Introduction to **Applied Data Science in Python**

QBS 101.5

Simon Stone[✤]*, Jeremy Mikecz*[✤]*, Carly Bobak*[✦]

[✤]*Research Data Services,* [✦]*Research Computing*

Dartmouth College

Applied Data Science in Python

Instructors

Carly Bobak, PhD

- Biomedical Informatics Specialist
- PhD in Quantitative Biomedical Sciences from Dartmouth College (2021)
- Teaches QBS 181: Data Wrangling
- Published papers on diverse public health issues, including TB, Covid, HIV, cancer, sepsis, smoking cessation, and obesity.
- Has two dogs who tend to crash QBS events

Jeremy Mikecz, PhD

- Research Data Science Specialist
- PhD in Latin American History, University of California
- Offers consultations and workshops on computational text analysis, data visualization, GIS and mapping, Python & R programming
- Published various articles and a book (in-press) showcasing how visualization and mapping can aid historical research

Dr. Simon Stone

- Research Data Science Specialist
- Doctoral degree in Electrical and Computer Engineering from Technische Universität Dresden
- Offers consultations and workshops on Data Science, Machine Learning, and Software Development
- Published papers on speech technology, sensor design, signal processing, and machine learning
- Freelance software developer by night

Applied Data Science in Python
Course materials

- Brand new class!
- Materials are created as we go along
- You can help shape them!
- Materials will consist of lecture slides and code-along notebooks

Class repository:

https://github.com/Simon-Stone/qbs-applied-data-science

Get the materials:

```
git clone https://github.com/Simon-Stone/qbs-applied-data-science
```

Update the materials:

```
git pull
```

Introduction

Data Science

Challenge:

Define *Data Science*!

Data science is the study of data to extract meaningful insights for business.

https://aws.amazon.com/what-is/data-science/

aws

Data science [...] uncover[s] actionable insights hidden in an organization's data.

https://www.ibm.com/topics/data-science

IBM

[Data science] models and analyzes key data to continually improve how businesses utilize data.

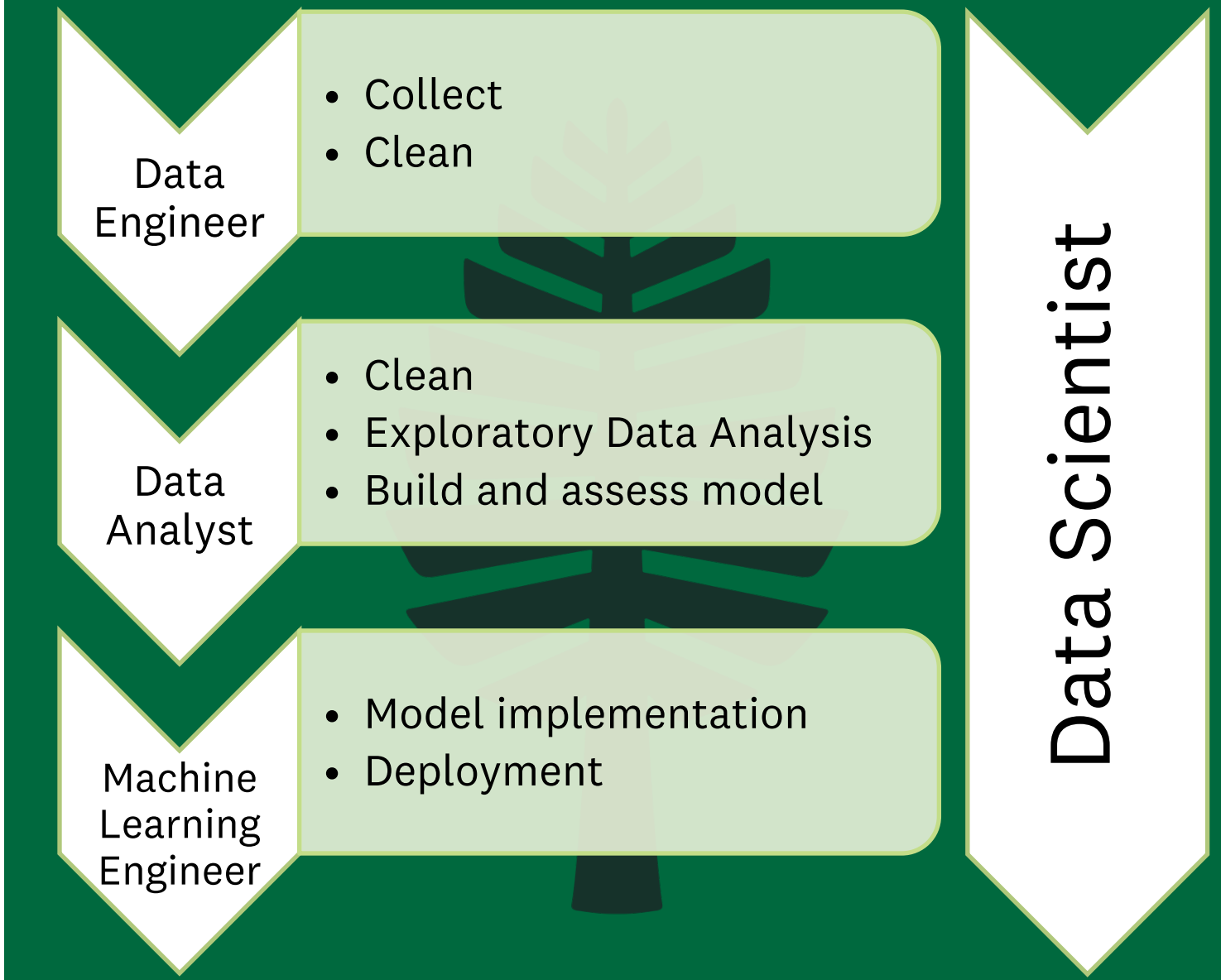
https://cloud.google.com/learn/training/machinelearning-ai

