Simple linear regression

Applied Data Science using R, Sessions 12 & 13

Prof. Dr. Claudius Gräbner-Radkowitsch
Europa-University Flensburg, Department of Pluralist Economics
www.claudius-graebner.com | @ClaudiusGraebner | claudius@claudius-graebner.com

Europa-Universität Flensburg

Europa-Universität Flensburg
International Institute of Management and Economic Education
Department of Pluralist Economics

Goals for today

I. Clarify the distinction between correlation and causation

II. Understand how the four steps of modelling data are operationalised within simple linear regression framework

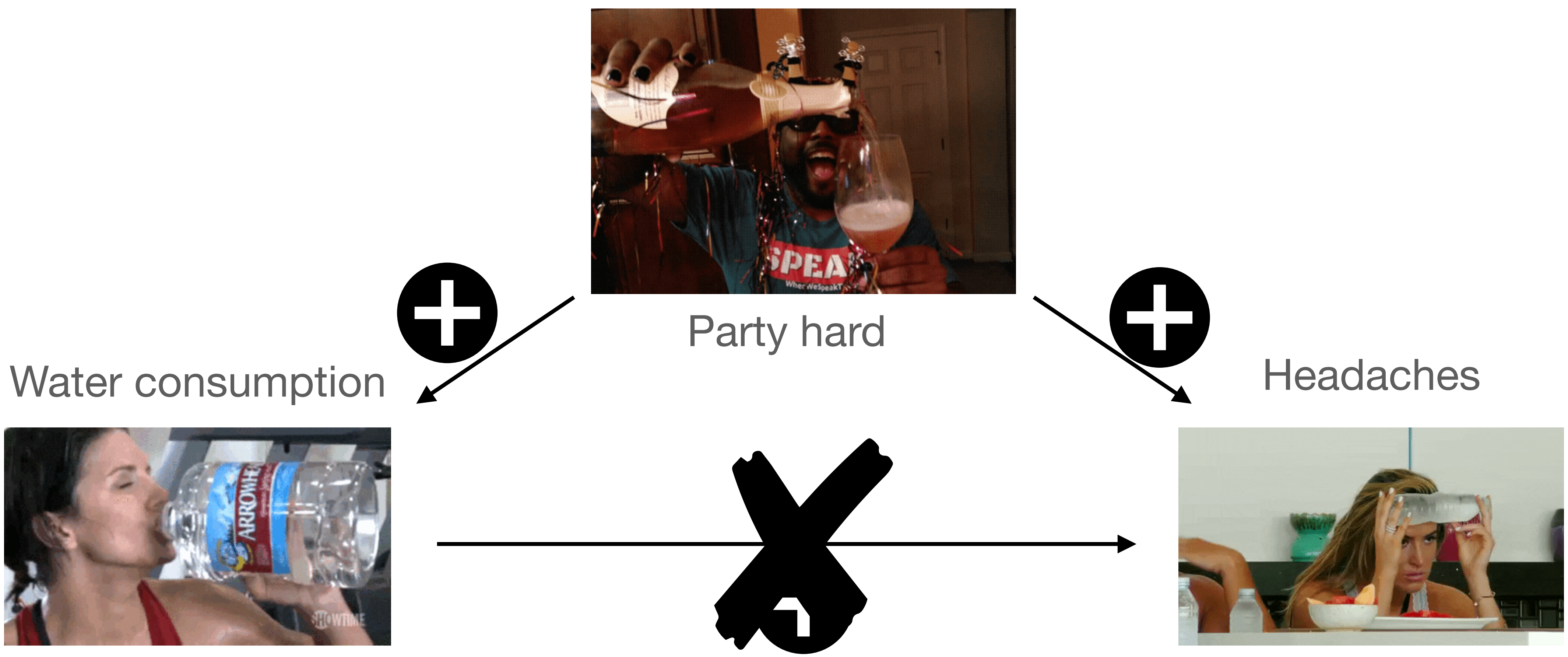
III. Understand the concept of ordinary least squares

IV. Learn how to conduct a simple lineare regression in R

Correlation & causation

Correlation and causation

- The distinction between correlation and causation is central for any applied (data) scientist
  - Correlation describes an **observed relationship**
  - Causation refers to an (unobservable) **cause-effect relationship**



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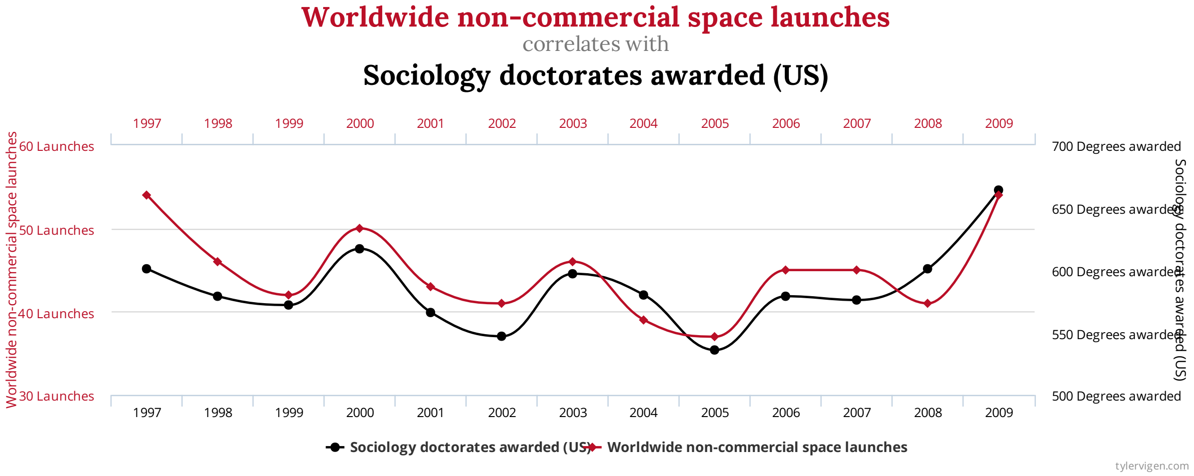
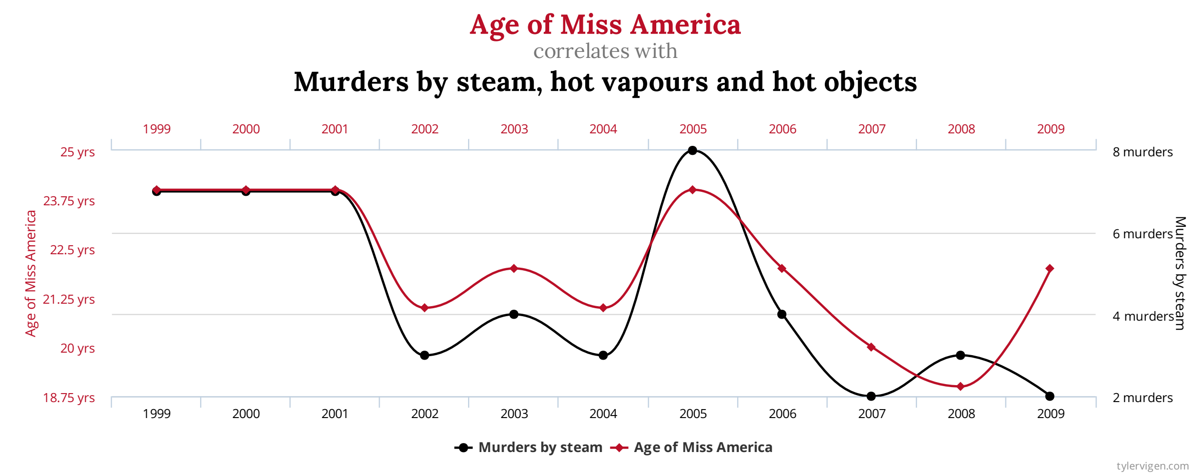
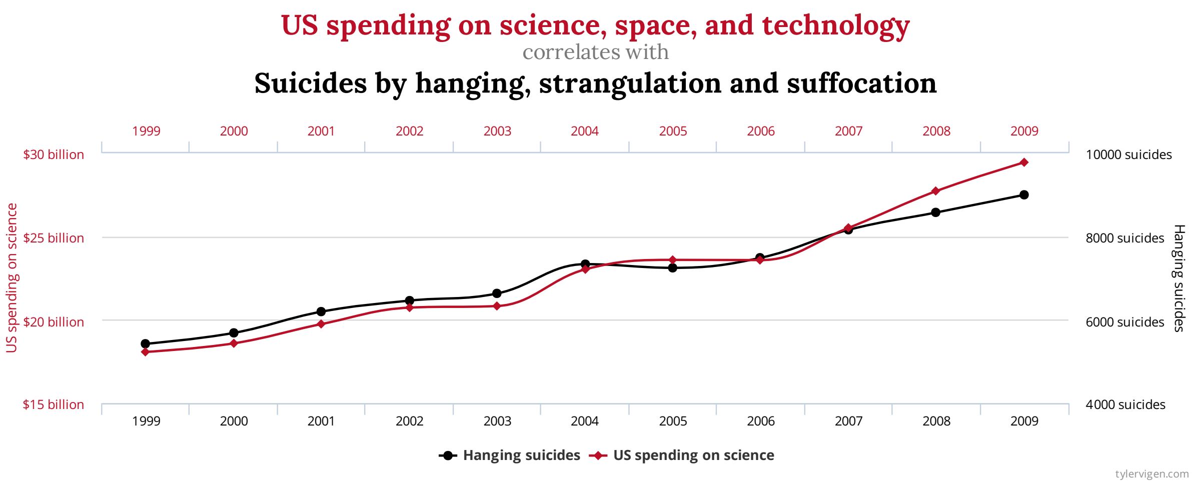
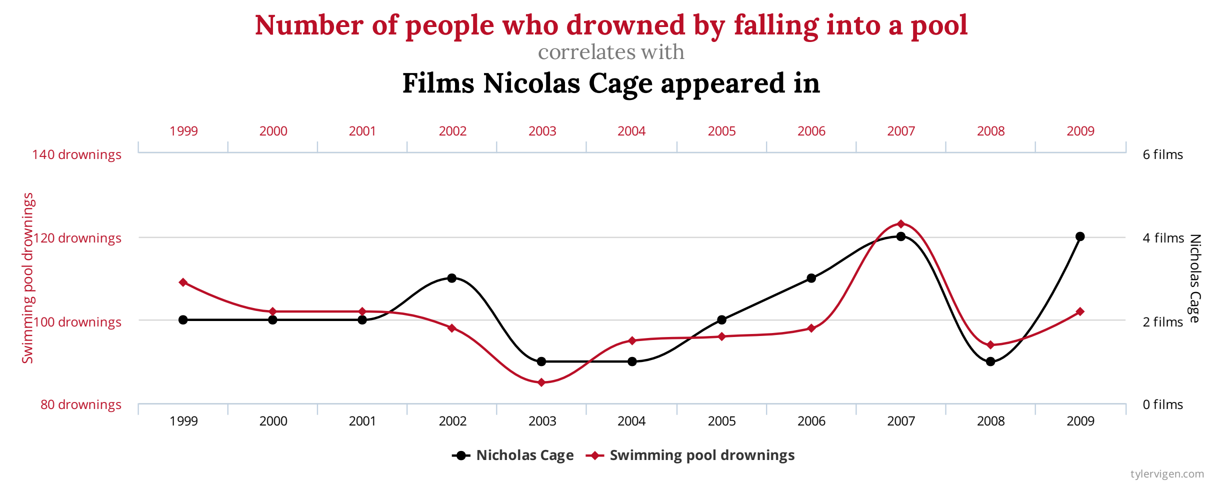








Correlation and causation

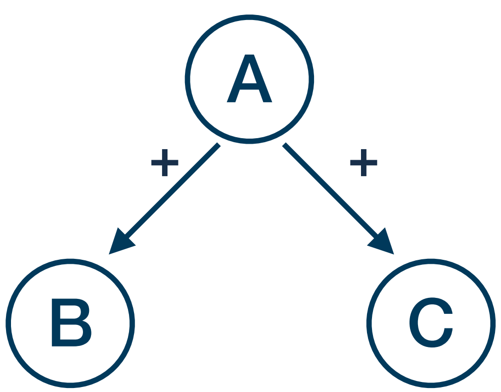
- The distinction between correlation and causation is central for any applied (data) scientist
  - Correlation describes an **observed relationship**
  - Causation refers to an (unobservable) **cause-effect relationship**
- If we observe correlation without causation as in the example we speak of a **spurious relationship** and (potentially) a **confounding variable**
- Knowledge about causality is important whenever we think about the effect of interventions
  - Here we need knowledge that goes **beyond our ability to predict**
  - We might be able to predict suicides by hanging or strangulation via US spending on aircraft, but cannot think about how to reduce them like this...

