DSC Capstone Sequence

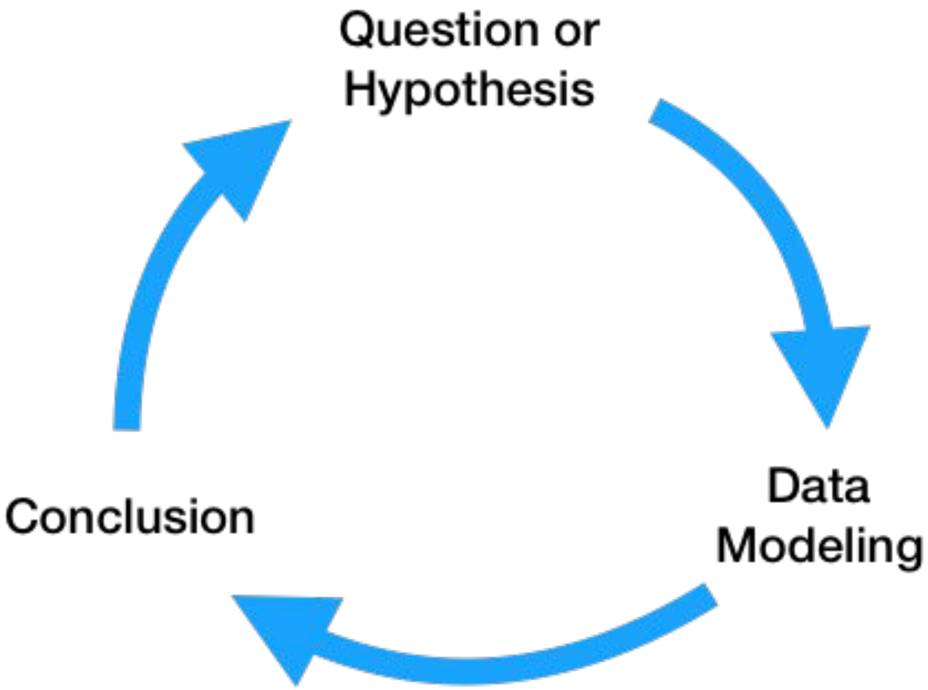
Lecture 03
Project Organization

Lecture Outline

- Goals of Data Science Software Development
- Anatomy of a Data Science Project
- Structuring a Data Science Project

The Goals of Data Science Software Development

Data Science Lifecycle

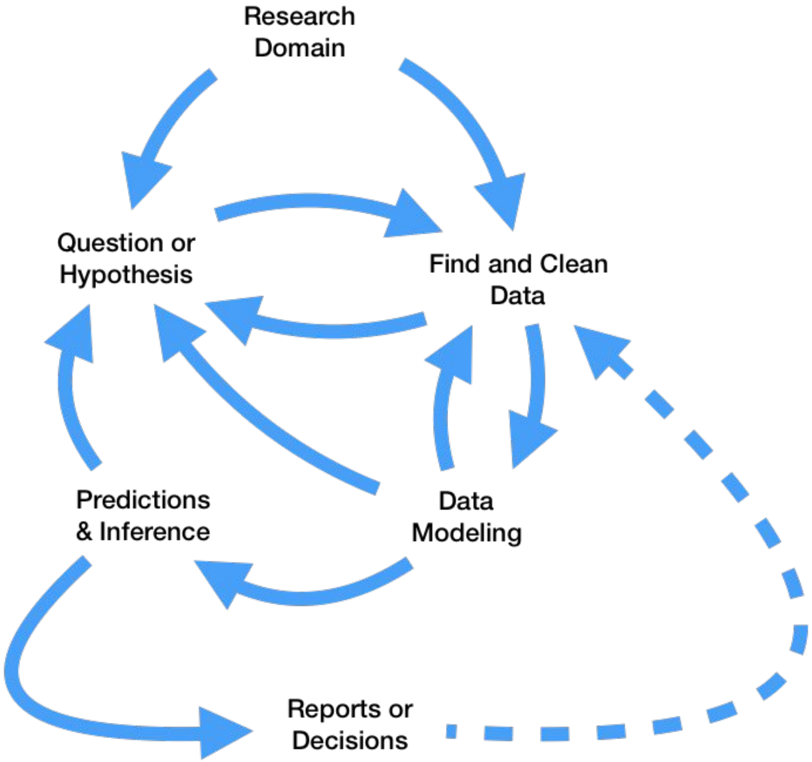


The code for an investigation must:

- Be flexibly written
- Clearly documented.
- Accessible to/Extensible for others.

