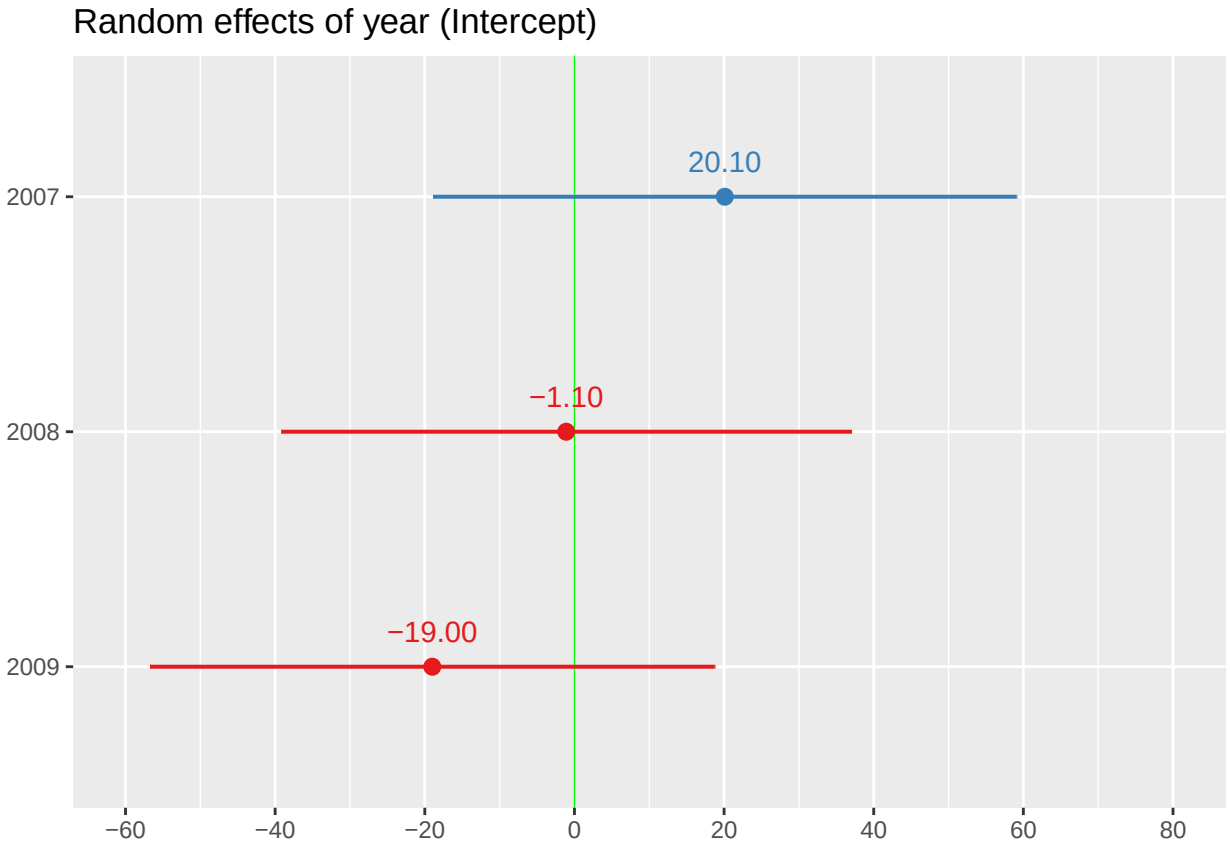
```
## `geom_smooth()` using formula = 'y ~ x'
## `geom_smooth()` using formula = 'y ~ x'
```



