Data Science 1

STAT/CS 287

Jim Bagrow, UVM Dept of Math and Statistics

LECTURE 22

Coding for (data) science

Fundamental challenges

My goals for writing scientific code
are, in order of decreasing importance:

1. Correctness
2. Clarity
3. Conciseness
4. Efficiency/speed

High-level and low-level challenges

Coding for (data) science

Fundamental challenges

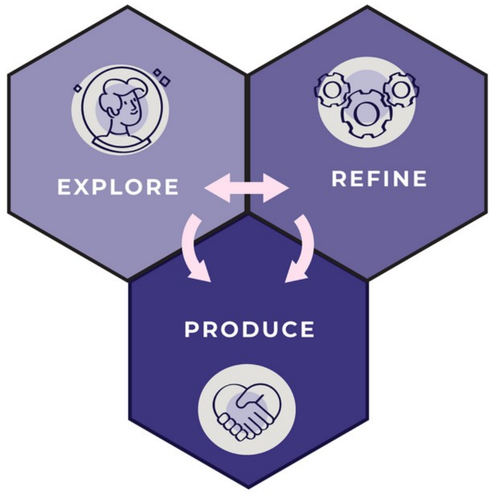
High-level

Low-level

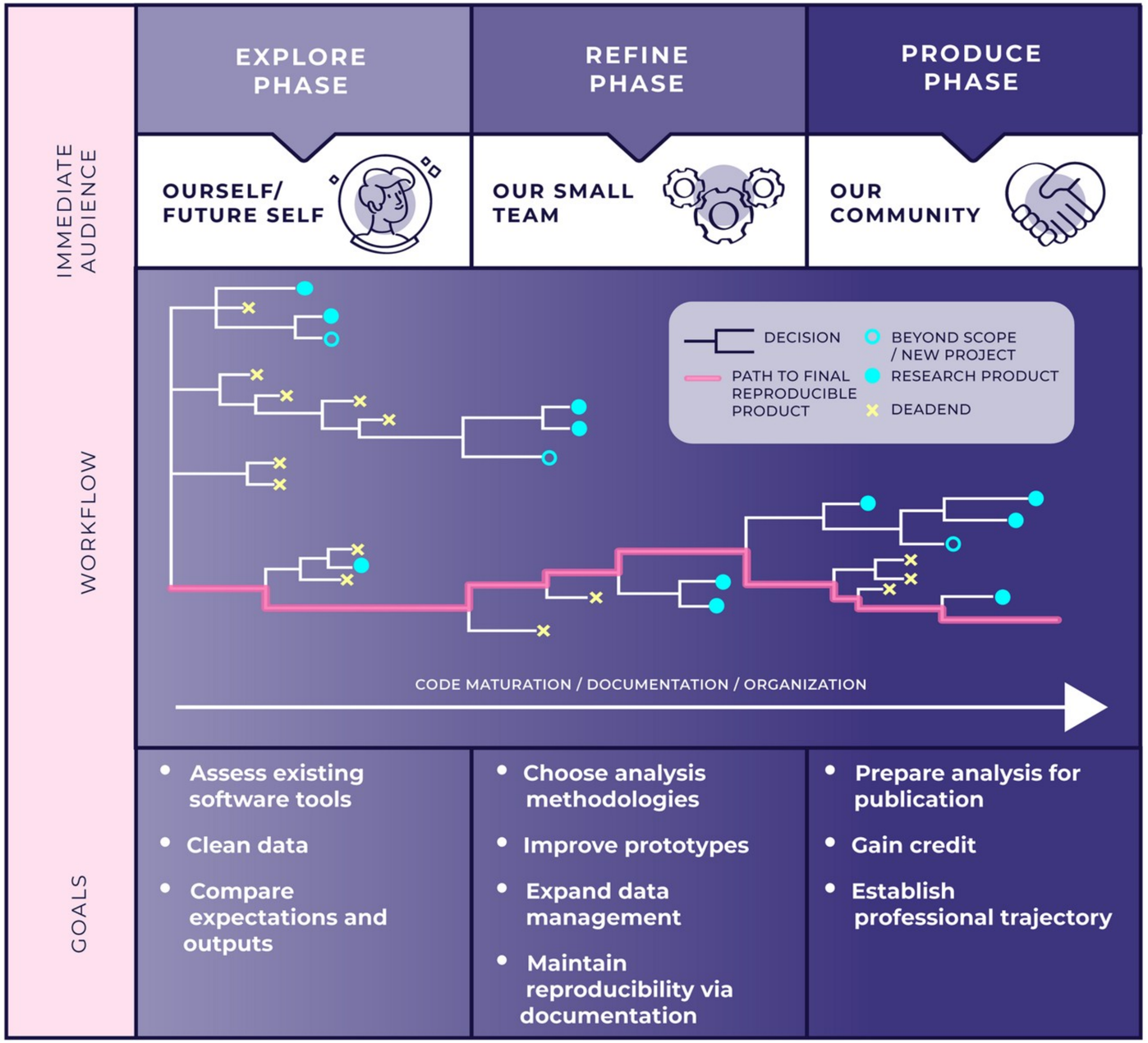
Coding for (data) sc

Fundamental challenges

High-level



Low-level



Stoudt, Vásquez, Martinez 2021

Coding for (data) science

Fundamental challenges

High-level

Low-level

pythontutor.com

Coding for (data) science

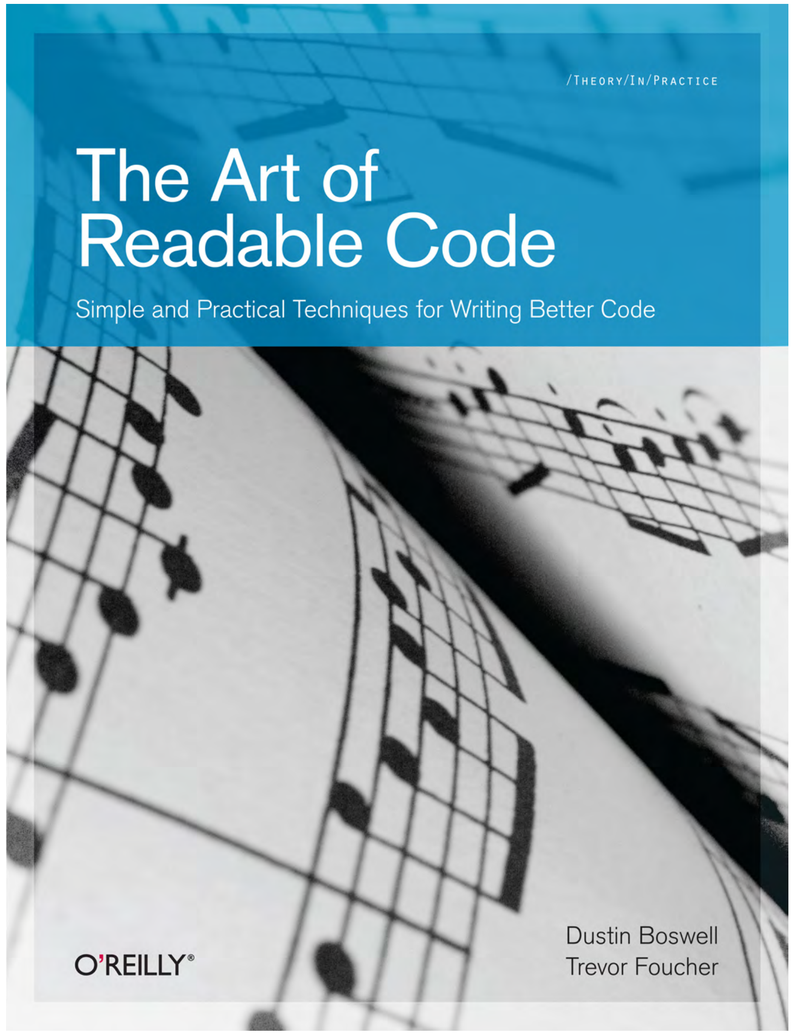
Fundamental challenges

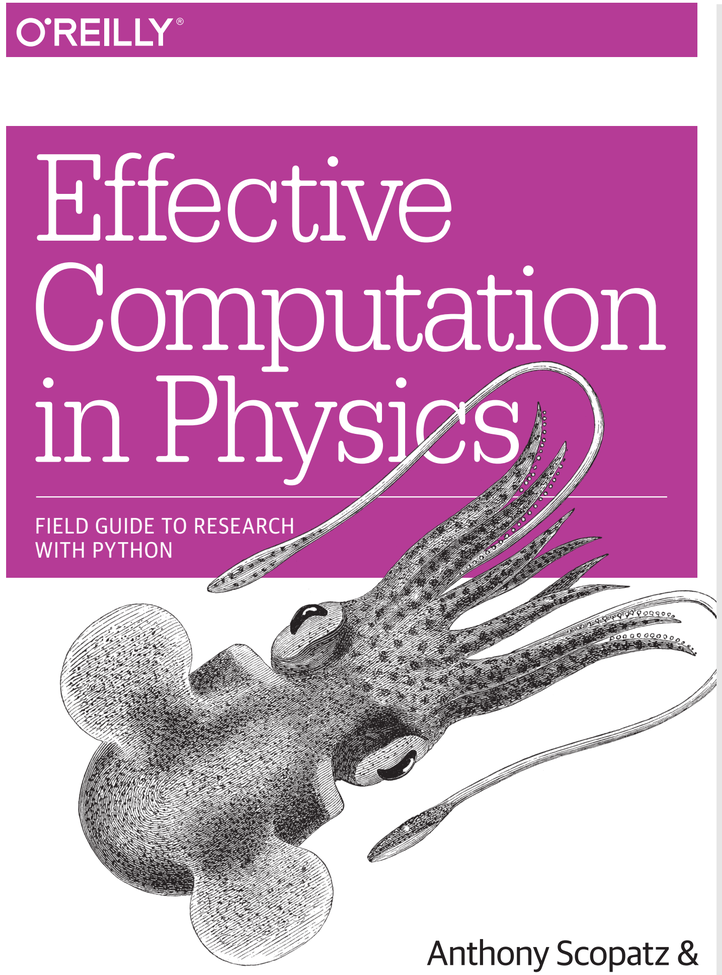
High-level

Low-level

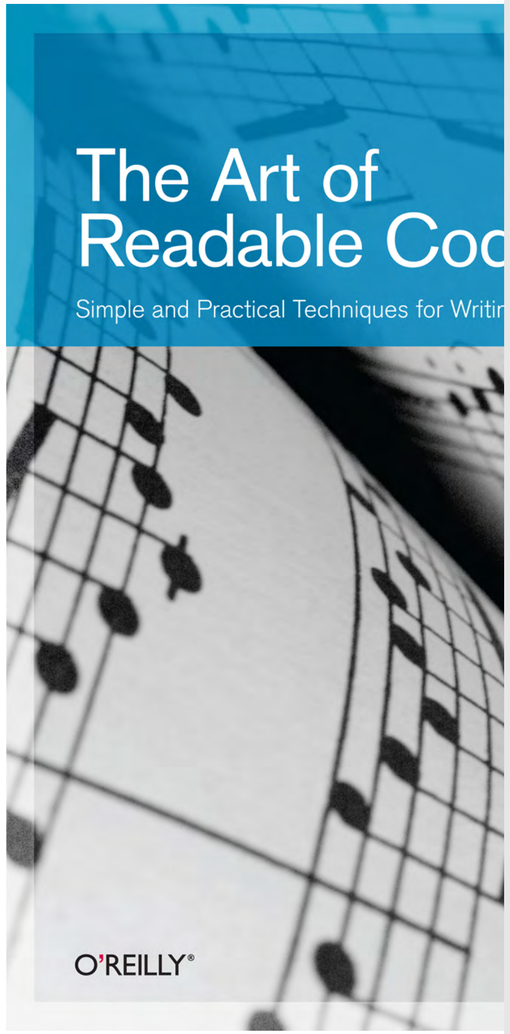
pythontutor.com

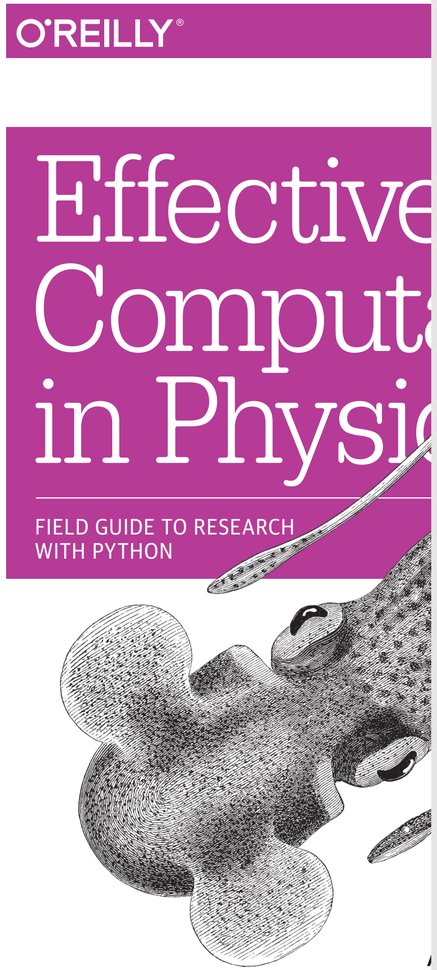
Some useful references





Some use s





James

Compare / Contrast

33 lines, 1583c

Compare / Contrast

```
for observation in dataset:
    if observation[0][1].lower() == 'bedford falls, new york':
        list1.append(observation)
    elif observation[0][1].lower() == 'derry, maine':
        list2.append(observation)
    elif observation[0][1].lower() == 'hill valley, california':
