Science Hacking 101:

Tips and tricks for writing good, shareable code

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Roadmap

1. The principle of simplicity
2. Coding: basic workflow, syntax, design
3. Storyboarding: creating “user stories”
4. Testing: when is it needed?
5. Debugging: tools, general strategies
6. Optimization: when? How?
7. Releasing your code
8. Summary

Simplicity

Simplicity

- **Simplicity**: the art of maximizing the amount of work *not* done.

- When in doubt, ask yourself: “what is the *simplest* way I can approach this part of the project?”

- You may need to design things the messy way first to understand all of the nuances. Then go back and think about the cleanest/simplest implementation. (Future you will appreciate it!)

- How does the principle of **simplicity** translate into good design practices?

Simplicity: code

- **Write everything once** and re-use. (***Modular*** programming; next slide)

- Consolidate the formats of inputs and/or use cases early (***funneling***; more on this later).

- **Fail fast**, before you've wasted the user's time. This also helps with debugging.

- **Minimize work for the *user*** when possible (e.g. set sensible defaults).

- Keep **syntax** and design clean, consistent, and free from clutter.

- **Simple** is often better than **fast**. (More on optimization later.)

Modular programming

- Idea: design code around *modules* that accomplish simple, general purpose tasks.

- Combine modules to accomplish more complex tasks.

- High-level functions should comprise (only) the main algorithm, with calls to lower-level modules to do anything complicated.

- Goal: someone reading your code should be able to quickly understand what your algorithm is, even for high-level functions.

- Modular programming helps minimize redundant code by facilitating re-use. It also facilitates optimization: optimizing one lower-level model will speed up all higher-level modules that depend on it!

Modular programming

- When you have multiple modules that do the similar things, consider:
  - Can I create a new lower-level module that my existing modules could call?
  - Could I create a more general-purpose module and consolidate my code?

Simplicity: packaging

- Keep focus **well-defined** and limited in scope. Ask: “what specific problems does my project solve, and what *doesn’t* it solve?”
    - Note: project scope can (and should!) evolve over time
- Keep folders and organization as flat as possible (more later)
- Modular designs facilitate development, maintenance, testing, and re-use/re-purposing

When to simplify

- If you are going to be using your code a lot, it's worth simplifying and cleaning it up.

- If you are going to be sharing your code, it's worth simplifying and cleaning it up.

- If you plan to re-visit your code later, or if you want other people to understand your code, it needs to be simple and clean.

- If you are writing a simple "one off" script that you are only going to use rarely (and that isn't going to be shared), a quick and dirty solution may be fine. Simple sometimes means: get something out quickly and easily.

Coding

Basic workflow

- You may want to use a variety of tools.

- Set up the package in PyCharm, Atom, or similar. Git integration and a nice debugger are key. Package management, syntax highlighting, code completion, etc. are also useful.
    - PyCharm has an especially nice debugger.

    - Atom (via plug-ins) supports collaborative coding, which is great for hackathon sessions.

- Once you have a prototype of the library ready, use Jupyter notebooks to run some tests. It's difficult to write serious packages purely in Jupyter— there's no great way of organizing or integrating across files.

Syntax

- Adhere to the **PEP8** style guide for Python code (or equivalent for other languages, when possible): https://www.python.org/dev/peps/pep-0008/.

- **Consistency**: within each type of named object (variables, functions, constants, loop iterators, etc.) use the same naming scheme and style. Keep names simple but descriptive.

- Use **spaces** around operators (e.g. `a += b * c`).

- Keep code **visually clean** by writing short lines and grouping related lines. Goal is to maximize code readability at a glance.

- **Use comments sparingly** but consistently to describe the API (for user-visible functions or complex internal functions) and to describe algorithms (if not obvious).

