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Tools I: Packaging and virtual-environments

Overview

Teaching: 4 min
Exercises: 6 min
Questions

- How to use a package manager to install third party tools and libraries

Objectives

- Use conda to install a reproducible environment

Python packages

- There are tens of thousands of python packages
- No need to reinvent the square wheel, it's already out there
- Contributing to existing packages makes it more likely your work will be reused
- Contributing to open-source packages is the best way to learn how to code

Virtual environments

- Virtual environments isolate a project's setup from the rest of the system
- It ensures different projects do not interfere with each other
- For instance, you may want simultaneously:
  - a production environment with tried and true version of your software and tensorflow 1.15
  - a development environment with shiny stuff and a migration to tensorflow 2.1

Package managers

Package managers help you install packages. Some help you install virtual environments as well. Better known python package managers include conda (https://docs.conda.io/en/latest/), pip (https://pip.pypa.io/en/stable/), poetry (https://python-poetry.org/)

	conda	**pip**	**poetry**
audience	research	all	developers
manage python packages	✅	✅	✅

	conda	pip	poetry
manage non-python packages	✅	❌	❌
choose python version	✅	❌	❌
manage virtual envs	✅	❌	✅
easy interface	❌	✅	❌
fast	❌	✅	✅

Rules for choosing a package manager

1. Choose one
2. Stick with it

We chose conda (https://docs.conda.io/en/latest/) because it is the de facto standard in science, and because it can natively install libraries such as fftw (https://anaconda.org/conda-forge/fftw), vtk (https://anaconda.org/conda-forge/vtk), or even Python, R, and Julia themselves.

It is also the de facto package manager on Imperial's HPC cluster (https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/support/applications/conda/) systems.

Example

Installing and using an environment

1. If you haven't already, see the setup guide (../setup) for instructions on how to install Conda and Visual Studio Code.
2. Download this zip archive (../code/course.zip) and extract it. Start Visual Studio Code and select "Open folder…" from the welcome screen. Navigate to the folder created from the archive and press "Select Folder".
3. From the side-bar select the file `environment.yml`. If you are prompted to install the Visual Studio Code Python extension then do so. The contents of `environment.yml` should match:

```
name: course
dependencies:
  - python==3.9
  - flake8
  - pylint
  - black
  - mypy
  - requests
```

4. Create a new virtual environment using conda:

   Windows users will want to open the app `Anaconda Prompt` from the Start Menu.

   Linux and Mac users should use a terminal app of their choice. You may see a warning with instructions. Please follow the instructions.

   Bash

   ```
   conda env create -f "path_to_environment.yml"
   ```

   You can obtain `path_to_environment.yml` by right clicking the file tab near the top of Visual Studio Code and selecting "Copy Path" from the drop-down menu. Make sure to include the quotation marks in the command. Right click on the window for your command line interface to paste the path.
5. We can now activate the environment:

   Bash

   ```
   conda activate course
   ```
6. And check Python knows about the installed packages. Start a Python interpreter with the command `python` then:

   Python

   ```
   import requests
   ```

   We expect this to run without any messages. You can see the location of the installed package with:

   Python

   ```
   requests.__file__
   ```

   Output

   ```
   'C:\\ProgramData\\Anaconda3\\envs\\course\\lib\\site-packages\\requests\\__init__.py'
   ```

   The file path you see will vary but note that it is within a directory called `course` that contains all of the files for the virtual environment you have created. Exit the Python interpreter:

Python

```
exit()
```

7. Finally, feel free to remove requests from `environment.yml`, then run

Bash

```
conda env update -f "path_to_environment.yml"
```

and see whether the package has been updated or removed.

Selecting an environment in Visual Studio Code

If you haven't already, see the setup guide (../setup) for instructions on how to install Visual Studio (VS) Code.

The simplest option for all platforms is to set the interpreter via the Command Palette:

- For Windows/Linux: Ctrl + Shift + P, and start typing "Python: Select interpreter"
- For macOS: Cmd + Shift + P, and start typing "Python: Select interpreter**

An entry should be present with the name `course`. It may take a few minutes to appear however.

If you already have a Python file open then it's also possible to set the interpreter using the toolbar at the bottom of the window.

Key Points

- There are tens of thousands of Python packages
- The choice is between reinventing the square wheel or reusing existing work
- The state of an environment can be stored in a file
- This stored environment is then easy to audit and recreate

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Tools II: Code Formatters

Overview

Teaching: 3 min
Exercises: 2 min
Questions

- How to format code with no effort on the part of the coder?

Objectives

- Know how to install and use a code formatter

Why does formatting matter?

- Code is read more often than written
- It's a menial task that adds cognitive load
- Ensures all code in a project is consistent, even if contributed by multiple authors
- Setting up a formatter in your editor takes 5 minutes
- Those 5 minutes are redeemed across the lifetime of the project

Rules to choose a code formatter

1. Choose one
2. Stick with it

We chose black (https://pypi.org/project/black/) because it has very few options with which to fiddle.

Formatting example

Using Visual Studio Code:

1. Open the file `messy.py`. Its contents should match:

Python

```
x = {  'a':37,'b':42,
'c':927}
y = 'hello '+       'world'
class foo  (     object  ):
  def f    (self   ):
       z =3
       return       y **2
   def g(self, x,
       y=42
       ):
      # pylint: disable=missing-docstring
      return x--y
def f  (   a ) :
   return      37+-a[42-a :  y*3]  # noqa: E203
```

2. Ensure that you have activated your “course” conda environment (see previous episode (http://localhost:4000/l1-01-tools-I/index.html#selecting-an-environment-in-visual-studio-code))
3. Make a trivial change to the file and save it: it should be reformatted automagically.
4. Use the `undo` function of VS Code to return the code to its unformatted state. Before saving again delete a ‘:’ somewhere. When saving, the code will likely not format. It is syntactically invalid. The formatter cannot make sense of the code and thus can’t format it.

Solution

After saving, the code should be automatically formatted to:

Python

```
x = {"a": 37, "b": 42, "c": 927}
y = "hello " + "world"


class foo(object):
    def f(self):
        z = 3
        return y ** 2

    def g(self, x, y = 42):
        # pylint: disable=missing-docstring
        return x - -y


def f(a):
    return 37 + -a[42 - a : y * 3]  # noqa: E203
```

Ah! much better!

Still, the sharp-eyed user will notice at least one issue with this code. *Formatting code does not make it less buggy!*

Key Points

- Code formatting means how the code is typeset
- It influences how easily the code is read
- It has no impact on how the code runs
- Almost all editors and IDEs have some means to set up an automatic formatter
- 5 minutes to set up the formatter is redeemed across the time of the project i.e. the cost is close to nothing

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Tools III: Linters

Overview

Teaching: 10 min
Exercises: 5 min
Questions

- How to make the editor pro-actively find errors and code-smells

Objectives

- Remember how to install and use a linter in vscode without sweat

What is linting?

