Lecture 9: Model fitting

C91AR: Advanced Statistics using R

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Contents

1 Session outline

- Today, we are going to examine methods for checking how well a model fits the data
- We are going to look at a few today outlined in Canduela and Raeside (2020)
- Discuss multicollinearity and how to check for it
- On Thursday I will run a code clinic where you can ask me any questions about R, to give you some extra support as your prepare the summative assessment.

2 Reproducibility & notation

```
# Set seed for reproducibility
set.seed(123)

# Change the output format
options(scipen = 999)
```

3 Load packages

```r
# Load packages
pacman::p_load(tidyverse,
               corrr,
               tidyplots,
               car) # for VIF
```

4 Data setup

```r
# Read in the data
handw <-
  read_csv("data_raw/heights_and_weights.csv",
           col_types = "dd")


# Add log transformed vectors to dataset
handw_log <-
  handw |>
  mutate(hlog = log(height_in),
         wlog = log(weight_lbs))

# load grades data for VIF
grades <-
  read_csv("data_tidy/grades.csv",
           col_types = "ddii")
```

5 R^2 Coefficient of determination

- To this point we have created a regression equation and used it to predict someone's weight given their height.
- But, we also want to know how good a fit our equation is given the data. To calculate this we use the ***coefficient of determination*** (R^2):

$$R^2 = \frac{\text{Sum of Squares Explained by Regression (SSR)}}{\text{Total Sum of Squares (before regression)(TSS)}} = \frac{\sum\limits_{i=1}^{n}(\hat{y}_i-\overline{y})^2}{\sum\limits_{i=1}^{n}(y_i-\overline{y})^2}$$

6 Calculating the total sum of squares

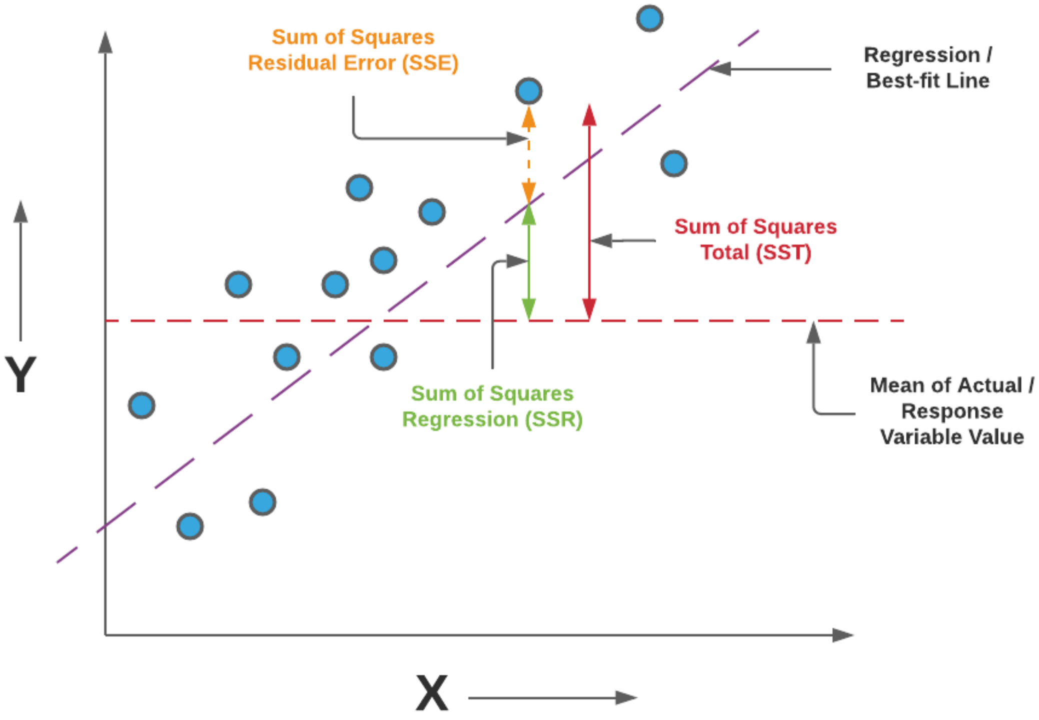
- The total sum of squares (TSS) in the dependent variable (i.e., weight) is split into two parts:
  - the part explained by sum of squares explain by regression (SSR), which is the sum of the squared differences between the predicted values ($\hat{y}_i$) and the mean of the response variable ($\overline{y}$)

