

# Delivering Data Science In Resources & Energy

Data Analysis II: Simple Predictions -Regression and statistical model building

DAY 5

15-Day Data Science Springboard

Dr Jeremy Mitchell & Dr Ying Yap, Data Mettle

**15 December 2021** 







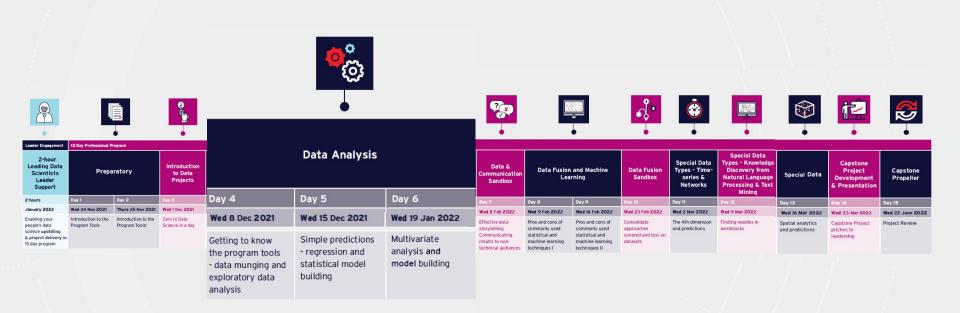




#### **Program Timeline**

DAY 4, 5 & 6: Data Analysis







#### **Q&A**, Issues & Announcements



#### **Before we Get Started**

- Resources & Tasks on Github.
- We'll start talking about projects a bit this afternoon, and help you start setting up yours
- Make notes about any ideas, perspectives or issues you encounter throughout the day.
- If you have aspects you'd like to go over throughout the day, feel free to post them to the general channel and we'll try to address the straightforward ones as we break.
- We'll come together to discuss before we close out this afternoon.



### **Schedule**

DAY 5



AWST	AEST	Agenda	Educator
07:30	09:30	Q&A, Issues & Announcements	
07:45	09:45	Models & Regression	Jeremy
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14:55	16:55	<u>Menti</u> Feedback	Tamryn
17:00	17:00	Close	



#### **Aims & Learning Outcomes**

DAY 5

#### Aims

- Perform statistical model building.
- Conduct regression.
- Generate simple predictions regression.

## **Learning Outcomes**

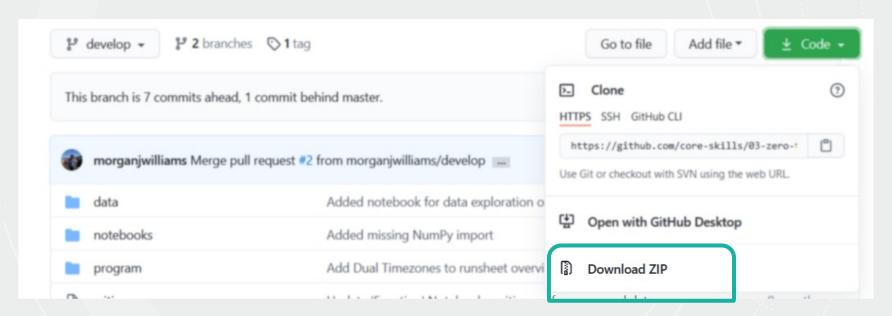
- Understand regression as the basis for prediction.
- Understand how outliers and noisy data affect results.
- Understand the impact of missing data and recall practical solutions to work with incomplete data sets.
- Understand how to choose between basic statistical models and evaluate their effectiveness (e.g. linear vs polynomial).
- Have an understanding of hierarchical models as a means of modelling connections between datasets or processes.