In order to adapt to successive iterations through the lifecycle.

The *Real* Data Science Lifecycle



Poorly developed code results in:

- Fewer iterations and slower progress on the project
- Higher likelihood of mistakes in the results
- Difficult to understand conclusions
- The project fading into obscurity...

Better code ⇒ higher chance of success

Tools/Libraries for Managing Project Components

Managing Project Components

Too many tools to learn! (and keep up with new developments!)

Instead, learn the core issues:

- What contract does one component need to speak to another?
- Maximize the isolation of each component to enable easy code changes.
- Know each component's relationship to the computational graph:
  - When to recompute a step...
  - When can steps run in parallel?
- How different components scale as the project/data grows in scope?
- Best use of ‘configuration files’ to manage and track iterations.

The Anatomy of a Data Science Project

How each lifecycle component interacts with code

Domain Research

Domain Research informs the bulk of a project's structure:

- Why you made certain design decisions
- The context behind the quantities of interest
- The subset and kind of data used
- The cleaning logic and any simplifications in modeling

Understanding these choices requires:

- Extensive narrative **documentation** (Notebooks; markdown; pdf)
- **Code comments** to explain specific instances requiring context

Question / Hypothesis

The question being investigated changes as a project evolves.

When the questions are similar:

- Write code parameterized to handle *all* questions simultaneously.
- Choice of parameters ⇔ a different question.
- Parameters are kept in configuration files (e.g. json, ini, cfg, yaml).
  - E.g. Configuration file is an instruction to run 10 instances of the investigation, for 10 different questions, simultaneously on 10 different servers (e.g. questions by year for 2010-2020)
- Strive to write (and rewrite) code to parameterize many possible questions!

Data ETL (extract-transform-load)

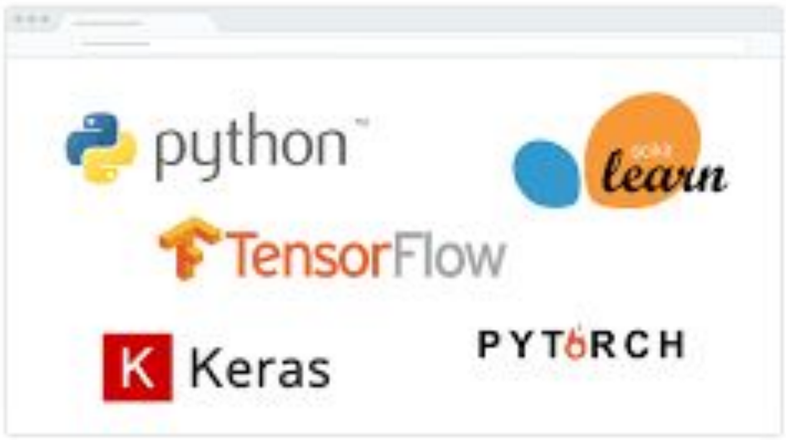
As a project evolves, the data may change or new data may be added…

- Keep schema and parameters in configuration (beware: magic numbers!)
- Is the source stable? (DB, API, Scrape)
  - Separate the data ingestion from any transformations
- Unnecessary computation wastes time and resources:
  - Problem: don't re-pull data because your cleaning code changed!
  - Answer: write intermediate files to disk (or a personal file store)
- Write processing code that is agnostic to the computer running it:
  - 'git clone => run' on your laptop or DataHub; scale up only when needed
  - Even better, is the intermediate data accessible from both? (and when do you want that?)

Model Building

Choosing the best model involves exploring *many* parameters!

- Keep track of parameters and results in configuration files.
- Use frameworks that enable 'pipelining' (e.g. sklearn, spark, tensorflow)
- Often need to scale-up processing on different servers



Continued Prediction / Inference

Once a model is built, a project often still lives on…

- Is the finished model being used for live predictions?
  - How does a scikit-learn model get called by a Java backend website?
  - `mdl.predict` may be called via HTTP-requests (RESTful interface).
- Model Quality Reporting:
  - If inference: is the project easily rerun on a new dataset? Can it be automated?
  - For live predictions: are the distributions of predictions stable? What is their quality? Can you create automated reporting?
- What if someone else uses the model? Does it work?
  - Package as a python module or in a Docker Container.