Linters enforce style rules (https://lintlyci.github.io/Flake8Rules/) on your code such as:

- disallow one letter variables outside of loops
- use `lower_snake_case` for variables
- use `CamelCase` for classes
- disallow nesting more than n deep
- detect code-smells (patterns that are often bugs, e.g. two functions with the same name)
- static type detection (mypy (http://mypy-lang.org/)) where we tell the editor what kind of objects (`dict` , `list` , `int` , etc) a function expects

Consistent styles make a code more consistent and easier to read, whether or not you agree with the style. Using an automated linter avoids bike-shedding since the linter is the final arbiter.

Why does linting matter?

- Code is read more often than written
- Setting up a linter in your editor takes 5 minutes
- Those 5 minutes are redeemed across the lifetime of the project
- Linters shortcut the `edit-run-debug and repeat` workflow

Rules for choosing linters

1. Choose a few
2. Stick with them

We chose:

- flake8 (https://pypi.org/project/black/) because it is simple
- pylint (https://www.pylint.org/) because it is (too?) extensive
- mypy (http://mypy-lang.org/) because it helps keep track of object types - check out the use of type hints (https://www.python.org/dev/peps/pep-0484/) in Python

Exercise

Setup VS Code:

1. Return to `messy.py` (now nicely formatted) in VS Code.
2. The output of the configured linters is shown displayed by coloured underlining in the editor, coloured vertical sections of the scroll bar and in the bottom status bar. Mouse over the underlined sections of the editor to see the reason for each.
3. Check the current errors (click on errors in status bar at the bottom).
4. Understand why each error is present and try to correct them.
5. Alternatively, try and disable them (but remember: *with great power*…). We've already disabled-one at the function scope level. Check what happens if you move it to the top of the file at the module level.

Key Points

- Linting is about discovering errors and code-smells before running the code
- It shortcuts the "edit-run-debug and repeat" workflow
- Almost all editors and IDEs have some means to setup automatic linting
- 5 minutes to setup a linter is redeemed across the time of the project i.e. the cost is close to nothing

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Data Structures

Overview

Teaching: 30 min
Exercises: 20 min
Questions

- How can data structures simplify codes?

Objectives

- Understand why different data structures exist
- Recall common data structures
- Recognize where and when to use them

What is a data structure?

```
data structure: represents information and how that information can be accessed
```

Choosing the right representation for your data can vastly simplify your code and increase performance.

Choosing the wrong representation can melt your brain. Slowly.

Examples:

The number `2` is represented with the integer `2`

Python

```
>>> type(2)
int
```

Acceptable behaviors for integers include `+`, `-`, `*`, `/`

Python

```
>>> 1 + 2
3
>>> 1 - 2
-1
```

On the other hand, text is represented by a string

Python

```
>>> type("text")
str
```

It does *not* accept all the same behaviours as an integer:

Python

```
>>> "a" + "b"
"ab"
>>> "a" * "b"
TypeError: can't multiply sequence by non-int of type 'str'
```

Integers *can* be represented as strings, but their behaviours would be unexpected:

Python

```
>>> "1" + "2"
"12"
```

With integers, `+` is an *addition*, for strings it's a *concatenation*.

Health impact of choosing the wrong data structure

- we could use `"1", "2", "3"` to represent numbers, rather than `1 , 2 , 3`
- we would have to reinvent how to add numbers, and multiply, and divide them e.g.

  ```
  str(int("1") + int("2"))
  ```

- the wrong data structures can make your code vastly more complicated
- also, the code would be much slower

Stay healthy. Stop and choose the right data structure for you!

📌 Priorities for Choosing Data Structures

We've discussed how the incorrect data structure can make your code more complicated and also give worse performance. Quite often these two factors are aligned - the right data structure will combine simple code with the best performance. This isn't always true however. In some cases simplicity and performance will be in tension with one another. A good maxim to apply here is **"Premature optimization is the root of all evil"**. This philosophy states that keeping your code simple and elegant should be your primary goal. Choosing a data structure based on performance or other considerations should only be considered where absolutely necessary.

Basic data structures

Different languages provide different basic structures depending on the purpose for which they were designed. We will consider here some of the basic data structures available in Python for which equivalents can be found in most other languages.

Lists

Lists are containers of other data:

Python

```
# List of integers
[1, 2, 3]
# List of strings
["a", "b", "b"]
# List of lists of integers
[[1, 2], [2, 3]]
```

Lists make sense when:

- you have more than one item of data
- the items are somehow related: Lists of apples and oranges are a code-smell (https://en.wikipedia.org/wiki/Code_smell)

  Python

  ```
  [1, 2, 3]  # might be the right representation
  ["a", 2, "b"]  # probably wrong
  ```

- the items are ordered and can be accessed

Python

```
>>> velocities_x = [0.3, 0.5, 0.1]
>>> velocities_x[1]  # e.g. could be velocity a point x=1
```

Beware! The following might indicate a list is the wrong data structure:

- apples and oranges
- deeply nested list of lists of lists

📌 Other languages

- C++:
  - std::vector (https://en.cppreference.com/w/cpp/container/vector), fast read-write to element i and fast iteration operations. Slow insert operation.
  - std::list (https://en.cppreference.com/w/cpp/container/list). No direct access to element i. Fast insert, append, splice operations.
- R: list (http://www.r-tutor.com/r-introduction/list)
- Julia: Array (https://docs.julialang.org/en/v1/manual/arrays/), also equivalent to numpy arrays.
- Fortran: array (https://www.tutorialspoint.com/fortran/fortran_arrays.htm), closer to numpy arrays than python lists

Tuples

Tuples are **short** and **immutable** containers of other data.

```
(1, 2)
("a", b")
```

Immutable means once that once created, elements cannot be added, removed or replaced:

Python

```
>>> shape = 2, 4
>>> shape
(2, 4)
>>> shape[1] = 4
TypeError: 'tuple' object does not support item assignment
```

Tuple make sense when:

- you need a short container with only a few elements
- the list does not need to be modified or should not be modified
- great for functions returning more than one *thing*

Beware! The following might indicate a tuple is the wrong data structure:

- the elements have no relationship (apples and oranges)
- more than four or five elements
- difficult to remember which element is what (is it `result[1]` I need or `result[2]`?)

📌 Other languages

- C++: std::tuple (https://en.cppreference.com/w/cpp/utility/tuple)
- R: cran package tuple (https://cran.r-project.org/web/packages/tuple/index.html)
- Julia: tuples and named tuples (https://docs.julialang.org/en/v1/base/base/#Core.NamedTuple)
- Fortran: Nope. Nothing.

Sets

Sets are containers where each element is *unique*:

Python

```
>>> set([1, 2, 2, 3, 3])
{1, 2, 3}
```

They make sense when:

- each element in a container must be unique
- you need to solve ownership issues, e.g. which elements are in common between two lists? Which elements are different?

Python

```
>>> set(["a", "b", "c"]).symmetric_difference(["b", "c", "e"])
{'a', 'e'}
```

Something to bear in mind with sets is that, depending on your language, they may or may not be *ordered*. In Python sets are unordered i.e. the elements of a set cannot be accessed via an index, but sets in other languages may allow this.

