Data Science Portfolio Projects to Rely On

Tips to organize and document a data science portfolio project

BACKGROUND

ACADEMIC TRAINING

B.Sc. in Physics

PhD in Medical Physics

Post-Doctoral Research in Physics





COMPUTING BACKGROUND

- MAPLE, FORTRAN, MATLAB
- R, PYTHON, SHELL scripts

DATA SCIENCE and PYTHON Training

Online Courses

- UDACITY Programming Foundations with Python
- Udemy Python for Data Science and ML Bootcamp

WeCloudData part-time Data Science with Python

WeCloudData Full time Diploma

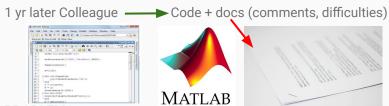
Documentation

Canadian Light Source (CLS) in Saskatoon, SK

- Particle Accelerator used in Applied Science Research
- Perform Science Experiments
- Collect Data

MATLAB → Analyze raw data Me -

- Deal with headers
 - Engineering data (Skip rows)
- Regular expressions (regexp)
- Perform Data Analysis
- 11 steps + Analysis based on your use-case

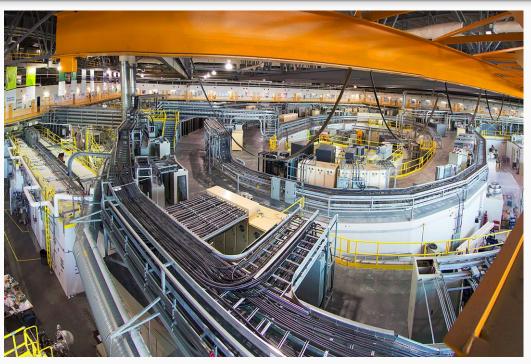




Database changes impacted headers, Step 8. and column structure failed

Colleague: Debug, MATLAB regexp, update 1 step in docs

Key Points: Documentation was present, Documentation was usable



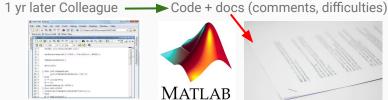
Documentation

Canadian Light Source (CLS)

- Applied Science Research Facility
- Perform Science Experiments
- Collect Data

Me → MATLAB → Analyze raw data

- Deal with headers
 - Engineering data (Skip rows)
- Regular expressions (regexp)
- Perform Data Analysis
- 11 steps + Analysis based on your use-case



PROBLEM:

Database changes impacted headers, Step 8. and column structure failed

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Data Science Portfolio Projects

Background: Research a topic, Identify the customer, Identify customer's needs

Analysis Workflow

- Extracting insights from real-world raw data
- Sharing insights with a customer
- Building solutions that offer direct value to a customer

Parts of our portfolio project follows the workflow used in industry applications

2016: https://www.dataguest.io/blog/build-a-data-science-portfolio/

Shared in Repository on on Github, GitLab, BitBucket, etc.







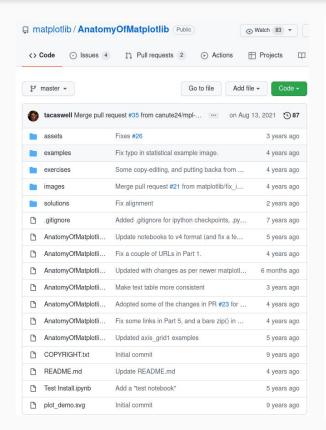
Benefits of Sharing **Documented** Data Science Portfolio Projects

- Easy for a reader to follow
- Easy for us to follow (quick iteration)
- Clear demonstration of above workflow (sharing, extracting, building)
 - Represents our implementation of a solution to a real-word problem

Structure of Contents in Portfolio Project

Blog Post How to share a portfolio:

2017: https://www.dataquest.io/blog/how-to-share-data-science-portfolio/



Introduction

This tutorial is a complete re-imagining of how one should teach users the matplotlib library. Hopefully, this tutorial may serve as inspiration for future restructuring of the matplotlib documentation. Plus, I have some ideas of how to improve this tutorial.

Please fork and contribute back improvements! Feel free to use this tutorial for conferences and other opportunities for training.