Conclusions / Decision / Report

Once a model is built to your satisfaction...

- Document and explain your results (e.g. in markdown).
- Justify any decisions made from the model
- Create reporting from the model
  - Update the reporting from new data, by rerunning project from scratch.
  - Email the compiled reporting (markdown=>HTML) automatically from a server.

Your project will fade into GitHub obscurity without good documentation!

Summary: Data Science Software Dev

A project should be:

- flexible for quick iterations
  - configuration vs code
- understandable to consumers/users of the output
  - thorough documentation and reports
- usable for developers/researchers extending your work
  - code/api documentation and deployability

Structuring a Data Science Project

Configuration vs. Code

Configuration vs Code

Isolate *code that does stuff* from the *parameters the code uses*.

- Code that is used by (multiple other) processes is called *library code*.
- *Configuration* consists of parameters that are passed into library code, and likely to change.
- When to abstract a piece of code to configuration depends on problem
    - Generalize, but don't over-generalize!

Where to place these files?

- Library code in py files; used by functions in scripts or notebooks
- Parameters as variables (imported by script or notebook)

Configuration vs Code

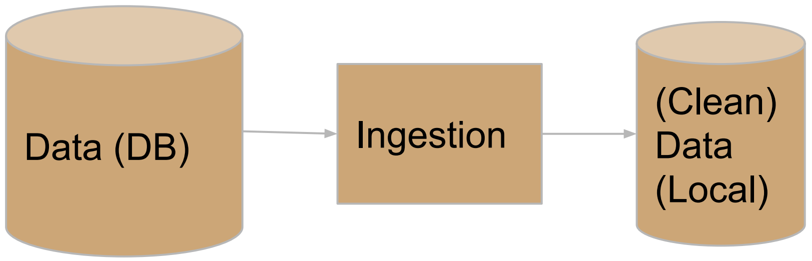
- Simple project separates:
  - library code, configuration
  - code that produces results/analysis (scripts / notebooks)
- More complicated projects have *directories* separating each of these!

```
Project
    |
    |----- code.py
    |----- config.txt
    |----- script.py
    |----- explore.ipynb
```

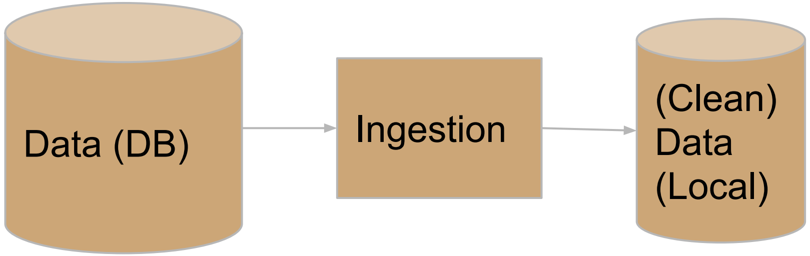
```
# Inside explore.ipynb / script.py
...
import code
params =
json.load(open('config.txt'))

code.run_process(**params)
```

Example: Data Ingestion

- Task: get data from internet to computer.
- Make it easy to (incrementally) change data ingested.
- Rerun to ‘refresh’ with new data.
- Run data pull on different servers to reproduce results



Data Ingestion: `etl.py`



- *Library code*: functions for use by other processes (nb, py files).
    - Good for interactive use; reusable.
    - Written as generically as practicable.
- Contains logic not necessary for a *consumer* of the project to know.
- Contains data collection logic other *developers* might want to expand on, when forking a project.
- Library code know nothing of what calls it!

```
Project
├── README.md
├── data-params.json
├── etl.py
└── run.py
```

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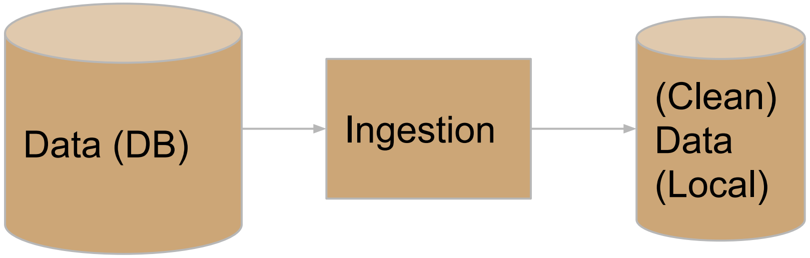
```
'''
etl.py contains functions used to download tables for different
teams and years.
'''

def get_season(team, year):
    '''
    return a table of season statistics for a
    given team and year.
    '''
    ...
    return ...


def get_data(years, teams, outdir):
    '''
    downloads and saves tables at the specified output
directory
    for the given years and teams.

    :param: years: a list of seasons to collect
    :param: teams: a list of teams to collect
    :param: outpath: the directory to which to save the data.
    '''
    ...
    return
```