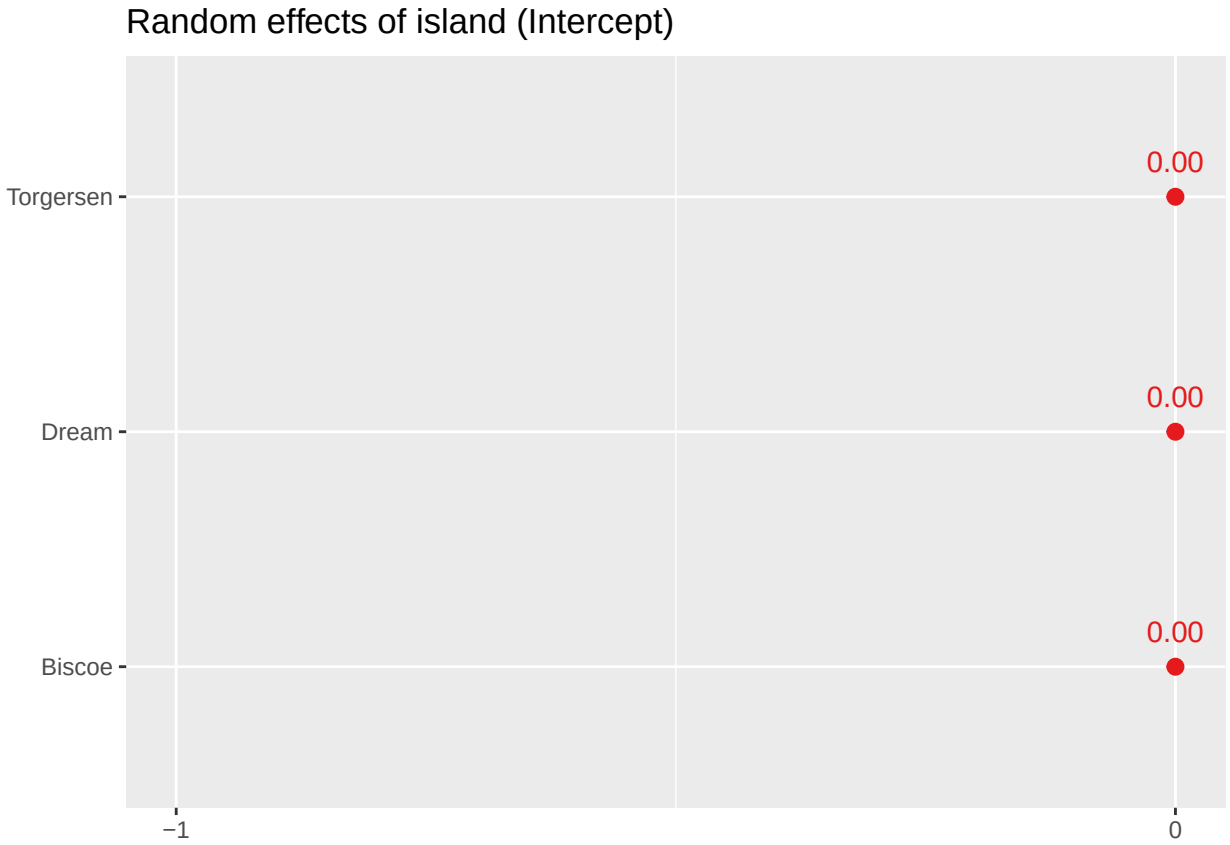

We also plot the random effects. Ideally, you want them centered around the middle line and crossing it, showing that there is no strong effect from these variables.

```
sjPlot::plot_model(model1, auto.label = FALSE, type = "re", # plots random effects
                   vline.color = "green", sort.est = TRUE, show.values = TRUE,
                   # add this to get the effects sorted for random effects
                   grid = FALSE)
```

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


Random effects of year (Intercept)
2007
2008
2009
20.10
−1.10
−19.00
−60
−40
−20
0
20
40
60
80

```
##
## [[2]]
```




We can extract the effect size of each variable by calculating how much the variance explained by the model drops when a given variable is removed.

```
# open an empty table to store the output
effect.table <-NULL %>% as.data.frame()

# extract a list with all the predictors
valid.names <- names(tmp)[!names(tmp) %in% c("To_Predict",
                                             "year",
                                             "island")]


# for each predictor
for(i in 0:length(valid.names)) {

  if(i == 0){
    # write the formula
    frm <- as.formula(paste("To_Predict ~ (1|year) + (1|island) +",
                            paste(valid.names, collapse = "+")))
    # feed it to the model
    model.tmp <- lmerTest::lmer(frm, data = tmp)

    #Determine R2:
    effect.table <- rbind(effect.table,
                          c("all factors",
                            caret::R2(predict(model.tmp), tmp$To_Predict)))
  }else{
```

```
    # write the formula
    frm <- as.formula(paste("To_Predict ~ (1|year) + (1|island) +",
                            paste(valid.names[-i], collapse = "+")))
    # feed it to the model
    model.tmp <- lmerTest::lmer(frm, data = tmp)

    #Determine R2:
    effect.table <- rbind(effect.table,
                          c(valid.names[i],
                            caret::R2(predict(model.tmp), tmp$To_Predict)))
  }}
```

```
## boundary (singular) fit: see help('isSingular')
## boundary (singular) fit: see help('isSingular')
## boundary (singular) fit: see help('isSingular')
## boundary (singular) fit: see help('isSingular')
## boundary (singular) fit: see help('isSingular')
```

```
# adjust column names
colnames(effect.table) <- c("Factor", "Var.exp")

# add a column for effect size
effect.table <- effect.table %>%
  # make the column numeric
  mutate(Var.exp = as.numeric(Var.exp),
         # effect size = gap of variance explained with the main model
         Effect.size = as.numeric(effect.table$Var.exp[1]) - Var.exp) %>%
  filter(Factor != "all factors") %>%
  mutate(Effect.size = round(Effect.size, digits = 4))

# visual check
effect.table %>% arrange(desc(Effect.size))
```

```
##              Factor   Var.exp Effect.size
## 1           species 0.8478408      0.0282
## 2               sex 0.8518421      0.0242
## 3 flipper_length_mm 0.8634357      0.0126
## 4     bill_depth_mm 0.8727494      0.0033
## 5    bill_length_mm 0.8733327      0.0027
```

- The R-square (R2), which represents the correlation between the actual values and the predicted values. The higher the R2, the better the model (can interpret it as a correlation coefficient).

```
caret::R2(predict(model1), tmp$To_Predict) %>% round(digits = 2)
```

```
## [1] 0.88
```

```
# r2marginal represents the variance explained by the fixed effects
# r2conditional represents the variance explained by the entire model (fixed + random effects)
MuMIn::r.squaredGLMM(model1)
```

```
## Warning: 'r.squaredGLMM' now calculates a revised statistic. See the help page.

##             R2m       R2c
## [1,] 0.8728317 0.8740358
```