The tutorial can be viewed on noviewer:

- · Part 0: Introduction To NumPv
- . Part 1: Overview of Matplotlib
- . Part 2: Plotting Methods
- . Part 3: How To Speak MPL
- · Part 4: Limits, Legends, and Layouts
- · Part 5: Artists
- · Part 6: mpl toolkits

Installation

All you need is matplotlib (v1.5 or greater) and jupyter installed. You can use your favorite Python package installer for this:

conda install matplotlib jupyter
git clone https://github.com/matplotlib/AnatomyOfMatplotlib.git
cd AnatomyOfMatplotlib
jupyter notebook

A browser window should appear and you can verify that everything works as expected by clicking on the Test Install.ipynb notebook. There, you will see a "code cell" that you can execute. Run it, and you should see a very simple line plot, indicating that all is well.

Repository in the matplotlib organization: https://github.com/matplotlib/AnatomyOfMatplotlib

```
README.md
requirements.txt
01_get_data.ipynb
02_clean_data.ipynb
03 eda.ipvnb
04_analyse_data.ipynb
src/
src/__init__.py
src/load_data.py
data/
data/raw/
data/processed/
```

- 1. README.md, requirements.txt, notebooks, extracted (custom) Python modules, data folders
- 2. Avoids notebooks that are too long (allows reader to stay interested in the contents)
- 3. Allows easier reuse of code
- 4. Helps keep code organized (avoids misplaced code cells)
- 5. Sets an appropriate context for visitor to the project (what is this project about, where to find code)

```
README.md
README.md
requirements.txt
                                                  Proiect title
                                                  Background, motivation, end-user, etc. for the the project
                                                   • Based on reading through whitepapers, research papers, etc.
01_get_data.ipynb
                                                  Add instructions for how to install Python packages and start jupyter
02 clean data.ipvnb
                                                  Example wording:
03 eda.ipvnb
                                                  To install all Python packages and start a Jupyter notebook, please run the following
04 analyse data.ipvnb
                                                  $ pip install -r requirements.txt
src/
                                                  $ jupyter notebook
src/__init__.py
                                                  How to run all the notebooks? Sequentially, based on their file names. Untitled12.ipynb
src/load data.pv
                                                  Example wording:
data/
                                                  Please run the notebooks in the following order
data/raw/
                                                  - 01_get_data.ipynb (to download the raw data)
data/processed/
                                                  -02 clean data.ipynb (to process the raw data)
                                                  - 03_eda.ipynb (to explore the processed data)
                                                  - 04_analyse_data.ipynb (to perform the quantitative analysis. eg. ML)
```

```
README.md
requirements.txt
01_get_data.ipynb
02 clean data.ipvnb
03 eda.ipvnb
04 analyse data.ipvnb
src/
src/ init .pv
src/load data.pv
data/
data/raw/
```

data/processed/

```
requirements.txt
```

pandas==1.35.0

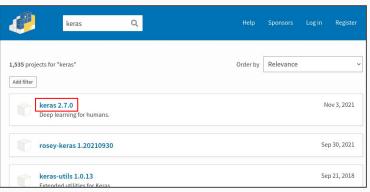
plotly==5.5.0

scipy==1.7.3

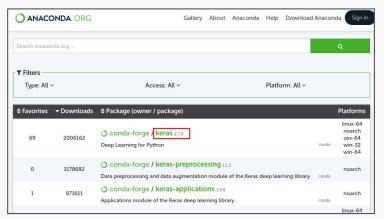
To get package version numbers

- o pip: https://pypi.org/
- o conda: https://anaconda.org/search

PyPI



Anaconda Search



```
README.md
                                  Clickable Section Headers (HTML Hyperlinks without href attribute)
requirements.txt
                                   <a id='get-data'>
01_get_data.ipynb
                                  ## 1. Get data
02 clean data.ipynb
                                   Table of Contents
03 eda.ipynb
                                        [Get data](#get-data)
04_analyse_data.ipynb
                                   2.
src/
                                  Divider / Horizontal Rule
src/__init__.py
src/load_data.py
                                   Footers for Navigation
data/
                                   <span style="float:left;">
data/raw/
                                       <a href="./01_dont_do_this.ipynb"> >> 02_get_data.ipynb</a>
data/processed/
                                   </span>
```

README.md requirements.txt 01_get_data.ipynb 02_clean_data.ipynb 03_eda.ipynb 04_analyse_data.ipynb src/ src/__init__.py src/load_data.py data/ data/raw/

data/processed/

01_get_data.ipynb

Download the raw data

Store raw data in a sub-folder -> data/raw/data_file_1.csv

Reduces chance of accidentally over-writing raw data with processed data





```
README.md
requirements.txt
01_get_data.ipynb
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04_analyse_data.ipynb
src/
src/__init__.py
src/load_data.py
data/
data/raw/
data/processed/
```

02_clean_data.ipynb

Process the raw data

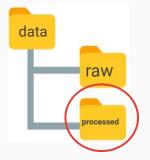
- Handle missing values
- Filter the data
- Drop invalid rows

- ...