$$\text{Sum of Squares Explained by Regression (SSR)} = \sum_{i=1}^{n} (\hat{y}_i - \overline{y})^2$$

- the part that is unexplained sum of squared errors (SSE), which is the squared difference between the observed values (y_i) and the predicted values ($\hat{y}_i$), since the relationship is never perfect and there are always some residuals.

$$\text{Sum of Squares Errors (SSE)} = \sum_{i=1}^{n} (y_i - \overline{y})^2$$

7 Where the R^2 values come from



8 R^2 Thresholds

$$R^2 = \frac{\text{Sum of Squares Explained by Regression (SSR)}}{\text{Total Sum of Squares (before regression)(TSS)}} = \frac{\sum\limits_{i=1}^{n}(\hat{y}_i-\overline{y})^2}{\sum\limits_{i=1}^{n}(y_i-\overline{y})^2}$$

- The coefficient of determination can take values between 0 and 1, but is commonly reported as a percentage, as it represent the proportion of the variation in the dependent variable (Y_i) which is explained by the predictor/independent variable (X_i).
- The higher the R^2 value (at least 70%) the better the model fit.
- A reasonable model fit would be more $R^2 >= 60\%$.

9 Exploring the Errors

- To assess the quality of the model further we need to look at the *errors* or *residuals* $(y_i - \hat{y}_i)$ after running the regression model.

- Model residuals should be **randomly scattered** with **no extreme values** and should have a **mean of zero**.

- Should these requirements not be met we would have to further investigate whether there is information in the residuals that could be covered by the model or be considered a cause for concern.

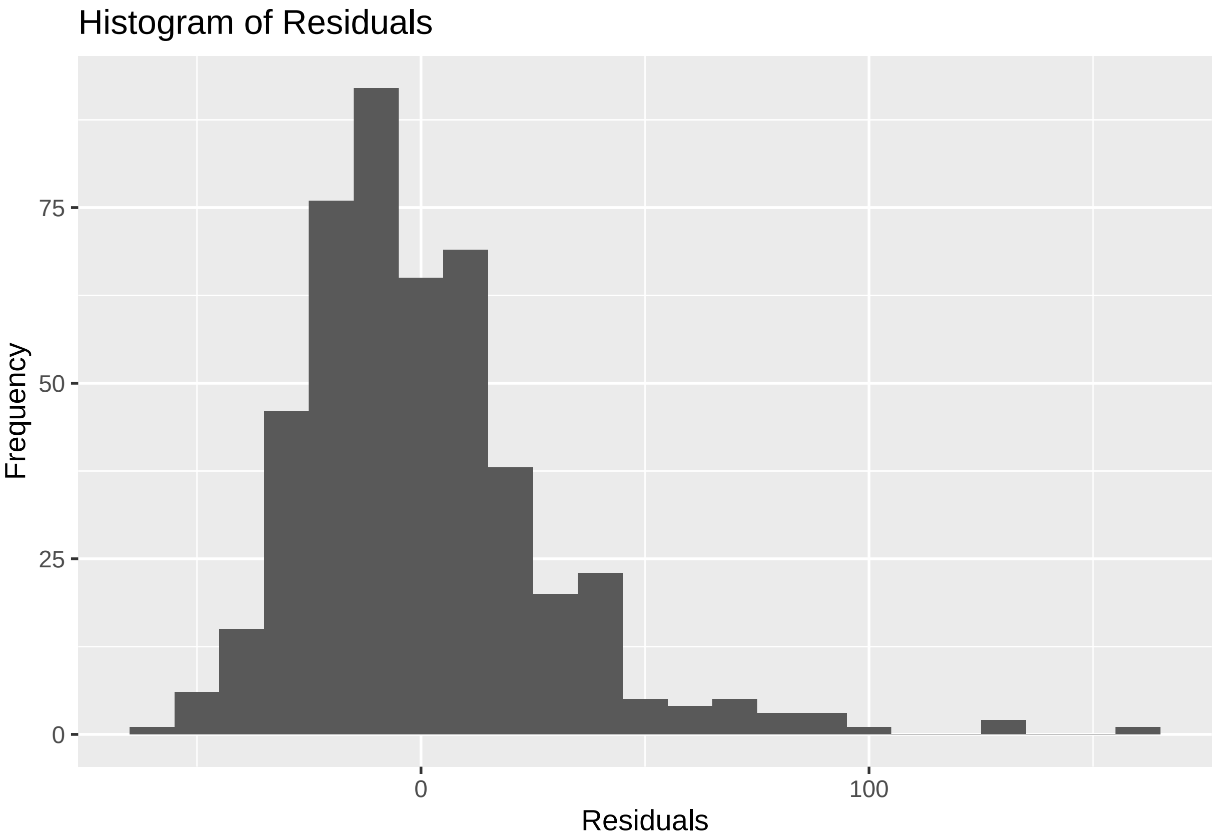
- A histogram of the residuals and normal probability plot can help you decide how well your residuals fit into the model.

