Simple linear regression

Applied data science with R

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What is simple linear regression?

Its at the foundation of many more advanced tool and very widely used!

Goals for today

- I. Understand what simple linear regression can be used for
- II. Understand the concept of ordinary least squares
- III. Learn how to conduct a simple lineare regression in R

The sequence of parametric modelling

The general sequence of parametric modelling

In the most general terms, modelling data using a parametric approach can be broken down into several steps:

Lets illustrate this via a short example

What is the relationship between beer consumption and beer price?

Theoretical law of demand: higher price comes with lower demand
 Obtain survey data on beer

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

consumption and beer prices!

Seems to be a linear relationship \rightarrow work with the family of linear models: $C = a + b \cdot p$

(Intercept) price -9.835 86.406

Simple linear regression

Modelling data - general workflow 1. Theoretical pre-considerations

- Important pre-considerations:
	- What is your subject of interest?
	- Do you want to engage in an prediction-oriented or explanatory analysis?
	- If the latter, what are your main hypothesis?
	- 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

- 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 \langle db1>81.7, 56.9, 64.1, 65.4, 6...$ price \langle \text{db1} \rangle 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
                \langledbl> 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

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

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

- 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:

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

- 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:

- The error term absorbs all effects on y not covered by $x \rightarrow$ 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)

- So far we have chosen a family of models: $y = \beta_0 + \beta_1 \cdot x$
	- 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:

- Most members of the linear family are clearly of the mark
- Fitting a model \sim choose the member of the family that fits the data best
	-

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

- 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 $\pmb{\beta}_0$ and $\pmb{\beta}_1$ ̂ ̂
- Such model gives a prediction for each value of *x*
	- We call this prediction a **fitted value** and denote it by $\hat{y} = \beta_0 + \beta_1 x$ ̂ ̂
- 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

- A good model has fitted values that are close to the actual values
- Choose the parameters such that the residuals are small
- Do not prioritise particular observations \rightarrow consider all residuals

- Can we simply sum up all the residuals?
	- We need to square the residuals first \rightarrow otherwise positive and negative residuals would cancel each other out
	- The sum of squared residuals is called the **RSS**: residual sum of squares

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

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

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

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

- Fitting a model: choose the 'best' member of a model family
	- Best fit is given by the model with the smallest RMSE \rightarrow the minimisation problem of ordinary least squares (OLS)

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

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

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

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~approx, data = beer_data_{red}+> moderndive::get_regression_table(linmod_c_price)
# A tibble: 2 \times 7Refer to sampling 
           estimate std_error statistic p_value lower_ci upper_ci
 term
                                                                  distribution<dbl><dbl><dbl> <dbl>
                                             <dbl><dbl>
  <chr>
                      4.32
                                20.0
                                                77.5
1 intercept 86.4\emptyset95.3
                                -7.15\emptyset-9.841.38
                                                -12.7-7.022 price
```


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

- $\bullet~$ 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 anything 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
- Keep in mind that we have used the following functions:
	- dplyr::glimpse(), skimr::skim(), lm() and moderndive::get regression table()

Linear regressions: some final remarks

- β_i and β_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 the **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

The sampling distribution

The sampling distribution of OLS estimates

- Reasoning analogous to examples from session on sampling theory
	- Standard error: measure for sampling distribution of estimate for price
- In reality: only one sample \rightarrow standard error must be estimated
- Consider a stylised example with a simulated population

The sampling distribution of OLS estimates

- Create a true population according to $y = \beta_0 + \beta_1 x + \epsilon$
	- With $N = 5000$, $\beta_0 = 1000$ and $\beta_1 = 3.5$:

- Now draw 500 samples with $n = 150$ and estimate the linear model
	- Obtain a β_0 and β_1 for each sample \rightarrow look at sampling distribution ̂ \overline{a}

The sampling distribution of OLS estimates The result of drawing 1000 samples with $n = 150$

The sampling distribution of OLS estimates Relation to the single estimation

Model evaluation

Evaluating models - assumptions

- We identified the best model by minimising the RMSE \rightarrow method of ordinary least squares (OLS)
	- Identifying the model this way is based on a number of assumptions
- Model evaluation: test of whether these assumptions were satisfied
- **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 \rightarrow 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
	-

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

Evaluating models - explanatory power

- TSS as the total variation in the outcome variable: $TSS = \sum_{i=1}^{n}$ $\sum_{i=1}^{n} (y_i - \bar{y})^2$
- 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:

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

- Residuals r : 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:
	- $TSS = \sum_{i=1}^{n} (Y_i \bar{Y})^2$
	- $RSS = \sum_{i=1}^{n} e_i^2$
	- $ESS = \sum_{i=1}^{n}$ $\sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2$ ̂
	- 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?

Linear regression and nonlinear relationships

Linear regression and nonlinear relationships

- Linear regression is a parametric approach
	- Focus on linear models → assumes a linear relationship

Meaning: **linearity** in parameters

- Fitting a linear model to nonlinear relationships is misleading, except…
	- …we transform the data to make the relationship linear

Model 1: *SuicideProb* = $\beta_0 + \beta_1 COH + \epsilon$ Model 2: *SuicideProb* = $\beta_0 + \beta_1 COH + \beta_2 COH^2 + \epsilon$

Linear regression and nonlinear relationships The Tukey-Anscombe Plot

- How to decide whether transformation was successful?
- The residuals should not show any structure \rightarrow Tukey-Anscombe Plot
	- x-Axis: predicted values (predict()), y-axis: residuals (residuals()):

Linear regression and nonlinear relationships Linearising exponential relationship with logs

Another very common transformation is taking logs \rightarrow linearises otherwise exponential relationships:

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Linear regression and nonlinear relationships Interpreting models with transformed variables: logs

- Not all relationships can be linearised
	- Sometimes linear regression is just not the right tool!
- Transformation of the variables must be considered in interpretation:

Linear regression and nonlinear relationships Interpreting models with quadratic terms

- Not all relationships can be linearised
	- Sometimes linear regression is just not the right tool!
- Transformation of the variables must be considered in interpretation:

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 \rightarrow method of **ordinary least squares**

Summary and outlook

- Using SLR makes sense if you are interested in a **linear relationship** between numerical variables
	- Thus, theoretical considerations and exploration of your data is necessary
	- Also: transforming your data might be needed to make relationship linear
- 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* & i*ndependent 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 β_0 and β_1 by minimising the RMSE for the data at hand ̂ ̂
	- Once estimated, we can use our model to create predictions: the fitted values $\hat{y} = \beta_0 + \beta_1 x$ ̂ ̂
- The deviations from the fitted and actual values are called residuals \rightarrow sample equivalent to the theoretical error term
- Once estimated, we can interpret the estimated values of our model
	- The model has **no causal interpretation** \rightarrow 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

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 \rightarrow 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:

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

Estimating a model using OLS Deriving the OLS estimator

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

• Since $\hat{y}_i = \beta_0 + \beta_1 \cdot x_i$ this equals have: ̂ ̂

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

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 $\rightarrow \beta_0$ and β_1 are identified ̂ ̂

Estimating a model using OLS Exercise: computing the OLS estimator manually

• Let us compute the estimated values β_0 and $\boldsymbol{\beta}_1$ for our example data set by hand ̂ ̂

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

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

$$
\begin{array}{ll}\n\text{1} & \text{data_set} \\
\text{2} & \text{data_set} \\
\text{3} & \text{alpha} \\
\text{4} & \text{alpha} \\
\text{5} & \text{alpha} \\
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$$

Estimating a model using OLS Exercise: computing the OLS estimator manually

> data_set

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 \rightarrow see session on regression diagnostics