📌 Other languages

- C++: std::set (https://en.cppreference.com/w/cpp/container/set)
- R: set functions (https://stat.ethz.ch/R-manual/R-devel/library/base/html/sets.html) that operate on a standard list.
- Julia: Set (https://docs.julialang.org/en/v1/base/collections/#Base.Set)
- Fortran: Nope. Nothing.

Dictionaries

Dictionaries are mappings between a key and a value (e.g. a word and its definition).

Python

```
# mapping of animals to legs
{"horse": 4, "kangaroo": 2, "millipede": 1000}
```

They make sense when:

- you have pairs of data that go together:

Python

```
# A list of tuples?? PROBABLY BAD!!
[
  ("horse", "mammal"),
  ("kangaroo", "marsupial"),
  ("millipede", "alien")
]
# Better?
{
  "horse": "mammal",
  "kangaroo": "marsupial",
  "millipede": "alien"
}
```

- given x you want to know its y: given the name of an animal you want to know the number of legs.
- often used as bags of configuration options

Beware! The following might indicate a dict is the wrong data structure:

- keys are not related to each other, or values are not related to each other

Python

```
{1: "apple", "orange": 2}
```

`1` not related to `"orange"` and `2` not related to `"apple"`

- deeply nested dictionaries of dictionaries of lists of dictionaries

Other languages

- C++: std::map (https://en.cppreference.com/w/cpp/container/map)
- R: cran package hash (https://cran.r-project.org/web/packages/hash/)
- Julia: Dict (https://docs.julialang.org/en/v1/base/collections/#Base.Dict)
- Fortran: Nope. Nothing.

Basic Data Structure Practice

You're writing a piece of code to track the achievements of players of a computer game. You've been asked to design the data structures the code will use. The software will need the following data structures as either a list, a dictionary or a set:

- A collection containing all possible achievements
- A collection for each player containing their achievements in the *order they were obtained* (assume no duplicates)
- A collection relating player names to their achievements

Implement the data structures as seems most appropriate and populate them with some example data. Now have a go at writing code for the following actions:

- get a player's achievements
- get a player's first achievement
- add a new achievement for a player
- get the number of achievements a player doesn't have yet
- get a collection of the achievements a player doesn't have yet
- find the achievements "player1" has that "player2" doesn't

If you picked the right structures, each action should be able to be implemented as a single line of code.

Solution

Python

```
all_achievements = {"foo", "bar", "baz"}

player_achievements = {
    "player1": ["foo", "baz"],
    "player2": [],
    "player3": ["baz"],
}

# get a player's achievements
player_achievements["player2"]

# get a player's first achievement
player_achievements["player1"][0]

# add a new achievement to a player's collection
player_achievements["player2"].append("foo")

# get the number of achievements a player doesn't have yet
len(all_achievements) - len(player_achievements["player2"])

# get a collection of the achievements a player doesn't have yet
all_achievements.difference(player_achievements["player1"])

# find the achievements player1 has that player2 doesn't
set(player_achievements["player1"]).difference(player_achievements["player2"])
```

Notice that for the last action we had to turn a list into a set. This isn't a bad thing but if we were having to do it a lot that might be a sign we'd chosen an incorrect data structure.

Advanced data structures

Whilst basic data structures provide the fundamental building blocks of a piece of software, there are many more sophisticated structures suited to specialised tasks. In this section we'll take a brief look at a variety of different data structures that provide powerful interfaces to write simple code.

Getting access to advanced data structures often involves installing additional libraries. As a rule of thumb, for any data structure you can think of somebody will already have published an implementation of it and its strongly recommended to use an available version rather than try to write one from scratch. We've discussed the best approach to managing dependencies for a project already.

Pandas Data Frames

The excellent and very powerful Panda's package is the go to resource for dealing with tabular data. Anything you might think of using Excel for Panda's can do better. It leans heavily on NumPy for efficient numerical operations whilst providing a high level interface for dealing with rows and columns of data via pandas.DataFrame (https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.DataFrame.html).

Python

```
# working with tabular data in nested lists

data = [
    ["col1", "col2", "col3"],
    [0, 1, 2],
    [6, 7, 8],
    [0, 7, 8],
]

# get a single row or column
row = data[0]
col = [row[data[0].index("col1")] for row in data]

# filter out rows where col1 != 0
[data[0]] + [row for row in data[1:] if row[0] == 0]

# operate on groups of rows based on the value of col1
for val in set([row[0] for row in data[1:]]):
    rows = [row for row in data[1:] if row[0] == val]

# vs

import pandas as pd

# many flexible ways to create a dataframe e.g. import from csv, but here we
# use the use the existing data.
dataframe = pd.DataFrame(data[1:], columns=data[0])

# get a single row or column
row = dataframe.iloc[0]
col = dataframe["col1"]

# filter out rows where col1 != 0
dataframe[dataframe["col1"] == 0]

# operate on groups of rows based on the value of col1
dataframe.groupby("col1")
```

Balltrees

A common requirement across many fields is working with data points within a 2d, 3d or higher dimensioned space where you often need to work with distances between points. It is tempting in this case to reach for lists or arrays but balltrees provide an interesting and very performant alternative in some cases. An implementation is provided in Python by the scikit-learn (https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.BallTree.html) library.

Python

```python
# Which point is closest to the centre of a 2-d space?

points = [
    [0.1, 0.1],
    [1.0, 0.1],
    [0.2, 0.2],
    [0.1, 0.3],
    [0.9, 0.2],
    [0.2, 0.3],
]
centre = [0.5, 0.5] # centre of our space

# Using lists

distances = []
for i, point in enumerate(points):
    dist = ((centre[0] - point[0])**2 + (centre[1] - point[1])**2)**0.5
    distances.append(dist)

smallest_dist = sorted(distances)[0]
nearest_index = distances.index(smallest_dist)

# vs

from sklearn.neighbors import BallTree

balltree = BallTree(points)
smallest_dist, nearest_index = balltree.query([centre], k=1)
```

Graphs and Networks

Another type of data structure that spans many different research domains are graphs/networks. There are many complex algorithms that can be applied to graphs so checkout the NetworkX library for its data structures (https://networkx.org/documentation/stable/tutorial.html).

Python

```python
edges = [
    [0, 1],
    [1, 2],
    [2, 4],
    [3, 1]
]

# Using lists

# get the degree (number of connected edges) of node 1

degree_of_1 = 0
for edge in edges:
    if 1 in edge:
        degree_of_1 += 1

# vs

import networkx as nx

graph = nx.Graph(edges)

# get the degree (number of connected edges) of node 1
graph.degree[1]

# easy to perform more advanced graph operations e.g.
graph.subgraph([1,2,4])
```

Custom data structures: Data classes

Python (>= 3.7) makes it easy to create custom data structures.

Python

```
>>> from typing import List, Text
>>> from dataclasses import dataclass
>>> @dataclass
... class MyData:
...   a_list: List[int]
...   b_string: Text = "something something"
>>> data = MyData([1, 2])
>>> data
MyData(a_list=[1, 2], b_string='something something')
>>> data.a_list
[1, 2]
```

Data classes make sense when:

- you have a collections of related data that does not fit a more primitive type
- you already have a class and you don't want to write standard functions like `__init__`, `__repr__`, `__ge__`, etc..