## **GitHub Content for Today**



#### github.com / core-skills / 05-simple-predictions

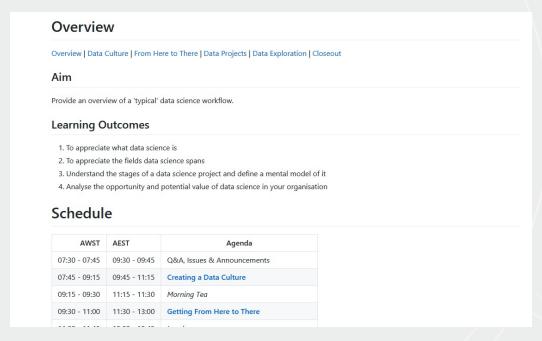




## **GitHub – Program Notes**



#### github.com / core-skills / 05-simple-predictions / program / 00\_overview.md





#### **Environment**



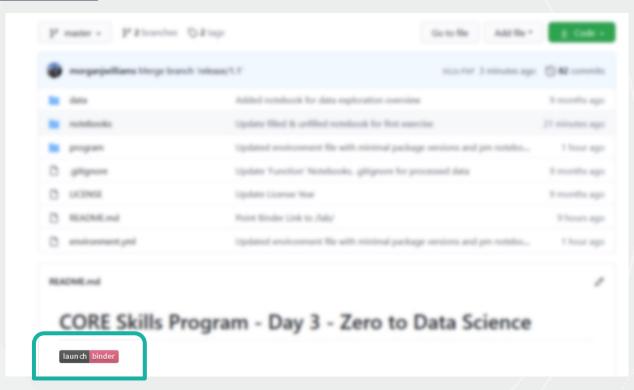
- Open an Anaconda Prompt
- Navigate to where you have the unzipped repository material

```
conda env create -f environment.yml # make new env
conda activate core05 # activate this env (Windows)
# make this available to Jupyter as a "kernel"
python -m ipykernel install --user --name=core05
jupyter lab # launch Jupyter lab
```



## **Binder Backup**







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#### **Discussion**

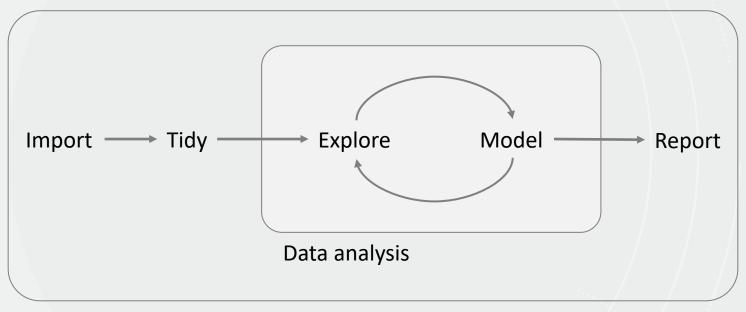


# What are the main steps of the data analysis workflow?



# Short introduction to data analytics and machine learning







## **Exercise: Explore a dataset using pandas and seaborn**



# Open am1-models-and-regression.ipynb

and go through exercise 1



# **Categories of machine learning**



scikit-learn.org/stable/tutorial/machine\_learning\_map/index.html



#### **Scikit-learn basics and API**



- Dataset in tidy format
- Basic API:
  - model = LinearRegression()
  - model.fit(x\_train, y\_train)
  - y\_pred = model.predict(x\_pred)



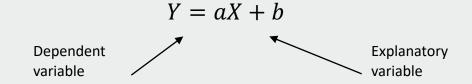


- The linear regression model is one of the most basic statistical models used in predictive analysis
- The model proceeds by fitting a linear equation to observed paired data to attempt to model the relationship between the two variables
- One variable is commonly referred as to the explanatory variable while the other is considered the dependent variable





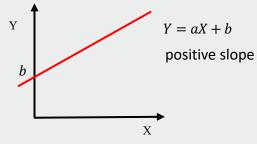
The equation of a line is

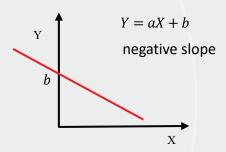


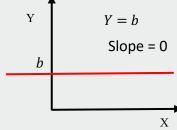
- a corresponds to the slope of the line and b to the intercept
- Parameters a and b need to be determined
- Different mathematical approaches can be used to determine the slope and the intercept. This leads to different types of regression