Google

Introduction
Data Science

Data Science is OSEMN!*

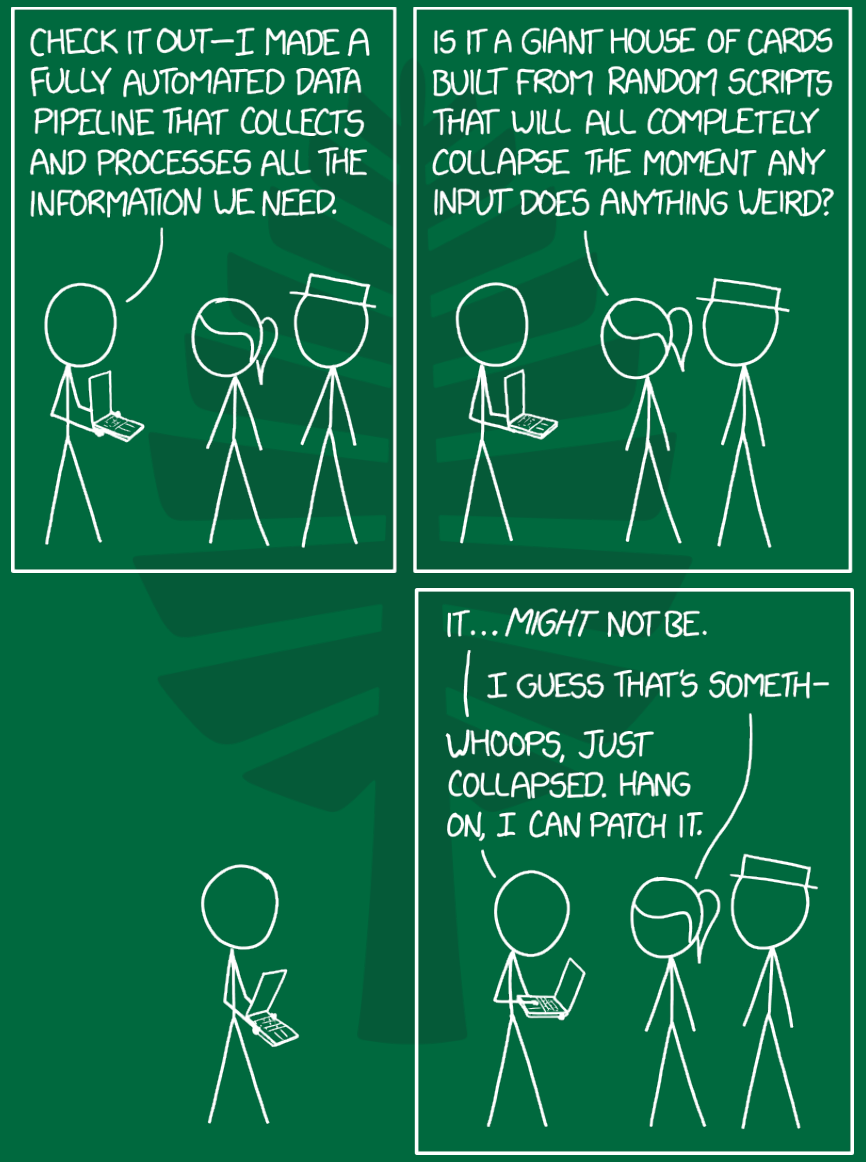
- 📥 Obtain
- 🧼 Scrub
- 🔎 Explore
- 🤖 Model
- ⁉️ iNterpret