Might need to combine with supplementary data before filtering

Store processed data in a sub-folder -> data/processed/cleaned_data.csv





```
README.md
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01_get_data.ipynb
02_clean_data.ipynb
03_eda.ipynb
04_analyse_data.ipynb
src/
src/__init__.py
src/load_data.py
data/
data/raw/
data/processed/
```

03_eda.ipynb

Explore the processed data

- Descriptive Statistics
- Visualisation



```
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data/
data/raw/
data/processed/
```

04_analyse_data.ipynb

Perform the quantitative data analysis

- Linear Regression
- Supervised Machine Learning
- Unsupervised Machine Learning
- Deep Learning
- ٠..



Modularize Python Code into src/

Avoids Long / Distracting Notebooks

Put common code into functions

Extract functions from notebook into custom Python modules

__init__.py: required to make Python treat the directories as containing packages to be imported: import numpy as np, from src.load_data import ...

Consider sub-folders for a larger code base

Can use multiple modules per folder

- eg. for visualization with matplotlib and plotly, may want
- visualize_matplotlib.py
- visualize_plotly.py

OPTION 1	OPTION 2
01_get_data.ipynb	01_get_data.ipynb
src/	src/
<pre>src/initpy</pre>	<pre>src/initpy</pre>
<pre>src/load_data.py</pre>	src/data/
<pre>src/create_features.py</pre>	<pre>src/data/initpy</pre>
src/visualize.py	<pre>src/data/load_data.py</pre>
	src/features/
	<pre>src/features/initpy</pre>
	<pre>src/features/create_features.py</pre>
	<pre>src/visualization/</pre>
	<pre>src/visualization/initpy</pre>
	<pre>src/visualization/visualize.py</pre>

Modularize Python Code into src/

BEFORE

Contents of 01_get_data.ipynb

```
import pandas as pd

df = pd.read_csv(url, nrows=200000, dtype={...})

df['date'] = pd.to_datetime(...)

df = df.drop(columns=['Unnamed: 7', 'Unnamed: 18'])

df = df.drop_duplicates(...)
```

OPTION 1

```
01_get_data.ipynb
src/
src/__init__.py
src/load_data.py
src/create_features.py
src/visualize.py
```

Modularize Python Code into src/

```
Contents of 01_get_data.ipynb
             import pandas as pd
             df = pd.read_csv(url, nrows=200000, dtype={...})
BEFORE
             df = df.drop duplicates(...)
             Contents of src/load_data.py
             import pandas as pd
 Define Function
             def get_data(url, dtypes_dict, nrows, drop_cols):
                df = pd.read_csv(url, nrows=nrows, dtype=dtypes_dict)
AFTER
                df['date'] = pd.to_datetime(...)
                df = df.drop(columns=drop cols)
                df = df.drop_duplicates(...)
                return df
```

OPTION 1

```
01_get_data.ipynb
src/
src/__init__.py
src/load_data.py
src/create_features.py
```

Contents of O1_get_data.ipynb

```
from src.load_data import get_data
```

```
df = get_data(url, {...}, 200000, ['Unnamed: 7, 'Unnamed: 18'])

Call Function in notebook
```

Documentation in a Data Science Notebook

Example Project

- 1. Analysis of Capital Bikeshare data
 - Washington, DC area (US)
- 2. Data is posted monthly
 - https://s3.amazonaws.com/capitalbikeshare-data/index.html
- 3. Steps in the workflow
 - Download Data
 - Use python to retrieve data
 - Process
 - Data Cleaning
 - Data Filtering
 - Visualise
 - EDA
 - Analyse
 - Feature Engineering
 - Machine Learning / Statistical Analysis