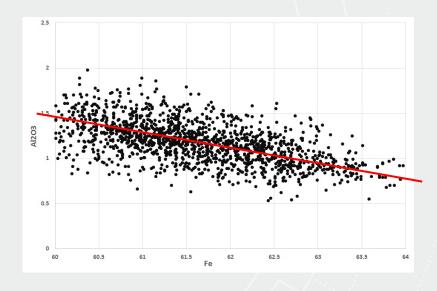






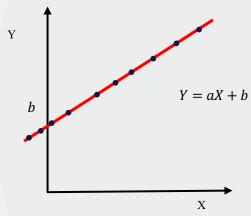


- Why do we want to fit a line?
- The scatterplot shows the paired data is scattered around a trend line
- The line is indicative of the average value of the dependent variable given the explanatory variable

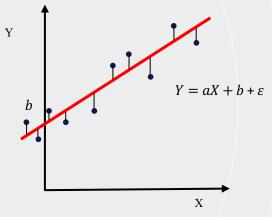








Values of X and Y are perfectly related

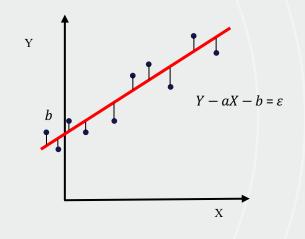


Values of X are known and it is assumed that Y=aX+b plus a random term  $\varepsilon$ 



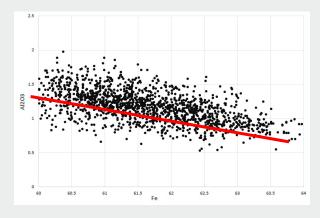


- A number of assumptions are made on the random error term  $\varepsilon$
- First assumption is that <u>on average</u> the error is equal to zero
- This ensures the model has no bias

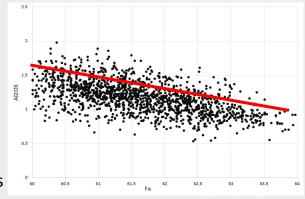








Positive bias

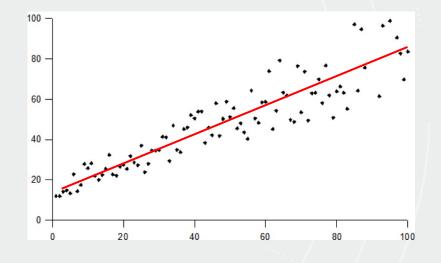


Negative bias





- Second assumption is that <u>the</u> <u>variance</u> of the random error term is constant
- This is know in statistics as homoscedasticity asummption
- Heteroscedasticity refers to the violation of this assumption





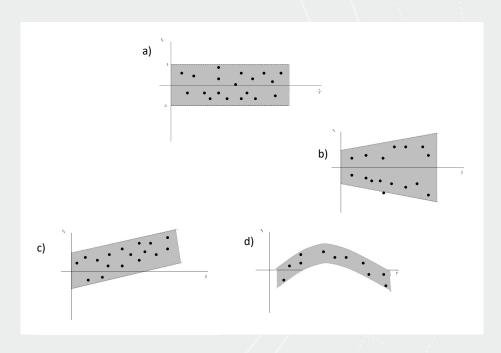


- Third assumption is that random error term is independent of both the explanatory and dependent variable
- Extremely important assumption and provides a way to assess the goodness of the linear model
- Scatterplot of the error with either the explanatory or the dependent variable should not show any clear pattern





- a) Appropriate
- b) homoscedasticity violated
- c) and d) are indicative that the linear regression model is not adequate







- Fourth assumption corresponds to the statistical distribution of the error component
- It is assumed that the distribution of the random error is Gaussian with mean equal to zero and variance  $\sigma^2$

$$\varepsilon \sim N(0, \sigma^2)$$

• The Gaussian assumption allows to derive all the theoretical properties of the linear regression model





#### Some of the theoretical properties are:

- The dependent variable has Gaussian distribution
   This allows to construct confidence intervals for the estimated values
- The slope a has Gaussian distribution

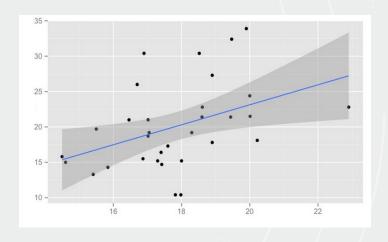
  This allows to use statistical tests to assess the "importance" of the explanatory variable

Statistical tests on the parameters are more important in multivariate problems





- Example of a linear regression model with confidence intervals
- Can you anticipate the behaviour of the residuals?
- Would you say the linear model is reasonable?