Syntax: naming styles

- `x` (single lowercase letter): loop iterators, minor scalar variables
- `X` (single uppercase letter): constants, matrices
- `lowercase`, `lowercase_with_underscores`: variables
- `UPPERCASE`, `UPPERCASE_WITH_UNDERSCORES`: usually constants
- `CamelCase`: classes
- `mixedCase`, `Capitalized_Words_With_Underscores`: no

Syntax: messy code

```
def AddSomeNumbers( my_data ):

  my_sum = 0 #keep track of the sum

for LoopIterator in range( len( my_data ) ):

  #add the next value to the sum

  my_sum += my_sum+my_data[ LoopIterator ]

return my_sum
```

Syntax: clean(er) code

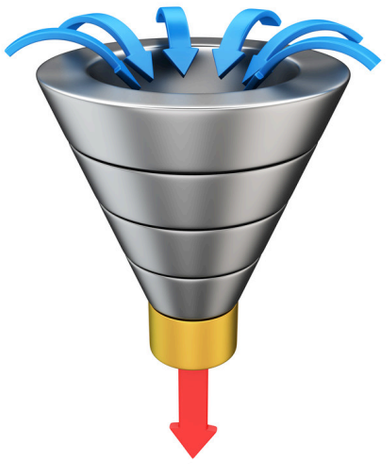
```
def sum(x):

    y = 0

for i in range(len(x)):

    y += x(i)

return y
```



Funneling

- Writing general purpose (modular) functions often requires supporting a variety of input formats

- To simplify package design, “funnel” data and arguments into a consistent format as early as possible

- This lessens the burden on internal functions and modules, with respect to the number of data formats and options they need to support

When should you funnel?

- If you check for formatting-related properties (e.g. class types, data dimensions, presence of particular arguments), this should be done **once** at the beginning of your function (and only in functions that the user interacts with directly).

- If you have a lot of “special cases” in your code, you may be able to simplify by funneling.

- Internal functions, or functions that only support one use case, probably come “pre-funneled.”

Funneling example

```
def brain_plotter(data, *args, **kwargs):
    [data, opts] = format_data(data, *args, **kwargs)

    analyzed = analyze_data(data, opts)

    plot(analyzed)
```

When to split {lines, functions, files, folders}

- **Lines** should be grouped if they are conceptually and/or syntactically related (import statements, performing a related series of calculations on similar data, etc.)

- **Make a separate function** if the group of lines is going to be used by other functions, or if it'll be repeated several times

- **Make a separate file** to organize all functions within a file around a low-level goal or task (e.g. display, i/o, data wrangling, etc.). Caveat: each file should be about a page long. Avoid creating many small files or few very large files.

- **Make a separate folder** to organize files around the same higher level goal (e.g. stats, plotting, interface, etc.). Try to keep the total number of folders small and the organization relatively flat. Avoid "mirrored" structure across different folders, unless that is a specific design feature (e.g. data format, tutorial format in this repo).

Storyboarding

TITLE SCREEN
FADE IN FROM BLACK
6 seconds

SPACE SHIP HOVERS FOR A MOMENT AND THEN FLYS TOWARDS A DISTANE EARTH
5 seconds

SPACE SHIP ON SURFACE OF MARS
4 seconds

SPACE SHIP FLYS OVER CITYSCAPE
5 seconds

ALIEN ENTERS INTO SPACE SHIP
4 seconds

PERSON ON GROUND SPOTS SPACE SHIP
6 seconds

Storyboards

- Describe “user stories” about different intended use cases. Try to imagine **why** the user is here and **what** they are trying to do.

- Help enforce a user-centric developer mindset.

- Provide a minimum viable set of formats and scenarios to support. This defines the project scope.

- Define a set of test cases that need to be checked.

- Be as specific as possible. If a use case doesn’t apply to a given story, it may need its own story...or it may be beyond the intended scope of the project.

Storyboards: examples

- Alice is a neurologist with a collection of structural MRI images. She wants to create detailed images to help her visually identify potential anatomical anomalies in her patients' brains.

- Bob is a psychologist with a collection of functional MRI images. He wants to make animations of brain activity changing over time during different experimental conditions so that he can add a slide to his Keynote presentation.

- Carol is a computer scientist who wants to apply pattern classifiers to structural and functional data from Neurovault. She wants to create a summary plot of which brain regions were most informative.