10 Histogram of model residuals

```r
# Create model for raw data
mod1 <-
  lm(weight_lbs ~ height_in,
     data = handw)

# Create residuals object
residuals_df <-
  mod1$residuals |>
  as_tibble() |>
  rename(residuals = value)

# Plot the data
ggplot(residuals_df, aes(x = residuals)) +
  geom_histogram(binwidth = 10) +
  labs(title = "Histogram of Residuals",
       x = "Residuals",
       y = "Frequency")
```



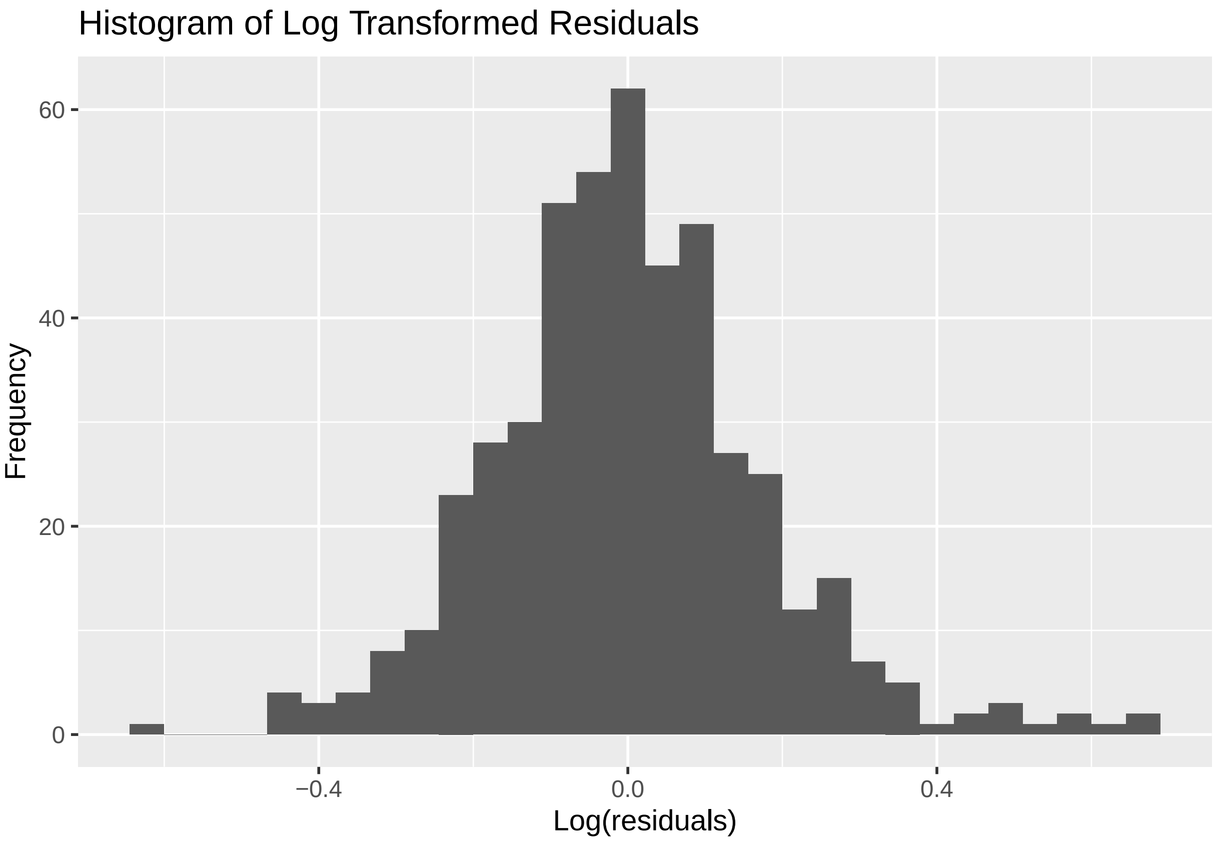
Are the residuals **randomly scattered** with **no extreme values**?