Correlation and causation

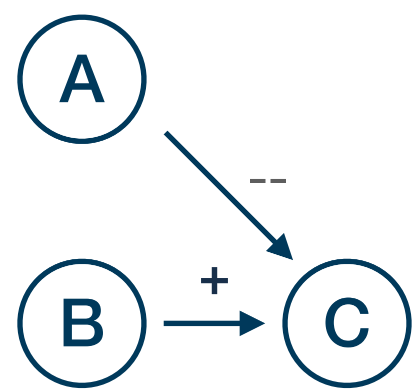
- Identifying causation is attractive but very hard
- It requires us to add theoretical hypotheses about cause-effect-relationships into a model
  - "No causes in, no causes out!"
  - This gives rise to **causal models** (which are often represented graphically)

Nancy Cartwright

- We do not engage in causal modelling, but note that event simply directed cycling graphs (DAGs) help you to sort your thoughts about causation



A: Party all night
B: Water consumption next morning
C: Headache next morning
→ Spurious relation betw. B and C



This is how there can be causation without observed correlation

Correlation and causation

- Identifying causation is attractive but very hard
- It requires us to add theoretical hypotheses about cause-effect-relationships into a model
  - "No causes in, no causes out!"
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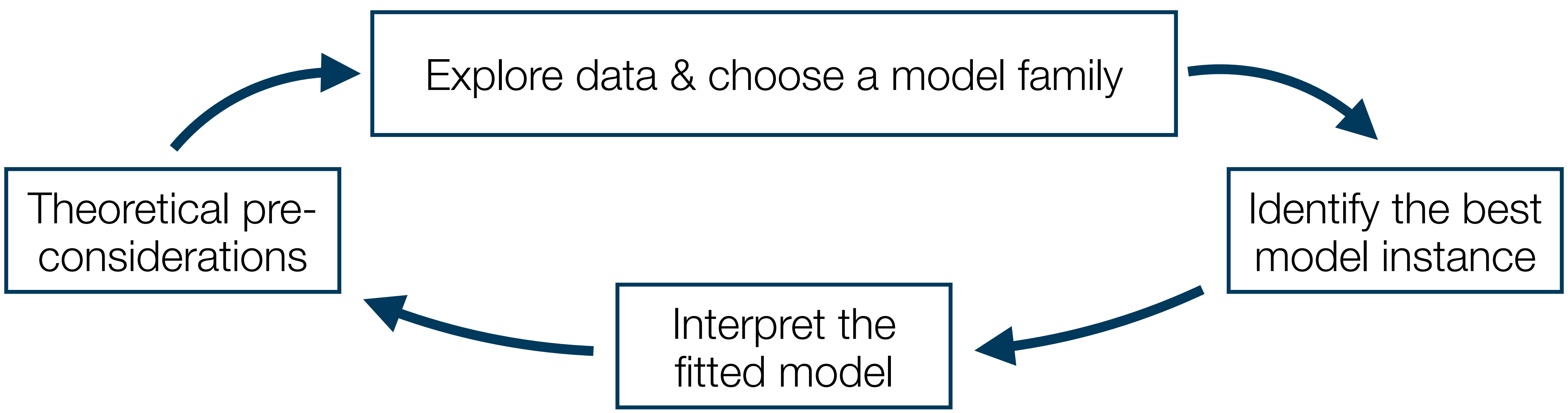
Nancy Cartwright

- We do not engage in causal modelling, but note that event simply directed cycling graphs (DAGs) help you to sort your thoughts about causation
- What you will do is how to ‘sort out’ or ‘control for’ variables being related to your variable of interest
  - Example: What is the relative association of migration background and income with criminal activity?

The sequence of modelling

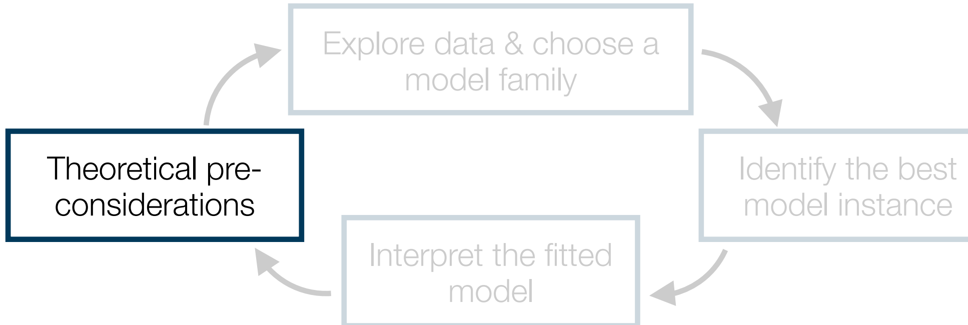
The general sequence of modelling

- In the most general terms, modelling data can be broken down into several steps:



- Applies roughly for both exploratory and explanatory analysis
- Note: sometimes you also choose several models and compare their fit
- Lets illustrate this via a short example

The general sequence of modelling
An example



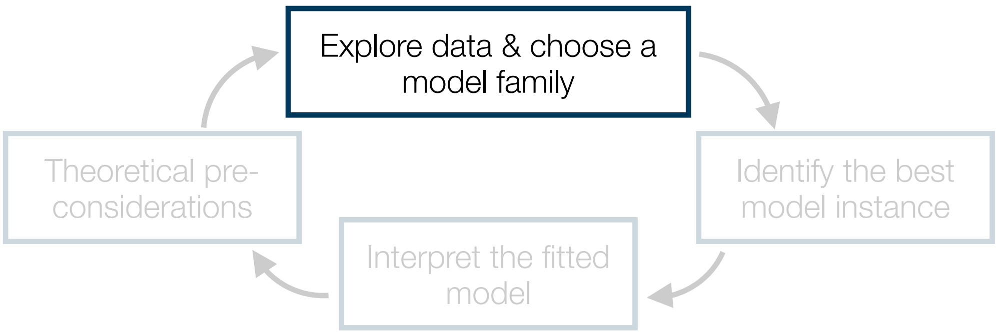
What is the relationship between beer consumption and beer price?

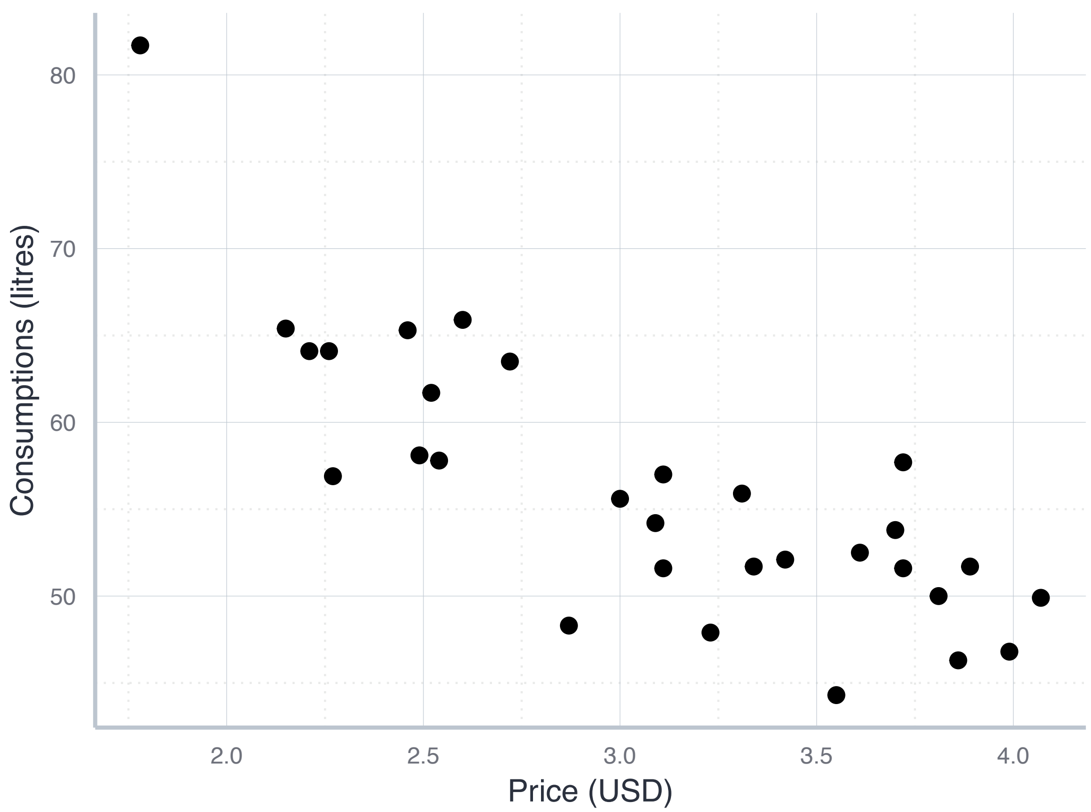
Theoretical law of demand: higher price comes with lower demand

$$D\left(p\right):\frac{\partial D\left(\cdot\right)}{\partial p}<0$$

Obtain survey data on beer consumption and beer prices!

The general sequence of modelling
An example

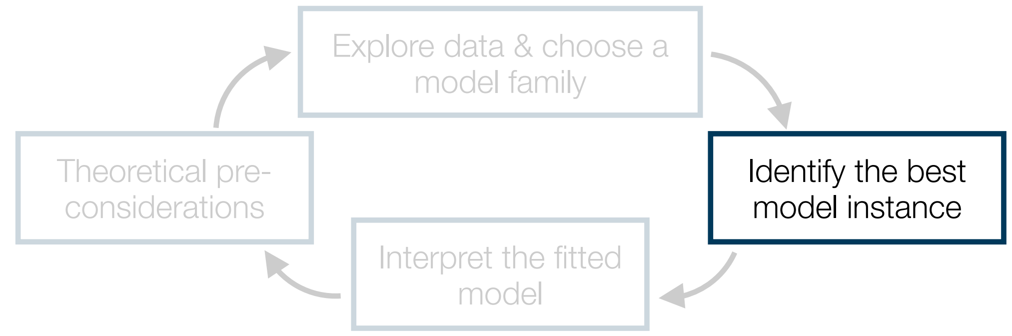




Seems to be a linear relationship → work with the family of linear models:

$$C = a + b \cdot p$$

The general sequence of modelling
An example

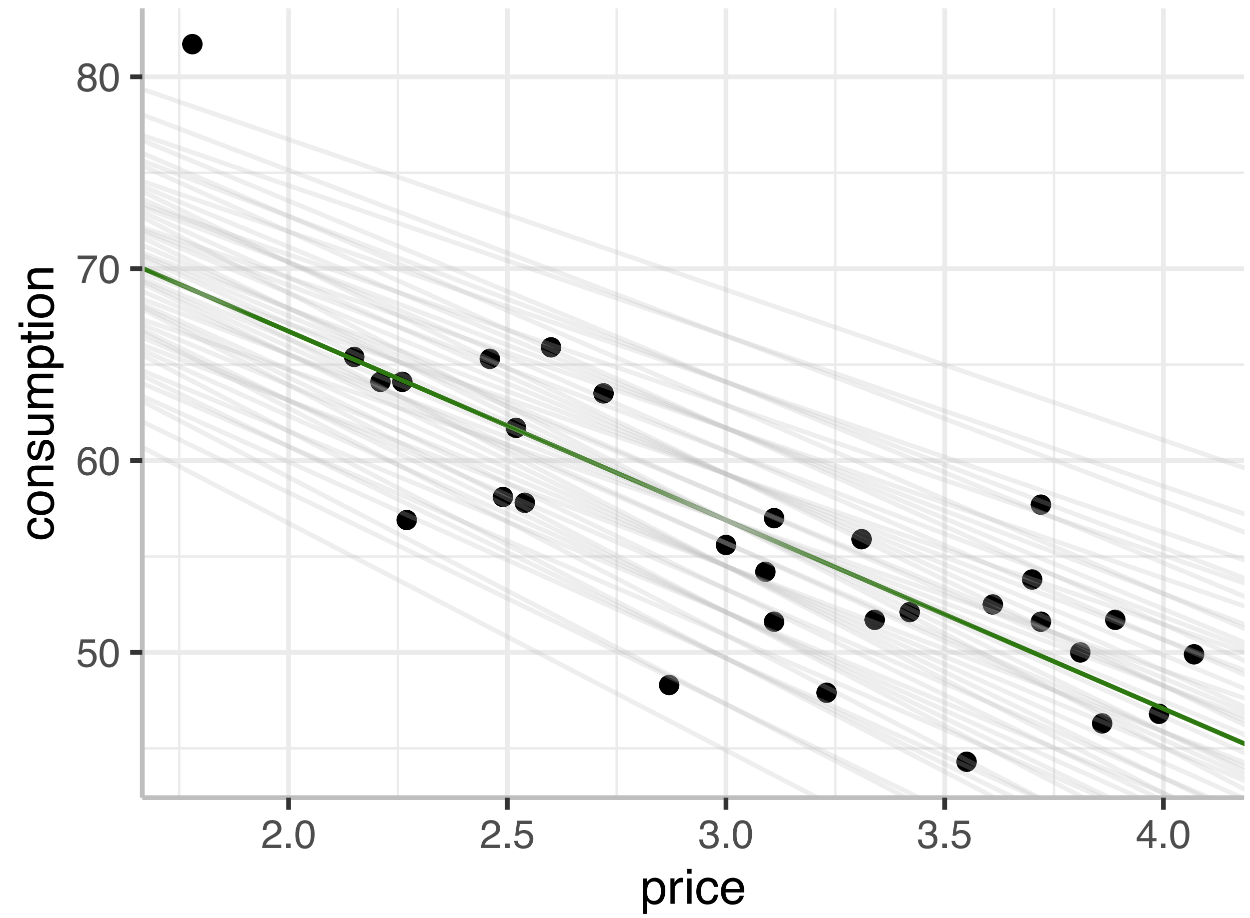


Two parameters:

$$C = a + b \cdot P$$

a and b

Choose parameter such that model describes data best

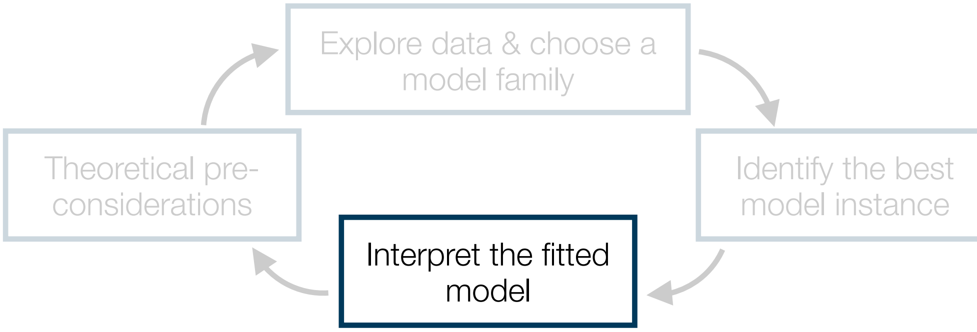


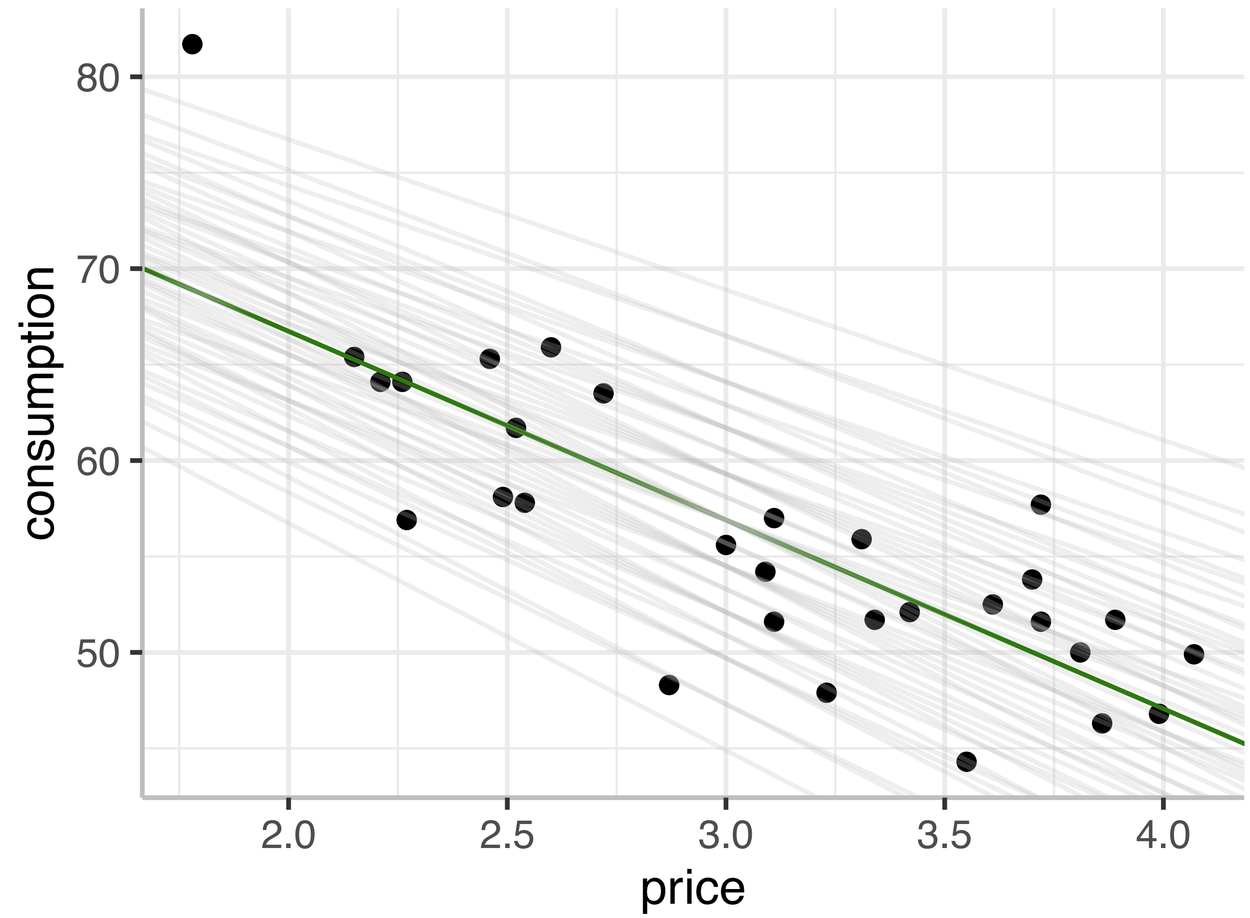

```
Call:
lm(formula = consumption ~ price, data = beer_data_red)

Coefficients:
(Intercept)        price
     86.406       -9.835
```

The general sequence of modelling
An example

```
> linmod_c_price <- lm(
+   formula = consumption~price, data = beer_data_red)
> moderndive::get_regression_table(linmod_c_price)
# A tibble: 2 x 7
  term      estimate
  <chr>        <dbl>
1 intercept     86.4
2 price        -9.84
```

For every increase of 1 unit in `price`, there is an **associated decrease** of, **on average**, 9.84 units of `consumption`.

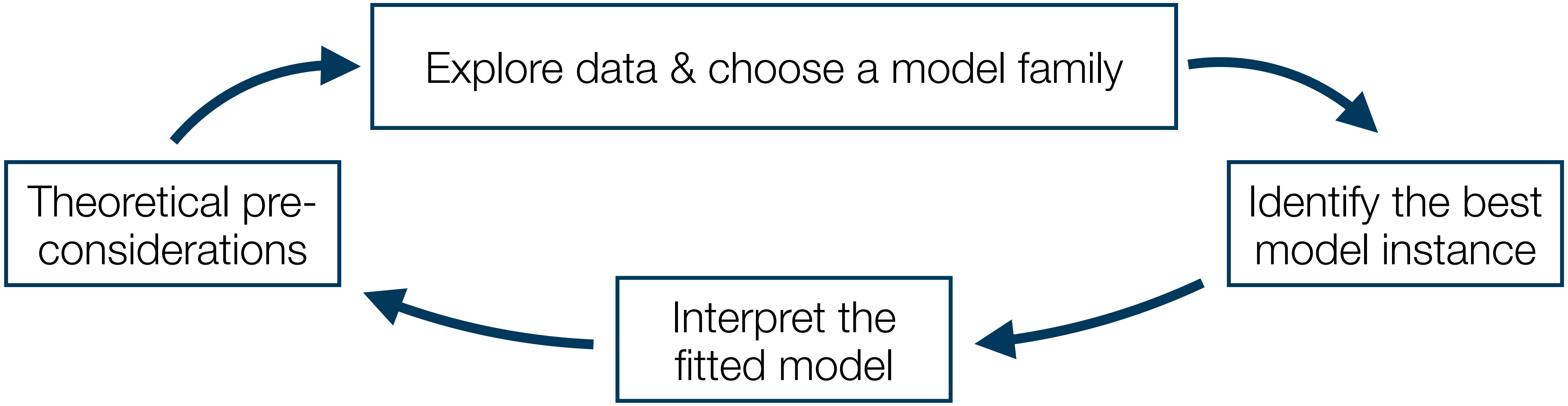




- We expand upon this example in the next section

Simple linear regression

Introduction



- We will mow go through these four steps for the modelling technique of **simple linear regression**
  - It its multiple variant, it is among the most widespread modelling techniques
  - It belongs to the class of **supervised machine learning**
  - While it can be used for exploratory purposes, its main strength lies in explanatory analysis

Modelling data - general workflow
1. Theoretical pre-considerations

- During the theoretical pre-considerations you think about the goal of your modelling exercise
    - What is your subject of interest?
    - Do you want to engage in an exploratory or explanatory analysis?
    - If the latter, what are your main hypothesis? If the former, what is the goal of exploration?
    - What is the data you need and how was it collected?
- **Example**:
    - We are interested in what drives beer consumption
    - We first want to explore the survey data we obtained to derive hypotheses, which we then want to test

Modelling data - general workflow
2. Data exploration and choice of family

- Based on our theoretical considerations we need to obtain data
- Then we need to inspect the data and think about how it could be modelled
- Assume we have a data set with survey results on beer consumption
    - First need to take a `glimpse` at the data set:

```
> glimpse(beer_data)
Rows: 30
Columns: 5
$ consumption  <dbl> 81.7, 56.9, 64.1, 65.4, 6…
$ price        <dbl> 1.78, 2.27, 2.21, 2.15, 2…
$ price_liquor <dbl> 6.95, 7.32, 6.96, 7.18, 7…
$ price_other  <dbl> 1.11, 0.67, 0.83, 0.75, 1…
$ income       <dbl> 25088, 26561, 25510, 2715…
```

- We have 30 observations of five variables, all of which are numeric
    - We should also have a look at common descriptive statistics

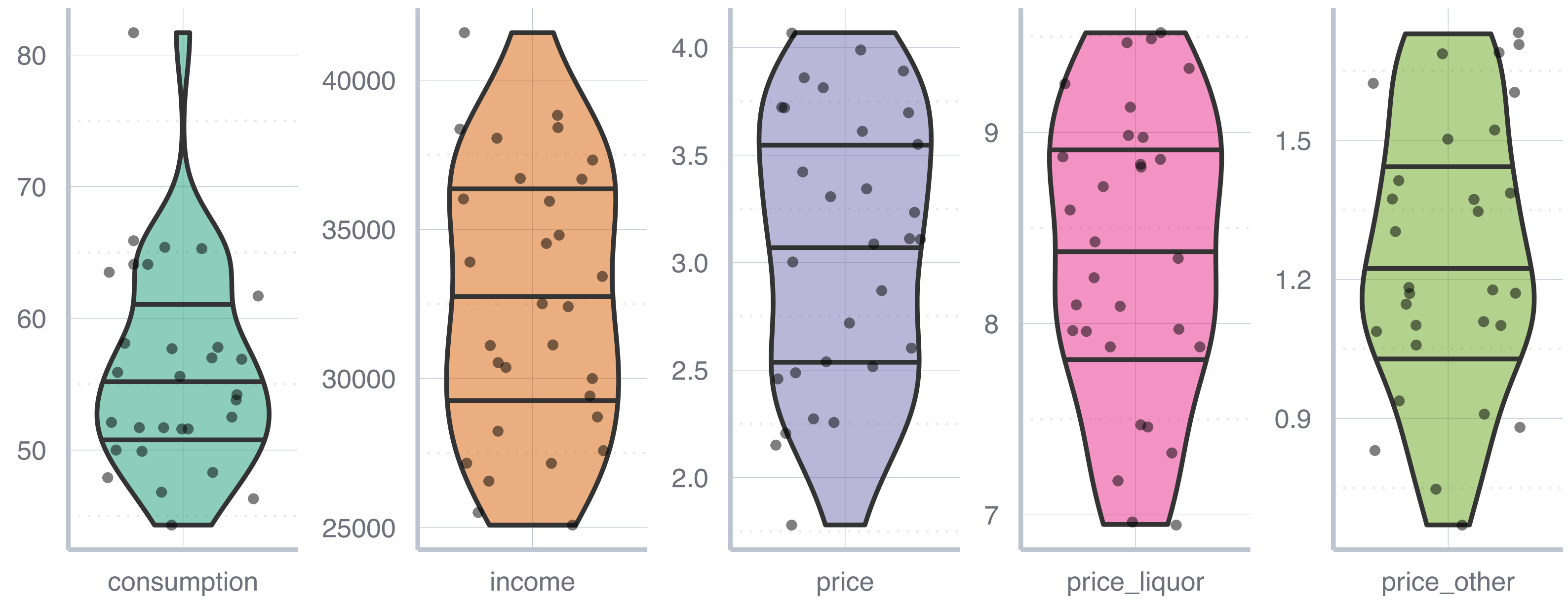
Note: `beer_data` is available as `DataScienceExercises::beer`

Modelling data - general workflow

2. Data exploration and choice of family

- The function `skimr::skim()` provides a nice statistical summary
  - We can complement this via some easy visualisations* (`geom_jitter()` and `geom_violin()`)

