Data Science Portfolio Projects to Rely On

Tips to organize and document a data science portfolio project

ELSTAN DESOUZA
WED JANUARY 19, 2022

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

Documentation

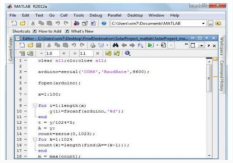
Canadian Light Source (CLS) in Saskatoon, SK

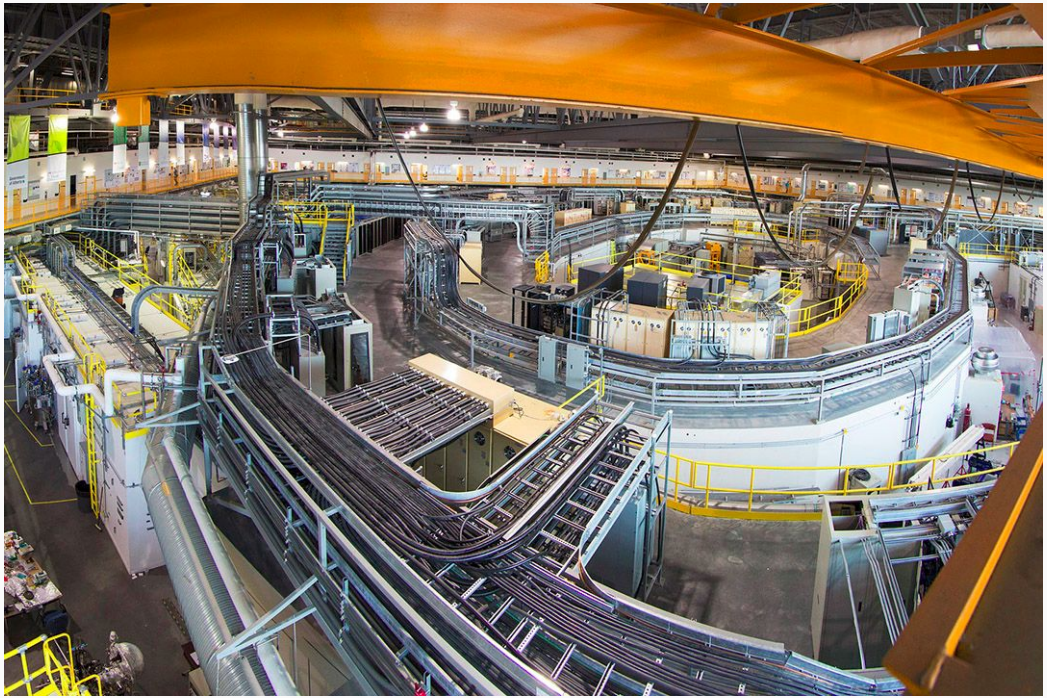
- Particle Accelerator used in Applied Science Research
- Perform Science Experiments
- Collect Data

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

1 yr later Colleague → Code + docs (comments, difficulties)





PROBLEMS:

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

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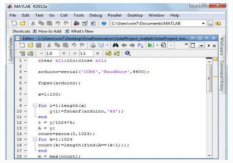

PROBLEM:

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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.dataquest.io/blog/build-a-data-science-portfolio/