11 Transformed data: residuals plot

```
# Create model for transformed data
mod2 <-
  lm(wlog ~ hlog,
     data = handw_log)

# Create residuals object
residuals_df <-
  mod2$residuals |>
  as_tibble() |>
  rename(residuals = value)
```

```
# Plot the data
ggplot(residuals_df, aes(x = residuals)) +
  geom_histogram(bins = 30) +
  labs(title = "Histogram of Log Transformed Residuals",
       x = "Log(residuals)",
       y = "Frequency")
```



Are the residuals **randomly scattered** with **no extreme values**?

12 Quantile quantile (Q-Q) plot

- A Q-Q plot compares the quantiles of the observed data to the quantiles of a theoretical distribution.
- It plots the observed quantiles on the y-axis and the theoretical quantiles on the x-axis.
- The primary purpose of a Q-Q plot is to visually assess how well the observed data fits a specified theoretical distribution.

- It helps identify deviations from the theoretical distribution, such as skewness, kurtosis, or other anomalies.
- In regression analysis and other statistical modeling, Q-Q plots are used to check the normality of residuals, which is an assumption for many statistical tests and models.

13 Interpreting a Q-Q plot

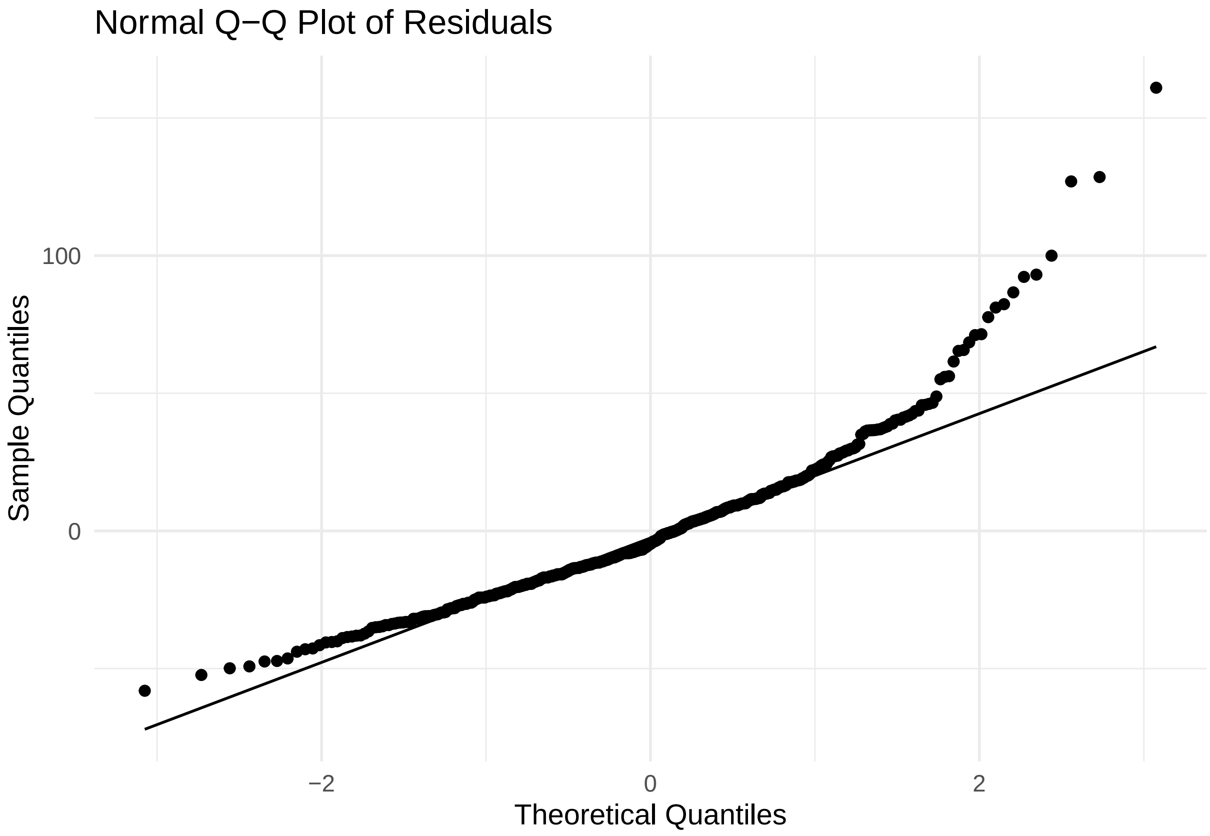
- If the data points lie approximately along a straight diagonal (45°) line, it suggests that the data follows the theoretical distribution.
- Deviations from the diagonal line indicate departures from the theoretical distribution. For example, a systematic curve might indicate skewness, while points that diverge at the ends might indicate heavy tails.

```r
# Extract residuals
residuals <-
  mod1$residuals

# Calculate theoretical quantiles
mod1_quantiles <-
  qqnorm(residuals, plot.it = FALSE)$x

# Create a data frame with residuals and theoretical quantiles
pp_df <-
  data.frame(
  residuals = residuals,
  theoretical_quantiles = mod1_quantiles
)

# Plot the Q-Q plot
ggplot(pp_df, aes(sample = residuals)) +
  stat_qq() +
  stat_qq_line() +
  labs(title = "Normal Q-Q Plot of Residuals",
       x = "Theoretical Quantiles",
       y = "Sample Quantiles") +
  theme_minimal()
```