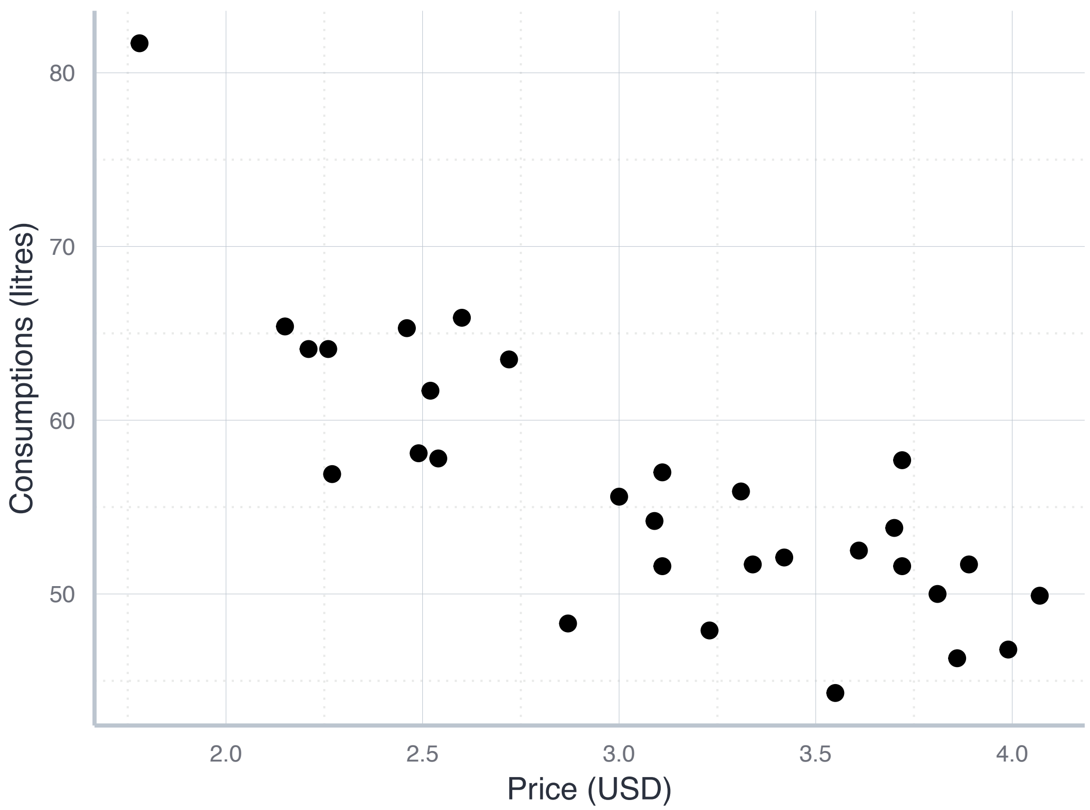
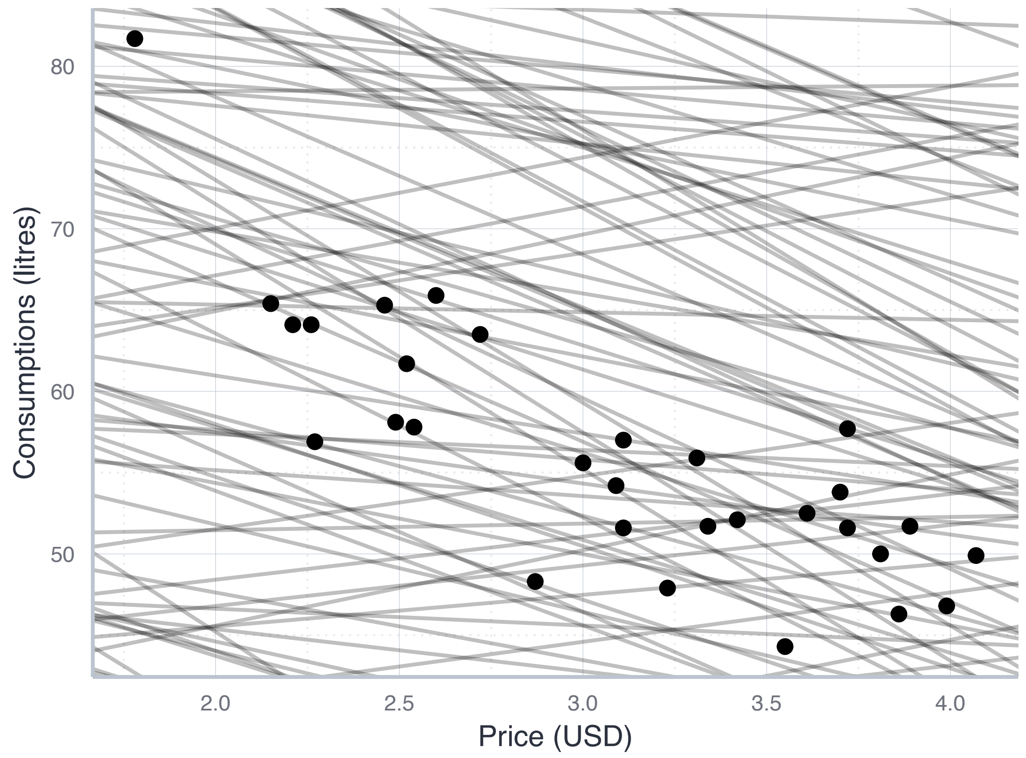
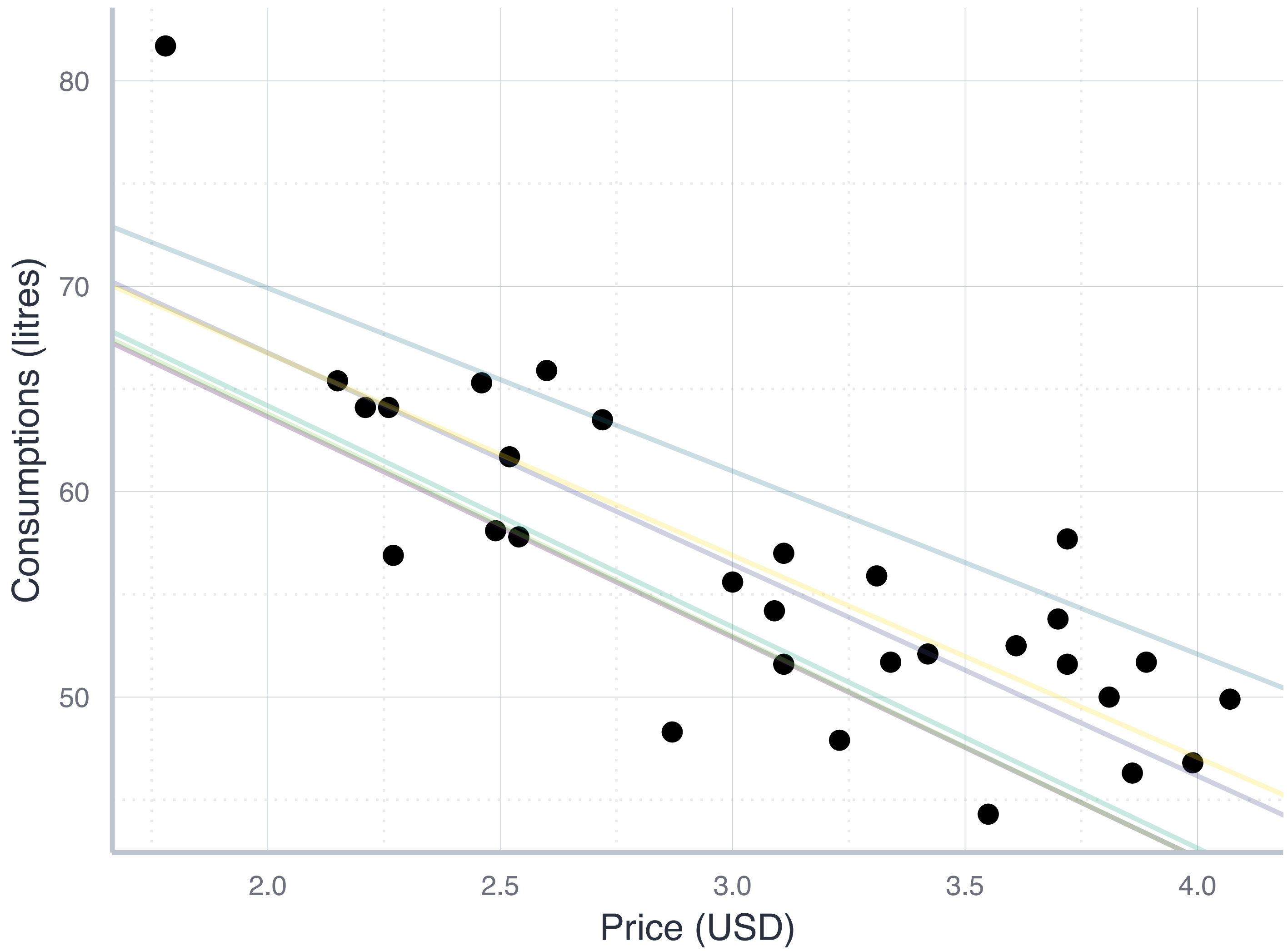
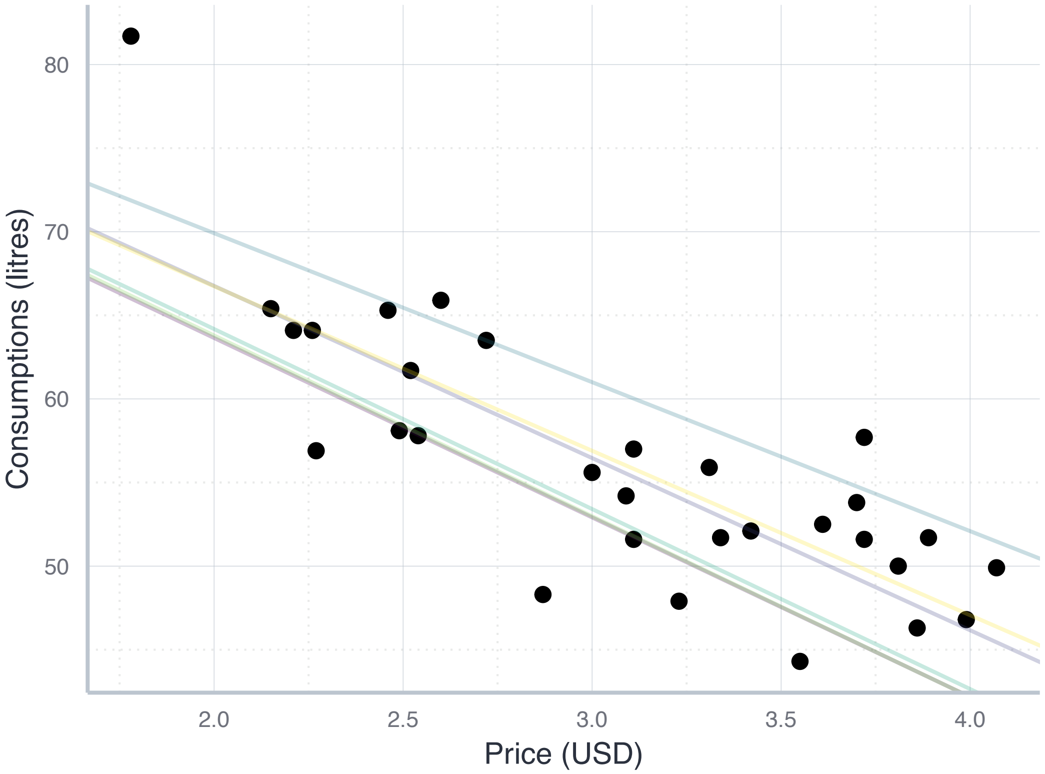
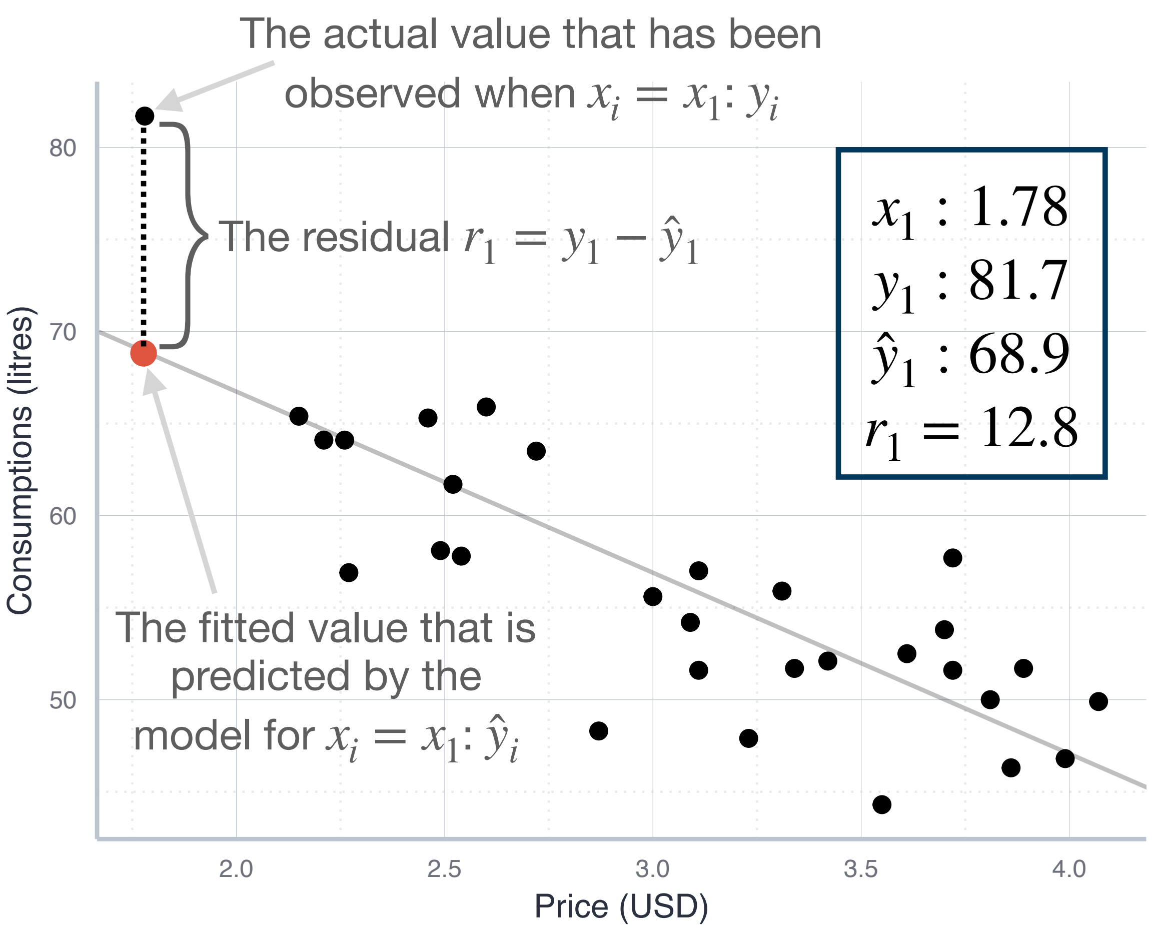
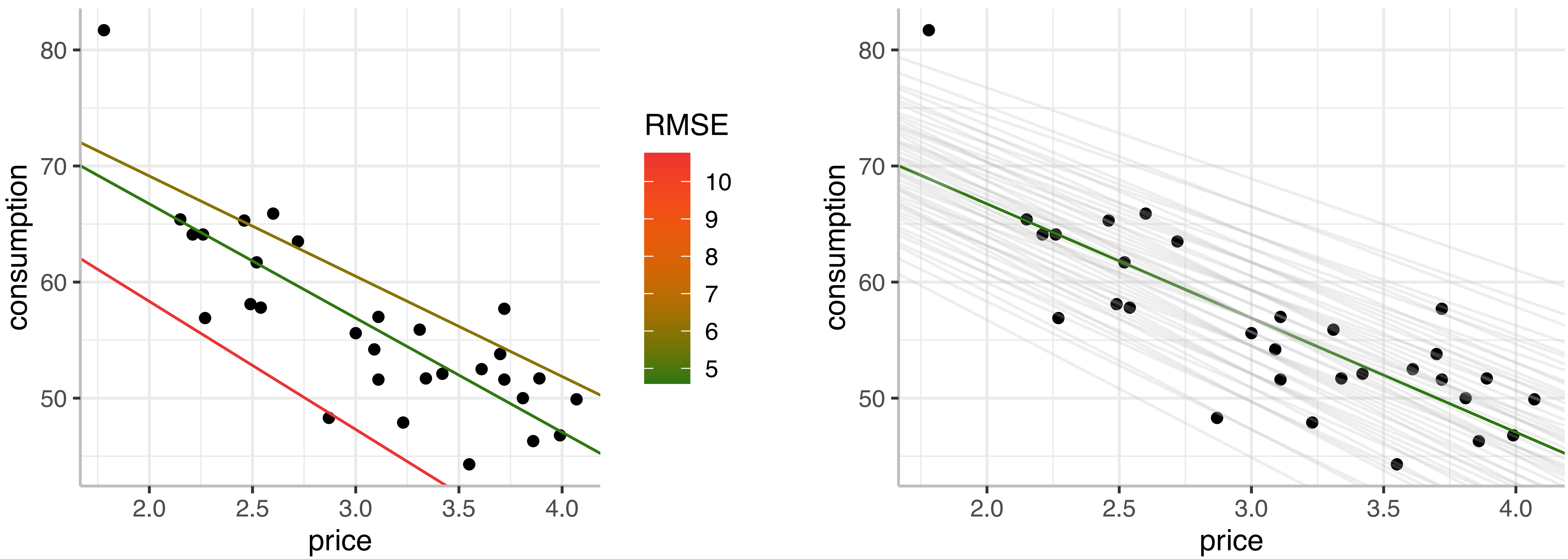
```
── Data Summary ────────────────────────
                           Values
Name                       beer_data
Number of rows             30
Number of columns          5
_______________________
Column type frequency:
  numeric                  5
________________________
Group variables            None
```




```
── Variable type: numeric ──────────────────────────────────────────────────────────
  skim_variable n_missing complete_rate    mean     sd    p0   p25   p50    p75  p100 hist
1 consumption           0             1    56.1   7.86  44.3  51.6  54.9   60.8  81.7
2 price                 0             1    3.08  0.642  1.78  2.53  3.11   3.68  4.07
3 price_liquor          0             1    8.37  0.770  6.95   7.9  8.38   8.94  9.52
4 price_other           0             1    1.25  0.298  0.67  1.09  1.18   1.48  1.73
5 income                0             1 32602.   4542. 25088 28888 32457 36516.  41593
```