        list3.append(observation)
    elif observation[0][1].lower() == 'stepford, connecticut':
        list4.append(observation)
    elif observation[0][1].lower() == 'questa verde, california':
        list4.append(observation)
    elif observation[0][1].lower() == 'haddonfield, illinois':
        list5.append(observation)

for observation in list1+list2+list3+list4+list5:
    if observation[0][1].lower() == 'bedford falls, new york':
        plt.plot(observation[2], observation[3])
        plt.title('Bedford Falls, New York')
    elif observation[0][1].lower() == 'derry, maine':
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values hardwired throughout code

33 lines, 1583c

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repetition, redundancy

33 lines, 1583c

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values hardwired into code,
many manually-defined data structures

33 lines, 1583c

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values hardwired throughout code

repetition, redundancy

unclear names

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repetition, redundancy

copy-paste errors

33 lines, 1583c

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```

```
1775    +dt_water_max5+jno_water_max6+jne_water_max6+jnt_water_max6+fo_water_max6\
1776    +fe_water_max6+ft_water_max6+mo_water_max6+me_water_max6+mt_water_max6\
1777    +ao_water_max6+ae_water_max6+at_water_max6+myo_water_max6+mye_water_max6\
1778    +myt_water_max6+jo_water_max6+je_water_max6+jt_water_max6+jyo_water_max6\
1779    +jye_water_max6+jyt_water_max6+auo_water_max6+aue_water_max6+aut_water_max6\
1780    +se_water_max6+st_water_max6+oo_water_max6+oe_water_max6+ot_water_max6\
1781    +no_water_max6+ne_water_max6+nt_water_max6+do_water_max6+de_water_max6\
1782    +dt_water_max6+jno_water_max7+jne_water_max7+jnt_water_max7+fo_water_max7\
1783    +fe_water_max7+ft_water_max7+mo_water_max7+me_water_max7+mt_water_max7\
1784    +ao_water_max7+ae_water_max7+at_water_max7+myo_water_max7+mye_water_max7\
1785    +myt_water_max7+jo_water_max7+je_water_max7+jt_water_max7+jyo_water_max7\
1786    +jye_water_max7+jyt_water_max7+auo_water_max7+aue_water_max7+aut_water_max7\
1787    +so_water_max7+se_water_max7+st_water_max7+oo_water_max7+oe_water_max7+ot_water_max7\
1788    +no_water_max7+ne_water_max7+nt_water_max7+do_water_max7+de_water_max7\
1789    +dt_water_max7+jno_water_max8+jne_water_max8+jnt_water_max8+fo_water_max8\
1790    +fe_water_max8+ft_water_max8+mo_water_max8+me_water_max8+mt_water_max8\