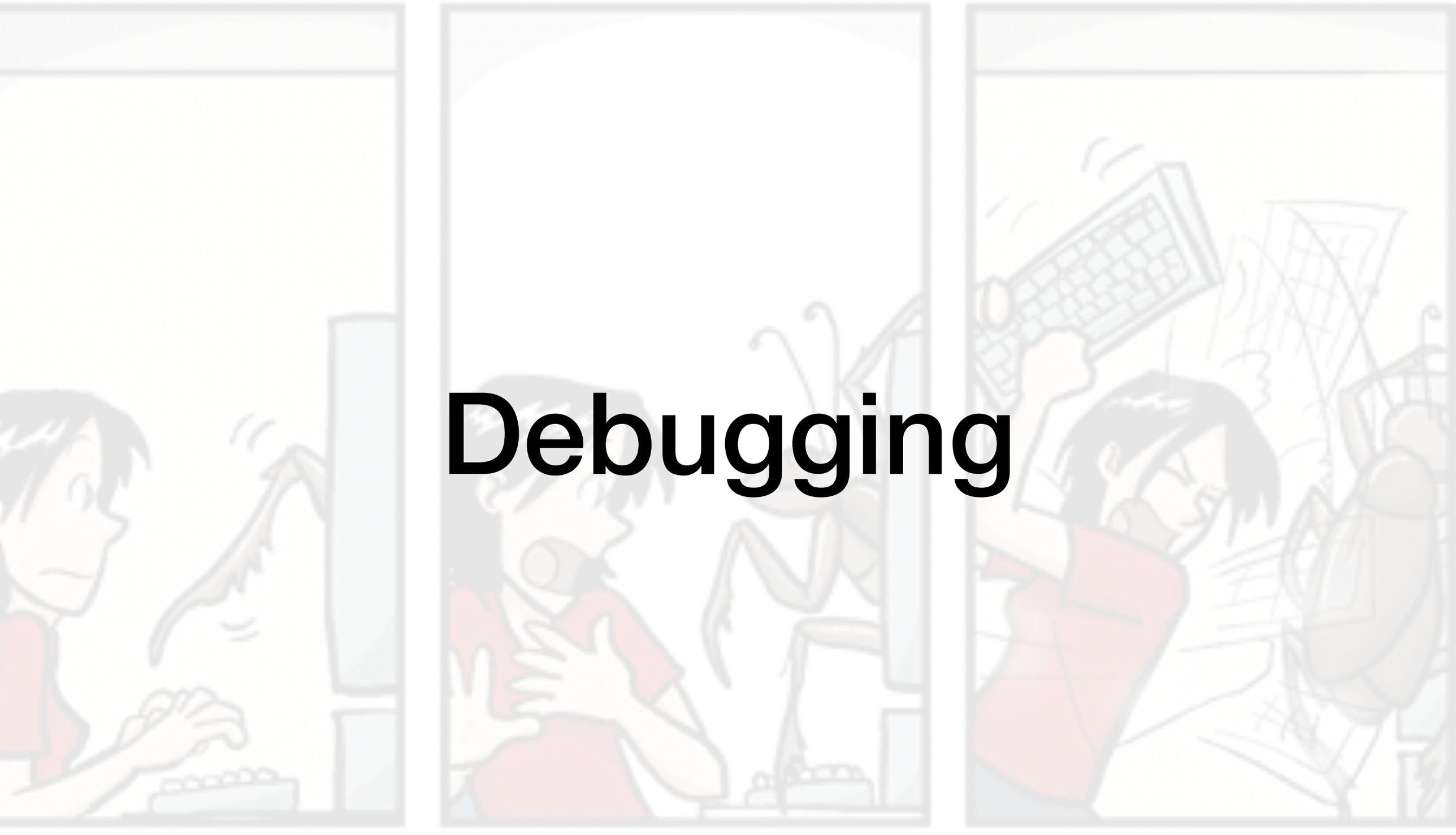
- Dave is a research assistant who wants to process functional MRI data in near real time as part of a neurofeedback experiment. He needs to read the data, preprocess the images, and predict the participant's mental state within a 2 second window.

Testing

What needs to be tested?

- Test each storyboard and recommended use case.
- As new storyboards are added, new tests are needed.
- Set up testing **early** to make your life easier in the long run— it's much easier to start simple and add/modify than to do everything at the end,
- Generate a variety of sample datasets and scripts that push on each place that your code might break.
- TravisCI (next week!)