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

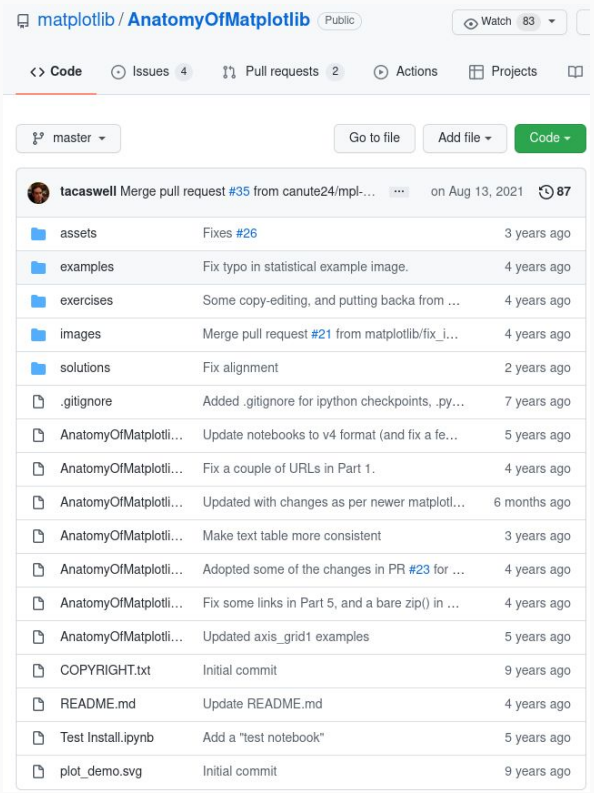
GitHub GitLab Atlassian Bitbucket

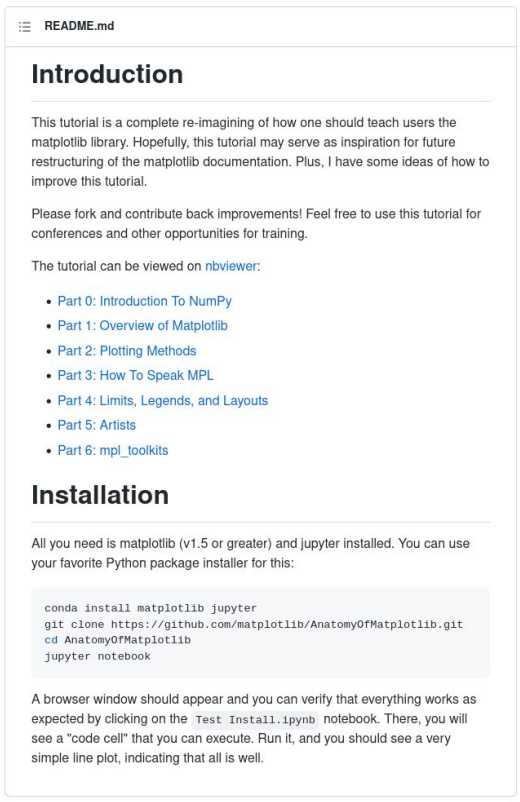
Benefits of Sharing **Documented** Data Science Portfolio Projects

- 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/





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

Use a Directory Structure for a Portfolio Project

```
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/
```

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)

Use a Directory Structure for a Portfolio Project

README.md

`requirements.txt`

`01_get_data.ipynb`

`02_clean_data.ipynb`

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`src/`

`src/__init__.py`

`src/load_data.py`

`data/`

`data/raw/`

`data/processed/`

README.md

1. Project title
2. Background, motivation, end-user, etc. for the the project
   - Based on reading through whitepapers, research papers, etc.
3. Add instructions for how to install Python packages and start jupyter

   Example wording:

   To install all Python packages and start a Jupyter notebook, please run the following

   ```
   $ pip install -r requirements.txt

   $ jupyter notebook
   ```

4. How to run all the notebooks? Sequentially, based on their file names. `Untitled12.ipynb` 

   Example wording:

   Please run the notebooks in the following order

   - `01_get_data.ipynb` (to download the raw data)

   - `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)

Use a Directory Structure for a Portfolio Project

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

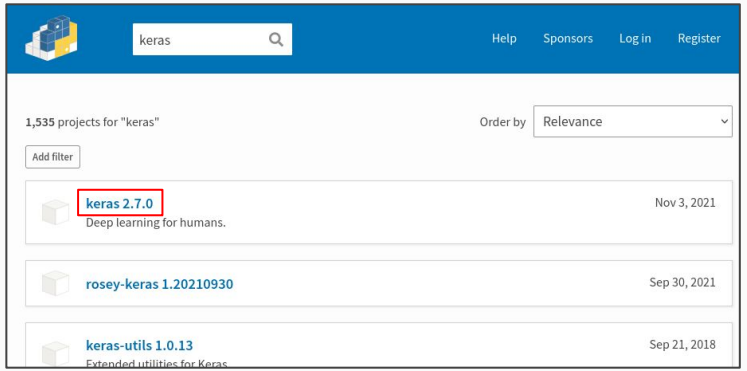
requirements.txt

```
pandas==1.35.0
plotly==5.5.0
scipy==1.7.3
```