It seems feasible and interesting to look at the relationship between `consumption`, `price` and `income`

Modelling data - general workflow
2. Data exploration and choice of family

- It seems feasible and interesting to look at the relationship between `consumption`, `price` and `income`
    - Economic theory would suggest a close relationship between them
    - Consumption and price do correlate with each other:
    - ```
      cor(
          x = beer_data$consumption,
          y = beer_data$price,
          method = "pearson"
      )
      ```
- `x` and `y` give the vectors, `method` the kind of correlation coefficient
    - If you do not remember the different kind of correlation coefficients, please review
- Beware: correlation only means association or co-movement, it **does not imply causation**! We should look at the relationship in more detail!
      ```

Modelling data - general workflow
2. Data exploration and choice of family

- To get more information and choose the right model family, it is always a good idea to **visualise** the data
  - Since both variables are numeric, we choose a scatter plot



- There seems to be a strong and **linear** relationship
- This suggests to choose the **family of linear models**
- It has the general form:

$$y = a + b \cdot x$$

Modelling data - general workflow
2. Data exploration and choice of family

- The family of linear models has the general form $y = a + b \cdot x$
- In the context of economic modelling, we use the following notation:

Parameters to be estimated

$$y = \beta_0 + \beta_1 x_1 + \epsilon$$

Dependent variable
(Synonyms: response variable, regressand,
explained variable, outcome variable)

Independent variable
(Synonyms: predictor, regressor,
explanatory variable, input variable)

Error term

- The **error term** absorbs all effects on **y** not covered by **x** → unobservable & probabilistic
- Everything on the left side of the = is called the left-hand-side (**LHS**)
- Everything on the right side of the = is called the right-hand-side (**RHS**)

Modelling data - general workflow

3. Fitting a model

- So far we have chosen a family of models: $y = \beta_0 + \beta_1 \cdot x$
  - It posits a linear relationship between the **dependent variable** y and the **independent variable** x → can be represented by a straight line
  - It has two parameters for which we need to choose particular values: β_0 and β_1
- Depending on the values for β_0 and β_1, these relationships can look very differently:



- We see that some of these different members of the linear family are clearly of the mark
- The job of fitting a model means to choose the member of the family that fits the data best → criterion needed!

Modelling data - general workflow
3. Fitting a model

- Fitting a model means to choose the 'best' member of a model family
  - How would you, for instance, evaluate the following models?



Modelling data - general workflow
3. Fitting a model



- Each of the model is a particular realisation of the general form $y = \beta_0 + \beta_1 x$
- If we talk about a particular model instance, where values for β_0 and β_1 were chosen, we write $\hat{\beta}_0$ and $\hat{\beta}_1$

- Such model gives a prediction for each value of x
  - We call this prediction a **fitted value** and denote it by $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$
- A good model would give fitted values $\hat{y}$ that are close to the true values y
  - Thus, a reasonable cost function would consider the difference between true and fitted values: the **residuals**

Modelling data - general workflow

3. Fitting a model



- A good model has fitted values that are close to the actual values
- To get the best model out of a family we should choose the parameters such that the residuals are small
- Since we do not prioritise particular observations, we consider all residuals

- Thus, we can get a measure for the ability of the model to represent the true values by summing up all residuals?
  - We need to square the residuals first → otherwise positive and negative residuals would cancel each other out
  - The sum of squared residuals is called the **RSS**: residual sum of squares

Modelling data - general workflow
3. Fitting a model

- The general approach in machine learning is to choose parameters by first defining a **cost function**, and then to minimise it
- A cost function maps the chosen parameters into a cost measure
  - Here we could use the RSS as a cost measure
  - More widespread is, however, the **Root Mean Squared Error** (RMSE):

$$RSS = \sum_{i=1}^{N} \left(y_i - \hat{y}_i\right)^2$$

$$MSE = \frac{\sum_{i=1}^{N} \left(y_i - \hat{y}_i\right)^2}{N}$$

$$RMSE = \sqrt{MSE} = \sqrt{\frac{\sum_{i=1}^{N} \left(y_i - \hat{y}_i\right)^2}{N}}$$

Modelling data - general workflow
3. Fitting a model

- Fitting a model means to choose the 'best' member of a model family
    - To evaluate these models we look at their RMSE → the best fit is given by the model with the smallest RMSE → the minimisation problem of **ordinary least squares** (OLS)



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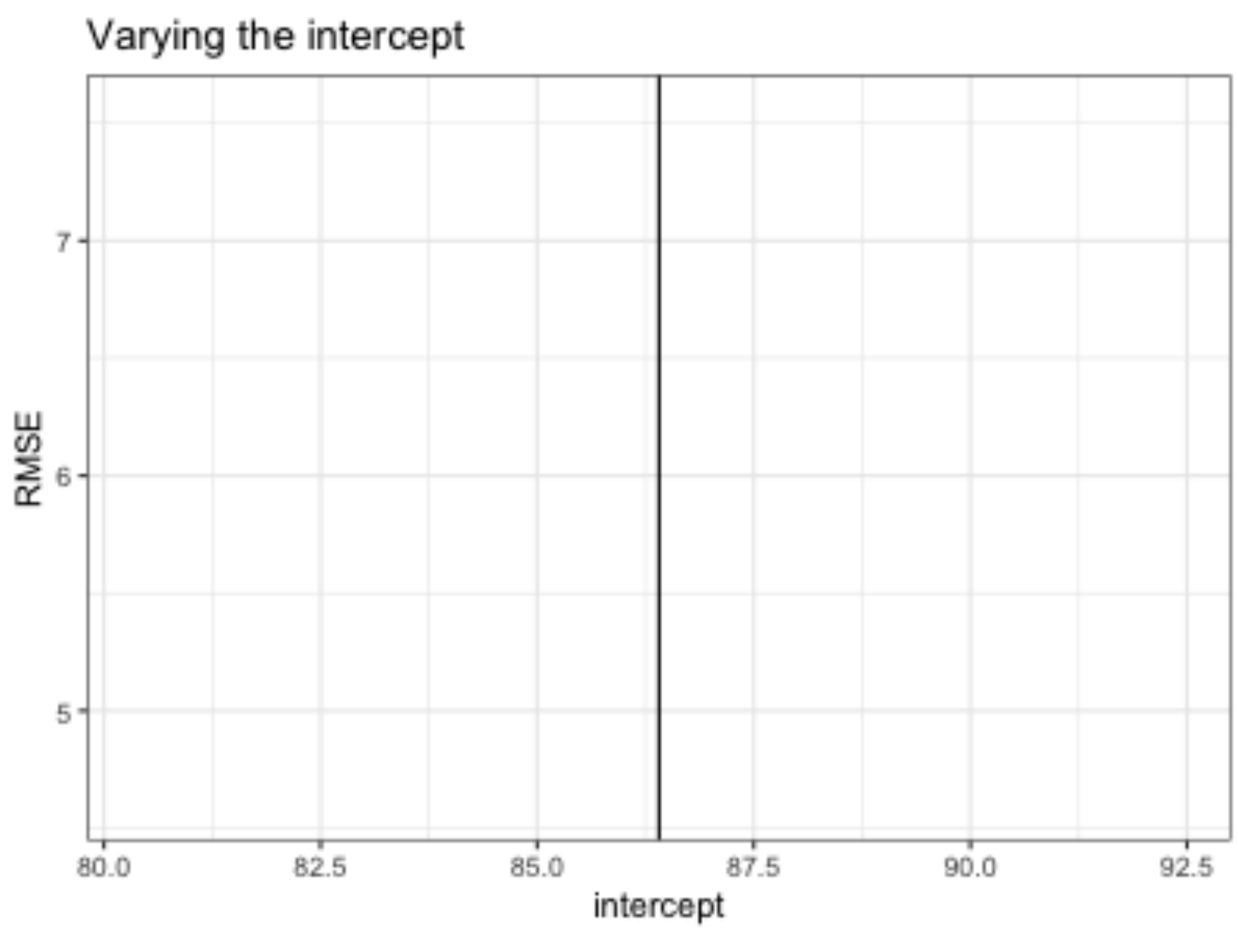