1791    +ao_water_max8+ae_water_max8+at_water_max8+myo_water_max8+mye_water_max8\
1792    +myt_water_max8+jo_water_max8+je_water_max8+jt_water_max8+jyo_water_max8\
1793    +jye_water_max8+jyt_water_max8+auo_water_max8+aue_water_max8+aut_water_max8\
1794    +so_water_max8+se_water_max8+st_water_max8+oo_water_max8+oe_water_max8+ot_water_max8\
1795    +no_water_max8+ne_water_max8+nt_water_max8+do_water_max8+de_water_max8\
1796    +dt_water_max8+jno_water_max9+jne_water_max9+jnt_water_max9+fo_water_max9\
1797    +fe_water_max9+ft_water_max9+mo_water_max9+me_water_max9+mt_water_max9\
1798    +ao_water_max9+ae_water_max9+at_water_max9+myo_water_max9+mye_water_max9\
1799    +myt_water_max9+jo_water_max9+je_water_max9+jt_water_max9+jyo_water_max9\
1800    +jye_water_max9+jyt_water_max9+auo_water_max9+aue_water_max9+aut_water_max9\
1801    +so_water_max9+se_water_max9+st_water_max9+oo_water_max9+oe_water_max9+ot_water_max9\
1802    +no_water_max9+ne_water_max9+nt_water_max9+do_water_max9+de_water_max9\
1803    +dt_water_max9+jno_water_max10+jne_water_max10+jnt_water_max10+fo_water_max10\
1804    +fe_water_max10+ft_water_max10+mo_water_max10+me_water_max10+mt_water_max10\
1805    +ao_water_max10+ae_water_max10+at_water_max10+myo_water_max10+mye_water_max10\
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tures