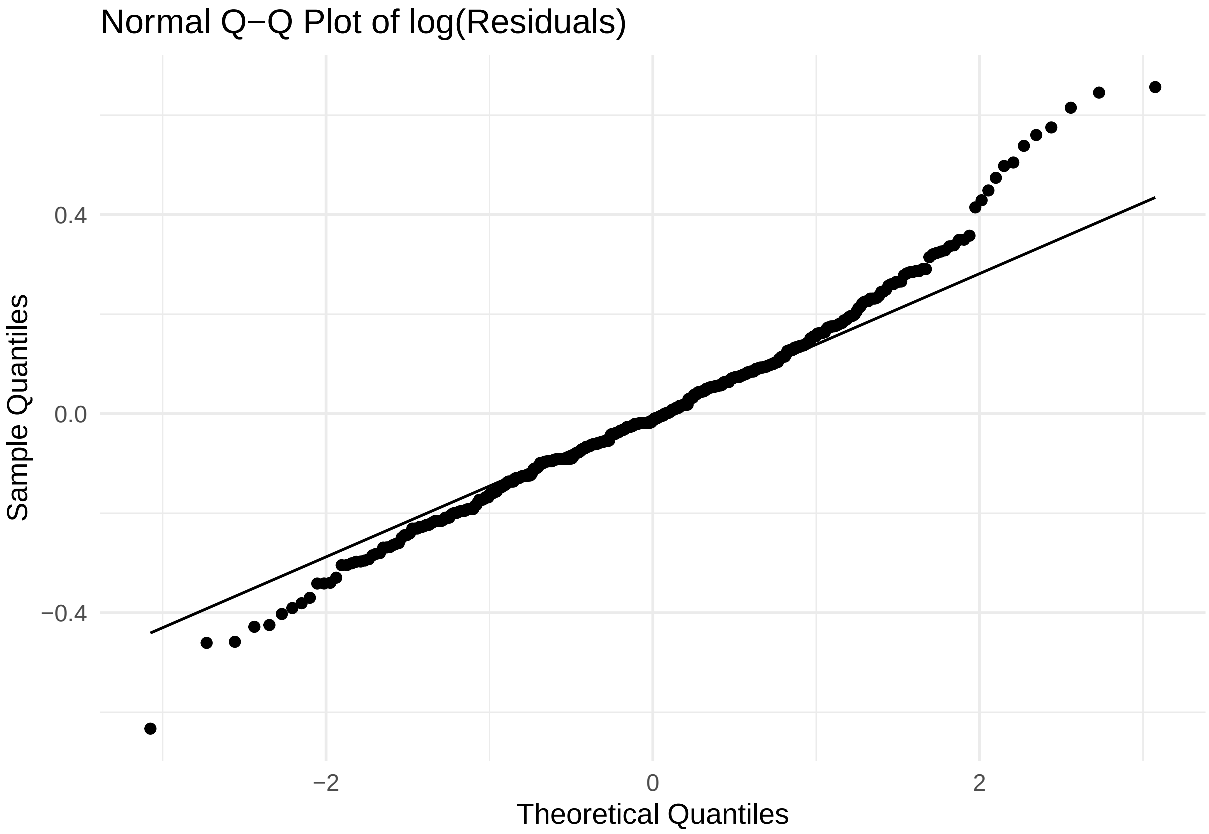
14 Transformed data: Normal PP plot

```
# Extract residuals
residuals <-
  mod2$residuals

# Calculate theoretical quantiles
mod2_quantiles <-
  qqnorm(residuals, plot.it = FALSE)$x

# Create a data frame with residuals and theoretical quantiles
pp_df <-
  data.frame(
  residuals = residuals,
  theoretical_quantiles = mod2_quantiles
)

# Plot the Q-Q plot
ggplot(pp_df, aes(sample = residuals)) +
  stat_qq() +
  stat_qq_line() +
  labs(title = "Normal Q-Q Plot of log(Residuals)",
       x = "Theoretical Quantiles",
       y = "Sample Quantiles") +
  theme_minimal()
```



15 Testing the Significance of the model and its coefficients

- We can use statistical tests to determine how well we are approximating the population parameters with those in our model. To do this we can use two methods:

- Analysis of variance (ANOVA): tests overall significance of the model

- *t*-test: test the individual significance of the coefficients.

16 Testing the overall significance of the model

- Testing the overall significance of the model evaluates how well the independent variables reliable predict the dependent variable.
- We can create hypotheses to make our statistical inferences:

H_0: The regression model does not explain a significant proportion of the variance in weight (our DV).