Data Ingestion: `data-params.json`

- Configuration: parameters for different investigations and experiments.
- E.g. Parameterize across time/space.
- Used by the *consumer* of the project. Shouldn't require a knowledge of the source code!
- Helps log the results of different experiments.

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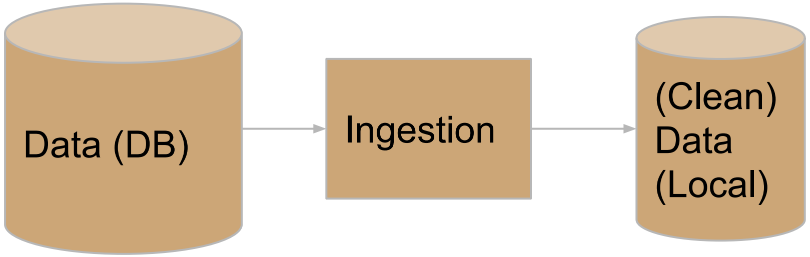
```json
{
    "years": [2015, 2016, 2017, 2018, 2019],
    "teams": ["sfo", "gnb"],
    "outpath": "data/raw"
}
```

Data Ingestion: `run.py`

- Script: Builds (common portions of) the project.
- Imports and runs library code: gives examples of *code usage*.
- Current: hand-made `run.py`
- Also possible to use specialized tools: python CLI (e.g. argparse), Makefiles, Maven, etc...




```
Project
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```

Data Ingestion: `run.py`

- Imports library code (`get_data`)
- Run as a script:
  - `python run.py data`
- Shebang: `#!/usr/bin/env python`
  - Specifies which python interpreter to use.
- `main` function strings together library functions with parameters in config.
- `__name__ == '__main__'...` returns true only when file is run as a script. Should only have minimal code inside.

```
#!/usr/bin/env python

import sys
import json

from etl import get_data


def main(targets):

    if 'data' in targets:
        with open('data-params.json') as fh:
            data_cfg = json.load(fh)

        # make the data target
        get_data(**data_cfg)

    return


if __name__ == '__main__':
    targets = sys.argv[1:]
    main(targets)
```

Structuring a Data Science Project

Templates and Cookie Cutter Data Science

Project Structure:

- As project grows, so does code complexity!
- As a project grows, it becomes unclear:
  - how code should be run...
  - what the code *does*...
  - if the code is correct...
- To simple to be realistic:

```
Project
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└── run.py
```

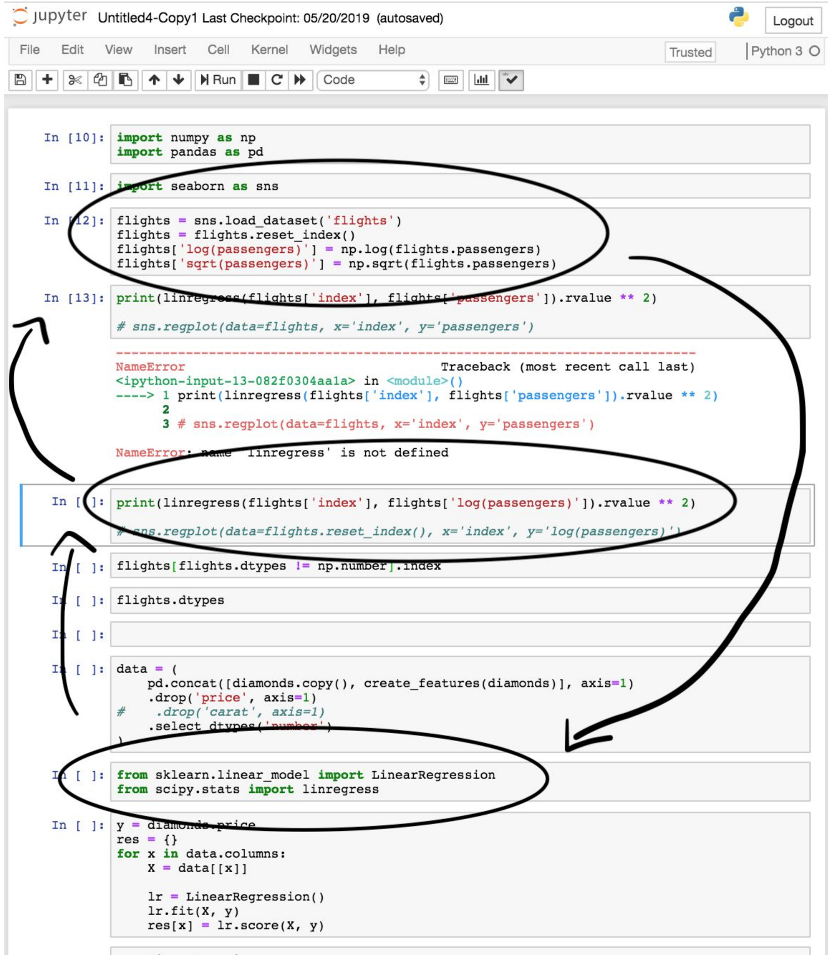

Why Care About Project Structure?

We're not talking about bikeshedding the indentation aesthetics or pedantic formatting standards — ultimately, data science code quality is about correctness and reproducibility.

Cookie Cutter Data Science

- Clear and consistent project organization encourages software development best-practices and readable code.
- Such habits yield more consistently correct code that's more easily fixed and adapted to other tasks.
- We will follow the opinions of [Cookie Cutter Data Science]()

An *Example* Project Template

```
├── .gitignore          <- files to keep out of version control (e.g. data/binaries)
├── run.py              <- run.py with commands like `make data` or `make train`
├── README.md           <- The top-level README for developers using this project.
├── data
│   ├── temp            <- Intermediate data that has been transformed.
│   ├── out             <- The final, canonical data sets for modeling.
│   └── raw             <- The original, immutable data dump.
├── notebooks           <- Jupyter notebooks (presentation only).
├── references          <- Data dictionaries, explanatory materials.
├── requirements.txt    <- For reproducing the analysis environment, e.g.
│                          generated with `pip freeze > requirements.txt`
├── src                 <- Source code for use in this project.
    ├── data            <- Scripts to download or generate data
    │   └── make_dataset.py
    ├── features        <- Scripts to turn raw data into features for modeling
    │   └── build_features.py
    ├── models          <- Scripts to train models and make predictions
    │   ├── predict_model.py
    │   └── train_model.py
    └── visualization   <- Scripts to create exploratory and results oriented viz
        └── visualize.py
```

Results are Derived from Immutable Raw Data

- Data is immutable: *never* edit raw data
    - Raw data is always (re)ingested from elsewhere.
    - File-path may be a *symbolic link* (shortcut), if stored locally.
    - **Raw data never changes => doesn't need version control! (.gitignore)**
- Final data is always reproducible from raw data (with run.py)
- Temp data holds data 'useful to keep around' for development, analysis, debugging, etc...

```
...
├── data
│   ├── temp            <- Intermediate data that has been transformed.
│   ├── out             <- The final, canonical data sets for modeling.
│   └── raw             <- The original, immutable data dump.
...
```

Notebooks are for Analysis and Communication

- Notebooks are great for communication, analysis, and initial development.
    - Use to create up-to-date, reproducible, static HTML reports.
- Complicated code in notebooks are hard to understand and don't work well with version control and collaboration.
- Notebooks should:
    - Mostly call library functions in src, with very simple code logic.
    - Never "copy-paste" code between notebooks -- if it's reusable, put it in a library function.
    - Name it something descriptive: `03-fraenkel-prelim-EDA.ipynb`

```
...
├── notebooks          <- Jupyter notebooks (presentation only).
...
```

Build from the Environment Up

- To reproduce a project from scratch, must also reproduce the computational environment on which it was run.
- requirements.txt contains all python libraries needed for running the project.
- `git clone project => mk virtualenv => pip install requirements.txt`
- When a project has more complicated requirements, may need to use container approach (e.g. Docker or Vagrant).

```
...
├── requirements.txt   <- For reproducing the analysis environment, e.g.
│                         generated with `pip freeze > requirements.txt`
...
```