Beware! The following might indicate a `dataclass` is the wrong data structure:

- you do need specialized `__init__` behaviours (just use a class)
- single huge mother of all classes that does everything (split into smaller specialized classes and/or stand-alone functions)
- a `dict`, `list` or `numpy` array would do the job. Everybody knows what a `numpy` array is and how to use it. But even your future self might not know how to use your very special class.

Exploring data structures

Take some time to read in more detail about any of the data structures covered above or those below:

- deques (https://docs.python.org/3/library/collections.html#collections.deque)
- named tuples (https://docs.python.org/3/library/collections.html#collections.namedtuple)
- counters (https://docs.python.org/3/library/collections.html#collections.Counter)
- dates (https://docs.python.org/3/library/datetime.html)
- enum (https://docs.python.org/3/library/enum.html) represent objects that can only take a few *values*, e.g. colors. Often useful for configuration options.
- numpy arrays (https://docs.scipy.org/doc/numpy/reference/generated/numpy.array.html) (multidimensional array of numbers)
- xarray arrays (http://xarray.pydata.org/en/stable/) (multi-dimensional arrays that can be indexed with rich objects, e.g. an array indexed by dates or by longitude and latitude, rather than by the numbers 0, 1, 2, 3)
- xarray datasets (http://xarray.pydata.org/en/stable/) (collections of named xarray arrays (http://xarray.pydata.org/en/stable/) that share some dimensions.)

Don't reinvent the square wheel.

Digital Oxford Dictionary, the wrong way and the right way

1. Implement an oxford dictionary with two `list` s, one for words, one for definitions:

```
barf: (verb) eject the contents of the stomach through the mouth
morph: (verb) change shape as via computer animation
scarf: (noun) a garment worn around the head or neck or shoulders for warmth
  or decoration
snarf: (verb) make off with belongings of others
sound: |
  (verb) emit or cause to emit sound.
  (noun) vibrations that travel through the air or another medium
surf: |
  (verb) switch channels, on television
  (noun) waves breaking on the shore
```

2. Given a word, find and modify its definition
3. Do the same with a `dict`
4. Create a subset dictionary (including definitions) of words rhyming with “arf” using either the two- `list` or the `dict` implementation
5. If now we want to also encode “noun” and “verb”, what data structure could we use?
6. What about when there are multiple meanings for a verb or a noun?

Dictionary implemented with lists

Python

```
from typing import List, Text, Tuple


def modify_definition(
    word: Text, newdef: Text, words: List[Text], definitions: List[Text]
) -> List[Text]:
    from copy import copy

    index = words.index(word)
    definitions = copy(definitions)
    definitions[index] = newdef
    return definitions


def find_rhymes(
    rhyme: Text, words: List[Text], definitions: List[Text]
) -> Tuple[List[Text], List[Text]]:
    result_words = []
    result_definitions = []
    for word, definition in zip(words, definitions):
        if word.endswith(rhyme):
            result_words.append(word)
            result_definitions.append(definition)
    return result_words, result_definitions


def testme():

    words = ["barf", "morph", "scarf", "snarf", "sound", "surf"]
    definitions = [
        "(verb) eject the contents of the stomach through the mouth",
        "(verb) change shape as via computer animation",
        (
            "(noun) a garment worn around the head or neck or shoulders for"
            "warmth or decoration"
        ),
        "(verb) make off with belongings of others",
        (
            "(verb) emit or cause to emit sound."
            "(noun) vibrations that travel through the air or another medium"
        ),
        (
            "(verb) switch channels, on television"
            "(noun) waves breaking on the shore"
        ),
    ]

    newdefs = modify_definition("morph", "aaa", words, definitions)
    assert newdefs[1] == "aaa"

    rhymers = find_rhymes("arf", words, definitions)
    assert set(rhymers[0]) == {"barf", "scarf", "snarf"}
    assert rhymers[1][0] == definitions[0]
    assert rhymers[1][1] == definitions[2]
    assert rhymers[1][2] == definitions[3]


if __name__ == "__main__":

    # this is one way to include tests.
    # the second session will introduce a better way.
    testme()
```

Dictionary implemented with a dictionary

Python

```
from typing import List, Text, Tuple, Mapping


def modify_definition(
    word: Text, newdef: Text, dictionary: Mapping[Text, Text]
) -> List[Text]:
    from copy import copy

    result = copy(dictionary)
    result[word] = newdef
    return result


def find_rhymes(
    rhyme: Text, dictionary: Mapping[Text, Text]
) -> Tuple[List[Text], List[Text]]:
    return {
        word: definition
        for word, definition in dictionary.items()
        if word.endswith(rhyme)
    }


def testme():

    dictionary = {
        "barf": "(verb) eject the contents of the stomach through the mouth",
        "morph": "(verb) change shape as via computer animation",
        "scarf": (
            "(noun) a garment worn around the head or neck or shoulders for"
            "warmth or decoration"
        ),
        "snarf": "(verb) make off with belongings of others",
        "sound": (
            "(verb) emit or cause to emit sound."
            "(noun) vibrations that travel through the air or another medium"
        ),
        "surf": (
            "(verb) switch channels, on television"
            "(noun) waves breaking on the shore"
        ),
    }

    newdict = modify_definition("morph", "aaa", dictionary)
    assert newdict["morph"] == "aaa"

    rhymers = find_rhymes("arf", dictionary)
    assert set(rhymers) == {"barf", "scarf", "snarf"}
    for word in {"barf", "scarf", "snarf"}:
        assert rhymers[word] == dictionary[word]


if __name__ == "__main__":

    testme()
```

More complex data structures for more complex dictionary

There can be more than one good answer. It will depend on how the dictionary is meant to be used later throughout the code.

Below we show three possibilities. The first is more deeply nested. It groups all definitions together for a given word, whether that word is a noun or a verb. If more often than not, it does not matter so much what a word is, then it might be a good solution. The second example flatten the dictionary by making “surf” the noun different from “surf” the verb. As a result, it is easier to access a word with a specific semantic category, but more difficult to access all definitions irrespective of their semantic category.

One pleasing aspect of the second example is that together things that are unlikely to change one one side (word and semantic category), and a less precise datum on the other (definitions are more likely to be refined).

The third possibility is a pandas (https://pandas.pydata.org/pandas-docs/stable/index.html) `DataFrame` with three columns. It’s best suited to big-data problems where individual words (rows) are seldom accessed one at a time. Instead, most operations are carried out over subsets of the dictionary.