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1798    +ao_water_max9+ae_water_max9+at_water_max9+myo_water_max9+mye_water_max9\
1799    +myt_water_max9+jo_water_max9+je_water_max9+jt_water_max9+jyo_water_max9\
1800    +jye_water_max9+jyt_water_max9+auo_water_max9+aue_water_max9+aut_water_max9\
1801    +so_water_max9+se_water_max9+st_water_max9+oo_water_max9+oe_water_max9+ot_water_max9\
1802    +no_water_max9+ne_water_max9+nt_water_max9+do_water_max9+de_water_max9\
1803    +dt_water_max9+jno_water_max10+jne_water_max10+jnt_water_max10+fo_water_max10\
1804    +fe_water_max10+ft_water_max10+mo_water_max10+me_water_max10+mt_water_max10\
1805    +ao_water_max10+ae_water_max10+at_water_max10+myo_water_max10+mye_water_max10\
1806    +myt_water_max10+jo_water_max10+je_water_max10+jt_water_max10+jyo_water_max10\
```

tures

33 lines, 1583c

Compare / Contrast

```python
for observation in dataset:
    if observation[0][1].lower() == 'bedford falls, new york':
        list1.append(observation)
    elif observation[0][1].lower() == 'derry, maine':
        list2.append(observation)
    elif observation[0][1].lower() == 'hill valley, california':
        list3.append(observation)
    elif observation[0][1].lower() == 'stepford, connecticut':
        list4.append(observation)
    elif observation[0][1].lower() == 'questa verde, california':
        list4.append(observation)
    elif observation[0][1].lower() == 'haddonfield, illinois':
        list5.append(observation)

for observation in list1+list2+list3+list4+list5:
    if observation[0][1].lower() == 'bedford falls, new york':
        plt.plot(observation[2], observation[3])
        plt.title('Bedford Falls, New York')
    elif observation[0][1].lower() == 'derry, maine':
        plt.plot(observation[2], observation[3])
        plt.title('Derry, Maine')
    elif observation[0][1].lower() == 'hill valley, california':
        plt.plot(observation[2], observation[3])
        plt.title('Hill Valley, California')
    elif observation[0][1].lower() == 'stepford, connecticut':
        plt.plot(observation[2], observation[3])
        plt.title('bedford falls, new york')
    elif observation[0][1].lower() == 'questa verde, california':
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        plt.title('bedford falls, new york')
    elif observation[0][1].lower() == 'haddonfield, illinois':
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        plt.title('bedford falls, new york')
```

33 lines, 1583c