Name	Date Modified	Size	Туре
2010-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:33:31 pm	2.41 MB	ZIP file
2011-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:45:30 pm	25.33 MB	ZIP file
2012-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:55:27 pm	43.46 MB	ZIP file
2013-capitalbikeshare-tripdata.zip	Mar 15th 2018, 07:16:26 pm	56.48 MB	ZIP file
2014-capitalbikeshare-tripdata.zip	Mar 15th 2018, 07:29:51 pm	66.50 MB	ZIP file
2015-capitalbikeshare-tripdata.zip	Mar 15th 2018, 10:04:26 pm	73.59 MB	ZIP file
2016-capitalbikeshare-tripdata.zip	Mar 15th 2018, 10:27:02 pm	78.23 MB	ZIP file
2017-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:25:30 pm	89.58 MB	ZIP file
201801-capitalbikeshare-tripdata.zip	Apr 30th 2018, 12:01:09 pm	3.87 MB	ZIP file
201802-capitalbikeshare-tripdata.zip	May 11th 2018, 04:47:35 pm	4.18 MB	ZIP file

```
Download the ChromeDriver 97.0,4692,71; https://chromedriver.chromium.org/downloads, This
         requires Google chrome version 97.0.4692.71.
         Download the bikeshare data from here: https://s3.amazonaws.com/capitalbikeshare-
         data/index.html
         Install Python libraries: selenium, pandas
In [1]: # !pip3 install selenium pandas
In [2]: import os
In [3]: from selenium.webdriver.chrome.options import Options
         from selenium import webdriver
         from selenium.webdriver.chrome.service import Service
In [4]: # Path to the Chrome webdriver on local system
        user name = os.getenv("USERNAME")
        webdriver path = f"/home/{user name}/chromedriver linux64/chromedriver"
         # Create ChromeDriver service object
        driver service object = Service(webdriver path)
         options = Options()
In [5]: driver = webdriver.Chrome(service=driver service object, options=options)
        Selenium Webdriver
         Download all the metadata
In [6]: driver.get("https://s3.amazonaws.com/capitalbikeshare-data/index.html")
                                                            Get table with list of files
        Web Scraping
In [7]: from selenium.webdriver.common.by import By
In [8]: container = driver.find element(By.XPATH, './/div[@class="container"]')
        table id = container.find element(By.XPATH, "//table[@class='hide-while-l
        header = container.find element(By.XPATH, "//table[@class='hide-while-loa
        headers = [h.text for h in header.find elements(By.CSS SELECTOR, "th")]
```

01_dont_do_this.ipynb

Name	Date Modified	Size	Type
2010-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:33:31 pm	2.41 MB	ZIP file
2011-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:45:30 pm	25.33 MB	ZIP file
2012-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:55:27 pm	43.46 MB	ZIP file
2013-capitalbikeshare-tripdata.zip	Mar 15th 2018, 07:16:26 pm	56.48 MB	ZIP file
2014-capitalbikeshare-tripdata.zip	Mar 15th 2018, 07:29:51 pm	66.50 MB	ZIP file
2015-capitalbikeshare-tripdata.zip	Mar 15th 2018, 10:04:26 pm	73.59 MB	ZIP file
2016-capitalbikeshare-tripdata.zip	Mar 15th 2018, 10:27:02 pm	78.23 MB	ZIP file
2017-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:25:30 pm	89.58 MB	ZIP file
201801-capitalbikeshare-tripdata.zip	Apr 30th 2018, 12:01:09 pm	3.87 MB	ZIP file
201802-capitalbikeshare-tripdata.zip	May 11th 2018, 04:47:35 pm	4.18 MB	ZIP file

```
In [9]: import pandas as pd
In [10]: # Scrape metadata
           mvlists = []
          for row in table id.find elements(By.CSS SELECTOR, "tr"):
               mylist = []
               zip file urls = []
               col idx = 0
               for cell in row.find elements(By.TAG NAME, "td"):
                   text = cell.text
                   if col idx == 0:
                       data zip url = cell.find element(By.CSS SELECTOR, "a").get at
Get table values
                       zip file urls.append(data zip url)
                   # Append contents of single row to empty list
                   mvlist.append(text)
                   col idx += 1
               df single row = pd.DataFrame.from records([{h: r for h, r in zip(head
               df single row["zip file url"] = zip file urls
               mylists.append(df single row)
          Data Processing
           Combine the data
Create DataFrame from scraped values
In [11]: df = pd.concat(mylists, ignore index=True)
In [12]: df.head(3)
Out[12]:
                            Name
                                     Date Modified
                                                        Type
                                                                                 zip file url
                                     Mar 15th 2018.
                                                         7IP
                                                                       https://s3.amazonaws.com
                2010-capitalbikeshare-
                                                   2.41
                        tripdata.zip
                                      06:33:31 pm
                                                                         /capitalbikeshare-data..
                2011-capitalbikeshare-
                                     Mar 15th 2018.
                                                                       https://s3.amazonaws.com
                        tripdata.zip
                                      06:45:30 pm
                                                          file
                                                                         /capitalbikeshare-data...
                2012-capitalbikeshare-
                                     Mar 15th 2018,
                                                  43.46
                                                         ZIP
                                                                       https://s3.amazonaws.com
                                      06:55:27 pm
                                                                         /capitalbikeshare-data
           Get data from 2021
Filter data to only get data from 2021
In [13]: df = df[df["Name"].str[:4] == "2021"].copy()
           df["date modified eod"] = pd.to datetime(df["Date Modified"])
```