Python

```
from typing import Text
from enum import Enum, auto
from dataclasses import dataclass
from pandas import DataFrame, Series


class Category(Enum):
    NOUN = auto
    VERB = auto


@dataclass
class Definition:
    category: Category
    text: Text


first_example = {
    "barf": [
        Definition(
            Category.VERB, "eject the contents of the stomach through the mouth"
        )
    ],
    "morph": [
        Definition(
            Category.VERB, "(verb) change shape as via computer animation"
        )
    ],
    "scarf": [
        Definition(
            Category.NOUN,
            "a garment worn around the head or neck or shoulders for"
            "warmth or decoration",
        )
    ],
    "snarf": Definition(Category.VERB, "make off with belongings of others"),
    "sound": [
        Definition(Category.VERB, "emit or cause to emit sound."),
        Definition(
            Category.NOUN,
            "vibrations that travel through the air or another medium",
        ),
    ],
    "surf": [
        Definition(Category.VERB, "switch channels, on television"),
        Definition(Category.NOUN, "waves breaking on the shore"),
    ],
}


# frozen makes Word immutable (the same way a tuple is immutable)
# One practical consequence is that dataclass will make Word work as a
# dictionary key: Word is hashable
@dataclass(frozen=True)
class Word:
    word: Text
    category: Text


second_example = {
    Word(
        "barf", Category.VERB
    ): "eject the contents of the stomach through the mouth",
    Word("morph", Category.VERB): "change shape as via computer animation",
    Word("scarf", Category.NOUN): (
        "a garment worn around the head or neck or shoulders for"
        "warmth or decoration"
    ),
    Word("snarf", Category.VERB): "make off with belongings of others",
    Word("sound", Category.VERB): "emit or cause to emit sound.",
    Word(
```

```
        "sound", Category.NOUN
    ): "vibrations that travel through the air or another medium",
    Word("surf", Category.VERB): "switch channels, on television",
    Word("surf", Category.NOUN): "waves breaking on the shore",
}

# Do conda install pandas first!!!
import pandas as pd

third_example = pd.DataFrame(
    {
        "words": [
            "barf",
            "morph",
            "scarf",
            "snarf",
            "sound",
            "sound",
            "surf",
            "surf",
        ],
        "definitions": [
            "eject the contents of the stomach through the mouth",
            "change shape as via computer animation",
            (
                "a garment worn around the head or neck or shoulders for"
                "warmth or decoration"
            ),
            "make off with belongings of others",
            "emit or cause to emit sound.",
            "vibrations that travel through the air or another medium",
            "switch channels, on television",
            "waves breaking on the shore",
        ],
        "category": pd.Series(
            ["verb", "verb", "noun", "verb", "verb", "noun", "verb", "noun"],
            dtype="category",
        ),
    }
)
```

Key Points

- Data structures are the representation of information the same way algorithms represent logic and workflows
- Using the right data structure can vastly simplify code
- Basic data structures include numbers, strings, tuples, lists, dictionaries and sets.
- Advanced data structures include numpy array and panda dataframes
- Classes are custom data structures

‹ (../l1-03-tools-III/index.html)

› (../l1-05-abstra

‹ (../l1-04-datastructures/index.html) Essential Software Engineering for Researchers (../) › (../l1-06-design

Structuring code

Overview

Teaching: 10 min
Exercises: 20 min
Questions

- How can we create simpler and more modular codes?

Objectives

- Explain the expression “separation of concerns”
- Explain the expression “levels of abstractions”
- Explain the expression “dataflow”
- Analyze an algorithm for levels of abstractions, separable concerns and dataflow
- Create focussed, modular algorithms

Intelligible code?

```
Intelligible: Able to be understood; comprehensible
```

Code is meant to be read by an audience who has infinite knowledge and an infinite capacity for misunderstanding:

- knows more about general relativity than Einstein
- given a point with coordinate `point[0], point[1], point[2]` , can’t remember whether whether `0` corresponds to `x` , `y` , or `z`

This audience is future-**you** reading past-**you**’s code.

Intelligible code aims to:

- avoid sources of confusion (what does index `0` reference?)
- lessen the cognitive load (ah! before using `c` don’t forget to call the function `nothing_to_do_with_c` because of historical implementation detail `z`).

Levels of abstraction

Scientific papers come with separate levels of details:

- abstract -> abstract concepts and no details
- body -> concrete concepts with some details
- appendix -> details only fit for a Ph.D. student

Similarly, code should be written with a structure separating different levels of details:

Python

```
def analyse(input_path):
    data = load_data(input_path)

    # special fix for bad data point
    data[0].x["january"] = 0

    results = process_data(data)
    return results
```

The “special fix” mixes levels of abstraction. Our top level function now depends on the structure of `data` . If the way data is stored changes (a low level detail) we now also need to change `analyse` which is a high level function directing the flow of the program.

Separable concerns

Scientific papers come with separate sections dealing with separate concerns, e.g.:

- `introduction` describes prior work
- `section I` describes the experimental setup
- `section II` describes the data analysis methods
- `section III` contains plots and a discussion of the results

Similarly, code should be written with a structure separating separable concerns:

Python

```
def main():
  # reading input files is one thing
  data = read_input(filename)

  # creating complex objects is another
  section_I = SectionI(data)

  # compute is still something else
  result_I = section_I.compute(some_value)

  # Saving data is another
  save(result_I)


def read_input(filename):
  """ Reads input data from file. """
  pass


def save(data, filename="saveme.h5"):
  """ Saves output data to file. """
  pass


class SectionI
  """ Runs experiment """
  def __init__(self, some_array):
      self.some_array = some_array

  def compute(self, y):
      """ Just does compute, nothing more, nothing less. """
      pass
```

In the code above we have made some choices:

- reading input files is separate from creating complex objects
- saving output files is separate from running computations
- objects are created in one go

A few examples of what **not** to do.

Mixing reading files and creating objects

Objects that do need files to be created are easy to create and re-create, especially during testing.

Python

```
class SectionI
    def __init__(self, some_array):
        self.some_array = array
        # BAD!! Now you need to carry this file around every time you want to
        # instantiate SectionI
        self.aaa = read_aaa("somefile.aaa")
```

Mixing computing stuff and IO

Below, it the compute has a hidden baggage: it can't operate without reading from file. It's not a pure function of `self`, `b`, and `filename`. Run it twice with exactly the same `self` and the same `b` and the same `filename`, and the results might still be different.

It creates file artifacts. Littering is a crime and hidden files are litter.

Python

```
class SectionI
    def run(self, b, filename="somefile.aaa"):
        # BAD!! hidden dependency on the content of the file
        aaa = read_aaa(filename)
        ...
        # BAD! Compute functions should not litter.
        save(result, "somefile")
        return result
```

Splitting concerns too far

It's unfortunately common to find objects that need to be created and setup in several steps. This is an anti-pattern (https://en.wikipedia.org/wiki/Anti-pattern) (We'll discuss patterns in a bit), i.e. something that should be avoided. Creating an object is one thing and one thing only. It should be fully usable right after creation.

Python

```
sectionI = SectionI(...)

# BAD! just put the initialization in SectionI.__init__
sectionI.setup(...)
results = sectionI.run(...)
```

📌 Paper vs code

Code should be organized the same way as the paper it will produce. If a concept X is described in one section, and concept Y in another, then X should be one function or class, and Y another.

That's because the primary purpose of paper and code is to communicate with other people, including your future self.