```python
locations = ['Bedford Falls, New York',
             'Derry, Maine',
             'Hill Valley, California',
             'Stepford, Connecticut',
             'Questa Verde, California',
             'Haddonfield, Illinois']

loc2obs = {}
for loc in locations:
    loc2obs[loc.lower()] = []

for observation in dataset:
    name = observation[0][1].lower()
    loc2obs[name].append(observation) # keyerror if unexpected loc

for location in locations:
    obs = loc2obs[location.lower()]
    times = obs[2]
    rates = obs[3]
    plt.plot(times, rates)
    plt.title(location)
```

21 lines, 577c

Compare / Contrast

Good practices

- DRY principle - *don't repeat yourself*
  - lean on functions, data structures (and know how the work)
  - avoid copy-paste
  - let the computer do the work
- isolate data from code
- use informative names
  - treat code as a written document
- Human working memory is limited
  - keep information local
- don't work blind (IPython, etc.)

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21 lines, 577c

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How to make the code

- work slowly, make incremental changes
- be prepared to revise
- optimize only when needed
- don't write code you don't need
  - code is only useful when it answers your questions

Research template

What about a "pipeline"?

Can you define a rough, reusable standard organization for (data) scientific investigations?

Pipeline or workflow:

```
[01-load data]
[02-process data]
[03-investigate Qs of interest]
[04-save results]
```

???

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???