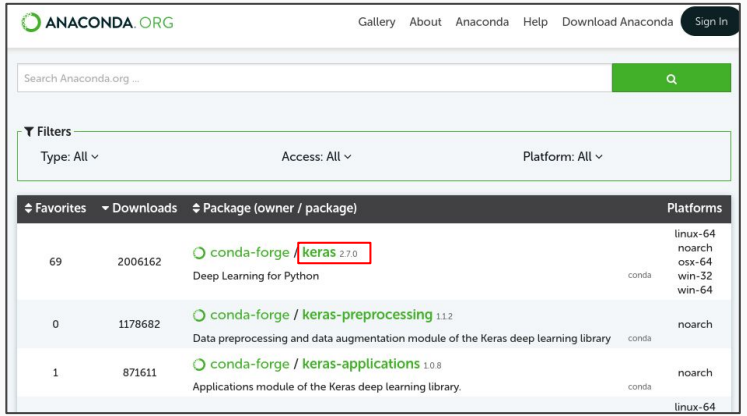
To get package version numbers

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

PyPI



Anaconda Search



Use a Directory Structure for a Portfolio Project

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/

Clickable Section Headers (HTML Hyperlinks without `href` attribute)

```
<a id='get-data'>

## 1. Get data
```

Table of Contents

```
1.  [Get data](#get-data)
2.  ...
```

Divider / Horizontal Rule

```
___
```

Footers for Navigation

```
<span style="float:left;">

    <a href="./01_dont_do_this.ipynb"> >> 02_get_data.ipynb</a>

</span>
```

Use a Directory Structure for a Portfolio Project

`README.md`

`requirements.txt`

`01_get_data.ipynb`

`02_clean_data.ipynb`

`03_eda.ipynb`

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`src/`

`src/__init__.py`

`src/load_data.py`

`data/`

`data/raw/`

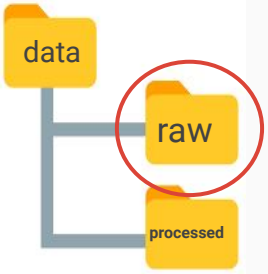
`data/processed/`

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



Use a Directory Structure for a Portfolio Project

`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/`

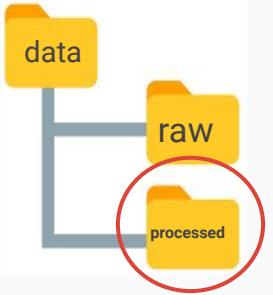
02_clean_data.ipynb

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`



Use a Directory Structure for a Portfolio Project

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```

03_eda.ipynb

Explore the processed data

- Descriptive Statistics
- Visualisation

Use a Directory Structure for a Portfolio Project

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```
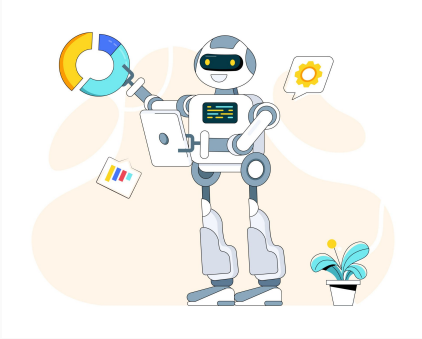

04_analyse_data.ipynb

Perform the quantitative data analysis

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



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/`
`src/__init__.py`	`src/__init__.py`
`src/load_data.py`	`src/data/`
`src/create_features.py`	`src/data/__init__.py`
`src/visualize.py`	`src/data/load_data.py`
	`src/features/`
	`src/features/__init__.py`
	`src/features/create_features.py`
	`src/visualization/`
	`src/visualization/__init__.py`
	`src/visualization/visualize.py`

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/`

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
```

AFTER

Define Function

Contents of src/load_data.py

```
import pandas as pd

def get_data(url, dtypes_dict, nrows, drop_cols):

    df = pd.read_csv(url, nrows=nrows, dtype=dtypes_dict)

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

    df = df.drop(columns=drop_cols)

    df = df.drop_duplicates(...)

    return df
```

Contents of 01_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	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

01_dont_do_this.ipynb

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")
```