Dataflow

A code is a sequence of transformations on data, e.g.:

1. data `measurements` is read from input
2. data `a` and `b` are produced from `measurements`, independently
3. data `result` is produced from `a` and `b`

The code should reflect that structure:

Python

```
def read_experiment(filename):
    ...
    return measurements


def compute_a(measurements):
    ...
    return a


def compute_b(measurements):
    ...
    return b


def compute_result(a, b):
    ...
    return result
```

1. One function to read `Experiment`
2. One function/class to compute `a` : It takes `measurements` as input and returns the result `a`
3. One function/class to compute `b` : It takes `measurements` as input and returns the result `b`
4. One function/class to compute `Result` : It takes `a` and `b` as input and returns the result `result` :

Here are things that should **not** happen:

Unnecessary arguments and tangled dependencies

Did we not say the result depends on `a` and `b` alone? The next programmer to look at the code (e.g. future you) won't know that. Computing `result` is no longer separate from `measurements` .

Python

```
# BAD! Unnecessary arguments. Now result depends on a, b, experiment
def compute_result(a, b, experiment):
    pass
```

Modifying an input argument

If possible avoid doing this.

Python

```
def compute_a(measurements):
    measurements[1] *= 2
    ...

def compute_b(measurements):
    measurements[1] *= 0.5
    ...
```

Now `compute_a` has to take place before `compute_b` because `compute_a` chose to modify it's argument, and thus `compute_b` was hacked to undo the damage. To get `b` the data is now forced to flow first through `compute_a` .

Some languages unfortunately are designed so sometimes you don't have any choice but to modify an input argument. Still, wherever possible avoid doing it.

Global variables

NEVER EVER EVER use global variables. They make the dataflow complex by essence.

Python

```
SOME_GLOBAL_VARIABLE = "a"

def compute_a(measurements):

    ...
    result *= SOME_GLOBAL_VARIABLE
    return result
```

Now the result of `compute_a` has a hidden dependency. It's never clear whether calling it twice with the same input (`measurements`) will yield the same result.

In general make sure that all variables have the most limited scope possible. If they're only needed within a single function define them there. Wherever possible treat variables with wide scope as constants (or make them actual constants if your language supports it) so you know they're not being modified anywhere.

📌 Dear Fortran 90 users

Module variables are global. They can be modified anywhere, anytime. It's best not to use them.

Disentangling a recipe

Disentangle the recipe below into separable concerns and level of details. Ensure the flow of ingredients from transform to transform to final dish is clear.

1. Write the solution as a recipe. Be sure to delete steps and information irrelevant to the recipe. Deleting code is GOOD! (if it's under version control)
2. Can you identify different levels of abstractions?
3. Can you identify different concerns?
4. Can you identify what is data and what are transformations of the data?
5. Write the solution as pseudo-code in your favorite language. Pseudo-code doesn't have to run, but it has to make sense. Or write a solution as a diagram, if that's your thing (e.g. UML (https://en.wikipedia.org/wiki/Unified_Modeling_Language), Sequence diagram (https://en.wikipedia.org/wiki/Sequence_diagram)).
6. Can you spot inconsistencies in the original recipe? That's what happens when code is copy-pasted. Invariably, versions diverge until each has set of unique bugs, as well as bugs in common.

```
### Tarte au Nutella

Poor the preparation onto the dough. Wait for it to cool. Once it is cool,
sprinkle with icing sugar.

The dough is composed of 250g of flour, 125g of butter and one egg yolk. It
should be blind-baked at 180°C until golden brown.

The preparations consists of 200g of Nutella, 3 large spoonfuls of crème
fraîche, 2 egg yolks and 20g of butter.

Add the Nutella and the butter to a pot where you have previously mixed the
crème fraîche, the egg yolk and the vanilla extract. Cook and mix on low heat
until homogeneous.

The dough, a pâte sablée, is prepared by lightly mixing by hand a pinch of
salt, 250g of flour and 125g of diced butter until the butter is mostly all
absorbed. Then add the egg yolk and 30g of cold water. The dough should look
like coarse sand, thus its name.

Spread the dough into a baking sheet. If using it for a pie with a pre-cooked
or raw filling, first cook the dough blind at 200°C until golden brown. If the
dough and filling will be cooked together you can partially blind-cook the
dough at 180°C for 15mn for added crispiness.

Enjoy! It's now ready to serve!
```

Key Points

- Code is read more often than written
- The structure of the code should follow a well written explanation of its algorithm
- Separate level of abstractions (or details) in a problem must be reflected in the structure of the code, e.g. with separate functions
- Separable concerns (e.g. reading an input file to create X, creating X, computing stuff with X, saving results to file) must be reflected in the structure of the code

‹ (../l1-04-datastructures/index.html)

› (../l1-06-design

Edit on GitHub (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/edit/gh-pages/_episodes/l1-05-abstractions.md) / Contributing (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/blob/gh-pages/CONTRIBUTING.md) / Source (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/) / Cite (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/blob/gh-pages/CITATION) / Contact (mailto:rse-team@imperial.ac.uk)

Using The Carpentries style (https://github.com/carpentries/styles/) version 9.5.3 (https://github.com/carpentries/styles/releases/tag/v9.5.3).

‹ (../l1-05-abstractions/index.html) Essential Software Engineering for Researchers (../) › (../l2-01-testing

Design Patterns

Overview

Teaching: 15 min
Exercises: 15 min
Questions

- How can we avoid re-inventing the wheel when designing code?
- How can we transfer known solutions to our code?

Objectives

- Recognize much-used patterns in existing code
- Re-purpose existing patterns as solutions to new problems

What is a design pattern?

```
software design patterns: typical solutions to common problems
```

Pros

1. It is easier to reuse known solutions than to invent them
2. Makes the code easier to understand for collaborators
3. Makes the code easier to maintain since patterns ought to be best-in-class solutions

Cons

1. Shoehorning: not all patterns fit everywhere
2. Patterns paper-over inadequacies that exist in one language but not another
    - the visitor (https://en.wikipedia.org/wiki/Visitor_pattern) pattern is popular in Java or C++, but useless in Julia (https://www.julia.org), thanks to multiple dispatch (https://en.wikipedia.org/wiki/Multiple_dispatch)
    - Haskell (https://www.haskell.org/)'s functional (https://en.wikipedia.org/wiki/Functional_programming) style makes the strategy (https://en.wikipedia.org/wiki/Strategy_pattern) pattern so obvious, it's not longer a pattern, it's the way things are done

Examples:

- Iterator (https://en.wikipedia.org/wiki/Iterator_pattern) pattern (see below) separates how to loop from what to do in a loop
- Dependency injection (https://en.wikipedia.org/wiki/Dependency_injection) (see below) makes it easier to create modular algorithms
- Resource allocation is acquisition (https://en.wikipedia.org/wiki/Resource_acquisition_is_initialization) idiom promotes creating fully functional objects in one go
- Factory (https://en.wikipedia.org/wiki/Factory_method_pattern) pattern separates creating object from the class of the object. It is used to unify or simplify the creation of similar objects into a single function.
- Adapter (https://en.wikipedia.org/wiki/Adapter_pattern) pattern interfaces one class to be used in an another
- More (https://en.wikipedia.org/wiki/Software_design_pattern) and more (https://refactoring.guru/design-patterns) and more (https://stackoverflow.com/) patterns
- And let's not forget anti-patterns (https://en.wikipedia.org/wiki/Anti-pattern#Software_engineering), i.e. patterns that should **not** be used

Iterator Pattern

Iterators separates *generating items over which to loop* from *doing the body of the loop*. It separates looping from computing.