```
├── README.md          <- The top-level README for contributors using this project.
├── .flake8            <- Standard config for Flake 8 linter (run `flake8 src` frequently)
├── data
|   ├── 00-external    <- Data from third party sources.
|   ├── 01-raw         <- The original, immutable data dump.
|   ├── 02-interim     <- Intermediate data from 00 or 01 that has been transformed.
|   └── 03-processed   <- The final, canonical data sets
|
├── methods-models     <- Trained and serialized models, model predictions, or model summaries
|                         Other analysis tools archived in separate subdirectories, kept as
|                         Git submodules, etc.
|
├── notebooks          <- Jupyter notebooks. Naming convention is a number (for ordering),
|                         the creator's initials, and a short `-` delimited description, e.g.
|                         `01.0-jpb-initial-data-exploration`.
|
├── references         <- Data dictionaries, manuals, papers, and all other explanatory materials.
|
├── reports            <- Generated analysis as HTML, PDF, LaTeX, etc.
|   └── figures        <- Generated graphics and figures to be used in reporting
|
├── setup.py           <- makes project pip installable (pip install -e .) so src can be imported
├── src                <- Source code for use in this project.
|   ├── __init__.py    <- Makes src a Python module
|   |
|   ├── data-gathering   <- Scripts to download or generate data.
|   |   └── make_dataset.py
|   |
|   ├── analysis-modeling <- Scripts to train models and then use trained models to make predictions
|   |   |                    (if there is a machine learning component to the project).
|   |   ├── predict_model.py
|   |   └── train_model.py
|   |
|   ├── data-processing  <- Scripts to process data, for example turn raw data into features for
|   |   |                   modeling.
|   |   └── build_features.py
|   |
|   ├── simulations      <- Scripts for performing simulations, if any.
|   |
|   └── visualization    <- Scripts to create exploratory and results oriented visualizations
