Structuring a DS Project

Lecture 3, DSC 180A

Announcements

Assignment 1 Comments: Comment on Grading; Code Review Friday.

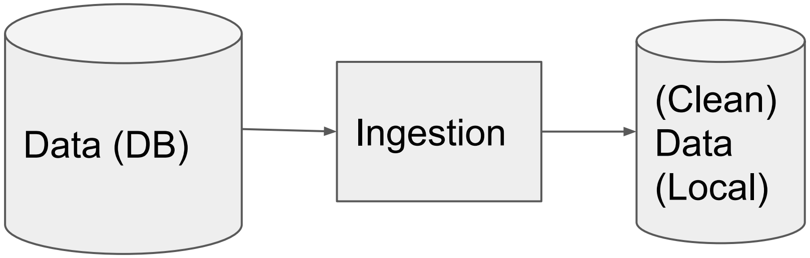
Working on projects:

- Work a little every day (things always go wrong!)
- Work in parallel on multiple pieces
- Don’t let a single step be a ‘blocker’.

Data Ingestion

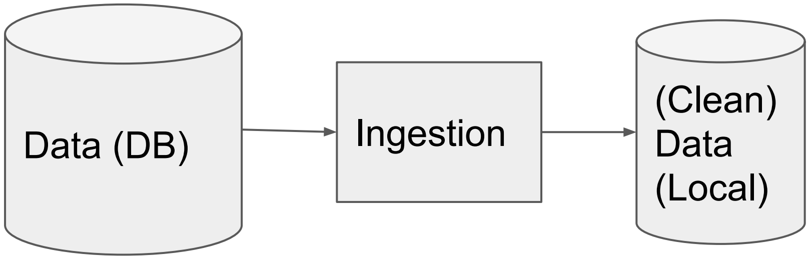
- Task: get data from internet to computer.
- Make it easy to (incrementally) change data ingested.
- Rerun to ‘refresh’ with new data.
- Run data pull on different servers to reproduce results

How to organize code to achieve this?



Data Ingestion: `etl.py`

- Library code: contains functions for importing by other processes.
- 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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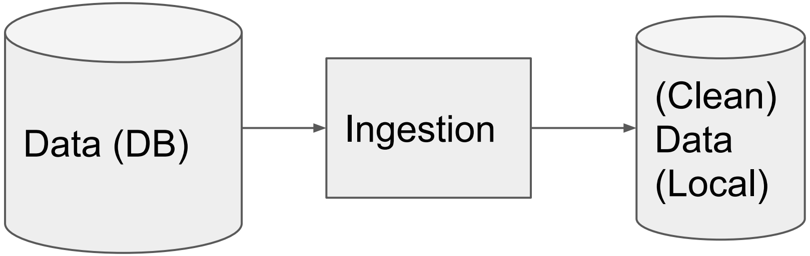
```
'''
etl.py contains functions used to download tables for different
teams and years.
'''

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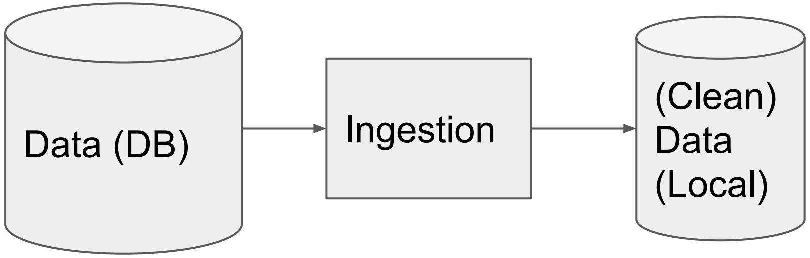
```
{
    "years": [2015, 2016, 2017, 2018, 2019],
    "teams": ["sfo", "gnb"],
    "outpath": "data/raw"
}
```

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...

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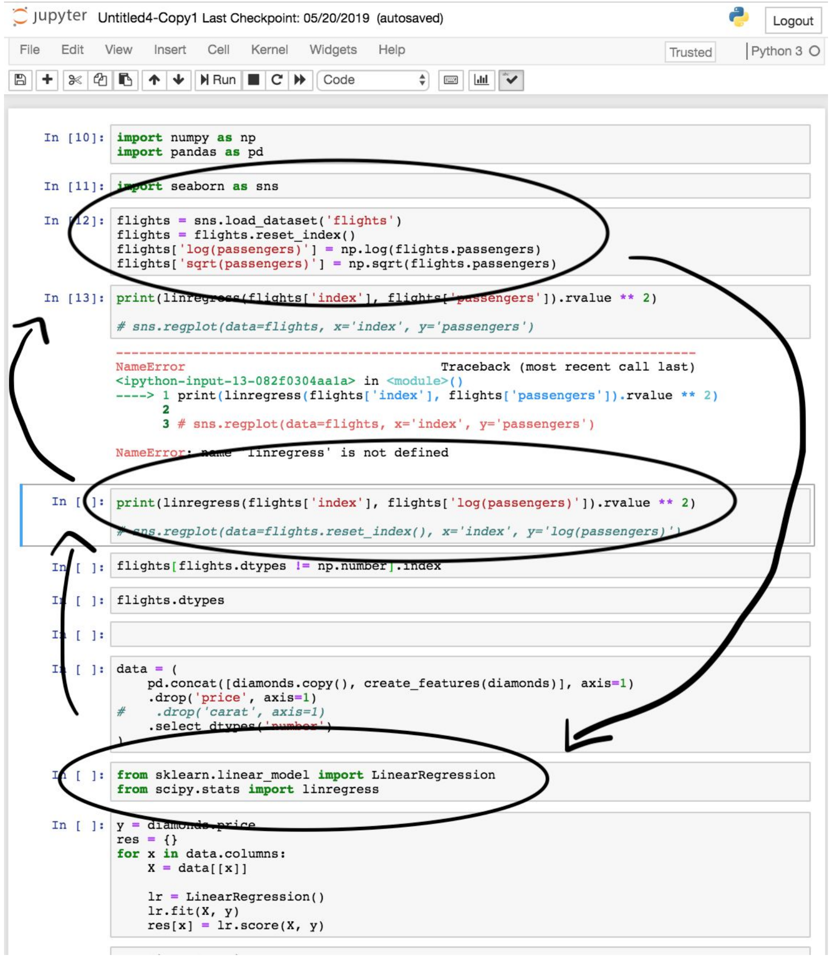
Data Ingestion: `run.py`

- 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)
```

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…



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.

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- 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.
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...
```