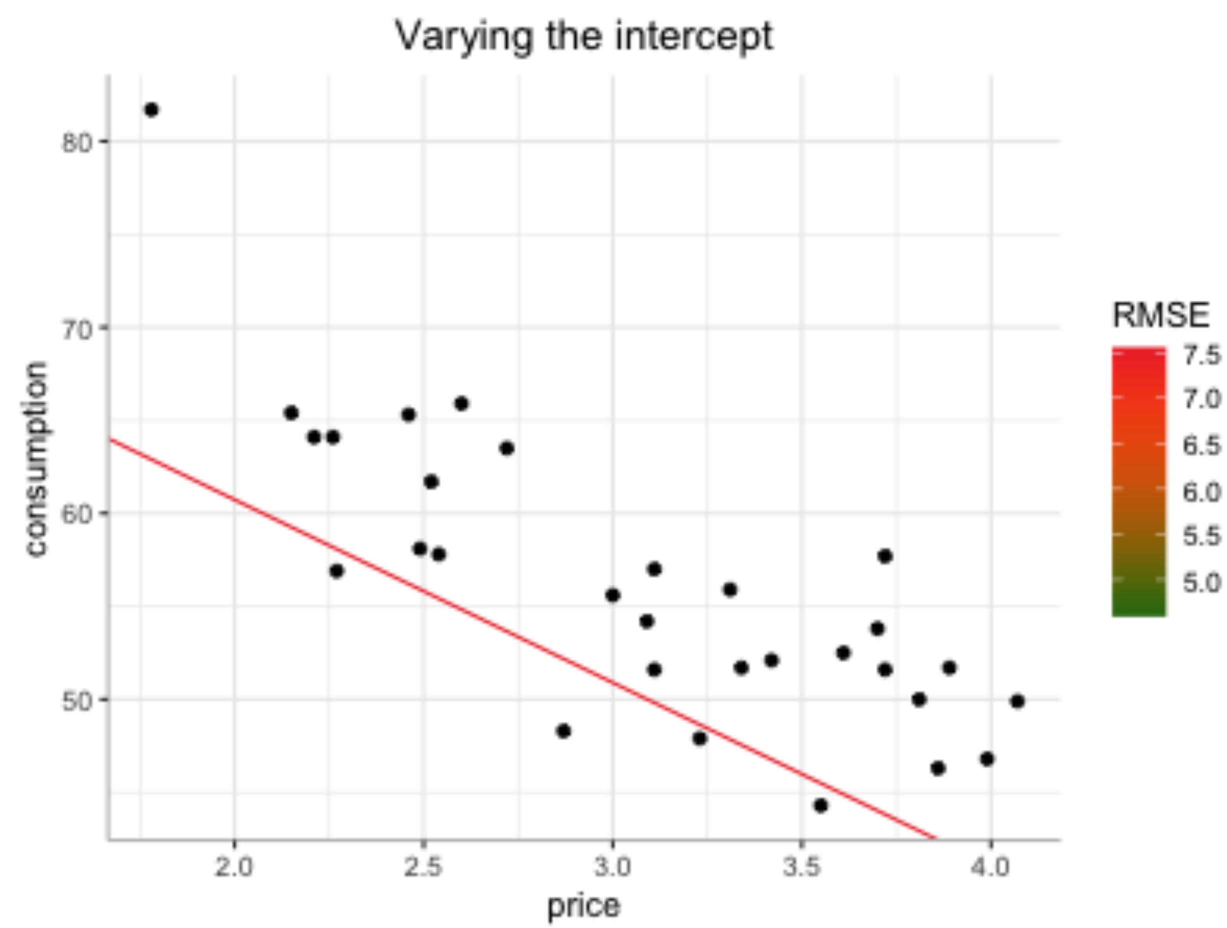

Modelling data - general workflow
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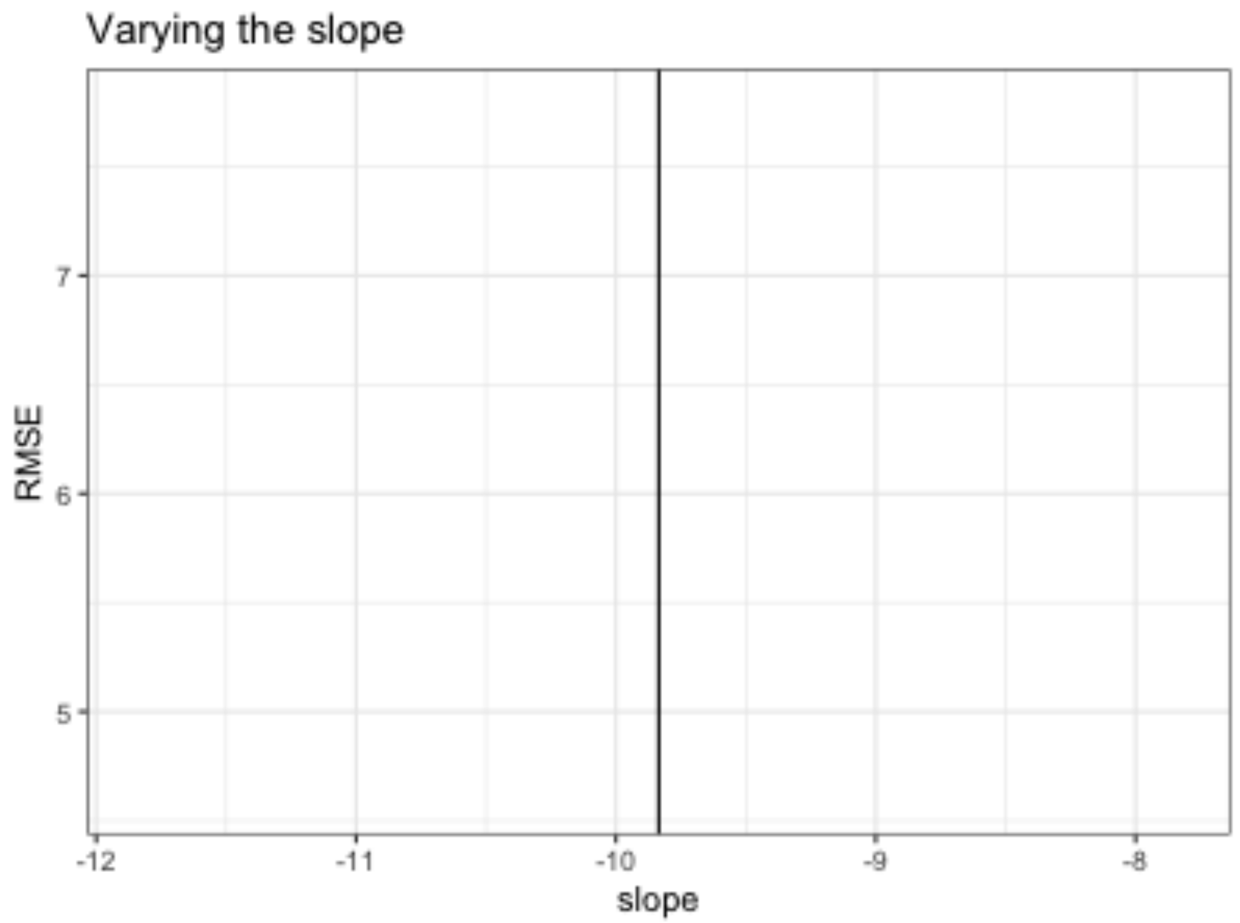

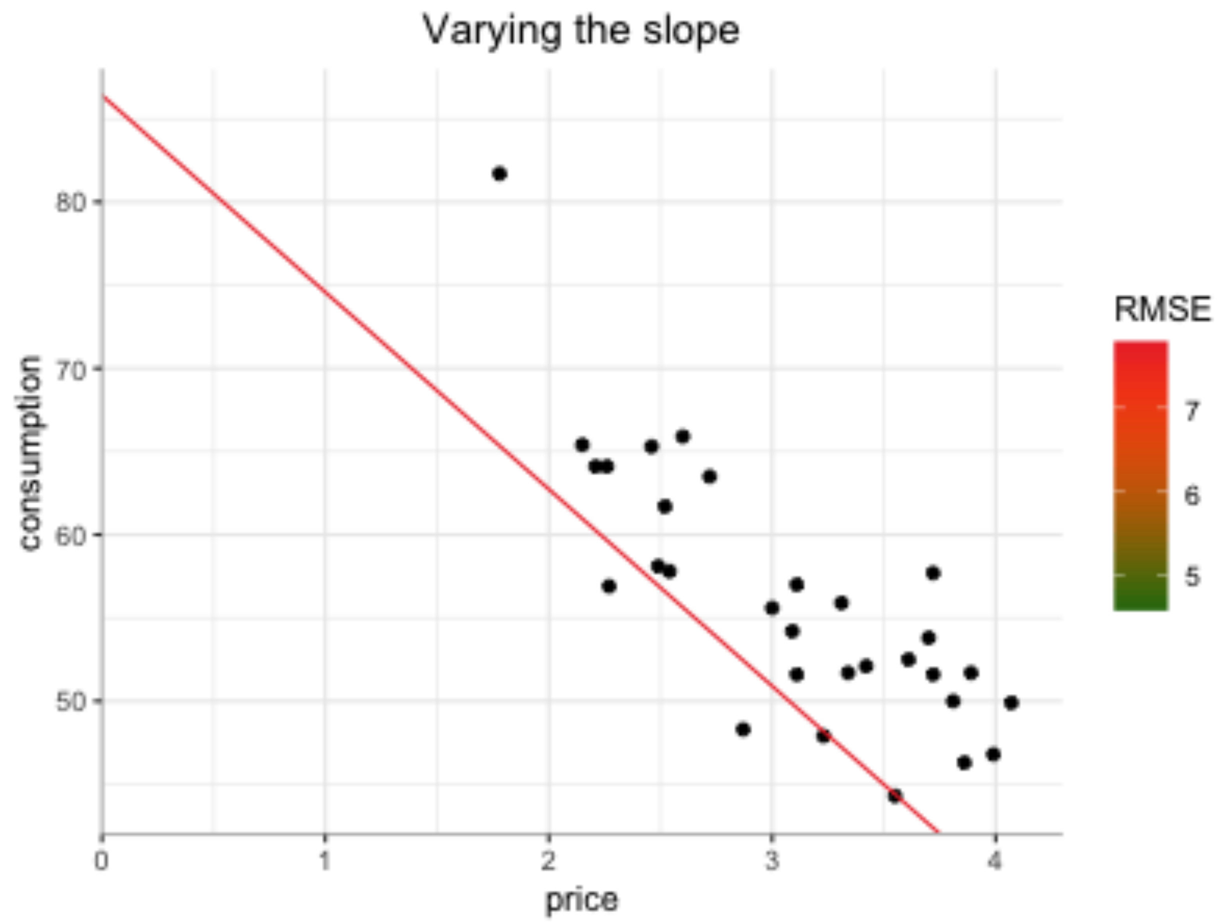

Modelling data - general workflow
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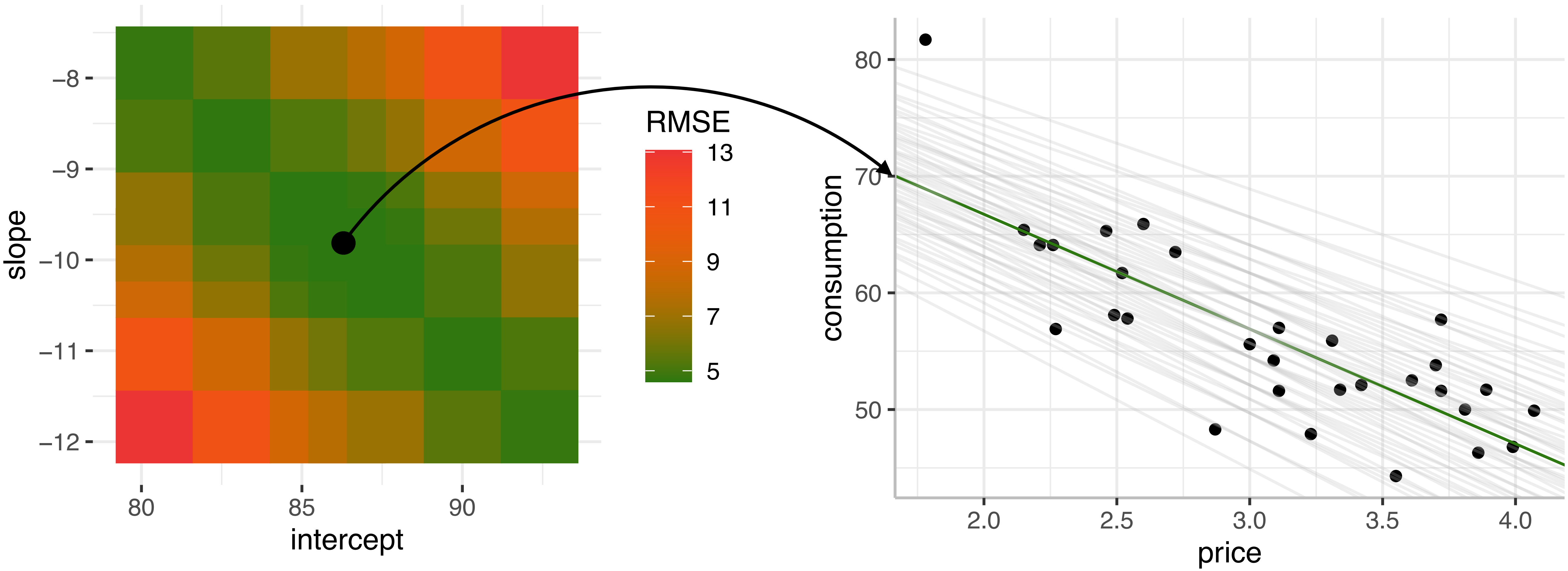


Note: For the linear case, the best model can actually computed using a formula!

Modelling data - general workflow
3. Fitting a model

- If the family of linear models is adequate for the modelling purpose at hand we can use the function `lm()` to find the model with the smallest RMSE:

```
lm(formula = consumption~price, data = beer_data_red)
```

The regression formula with the dependent variable on the LHS, and the independent variable on the RHS of the ~

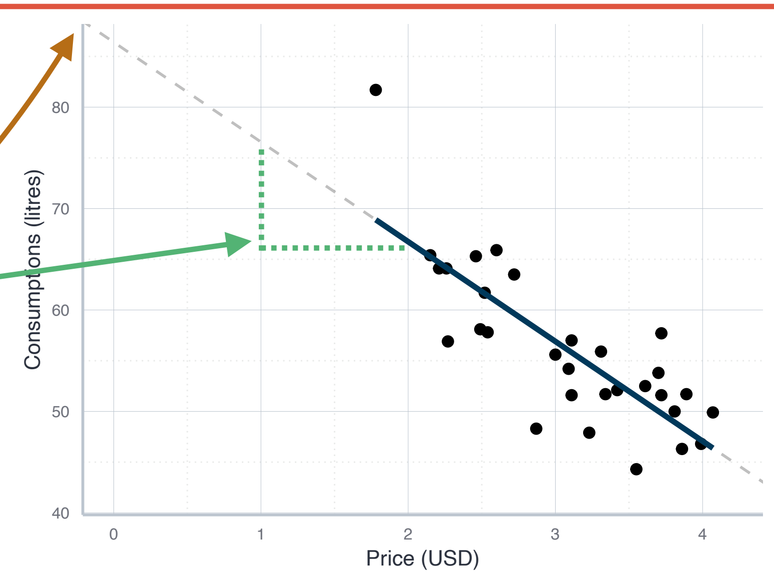
The data set used; the variables in the formula must correspond to the variables in the data set

```
> head(beer_data_red, 2)
# A tibble: 2 × 2
  consumption price
        <dbl> <dbl>
1        81.7  1.78
2        56.9  2.27
```

- The immediate output of `lm()` is already quite informative:

```
Call:
lm(formula = consumption ~ price, data = beer_data_red)

Coefficients:
(Intercept)        price
     86.406       -9.835
```



Modelling data - general workflow
4. Evaluate and interpret the model

- Usually we want to have more information about our regression result than the function `lm()` provides
    - The classical option is to call `summary()` on the resulting object
- A neat alternative is `moderndive::get_regression_table()`

```
> linmod_c_price <- lm(
+   formula = consumption~price, data = beer_data_red)
> moderndive::get_regression_table(linmod_c_price)
# A tibble: 2 × 7
  term      estimate std_error statistic p_value lower_ci upper_ci
  <chr>        <dbl>     <dbl>     <dbl>   <dbl>    <dbl>    <dbl>
1 intercept    86.4       4.32     20.0        0     77.5    95.3
2 price        -9.84      1.38     -7.15       0    -12.7    -7.02
```

Subject to later sessions!