01_dont_do_this.ipynb

```
In [ ]:
In [14]: df.head(3)
Out[14]:
                                      Date
                                                                      zip file url date modified eod
                          Name
                         202101-
                                    Feb 4th
                                                  ZIP
                                                          https://s3.amazonaws.com
                                                                                      2021-02-04
                  capitalbikeshare-
                                     2021.
                                             MB
                                                   file
                                                            /capitalbikeshare-data...
                                                                                        16:55:29
                       tripdata.zip 04:55:29 pm
                         202102-
                                    Mar 9th
                                            2.78
                                                  7IP
                                                                                      2021-03-09
                                                          https://s3.amazonaws.com
                  capitalbikeshare-
                                                            /capitalbikeshare-data...
                                                                                        19:07:41
                       tripdata.zip 07:07:41 pm
                        202103-
                                            5.88 ZIP
                                                          https://s3.amazonaws.com
                                                                                      2021-04-08
                  capitalbikeshare-
                                             MB
                                                            /capitalbikeshare-data...
                                                                                        10:31:40
In [15]: driver.quit()
 In [ ]:
           Download the data
                              Download data from 2021
In [18]: from io import BytesIO
           from urllib.request import urlopen
           from zipfile import ZipFile
In [19]: %%time
           for , row in df.iterrows():
               zipurl = row["zip file url"]
               # Extract without saving
               with urlopen(zipurl) as zipresp:
                    with ZipFile(BytesIO(zipresp.read())) as zfile:
                         zfile.extractall(f'data/raw')
           CPU times: user 1.87 s, svs: 541 ms, total: 2.41 s
           Wall time: 11.3 s
```

```
Download the ChromeDriver 97.0.4692.71: https://chromedriver.chromium.org/downloads. This
         requires Google chrome version 97.0.4692.71.
         Download the bikeshare data from here: https://s3.amazonaws.com/capitalbikeshare-
         data/index.html
         Install Python libraries: selenium, pandas
In [1]: # !pip3 install selenium pandas
In [2]: import os
In [3]: from selenium.webdriver.chrome.options import Options
         from selenium import webdriver
         from selenium.webdriver.chrome.service import Service
In [4]: # Path to the Chrome webdriver on local system
         user name = os.getenv("USERNAME")
        webdriver path = f"/home/{user name}/chromedriver linux64/chromedriver"
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         options = Options()
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         Selenium Webdriver
         Download all the metadata
In [6]: driver.get("https://s3.amazonaws.com/capitalbikeshare-data/index.html")
         Web Scraping
In [7]: from selenium.webdriver.common.by import By
In [8]: container = driver.find element(By.XPATH, './/div[@class="container"]')
         table id = container.find element(By.XPATH, "//table[@class='hide-while-l
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         headers = [h.text for h in header.find elements(Bv.CSS SELECTOR. "th")]
```