VS

H_1: The regression model does explain a significant proportion of the variation in weight.

And we test the above using the F-distribution.

17 ANOVA for regression modelling

ANOVA for regression

Source of	Sum of Squares	Degrees of Freedom	Mean Square	
Variation	(SS)	(df)	(MS)	F-Statistic (F)
Model	$\text{SS}_{\text{model}} = \sum_{i=1}^{n} (\hat{y}_i - \bar{y})^2$	k	$\text{MSR} = \frac{\text{SSR}}{k}$	$\frac{\text{MSR}}{\text{MSE}}$
Residual	$\text{SS}_{\text{residual}} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$	$n - k - 1$	$\text{MSE} = \frac{\text{SSE}}{n-k-1}$	
Total	TSS = $SSR + SSE = \sum_{i=1}^{n} (y_i - \bar{y})^2$	$n - 1$		

ANOVA for regression: key

- n = total number of observations
- k = total number of independent variables
- y = the observed values
- $\bar{y}$ = mean of the dependent variables
- $\hat{y}_i$ = the estimated values

18 ANOVA for log transformed model

Remember: `mod2 <- lm(wlog ~ hlog, data = handw_log)`

```
# Run an ANOVA on our log transformed model
anova_results <-
  anova(mod2)


print(anova_results)
```

```
## Analysis of Variance Table
##
## Response: wlog
##            Df  Sum Sq Mean Sq F value                Pr(>F)    
## hlog        1 182.622 182.622  5801.8 < 0.00000000000000022 ***
## Residuals 473  14.888   0.031                                  
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```r
# Calculate TSS
ss_model <-
  anova_results["hlog", "Sum Sq"]

ss_residual <-
  anova_results["Residuals", "Sum Sq"]

tss <-
  ss_model + ss_residual

print(tss)
```

```
## [1] 197.5102
```

19 Interpreting the results of ANOVA

- We can see from the output that `hlog` that the slope of the line is significant difference from 0, where $p < 0.001$.
- Thus we reject the null hypothesis (H_0).

20 Multicollinearity

- Multicollinearity occurs when **two or more predictor variables** in a regression model are highly correlated.
- It can cause problems in estimating the coefficients of the regression model, leading to unreliable and unstable estimates.
- High multicollinearity inflates the standard errors of the coefficients, making it difficult to determine the individual effect of each predictor.

21 Variance Inflation Factor (VIF)

- VIF quantifies the extent of multicollinearity in a regression model.
- It measures how much the variance of a regression coefficient is inflated due to multicollinearity.

$$\text{VIF}_j = \frac{1}{1 - R_j^2}$$

- VIF_j = the variance inflation factor for variable j - R_j^2 is the R^2 of the regression of variable j over the rest of the variables

22 VIF parameters

- VIF near to 1 indicate no or little correlation between predictor variable j and the other predictors.
- VIF values above 4 suggests that multicollinearity may be inflating a coefficient values due to strong predictor correlations
- If VIF $>$ 10 then multicollinearity is serious, pointing to unreliable parameter estimates.

23 Checking the multicollinearity of our grades regressopn model

```r
# Grades predicted by GPA, lectures attended, and number of VLE downloads
model <-
  lm(grade ~ GPA + lecture + nclicks, grades)

# Calculate VIF values
vif_values <-
  vif(model)

# Display VIF values
print(vif_values)
```

```
##      GPA  lecture  nclicks
## 1.277344 1.337824 1.183668
```

What can you infer from the output?

24 Roundup

- Today we looked at ways to check the fit of your regression model
- These are important for validating your analytical approach
- When you have more than one predictor, you need to be aware of multicollinearity
- In Thursdays lab we will begin our revision of the course.

References

Canduela, Jesus, and Robert Raeside. 2020. *The Quantitative Researcher*. Heriot-Watt University. www.hw.ac.uk/ebs.