*pronounced “awesome” - /ˈɔ.səm/
https://www.datascience-pm.com/osemn

Outline

- 🎬 Introduction
- 📅 Schedule
- 🎓 Learning Objectives
- ❄️ What makes a Data Science project special?
- 🐍 What makes a Python project special?
- 🛠️ Tools of the Trade
- 🥜 Summary
- 💻 Assignment



Munroe, R. (n.d.). *Data Pipeline*. xkcd. https://xkcd.com/2054/ (CC BY-NC 2.5)

Learning Objectives

1. **Complete a data science project** through the process of finding, cleaning, compiling, exploring, analyzing, visualizing, and modeling data.
2. **Become proficient at writing and applying Python** code to complete these data science steps.
3. **Practice effectively communicating** (and providing critical feedback on) data science research.
4. Apply the principles of **reproducible research** throughout the data science lifecycle.

Format

Class times and location:

- Monday, 4 pm – 5:30 pm
- Wednesday, 4 pm – 5:30 pm
- Remsen 312

- Classes will consist of lectures, code-alongs, hands-on project work, or a mix of all the above
- There will be assignments to continue the engagement with each week's content
- At the end of each Wednesday class, there is time for project check-ins, show & tell, or troubleshooting
- Each student is expected to hand in a final project

Format
Final Project

Project requirements:

- Devise a business or research question that can be answered through data
- Identify a suitable dataset
- Implement all major steps of a data science project to find an answer to the chosen question

Deliverables:

- Project pitch (details to come)
- Fully reproducible project repository
- Final presentation

Schedule

Week 1 (June 26 & June 28): Getting Started with Applied Data Science & Python

- Introduction to Applied Data Science with Python
- Data Wrangling

Week 2 (July 3 & July 5): Texts, Maps, and Graphs

- Data Visualization
- NLP I

Week 3 (July 10 & July 12): Texts as Data

- NLP II
- NLP III

Week 4 (July 17 & July 19): Machine Learning

- Scikit-learn
- PyTorch

Week 5 (July 24 & July 26): Project Work

- Project proposals due (Monday July 24)
- *No class meetings*

Week 6 (July 31 & August 2):

- *No class meetings*

Week 7 (August 7 & August 9): Collaboration and Documentation

- Documenting, Sharing and Evaluating Code
- Peer Review

Week 8 (August 14 & August 16): Code Revision Work

- *No Class Meetings*

Week 9 (August 21 & August 23):

- Final Presentations and revised code due (Wed. Aug 23)

Policy on Generative AI

Use of generative AI is generally accepted in this course if it meets the following requirements:

- You are expected to take full ownership of your work, including the use of generative AI
- You need to be able to understand and reflect any output of generative AI you want to include in your work
    - “It’s a tool, you’re its master!”
- Just like with code taken from other sources (e.g., Stack Overflow), any code other than your own must be cited (see Week 7: Documentation)
- You are expected to be able to explain and discuss every line of code in your final project

Applied Data Science with Python

What makes a Data Science project special

Typical project has **two phases**:

1. Exploration phase

   🧭 Explore data, imputations, feature engineering, model selection

2. Reporting and “deployment” phase

   📊 Generate result tables and graphs, refactor code, export trained models

Subject matter domains differ, tasks are similar

   🤹 Multiple stakeholders to consider, “interrogate”, and convince

Applied Data Science with Python

What makes a Python project special

💪 Powerful language with incredible community and industry support

- Often large number of (inter-)dependencies

🚀 Rapid prototyping

🖥️ (Mostly) cross-platform compatible on Windows, Mac OS, Linux

😵 Sprawling, sometimes confusing ecosystem

😫 Deployment / reproducibility can be challenging

Applied Data Science with Python
Tools of the Trade

- Integrated Development Environment (IDE) for writing code
- Command line scripts for project setup and configuration
- Jupyter notebooks for prototyping and reporting
- Version control for code (and sometimes data)

Not part of this course:

- Cloud infrastructure (Amazon Web Services, Google Cloud, Microsoft Azure)

Tools of the Trade
Anti-patterns

"A commonly-used process, structure or pattern of action that, despite initially appearing to be an appropriate and effective response to a problem, has more bad consequences than good ones."

*Gang of Four**

* Gamma, E., Helm, R., Johnson, R., Vlissides, J. (1995). *Design patterns: elements of reusable object-oriented software*. Boston, MA, USA: Addison-Wesley Longman Publishing Co., Inc.. ISBN: 0-201-63361-2

- Not using an IDE
- Not organizing your project in one place
- Using a too simple or too elaborate project setup
- Overusing Jupyter notebooks (sometimes scripts are better)
- Not managing your Python environment

Tools of the Trade

Recommended Setup for this class

Recommended **Python distribution**:

- 🐍 Vanilla Python 3.8 or newer: https://www.python.org/

Recommended **IDE**:

-  Visual Studio Code: https://code.visualstudio.com/

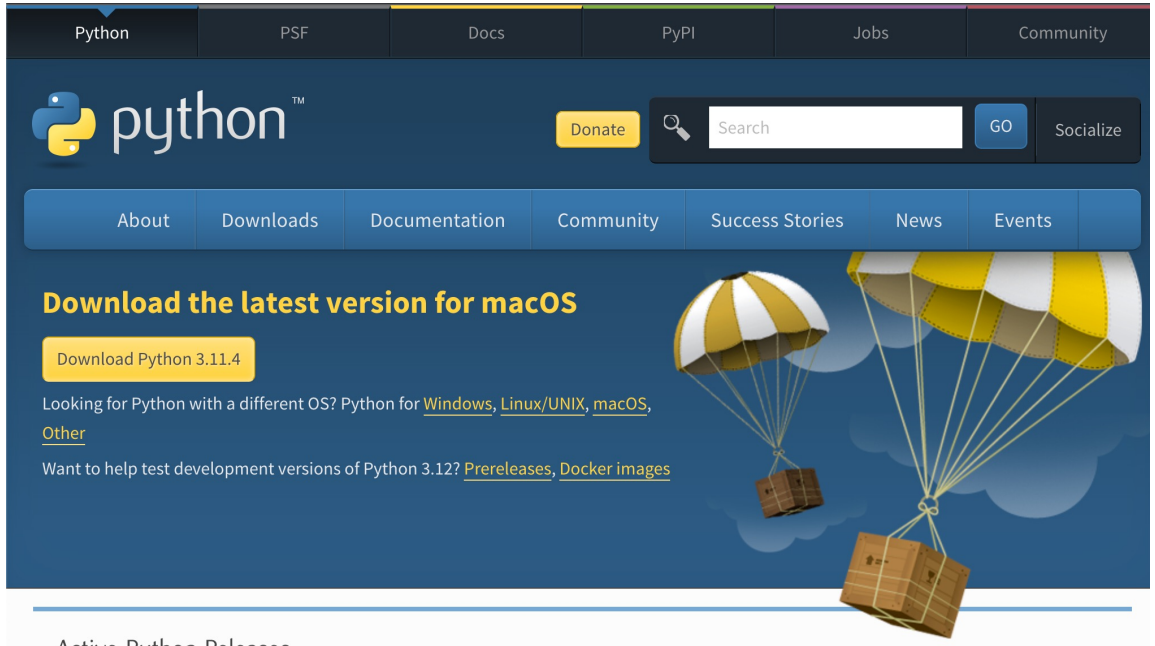
Recommended **version control** hosting platform