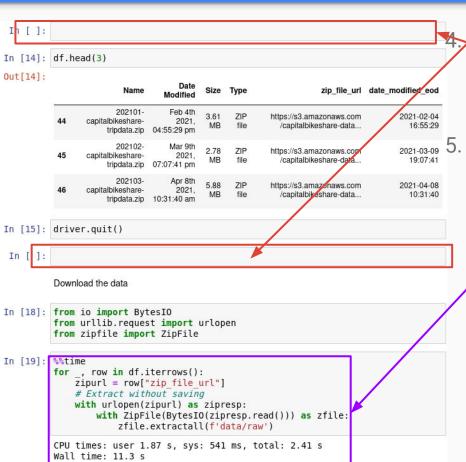
Problems with 01_dont_do_this.ipynb

- 1. No table of contents, No Intro section, No Title
 - a. Notebook requirements can be included in Intro section
- 2. Python requirements should be in requirements.txt

3. import statements

- a. Scattered across notebook
- b. Not sorted (https://www.python.org/dev/peps/pep-0008/#imports)
 - i. Python standard libraries
 - ii. Third party libraries
 - iii. Our custom modules from src/

Problems with 01_dont_do_this.ipynb



Blank cells are not necessary

- Distracting to reader
- Reader doesn't know if author meant to add code in these cells

5. Long-running cells with a loop

- Add a print statement to see output in each iteration

Process Data - Document Future Changes to Data

Accepted Methods of payment

- O How to handle changes?
- o 2 unique values becomes 1 unique value
- Keep / Drop all stations where changes have been made?
- What have others in this field done? Refer to our background research.
- Add Documentation to Notebook...









Analysis (ML) - Document Data Availability / Client Constraints

1. Use-Case: Predict number of bikeshare departures per station to rebalance a station

2. Client Requirements

- We can read about these in whitepapers, Journals, blog posts, etc.
- Predict 7 days of bikeshare trips departing / arriving per station
- Client will use predictions to re-balance bikes at stations
 - Need to deliver predictions ahead of time (client can plan staffing, inventory, etc.)

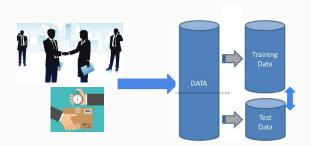
3. **Constraints:** When will data be available to use?

- o 2021-12-01 2021-12-31 data is posted on 2022-01-06; if client needs ML predictions on 2022-01-04?
- If latest data is not uploaded in time, be ready to use older data (ending on 2021-11-30)
- ML Model performance might be worse

4. How to choose validation and test splits?

- Test split to evaluate ML model's performance, Validation split to compare models, hyperparameters
- Validation and test split must be chosen following
 - Client Requirements, Constraints





Analysis (ML) - Document Data Availability / Client Constraints

1. Use-Case: Predict number of bikeshare departures per station to rebalance a station

2. Client Requirements (README.md)

- We can read about these in whitepapers, Journals, blog posts, etc.
- Predict 7 days of bikeshare trips departing from each station
- Client will use predictions to re-balance bikes at stations
 - Need to deliver predictions ahead of time (client can plan staffing, inventory, etc.)

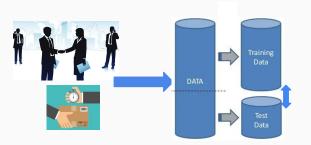


- o 2021-12-01 2021-12-31 data is posted on 2022-01-06; if client needs ML predictions on 2022-01-04?
- o If *latest* data is not uploaded in time, be ready to use older data (ending on 2021-11-30)
- ML Model performance might be worse

4. How to choose validation and test splits? (Notebook)

- Test split to evaluate ML model's performance, Validation split to compare models, hyperparameters
- Validation and test split must be chosen following
 - Client Requirements, Constraints





Additional Helpful Links

- Github Repository Used here
 - https://github.com/elsdes3/portfolio-documentation-tips
- 2. Jupyter notebook utilities
 - TOC manually:
 - i. https://moonbooks.org/Articles/How-to-create-a-table-of-contents-in-a-jupyter-notebook-/
 - ii. https://sebastianraschka.com/Articles/2014_ipython_internal_links.html
 - TOC Jupyter extension:
 https://jupyter-contrib-nbextensions.readthedocs.io/en/latest/nbextensions/toc2/README.html
- 3. Other Files to include in a Portfolio Project
 - o .gitignore: https://www.toptal.com/developers/gitignore (enter Python in search box)
 - o papermill: https://papermill.readthedocs.io/en/latest/
 - o Open Source LICENSE: https://towardsdatascience.com/a-data-scientists-guide-to-open-source-licensing-c70d5fe4207

THANK YOU

Q & A, DISCUSSION



https://github.com/elsdes3

https://twitter.com/elsdes3