Modelling data - general workflow

4. Evaluate and interpret the model

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> linmod_c_price <- lm(
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2 price        -9.84      1.38     -7.15       0    -12.7    -7.02
```

Subject to later sessions!

- The intercept is often practically irrelevant: hypothetical consumption when $price = 0$
- The coefficient of price (or any explanatory variable) is more important:

> For every increase of 1 unit in `price`, there is an **associated decrease** of, **on average**, 9.84 units of `consumption`.

- Our model is only about association, not about causation
- Our model does not say anymething about particular comparisons, but the average over all possible cases

Your turn!

- Consider the data set `DataScienceExercises::beer`, but focus on the relationship between `consumption` and `income`
- Go through all the relevant steps for conducting a regression:
  1. Theoretical pre-considerations
  2. Data exploration and choice of a model family
  3. Fit the model
  4. Evaluate and interpret your model
- Keep in mind that we have used the following functions:
  - `dplyr::glimpse()`, `skimr::skim()`, `lm()` and `moderndive::get_regression_table()`
- *Note: To add a regression line to a* `ggplot` *you may use* `geom_smooth(method="lm", se=FALSE)`

Linear regressions: some final remarks

- β_i and $\hat{\beta}_i$ are different: the former is the **true value**, the latter the **estimate**
  - This distinction refers to the fundamental distinction between a **population** and a **sample**
  - Similarly: residuals as the **sample equivalent** to the population error term
  - We will discuss this in more detail after our session on sampling
- In this context we also need to distinguish n **estimator** and the **estimate**
  - An estimator is way to compute the estimate: its a formula or an algorithm
  - The estimate is the result of this procedure: for each sample, it corresponds to a single number

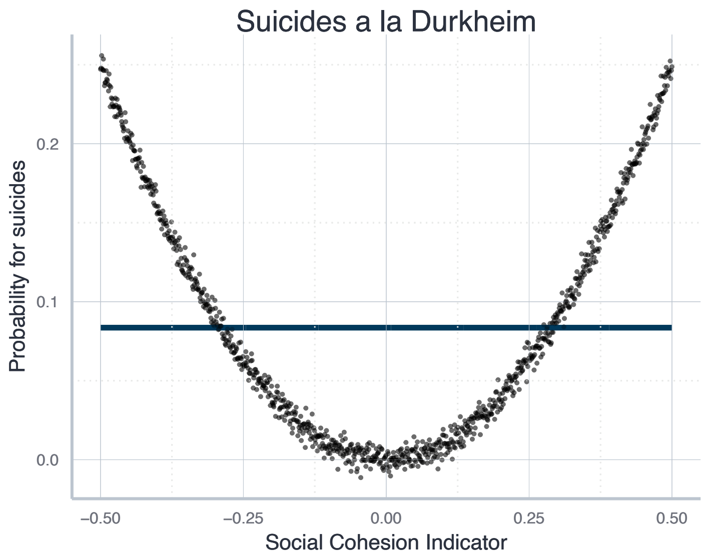
Model evaluation

Evaluating models - assumptions

- We identified the best model by minimising the RMSE → the method of ordinary least squares (OLS)
    - Identifying the model this way is based on a number of assumptions
- Part of any model evaluations should be the test of whether these assumptions were satisfied in the case at hand
    - We will have a specific session about how to do this
- **Example**: one central assumption of the simple OLS regression is that the relationship between the two variables is **linear**
- What would happen if this assumption was not met?

Evaluating models - assumptions

- The French sociologist Emile Durkheim distinguished two types of suidices:
  - Moral confusing and a lack of social embeddednes in modern societies
  - Neglect of individual desires in archaic societies
- This could be summarised in a u-shaped relationship between social cohesion and the likelihood of suicides



- This is not a linear relationship, and fitting a linear model would lead to very misleading results
  - Here the estimate for β_1 would be zero → suggests no systematic relationship
- Its always important to visualise the data and then choose the right family

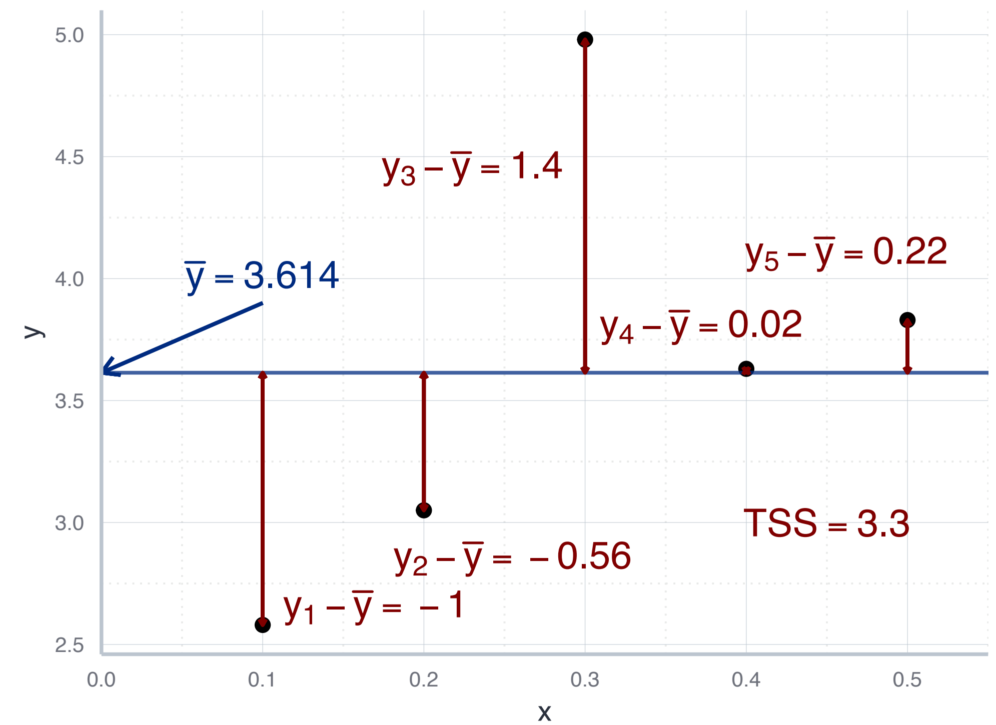
Evaluating models - explanatory power

- We will learn more about the underlying assumptions and how to test for them in a later session
- At this point we want to focus on one additional measure for the goodness of fit of a model: its R^2
  - The R^2 measures how much variation in the explained variable can be explained by the variation of the explanatory variable
  - Lets look at an artificial example:

```
datensatz
```

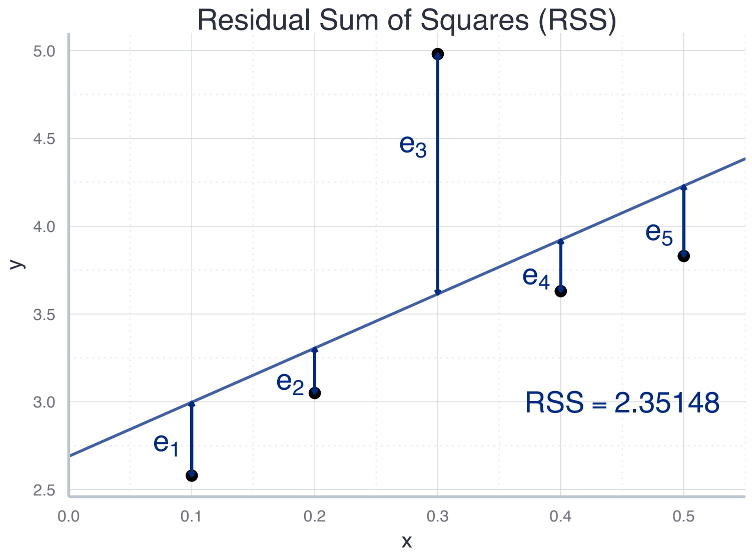
```
#>     x    y
#> 1 0.1 2.58
#> 2 0.2 3.05
#> 3 0.3 4.98
#> 4 0.4 3.63
#> 5 0.5 3.83
```

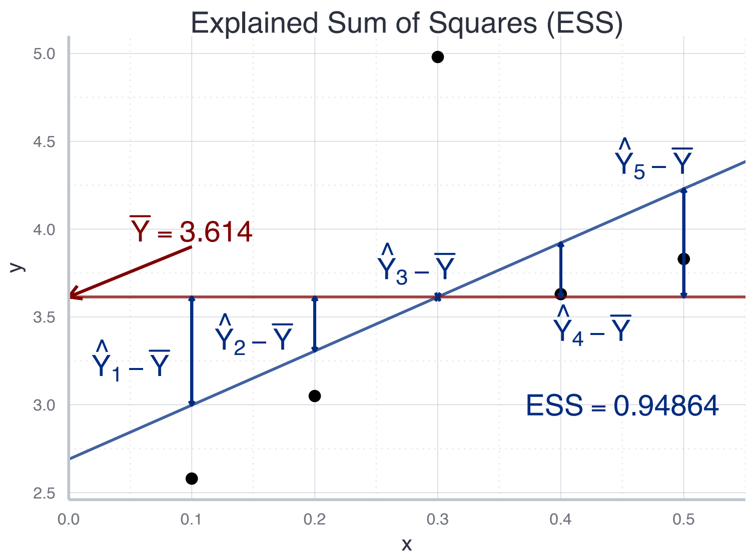
- How to measure the total variation in the explained variable?
  - Deviations from its mean value: total sum of squares:
  - $TSS = \sum_{i=1}^{n} (Y_i - \bar{Y})^2$



Evaluating models - explanatory power

- TSS as the total variation in the outcome variable: $TSS = \sum_{i=1}^{n} (Y_i - \bar{Y})^2$
- We separate the total variation into two parts:





- **Explained sum of squares** (ESS): the variation explained by our model
- **Residual sum of squares** (RSS): the variation left unexplained
- RSS: the sum of squared residuals:

$$RSS = \sum_{i=1}^{n} e_i^2$$

  - Residuals e: observable counterpart to the error term ϵ
- ESS: squared deviations between the fitted values and $\bar{y}$:

$$ESS = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2$$

Evaluating models - explanatory power

- We separate the total variation into two parts:

$$TSS = ESS + RSS$$

- The R^2 is defined as the share of explained variation:

$$R^2 = \frac{ESS}{TSS} = 1 - \frac{RSS}{TSS}$$

- In general, a higher R^2 comes with higher explanatory power
- A very high R^2, however, should also make you suspicious
- But in general, its a good indication for the usefulness of your model

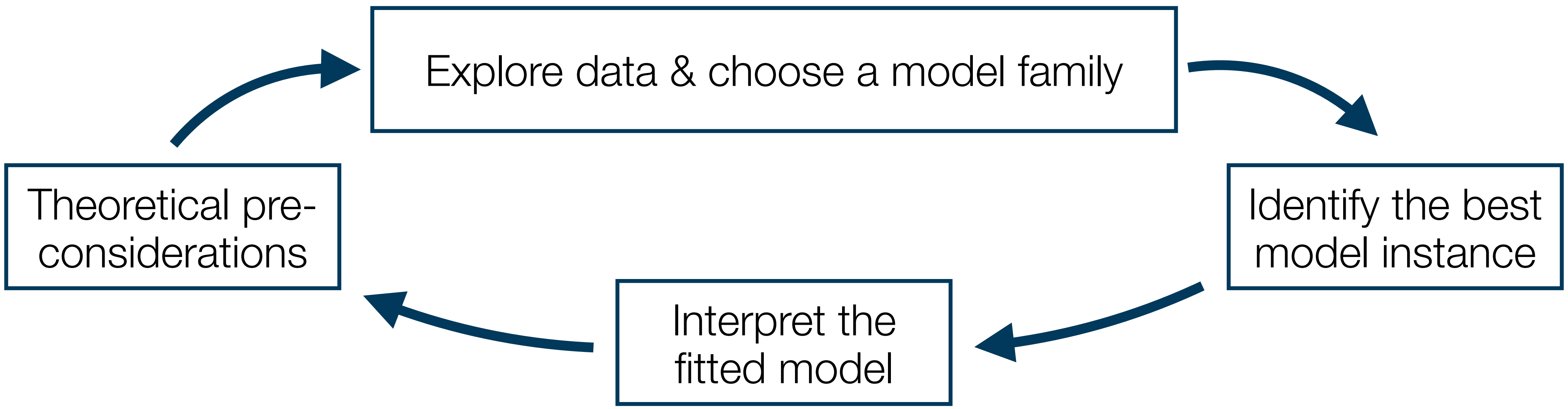
Exercise: computing R^2

- Consider again our example of beer consumption and the linear model you fitted before (i.e. on beer consumption and income).
  - Now compute the R^2 of your model by hand.
- Remember:
  - $TSS = \sum_{i=1}^{n} (Y_i - \bar{Y})^2$
  - $RSS = \sum_{i=1}^{n} e_i^2$
  - $ESS = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2$
  - Any `lm`-object has the elements `residuals` and `fitted.values`, through which you can obtain the respective vectors
- How can you interpret your R^2?
- Bonus: compare it to the R^2 of the model including price instead of income. How would you interpret this?

Summary & outlook

Summary and outlook

- We applied the general **workflow** of empirical modelling in the context of simple linear regression:



- The idea is to use the **family of linear models** with **two variables**
- Thus, SLR is used to study the association of two numerical variables
- The idea is to fit a regression line that minimises the squared differences between the actual and fitted values → method of **ordinary least squares**

Summary and outlook

- Using SLR makes sense if you are interested in a **linear relationship** between numerical variables
  - Thus, prior theoretical considerations and descriptive exploration of your data is necessary
- SLR is built upon the **family of linear models**, which in the context of economic applications is specified as $y = \beta_0 + \beta_1 x_1 + \epsilon$
  - In this context we introduced the concepts of the *LHS* and *RHS* of a regression equation, as well as the terms *parameters*, *dependent* & *independent variables*, and the *error term*
- We defined the best model instance of the family of linear models as the one that has the smallest **RMSE** for the data at hand
  - To find the particular model, we used the method of **OLS**

Summary and outlook

- OLS produces concrete **estimates** $\hat{\beta}_0$ and $\hat{\beta}_1$ by minimising the RMSE for the data at hand
    - Once estimated, we can use our model to create predictions: the **fitted values** $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$
- The deviations from the fitted and actual values are called **residuals** → sample equivalent to the theoretical error term
- Once estimated, we can interpret the estimated values of our model
    - The model has **no causal interpretation** → its about associations
- The OLS method is built upon **assumptions**, which we need to check for each application
- There are other tools to assess our estimated model, such as its R^2

Summary and outlook

- Next time we will extend the approach of simple linear regression and learn about **multiple** linear regression
  - We study not the relationship between two, but between many variables
  - This will allow us to isolate the relationship between two variables from the confounding effects of other variables
  - After this, we consider the process of taking samples from bigger populations theoretically, and then learn how to assess the quality of our regression models

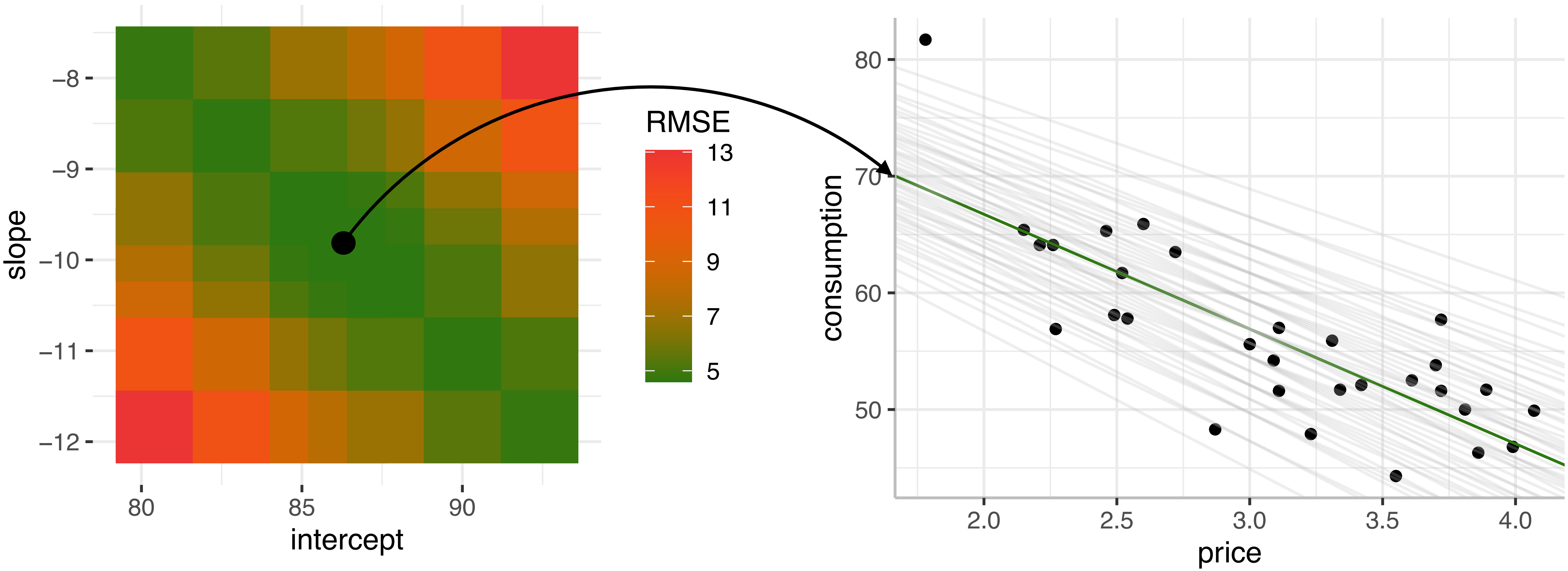
Tasks until next time:

1. Fill in the **quick feedback survey** on Moodle
2. Read the **tutorials** posted on the course page
3. Do the **exercises** provided on the course page and **discuss problems** and difficulties via the Moodle forum

Appendix: Ordinary Least Squares (OLS) estimation

Estimating a model using OLS

- Above we argued that estimating a linear model means to identify the model instance with the smallest RMSE
  - Now we look at how this is being done in practice → the OLS method



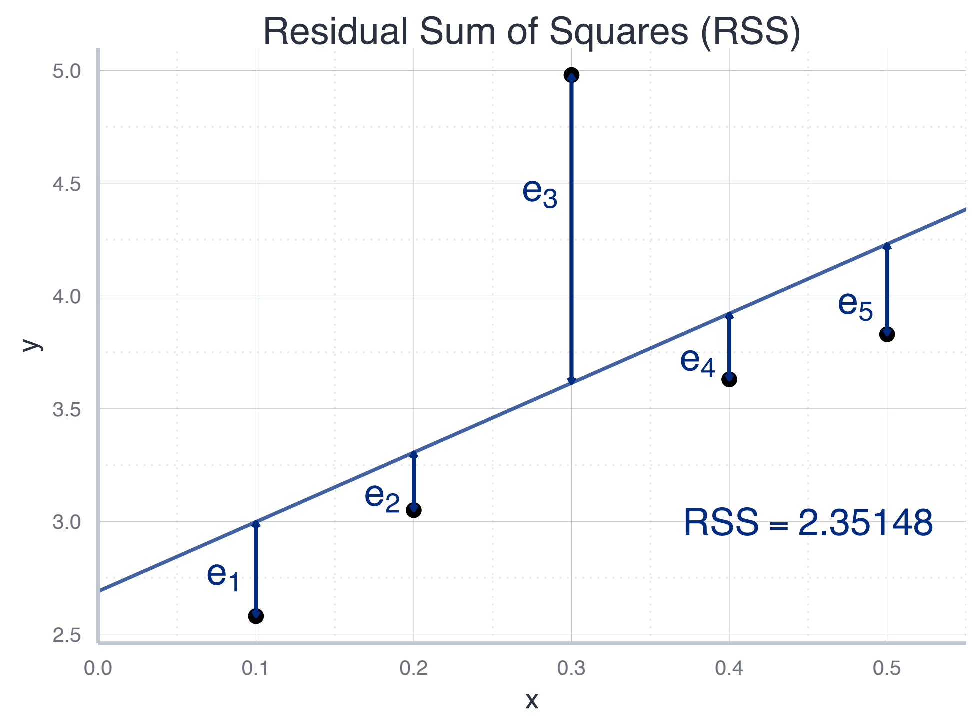
Estimating a model using OLS
The general idea

- In principle we could minimise the loss function numerically
  - But this is very inefficient and dangerous
- For the linear case, the best model can be derived analytically
  - This also allows us to derive some further properties of the model
- The idea is to choose β_0 and β_1 such that the RSS gets minimised

$$RSS = \sum_{i=1}^{n} e_i^2$$

- Put mathematically:

$$\hat{\beta}_0, \hat{\beta}_1 = \text{argmin}_{\beta_0, \beta_1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$



Estimating a model using OLS
Deriving the OLS estimator

$$\hat{\beta}_0, \hat{\beta}_1 = \text{argmin}_{\beta_0, \beta_1} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

- Since $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_i$ this equals have:

$$\hat{\beta}_0, \hat{\beta}_1 = \text{argmin}_{\beta_0, \beta_1} \sum_{i=1}^{n} (y_i - \hat{\beta}_0 + \hat{\beta}_1 \cdot x_i)^2$$

- With a little bit of algebra we can rearrange this expression to:

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n} (x_i - \bar{x})^2} \quad \text{and} \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

- All the variables are included in our data → $\hat{\beta}_0$ and $\hat{\beta}_1$ are identified

Estimating a model using OLS

Exercise: computing the OLS estimator manually

- Let us compute the estimated values $\hat{\beta}_0$ and $\hat{\beta}_1$ for our example data set by hand

$$\hat{\beta}_1 = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

```
> data_set
# A tibble: 5 × 2
      x     y
  <dbl> <dbl>
1   0.1  2.58
2   0.2  3.05
3   0.3  4.98
4   0.4  3.63
5   0.5  3.83
```

- $\bar{x} = 0.3$
- $\bar{y} = 3.614$
- $\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) = (0.1 - 0.3)(2.58 - 3.614) + \ldots = 0.308$
- $\sum_{i=1}^{n}(x_i - \bar{x})^2 = (0.1 - 0.3)^2 + (0.2 - 0.3)^2 + \ldots = 0.1$
- $\hat{\beta}_1 = \frac{0.308}{0.1} = 3.08$
- $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x} = 3.614 - 3.08 \cdot 0.3 = 2.69$

Estimating a model using OLS

Exercise: computing the OLS estimator manually

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      x     y
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- $\bar{x} = 0.3$
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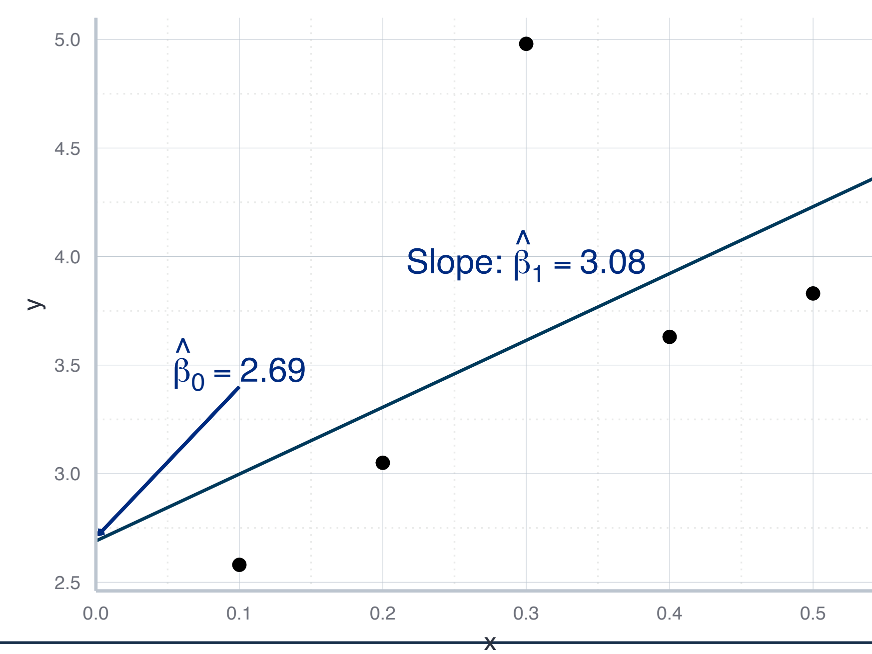
- $\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y}) = (0.1 - 0.3)(2.58 - 3.614) + \ldots = 0.308$
- $\sum_{i=1}^{n}(x_i - \bar{x})^2 = (0.1 - 0.3)^2 + (0.2 - 0.3)^2 + \ldots = 0.1$
- $\hat{\beta}_1 = \frac{0.308}{0.1} = 3.08$
- $\hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x} = 3.614 - 3.08 \cdot 0.3 = 2.69$

- Let us now verify our result by computing $\hat{\beta}_0$ and $\hat{\beta}_1$ using `lm()`:

```
Call:
lm(formula = y ~ x, data = data_set)

Coefficients:
(Intercept)            x
       2.69         3.08
```



Estimating a model using OLS
Final remarks on the OLS method

- The OLS estimation method has some great mathematical properties
  - E.g., if you can only obtain a sample of the population of interest, the estimates obtained via OLS are **unbiased** and **efficient**
- These properties hing, however, on some **assumptions**, e.g. a linear relationship between y and x
  - In practice you always need to test whether your assumptions are met
  - Otherwise there is no way to tell whether the estimates obtained via OLS are not terribly misleading → see session on **regression diagnostics**