- GitHub: https://www.github.com

Tools of the Trade
Python

- Recommended minimum **version 3.8+**
- Installer from python.org recommended
- Recommended **environment management**:
  - Using Python's built-in virtualenv: https://docs.python.org/3/library/venv.html
  - Install packages into virtual environment
  - Document project requirements using:

```
pip freeze > requirements.txt
```



Active Python Releases

For more information visit the Python Developer's Guide.

Python version	Maintenance status	First released	End of support	Release schedule
3.12	prerelease	2023-10-02 (planned)	2028-10	PEP 693
3.11	bugfix	2022-10-24	2027-10	PEP 664
3.10	security	2021-10-04	2026-10	PEP 619
3.9	security	2020-10-05	2025-10	PEP 596
3.8	security	2019-10-14	2024-10	PEP 569
3.7	security	2018-06-27	2023-06-27	PEP 537

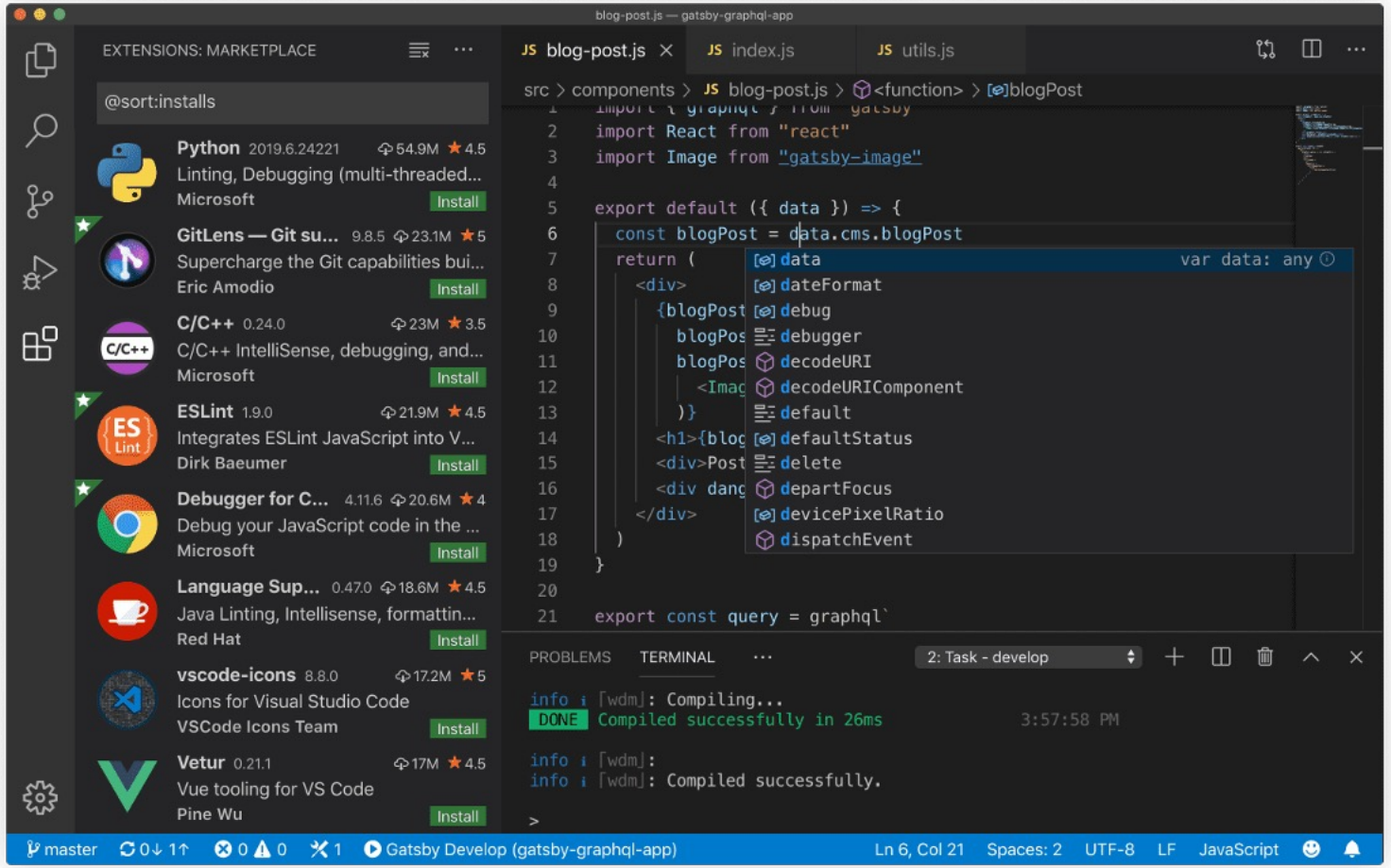
https://www.python.org/downloads/

Tools of the Trade
Python

- Python is supported by Jupyter notebooks
- Notebooks are a convenient way to combine code, text, and images in a single file
- Notebooks are great for developing a narrative in your analysis
- Notebooks are not a good choice for project setup, config, or model deployment
- Use regular Python scripts (*.py) for that

Tools of the Trade
Visual Studio Code

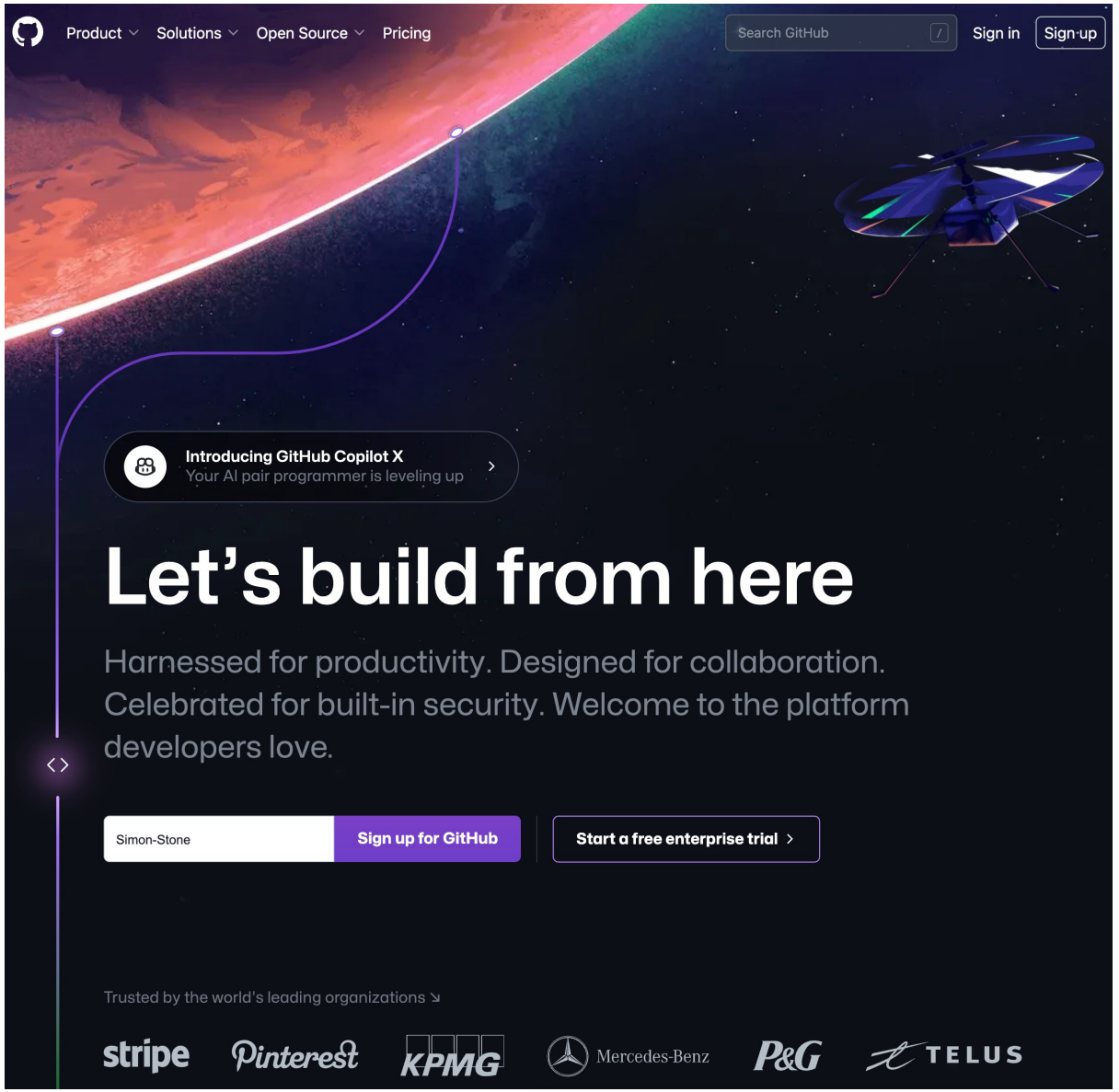
- Cross-platform (Windows, Mac, Linux)
- Open source
- Lightweight (no project files required)
- Support for all sorts of languages
- Syntax highlighting and autocomplete
- Extensible in millions of ways
- Natively supports Jupyter notebooks
- Git built-in
- Easy to get started
- Many powerful advanced features