For instance, we want to loop over all items in `xs` and `ys`:

Python

```
for x in xs:
    for y in ys:
        compute(x, y)
```

The code above can be transformed to:

Python

```
from itertools import product

for x, y in product(xs, ys):
    compute(x, y)
```

Behind the scenes, itertool (https://docs.python.org/3.8/library/itertools.html)'s `product` returns an iterator (https://docs.python.org/3/library/stdtypes.html#iterator-types), i.e. something we can loop over.

Using `product` is both simpler and more general. Now the number of nested loops can be determined at runtime. It is no longer hard-coded.

Python

```
>>> from itertools import product
>>> list_of_lists = [[1, 2], [3, 4]]
>>> for args in product(*list_of_lists):
...     print(args)
(1, 3)
(1, 4)
(2, 3)
(2, 4)
>>> list_of_lists = [[1, 2], [3, 4], [5, 6]]
>>> for args in product(*list_of_lists):
...     print(args)
(1, 3, 5)
(1, 3, 6)
(1, 4, 5)
(1, 4, 6)
(2, 3, 5)
(2, 3, 6)
(2, 4, 5)
(2, 4, 6)
```

Generators: iterators made easy

Generators create iterators using syntax that is similar to the standard loop:

Python

```
for x in xs:
    for y in ys:
        print(f"some complicated calculation with {x} and {y}")
```

We can *lift* the loops out of the code and create a generator:

Python

```
def my_generator(xs, ys):
  for x in xs:
      for y in ys:
          yield x, y
          print(f"I am in my_generator {x}, {y}")
```

And then loop with an iterator which python creates auto-magically:

Python

```
>>> for x, y in my_generator([1, 2], ["a", "b"]):
...     print(f"some complicated calculation with {x} and {y}")
some complicated calculation with 1 and a
I am in my_generator 1, a
some complicated calculation with 1 and b
I am in my_generator 1, b
some complicated calculation with 2 and a
I am in my_generator 2, a
some complicated calculation with 2 and b
I am in my_generator 2, b
```

In practice, Python runs through the code in `my_generator` and returns a new element each time it hits yield. The next time it is called, it restarts from the line *right after* `yield` .

When to use generators?

1. To separate complex loops from complex calculations in the loop
2. Complex loops that occur multiple times in the code (copy-paste is a foot gun).
3. When running out of memory, generators allow you be lazy (https://en.wikipedia.org/wiki/Lazy_evaluation)
4. Use iterators when the language does not allow for generators (e.g. c++ (https://en.cppreference.com/w/cpp/iterator/iterator)).

Exercise

Power of two iterator

What does this print out?

Python

```
def powers_of_two(xs):
    for x in xs:
        yield 2**x

for x in powers_of_two([2, 4, 3, 2]):
    print(x)
```

Solution

```
4
16
9
4
```

Interleaved power of two and squares

How about this? Where does the function return two on after the first element, what about after the second element?

Python

```
def interleaved(xs):
    for x in xs:
        yield 2 ** x
        yield x ** 2

for x in interleaved([2, 4, 3, 2]):
    print(x)
```

Solution

```
4
4
16
16
8
9
4
4
```

Sequential power of two and squares

What is the output sequence in this case?

Python

```
def sequential(xs):

  for x in xs:
      yield 2 ** x

  for x in xs:
      yield x ** 2

for x in sequential([2, 4, 3, 2]):
    print(x)
```

Solution

```
4
16
8
4
4
16
9
4
```

How to use the iterator pattern

What to look for:

- Complex loops
- Complex loops that occur multiple times in the code
- Complex loops that occur multiple times in the code with only slight variations

What to do:

- Lift the loop into a generator function and make any parameter an input argument of the generator function.

Other languages

- c++: create a class with the following methods:

```C++
class Iterator {
  // pre-increment
  // note: const is optional, but a priori, its a good idea.
  Iterator operator++() const;
  // or post-increment. or both.
  // note: const is optional, but a priori, its a good idea.
  Iterator operator++(int) const;

  // dereference, to access the "yielded" values
  T operator*();
  // optionally, const dereference
  const T operator*() const;

  // comparison to other iterator
  bool operator!=(const Iterator &) const;
}
```

  Then use in loop:

```C++
for(Iterator i(...), end(...); i != end; ++i)
    compute(*i);
```

- R: CRAN package iterators (https://cran.r-project.org/web/packages/iterators/index.html)
- Julia: iterator interface (https://docs.julialang.org/en/v1/manual/interfaces/#man-interface-iteration-1)
- Fortran: of course not

Dependency Injection, or how to make algorithms tweakable

It's not unusual to want to change an algorithm, but only in one or two places:

```Python
def my_algorithm(some_input):
    return [
        uncornify(webby)
        for webby in deconforbulate(some_input)
    ]
```

Say that rather than loop over `deconforbulate` objects, you need to loop over `undepolified` objects.

Here's one *bad* solution:

```Python
def my_awful_copy_paste_non_solution(some_input):
    return [
        uncornify(webby)
        for webby in undepolified(some_input)
    ]
```

Here's a slightly better one:

```Python
```

```
def my_somewhat_better_solution(some_input, is_deconfobulated: bool = True):
    if is_deconfobulated:
      generator = deconforbulate
    else:
      generator = undepolified

    return [
        uncornify(webby) for webby in generator(some_input)
    ]
```

But it doesn't scale!

Your supervisor just popped in and wants you to try and loop over `unsoupilate`d, `resoupilate`d, and `gunkifucate`d objects, and probably others as well. Using the pattern above, we have to modify the algorithm each and every time we add a new tweak.

This scenario is based on multiple past and future real-life stories.

Thankfully, the dependency-injection design pattern can come to the rescue!

Python

```
from typing import Callable, Optional

def the_bees_knees_solution(some_input, generator: Optional[Callable] = None):
    if generator is None:
        generator = deconforbulate

    return [
        uncornify(webby) for webby in generator(some_input)
    ]
```

Now the algorithm is independent of the exact generator (Yay! Separation of concerns!). It can be used without modification with any generator that takes `obstrucated`-like objects.

Other languages

- c++: The tweakable element is any function object (https://en.cppreference.com/w/cpp/utility/functional) or function. The algorithm takes std::function (https://en.cppreference.com/w/cpp/utility/functional/function) as argument (simpler code, faster compilation, possibly slower performance). Or use a template argument (https://en.cppreference.com/w/cpp/language/template_parameters) (slower compilation, no performance hit, often leads to complicated code).
- R: just pass the function, like in Python.
- Julia: just pass the function, like in Python.
- Fortran: The Fortran 2003 standard introduced procedure pointers (http://fortranwiki.org/fortran/show/Procedure+pointers). Since it has only been 17 years, Fortran 2003 compilers can be patchy, buggy, and under-performant. Use at your own risk.

