Decoupled code

Good research code

Patrick Mineault

Lesson 2

Keep things decoupled

Spaghetti code

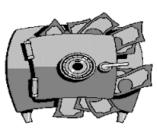
Development AntiPattern:

Spaghetti Code

Spa-ghet-ti code [Slang] an undocumented piece of software source code that cannot be extended or modified without extreme difficulty due to its convoluted structure.



Un-structured code is a liability



Well structured code is an investment.

Do you know when your code smells?

- ► Maybe your code is written in a way where you're doing a little bit of everything all at once
- ► e.g. wave_clus
 - very useful software to sort spikes
 - has a GUI in Matlab GUIDE
 - ► GUIDE makes it exceptionally hard to write good code
 - ► Picked it because it's real code
- This stuff can happen in Matlab or in Python!

Sample code

Link.

What's going here?

This is a callback for a function in a GUI for spike sorting.

- ► Does many things at once
 - ► Manipulates the GUI
 - Modifies data
 - ► Reads a jpg file?
- Uses magic numbers and magic columns
- Uses various string formatting functions and eval
- ► Big function
- Not complex, but it's complicated

Tightly coupled

- ► When code does a lot of unrelated things at once, it becomes very hard to reason about.
- ▶ Let's say your results are weird, are they weird because. . .
 - ▶ the data is bad?
 - you're loading the data wrong?
 - your model is incorrectly implemented?
 - your model is inappropriate for the data?
 - you statistical tests are inappropriate for the data distribution?

Uncouple and simplify

- ► Keep each of the boxes separate with minimal interface
 - Separation of concerns:
 - Example: your data loading function should just load data
 - Your computation functions shouldn't load data, they should just compute
- ► Make each of the boxes small
 - Don't make giant monolithic functions
 - ► Make functions which are small
 - ► A screen's worth, 80 columns, 50 lines
- Avoid side effects, prefer pure functions

What's a side effect?

In computer science, an operation, function or expression is said to have a side effect if it modifies some state variable value(s) outside its local environment, that is to say has an observable effect besides returning a value (the main effect) to the invoker of the operation. State data updated "outside" of the operation may be maintained "inside" a stateful object or a wider stateful system within which the operation is performed. Example side effects include modifying a non-local variable, modifying a static local variable, modifying a mutable argument passed by reference, performing I/O or calling other side-effect functions. (Wikipedia)

Side effects

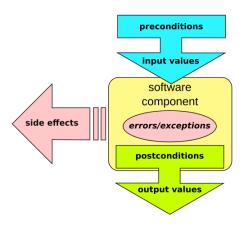


Figure 2: From Wikipedia

A function with side effects

```
Q: what will be printed?
def reversi(arr):
    """Reverses a list."""
    for i in range(len(arr) // 2):
        arr[-i - 1], arr[i] = arr[i], arr[-i - 1]
    return arr
>>> a = [0, 1, 2]
>>> b = reversi(a)
>>> print(b)
>>> print(a)
```

A function which changes its arguments

```
n [12]: def reversi(arr):
        """Reverses a list."""
   ...: for i in range(len(arr) // 2):
                arr[-i - 1], arr[i] = arr[i], arr[-i - 1]
   ...: return arr
[n [13]: a = [0, 1, 2]
in [14]: b = reversi(a)
  [15]: print(b)
[2, 1, 0]
  [16]: print(a)
[2, 1, 0]
```

Figure 3: This function mutates its arguments

Side effects

- ► Modifying arguments
- ► Printing
- ► Making API calls
- ► Changing globals

Side effects are not the best

- lacktriangle Stuff happens outside of the normal flow from arguments ightarrow return value
- ▶ Need to know state of function to understand it
- ► Hard to test
- ► Let's box them
 - You can use closures or classes to encapsulate state

Demo

- ▶ fib.py
- Fibonacci sequence, F(n) = F(n-1) + F(n-2)
- ▶ Memoization

Learn more about your language

- Sometimes (but not always!), code smells come from lack of knowledge
 - ► E.g. using magic column numbers in a raw numpy array rather than named columns in pandas because you don't know pandas
 - Using unnamed dimensions in numpy rather than xarray
 - ► Using + and bespoke casting for string formatting rather than the one true solution, the f-string
- ► Take time to learn more about the language you use
- ► Coming from Matlab? I have three tutorials: [1], [2], [3]

Enough theory!

Let's de-couple CKA!

Background on centered kernel alignment

Q: how can we compare how different brain areas and artificial neural networks represent the world?

A: Choose a standard battery of stimuli, measure responses across systems, compare the responses between the systems. Many approaches, including:

- ► forward encoding models (e.g. ridge regression)
- canonical correlation analysis (CCA)
- representational similarity analysis (RSA).

CKA

Kornblith et al. (2019) propose a new method to compare representations. You can think of it as a generalization of the (square of the) Pearson correlation coefficient, but with matrices instead of vectors.

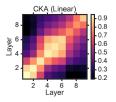


Figure 4: Alignment between layers of two neural nets initialized with different seeds

Importantly, CKA is not implemented in scipy or sklearn, github gives very few hits $^1...$ it's real research code!

Centered kernel alignment

- ▶ We collect the responses of each system to our battery of n stimuli into matrices X, Y.
- $ightharpoonup \mathbf{X}$, \mathbf{Y} have shape $n \times k$, $n \times l$, and k and l are not necessarily the same.
- ► Center **X**, **Y** so each column has 0 mean, then:

$$CKA(\mathbf{X}, \mathbf{Y}) = \frac{||\mathbf{X}^T \mathbf{Y}||_2^2}{||\mathbf{X}^T \mathbf{X}||_2||\mathbf{Y}^T \mathbf{Y}||_2}$$

- ► Min 0, max 1
- ▶ Check: if **X** and **Y** are one-dimensional, then $CKA = \rho(\mathbf{X}, \mathbf{Y})^2$.

Open discussion

Q: What's not ideal about this code? research_code.cka_not_great.py

Pain points

- ▶ IO, computation and plotting are all in one big blob
- Solution: isolate the computation in its own function independent of IO
- Put the controller in the main function, hide behind __name__
 == " main "
 - Avoids module variables in Python
 - ► Makes the code importable

Live coding!

(the result is cka_step2.py)

You can apply this advice at a project-wide level as well

Advice from van Vliet (2020):

- 1. Each analysis step is one script
- 2. A script either processes a single experimental replicate, or aggregates across replicates, never both.
- 3. One master script to run the entire analysis
- 4. Save all intermediate results
- 5. Visualize all intermediate results
- 6. Each parameter and filename is defined only once
- 7. Distinguish files that are a part of the official pipeline

Decoupling configuration

- Keep your configuration our of your code
 - ▶ Use argparse to specify options via the command line
 - Keep configuration options located in an importable config.py file
 - ▶ Use python-dotenv to store secrets in a .env file

Lesson 2

- ► Keep things decoupled
- By keeping things decoupled, you can think about one part of your program at a time
- ► Save your WM slots
- ► Your 5-minute exercise: take existing code and wrap it in main