https://code.visualstudio.com/

Tools of the Trade
GitHub

- Web-based platform for individuals and teams to collaboratively develop software projects
- Uses the Git version control system
- Also offers tools and services for
  - project management,
  - continuous integration and deployment,
  - documentation
- Building up portfolio of projects on GitHub can benefit your job applications



https://www.github.com/

Tools of the Trade
GitHub

- Repository structure:
  - Many templates available on the internet:
    - http://drivendata.github.io/cookiecutter-data-science/
    - https://gist.github.com/ericmjl/27e50331f24db3e8f957d1fe7bbbe510
- Try them out, learn what works, adjust and adapt to fit your flow
- Consider creating a GitHub template repo

Tools of the Trade
GitHub

- An example structure you can use in this class:
- Tour of the example repo
- Not all of this will be helpful in every project

```
├── data/
│   ├── raw/
│   ├── processed/
│   └── cleaned/
├── models/
├── notebooks/
│   ├── 01-first-logical-notebook.ipynb
│   ├── 02-second-logical-notebook.ipynb
│   ├── prototype-notebook.ipynb
│   └── archive/
│           └── no-longer-useful.ipynb
├── projectname/
│   ├── projectname/
│         | ├── __init__.py
│         | ├── config.py
│         | ├── data.py
│         | ├── utils.py
│   └── setup.py
├── results/
├── scripts/
│   ├── script1.py
│   ├── script2.py
│   └── archive/
│      └── no-longer-useful.py
├── .gitignore
├── README.md
└── requirements.txt
```