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")]
```

Get table with list of files

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
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201802-capitalbikeshare-tripdata.zip	May 11th 2018, 04:47:35 pm	4.18 MB	ZIP file

01_dont_do_this.ipynb

In [9]:
```
import pandas as pd
```

In [10]:
```
# Scrape metadata
mylists = []
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
            zip_file_urls.append(data_zip_url)
        # Append contents of single row to empty list
        mylist.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)
```

Get table values

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	Size	Type	zip_file_url
0	2010-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:33:31 pm	2.41 MB	ZIP file	https://s3.amazonaws.com/capitalbikeshare-data...
1	2011-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:45:30 pm	25.33 MB	ZIP file	https://s3.amazonaws.com/capitalbikeshare-data...
2	2012-capitalbikeshare-tripdata.zip	Mar 15th 2018, 06:55:27 pm	43.46 MB	ZIP file	https://s3.amazonaws.com/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"])
```

In [ ]:

In [14]:
```
df.head(3)
```

Out[14]:

	Name	Date Modified	Size	Type	zip_file_url	date_modified_eod
44	202101-capitalbikeshare-tripdata.zip	Feb 4th 2021, 04:55:29 pm	3.61 MB	ZIP file	https://s3.amazonaws.com/capitalbikeshare-data...	2021-02-04 16:55:29
45	202102-capitalbikeshare-tripdata.zip	Mar 9th 2021, 07:07:41 pm	2.78 MB	ZIP file	https://s3.amazonaws.com/capitalbikeshare-data...	2021-03-09 19:07:41
46	202103-capitalbikeshare-tripdata.zip	Apr 8th 2021, 10:31:40 am	5.88 MB	ZIP file	https://s3.amazonaws.com/capitalbikeshare-data...	2021-04-08 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, sys: 541 ms, total: 2.41 s
Wall time: 11.3 s
```

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`

In [ ]:

In [14]:
```
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```

Out[14]:

	Name	Date Modified	Size	Type	zip_file_url	date_modified_eod
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In [15]:
```
driver.quit()
```

In [ ]:

Download the data

In [18]:
```
from io import BytesIO
from urllib.request import urlopen
from zipfile import ZipFile
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In [19]:
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%%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, sys: 541 ms, total: 2.41 s
Wall time: 11.3 s
```

4. 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

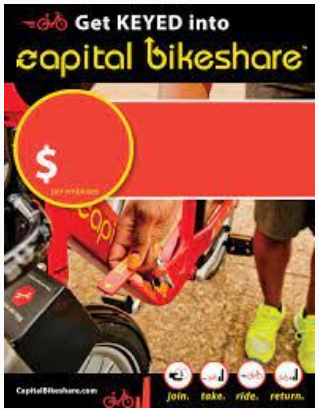
Accepted Methods of payment

- How to handle changes?
- 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...**

Now: `["KEY", "CREDITCARD"]`

Future(?): `["KEY", "CREDITCARD"]`

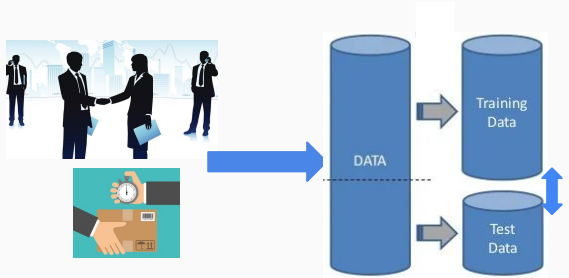
Future(?): `["CREDITCARD"]`



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?
   - 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.)