Debugging



Debugging: tips and tricks

- **Section out the one thing you're trying to fix and make it easy and fast to run (i.e. "get to that point" in the execution pipeline).**

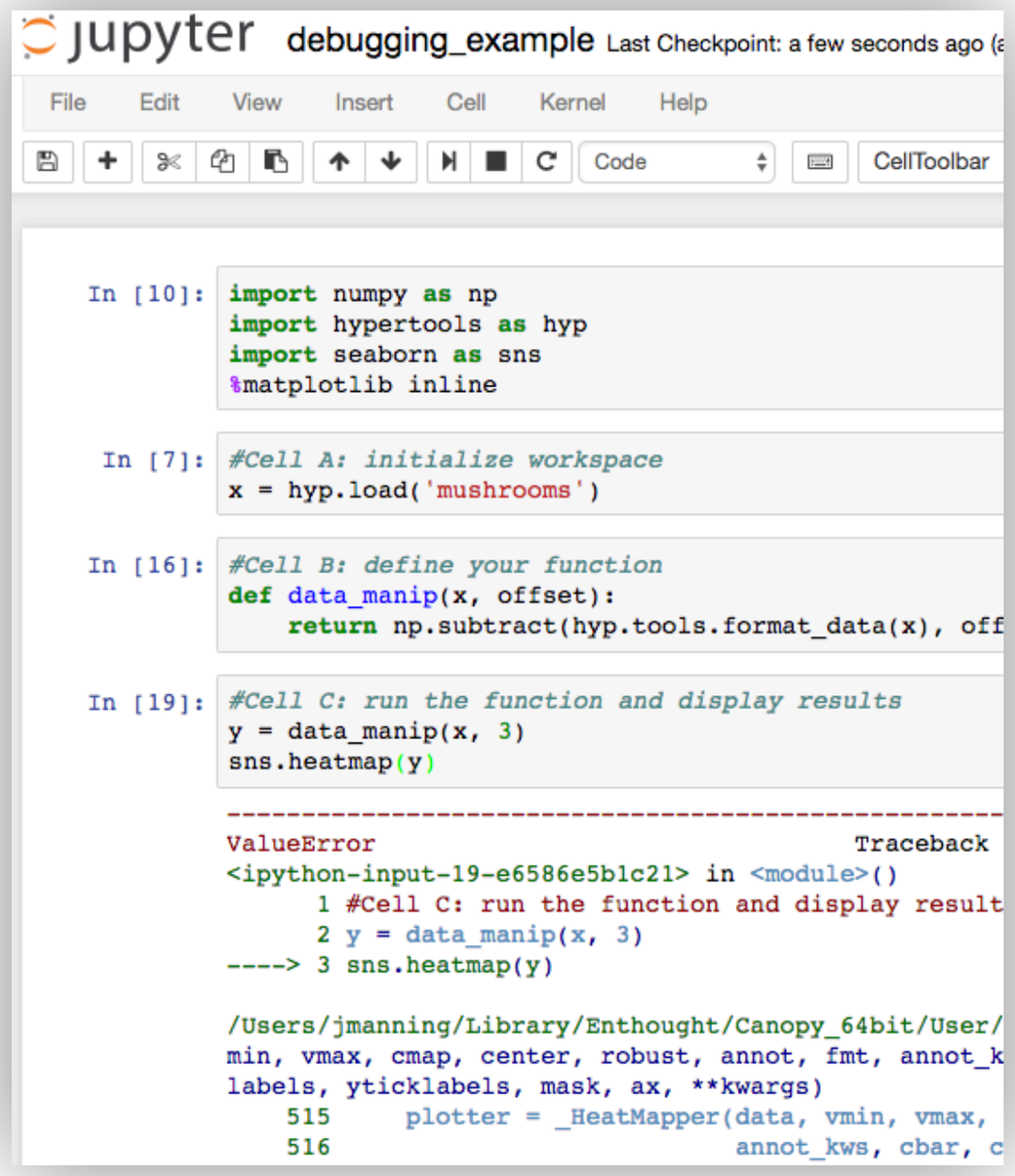
- Use small test datasets to allow you to run your tests quickly.

- Minimize the amount you need to do to re-run your test case (e.g. re-typing, re-starting, etc.). For a tricky debugging session you might be running the same code hundreds of times. Make this easy!