https://github.com/Simon-Stone/data-science-project-repo

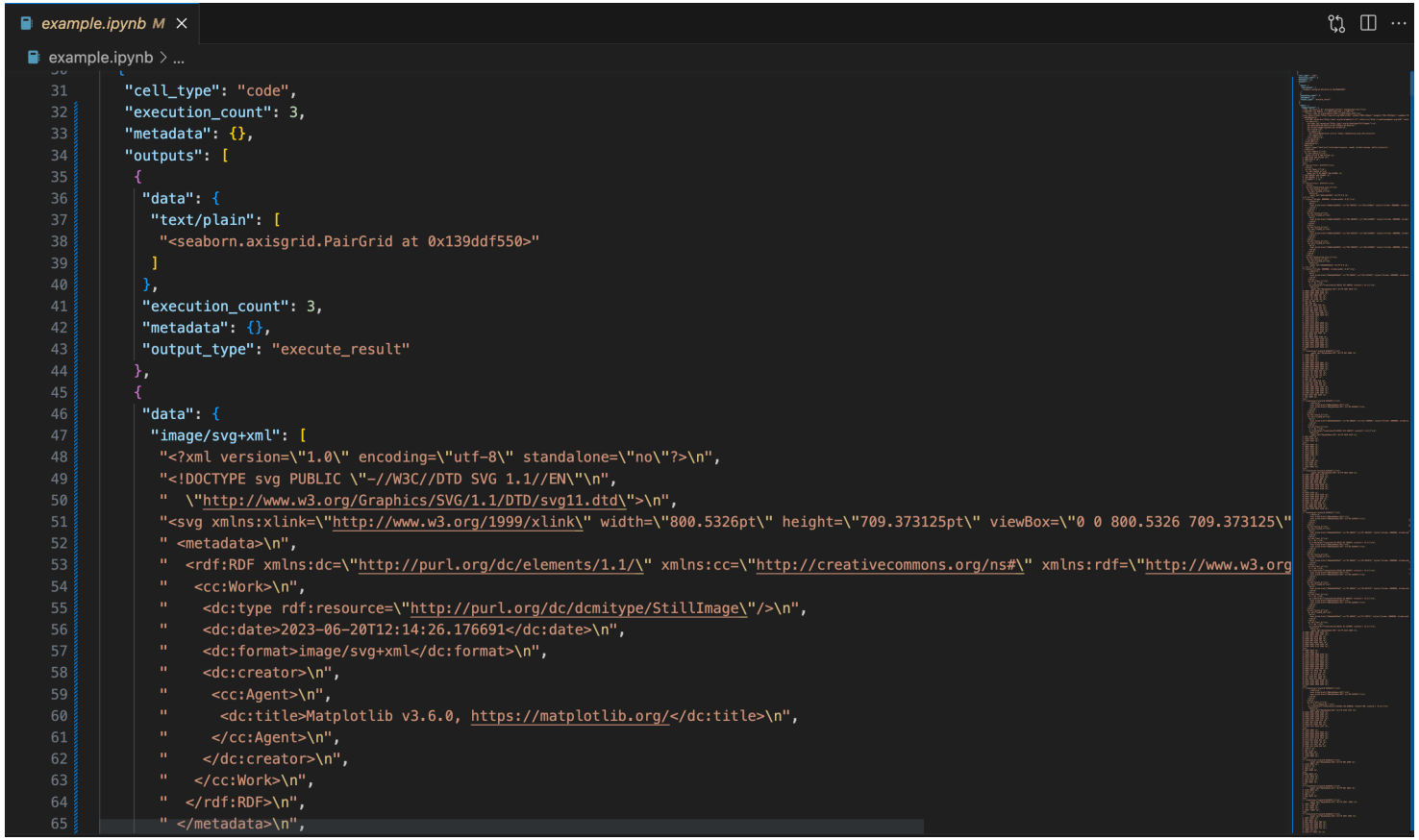
Tools of the Trade
Bonus tip: Jupyter notebooks in Version Control

The problem:

- Jupyter notebooks contain metadata, binary blobs, or other artifacts from execution
- Git tracks changed lines in text files
- Diffs become almost meaningless

Solution:

- Always clear the output before committing
- Use pre-commit hooks
- Use `nbstripout` (https://github.com/kynan/nbstripout)



Assignment

- Set up a skeleton project repository
- Start thinking about a ”business/research question” you want to explore in your project
- Start thinking about the kind of data you want to work with
- Start looking for corresponding data
  - Is it already available as a dataset? API? Possible and allowed to scrape?

Thank you