3. **Constraints:** When will data be available to use? **(README.md, Notebook)**
   - 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? **(Notebook)**
   - Test split to evaluate ML model's performance, Validation split to compare models, hyperparameters
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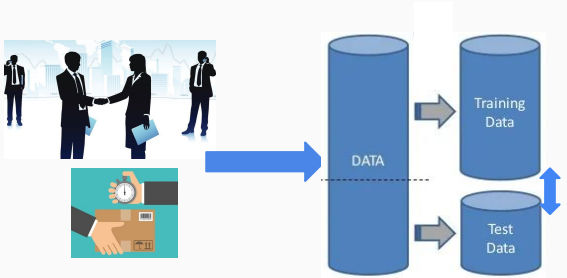

Additional Helpful Links

1. 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
    - .gitignore: https://www.toptal.com/developers/gitignore (enter Python in search box)
    - papermill: https://papermill.readthedocs.io/en/latest/
    - Open Source LICENSE: https://towardsdatascience.com/a-data-scientists-guide-to-open-source-licensing-c70d5fe4207

THANK YOU

Q & A, DISCUSSION

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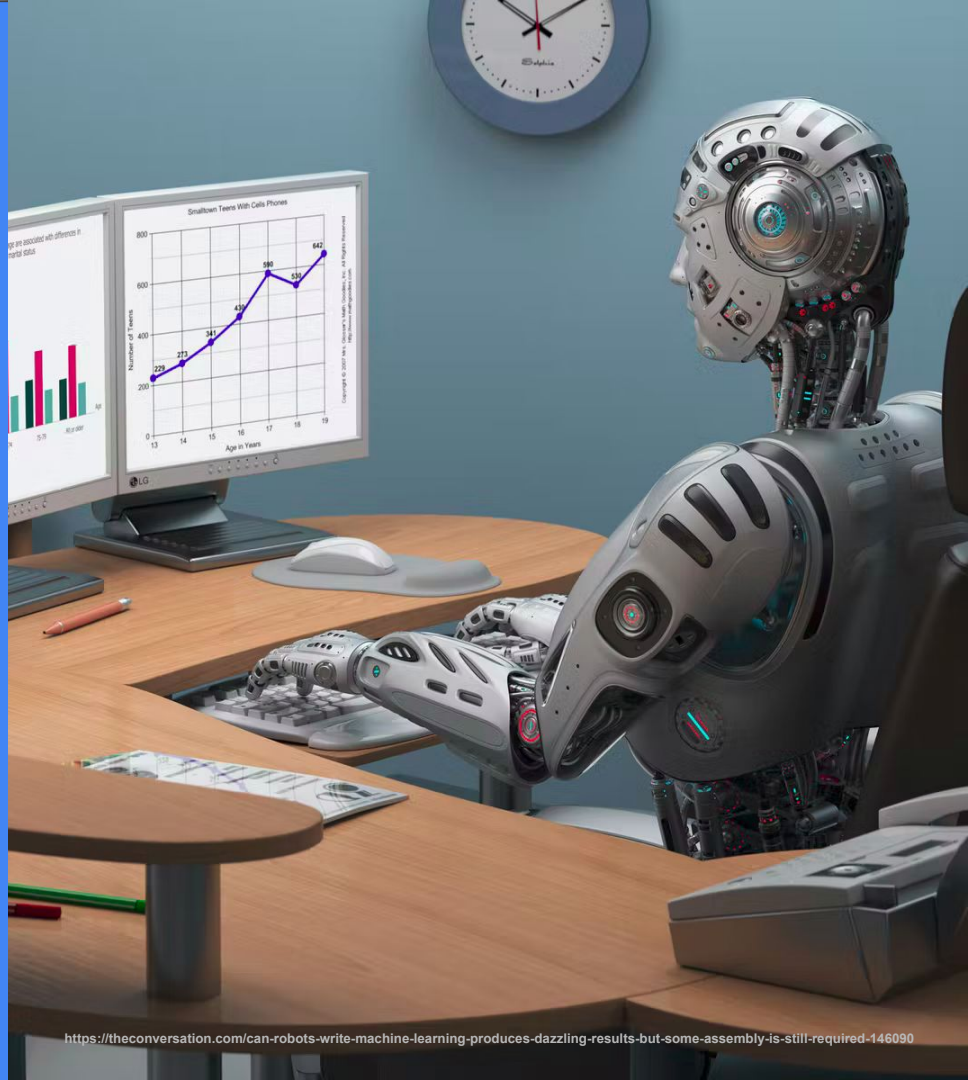
https://github.com/elsdes3

https://twitter.com/elsdes3



https://theconversation.com/can-robots-write-machine-learning-produces-dazzling-results-but-some-assembly-is-still-required-146090