# **Exercise: Linear regression with scikit-learn**



# Return to am1-models-and-regression.ipynb

and go through exercise 2



# **Exercise: Perturbing perfect linear data**



# Return to am1-models-and-regression.ipynb

and go through exercise 3



## A look at $R^2$



- $R^2$  is also known as coefficient of determination
- $R^2$  is used as a goodness of fit measure for linear regression models, i.e. to determine how well the regression model fits the data

$$R^2 = 1 - \frac{\sum \varepsilon_i^2}{\sum (y_i - \bar{y})^2}$$

Proportion of the variance in the dependent variable that the explanatory variable explains



#### A look at $\mathbb{R}^2$



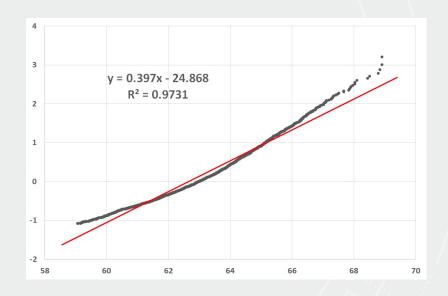
- $R^2$  has limitations and therefore should not be the only criteria used to assess the goodness of the linear regression model
- Some of its limitations are:
  - Does not account for the number of paired data used
  - Does not indicate if the explanatory variable used is appropriate
  - Does not indicate if the regression used is appropriate
  - Does not indicate if the model is biased



# A look at $R^2$



A biased model can have a high  $\mathbb{R}^2$  value!

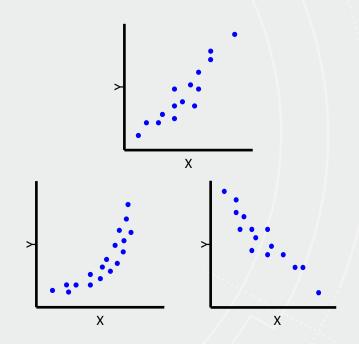




# **Correlation and Independence**



- Traditional correlation is a measure of the <u>linear relationship</u> between two variables
- A correlation value equal to zero does not mean the variables are not related





# **Correlation and Independence**



- The concept of statistical independence is given by the factorisation of the joint probability distribution as the product of the marginal distributions
- This means that knowing the value of one of the variables does not tell anything about the value of the other variable
- Independence implies no correlation but the reverse is not true



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## If you don't have a dataset



UCI Machine Learning Repository:

archive.ics.uci.edu/ml/index.php

Kaggle datasets:

www.kaggle.com/datasets



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## **High-level Takeaways From Today**



- Understand regression as the basis for prediction.
- Understand how outliers and noisy data affect results.
- Understand the impact of missing data and recall practical solutions to work with incomplete data sets.
- Understand how to choose between basic statistical models and evaluate their effectiveness (e.g. linear vs polynomial).
- Have an understanding of hierarchical models as a means of modelling connections between datasets or processes.



# **High-level Takeaways From Today**



Your thoughts?





# **Capstone Projects**



## **Update**

How you are shaping up your Project

#### Action

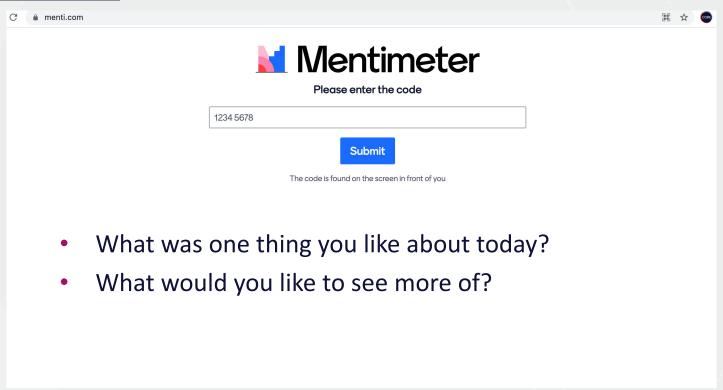
- Milestone #1 → L0 in Momentum
- If not done already, update your Working Project Title & Short Project Statement (Problem/Solution/Plan) here.
- Update your Leader





## Menti









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