|       └── visualize.py
|
└── stats              <- Store intermediary analyses results, data for plotting, etc.
```

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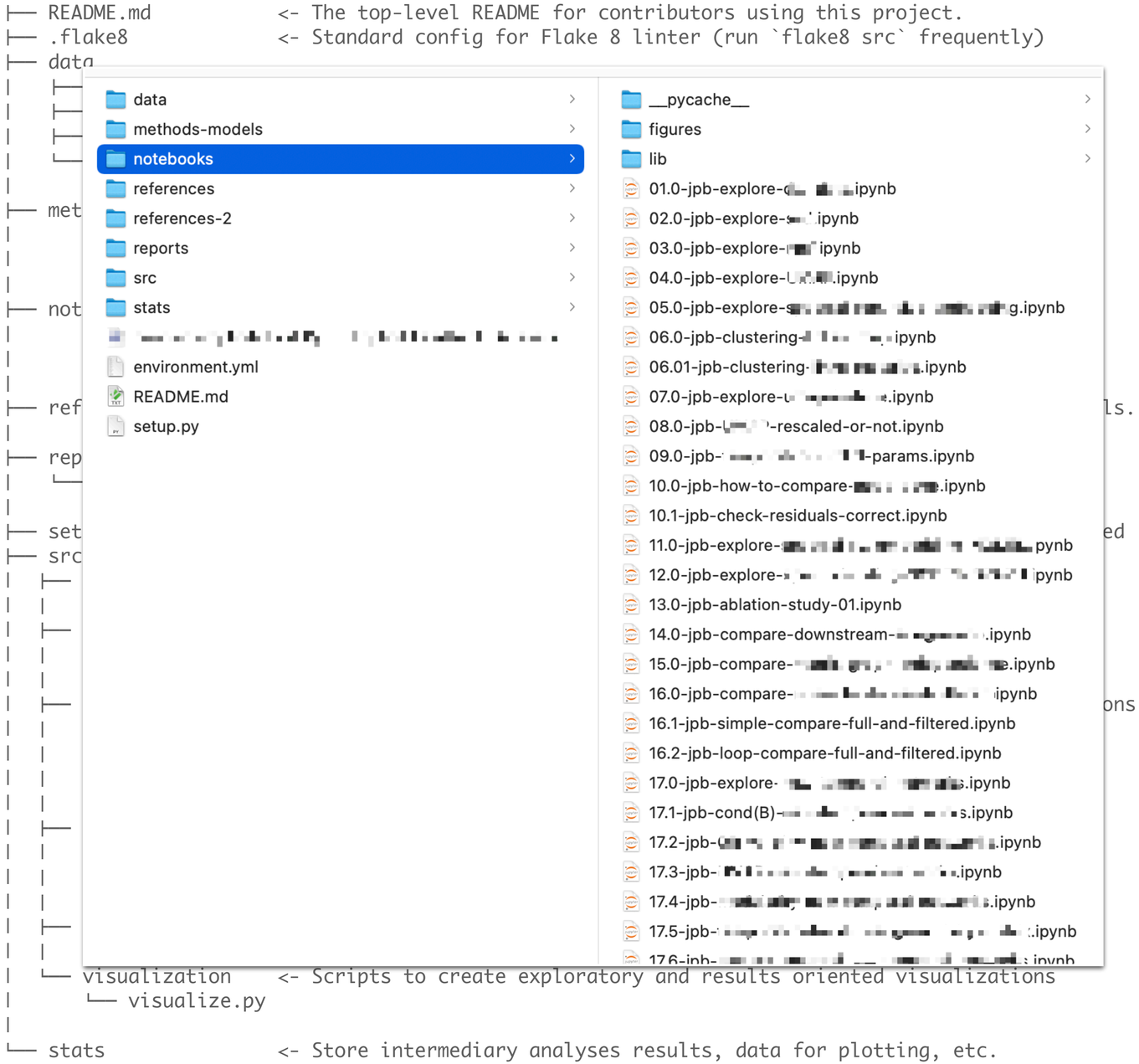

Research template

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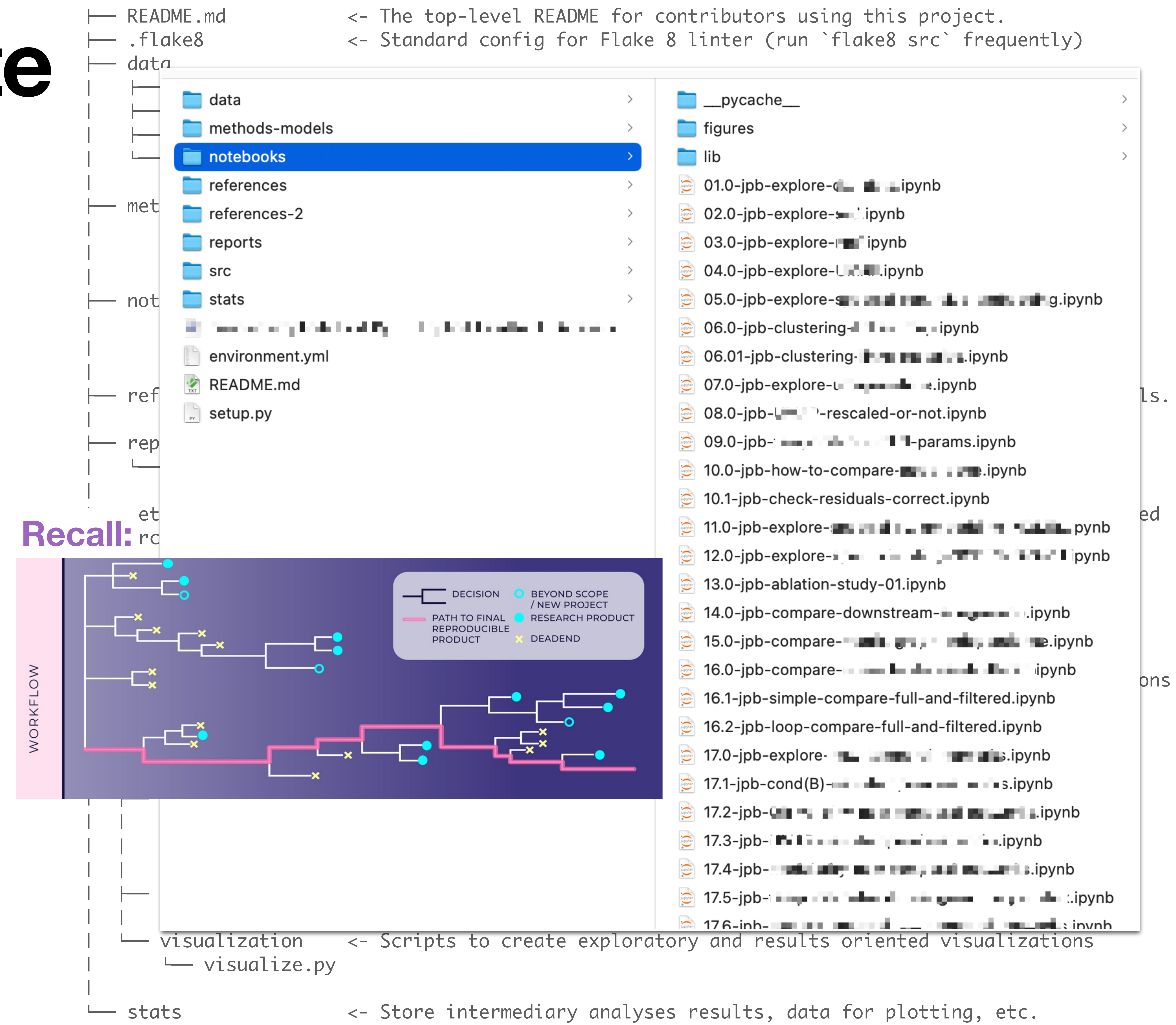
(Can something like this help with the explore-refine-produce loop?)



Team exercise | Coding for (data) science

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Plan

1. Break out into your teams
2. Teams choose a team manager
   - keeps discussions on track, makes sure everyone has a turn
3. Each team member in turn:
   - presents their code file(s) for one assignment, what they did and why, what they struggled with, etc.
   - others follow along, taking notes
   - hold a (construction) discussion about the code
   - ~10min per team member, depending on team size and time
4. Any remaining time: work on a research template

- *Ask me questions at any time*

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Deliverables

Team — design a general data science "workflow" template

Individual — Written reflection:

1. My code (~1 page):
   - Could I accomplish as much or more with less?
   - Opportunities for functions, (better) data structures?
   - Defensive data analysis - what will my code do when given bad data? If the data changed?
   - How easily can team members understand my code?
2. Each team member's code (~1 page total):
   - Summary of their work compared to yours
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   - What approach did they take to the problem that I can use in the future? That is, what's a takeaway I see from their code?
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Logistics

Attendance — taken at end

Files — on Blackboard (coming soon)

Due — last day of classes (see Blackboard)

Grading — bonus:

- Replaces lowest quiz or HW grade, whichever helps more, after lowest grade(s) dropped and only if it helps final grade