- Ideally identify the simplest scenario where your bug shows up, and just try to fix that (this is sometimes tricky).

Debugging: Jupyter

- Good for rapid debugging
- Basic setup:
  - Initialize/reset your workspace in cell A
  - Define your function in cell B (this is what you'll be modifying)
  - Run the function and display results in cell C
  - To debug, run A, then B, then C



Debugging: PyCharm

- Good for complex bugs
- Full tutorial: https://www.jetbrains.com/help/pycharm/part-1-debugging-python-code.html
- Set up Python environment and packages
- Set up breakpoints
- Add a “debug” script for your file
- Use console to interact with (and fix) your code as it’s running

```
    def demo(self, a, b, c):
        d = b ** 2 - 4 * a * c
        if d > 0:
            disc = math.sqrt(d)
            root1 = (-b + disc) / (2 * a)
            root2 = (-b - disc) / (2 * a)
            return root1, root2
        elif d == 0:
            return -b / (2 * a)
        else:
            return "This equation has no roots"


if __name__ == '__main__':
    solver = Solver()

    while True:
        a = int(input("a: "))
        b = int(input("b: "))
        c = int(input("c: "))
        result = solver.demo(a, b, c)
        print(result)
```

Optimization

When should you optimize?

- Function that will run many times (e.g. “work horse” functions). Time savings are proportional to the number of runs.

- Single-use functions with time requirements (e.g. real-time control) or that take an inconveniently long time.

- Major points of user interaction (e.g. importing a library, reading/writing data, making figures, etc.).

How do you optimize?

- Algorithmically: think through each possible workflow and try to minimize the number of steps that run. **Reduce redundancies** by eliminating repeated steps, pre-computing re-used values, etc.

- Go **back to basics** (as specifically as possible): try to think about how exactly your code is being executed, how data gets read/written, etc. Try to find the slowest steps.

- Focus on **bottlenecks**: identify the slowest part of your code, then move on to the next slowest, etc. until it is “fast enough”

- **Check if a solution already exists**— other libraries, Google/Stack exchange, CS textbooks, code recipes, etc.

- Can your code be **parallelized**? (Multithreading, multiprocessing)

Profiling your code

- In Jupyter notebooks, use `timeit` to analyze the run time of a single cell. This can help identify what's slow.

- The PyCharm profiler is good for more detailed reports: https://www.jetbrains.com/help/pycharm/optimizing-your-code-using-profilers.html

  - Set up is similar to creating debugging scripts

Vectorizing

- Loops can often be translated into matrix multiplications
- There is an art to doing this well
- Get to know `lambda` functions and `map`
- Look for existing solutions to similar problems

Vectorizing: example

```
result = np.zeros(x.shape[0])

for i in range(x.shape[0]):

  results[i] = my_function(x[i])
```

Vectorizing: example

```
result = np.array(list(map(my_function, x)))
```

Releasing your code

Your code is ready to be shared when…

- Your code is on GitHub
- Your project well-organized and the syntax is clean
- You have set up automated tests
- You have documented the intended use cases, selected a license, etc.
- Your co-authors approve release

Selecting a license

- When in doubt, choose the MIT License

- If you want to get into the nitty gritties, start here: https://choosealicense.com/

Documentation

- Documentation is about empathizing with your users and future developers (including yourself!)
- Think about the storyboards and intended use cases
- Consider a “gallery of use cases” centered around your storyboards
- Write clearly, explain fully (but simply), cite resources that provide more information (including credit for other people’s ideas)
- Include guidelines for contributing and citing your work
- Sphinx, Readthedocs (another week)

Publicizing your release

- Announce via Twitter!
- Make use of the classic science communication tools: posters, papers, talks, etc.
- Consider writing a blog post (e.g. Kaggle) or web-friendly demo (e.g. Distill)
- Organize a hackathon or tutorial
- Word of mouth

Summary

Take-home messages

- **Simplicity** above all else
- Use **storyboards** to
  - Organize your thoughts
  - Consider theory of mind of the *user*
  - Consider theory of mind of the *developer*
- **Funnel** early, **fail early**, and keep the design **modular**