How to use dependency-injection

What to look for:

- algorithms that have been copy-pasted
- slight variations of the same algorithm

What to do:

- Separate levels of details and concerns in the algorithm
- Write the algorithm as seperate functions/class for each level of details and concern
- Identify the "tweakable" concerns that need to be changed easily
- Make the "tweakable" concerns an argument of the algorithm

Iterating over points in a ring

Create an iterator and/or a generator that lifts the loop over points in a two-dimensional ring:

Take this code:

Python

```
from math import sqrt

points = [[1, 2], [0, 0], [-2, 0], [-2, 3], [-3, -4], [4, 0], [5, 5]]
radius = 3.5
width = 1.0

inner = radius - 0.5 * width
outer = radius + 0.5 * width
for point in points:
    distance = sqrt(point[0] * point[0] + point[1] * point[1])
    if distance >= inner and distance <= outer:
        print(f"Some complicated calculation at {point}")
```

and create a generator function `points_in_ring`:

Python

```
for point in points_in_ring(points, radius, width):
    print(f"Some complicated calculation at {point}")
```

At this point, `points_in_ring` uses the Euclidian distance (https://en.wikipedia.org/wiki/Euclidean_distance) to figure out what is in the ring. Using dependency-injection, make `points_in_ring` capable of using any sensible distance (say the Manhattan norm (https://en.wikipedia.org/wiki/Norm_(mathematics)#Taxicab_norm_or_Manhattan_norm)):

Python

```
def manhattan(point: List[float]) -> float:
    return sum(abs(x) for x in point)


for point in points_in_ring(points, radius, width, norm=manhattan):
    print(f"Some complicated calculation at {point}")
```

NOTE:

- `points_in_ring` can be used over and over across the code
- it is parametrized by radius and width
- it make the loop self-descriptive
- it is more memory efficient (lazy evaluation (https://en.wikipedia.org/wiki/Lazy_evaluation)) than a list
- it is almost always better than creating and keeping in sync a second list holding only points in a ring (compute is cheap)
- it makes it possible to test/debug the loop alone, without worrying about the compute inside the loop

Ring generator

Python

```python
from math import sqrt
from typing import Iterable


def points_in_ring(points: Iterable, radius: float, width: float) -> Iterable:
    inner = radius - 0.5 * width
    outer = radius + 0.5 * width
    for point in points:
        distance = sqrt(point[0] * point[0] + point[1] * point[1])
        if distance >= inner and distance <= outer:
            yield point


points = [[1, 2], [0, 0], [-2, 0], [-2, 3], [-3, -4], [4, 0], [5, 5]]

for point in points_in_ring(points, radius=3.5, width=1.0):
    print(f"Some complicated calculation at {point}")
```

Ring generator with tweakable norm

Python

```python
from math import sqrt
from typing import Iterable, List, Optional, Callable


def euclidean(point: List[float]) -> float:
    return sqrt(sum((x * x) for x in point))


def manhattan(point: List[float]) -> float:
    return sum(abs(x) for x in point)


def points_in_ring(
    points: Iterable,
    radius: float,
    width: float,
    norm: Optional[Callable] = None,
) -> Iterable:
    if norm is None:
        norm = euclidean

    inner = radius - 0.5 * width
    outer = radius + 0.5 * width
    for point in points:
        distance = norm(point)
        if distance >= inner and distance <= outer:
            yield point


points = [[1, 2], [0, 0], [-2, 0], [-2, 3], [-3, -4], [4, 0], [5, 5]]

for point in points_in_ring(points, radius=3.5, width=1.0, norm=manhattan):
    print(f"Some complicated calculation at {point}")
```

Key Points

- Many coders have come before
- Transferable solutions to common problems have been identified
- It is easier to apply a known pattern than to reinvent it, but first you have to spend some time learning about patterns.
- Iterators and generators are convenient patterns to separate loops from compute and to avoid copy-pasting.
- Dependency injections is a pattern to create modular algorithms

‹ (../l1-05-abstractions/index.html)

› (../l2-01-testing

Edit on GitHub (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/edit/gh-pages/_episodes/l1-06-design_patterns.md) / Contributing (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/blob/gh-pages/CONTRIBUTING.md) / Source (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/) / Cite (https://github.com/ImperialCollegeLondon/grad_school_software_engineering_course/blob/gh-pages/CITATION) / Contact (mailto:rse-team@imperial.ac.uk)

‹ (../l1-06-design_patterns/index.html) Essential Software Engineering for Researchers (../) › (../l2-02-testing_

Testing Overview

Overview

Teaching: 15 min
Exercises: 5 min
Questions

- Why test my software?
- How can I test my software?
- How much testing is 'enough'?

Objectives

- Appreciate the benefits of testing research software
- Understand what testing can and can't achieve
- Describe various approaches to testing, and relevant trade-offs
- Understand the concept of test coverage, and how it relates to software quality and sustainability
- Appreciate the benefits of test automation

Why Test?

There are a number of compelling reasons to properly test a research code:

- Show that physical laws or mathematical relationships are correctly encoded
- Check that code works when running on a new system
- Make sure new code changes do not break existing functionality
- Ensure code correctly handles edge or corner cases
- Persuade others your code is reliable
- Check that code works with new or updated dependencies

Whilst testing might seem like an intimidating topic the chances are you're already doing testing in some form. No matter the level of experience, no programmer ever just sits down and writes some code, is perfectly confident that it works and proceeds to use it straight away in research. Instead development is in practice more piecemeal - you generally think about a simple input and the expected output then write some simple code that works. Then, iteratively, you think about more complicated example inputs and outputs and flesh out the code until those work as well. When developers talk about testing all this means is formalising the above process and making it automatically repeatable on demand.

This has numerous advantages over a more ad hoc approach:

- Provides a record of the tests that have been carried out
- Faster development times - get feedback on changes quickly
- Encourages writing more modular code
- Ensures breakages are caught early in development
- Prevent manual testing mistakes

As you're performing checks on your code anyway it's worth putting in the time to formalise your tests and take advantage of the above.

A Hypothetical Scenario

Your supervisor has tasked you with implementing an obscure statistical method to use for some data analysis. Wanting to avoid unnecessary work you check online to see if an implementation exists. Success! Another researcher has already implemented and published the code.

You move to hit the download button, but a worrying thought occurs. How do you know this code is right? You don't know the author or their level of programming skill. Why should you trust the code?

Now turn this question on its head. Why should your colleagues or supervisor trust any implementation of the method that you write? Why should you trust work you did a year ago? What about a reviewer for a paper?

This scenario illustrates the sociological value of automated testing. If published code has tests then you have instant assurance that its authors have invested time in the checking the correctness of their code. You can even see exactly the tests they've tried and add your own if you're not satisfied. Conversely, any code that lacks tests should be viewed with suspicion as you have no record of what quality assurance steps have been taken.

Types of Testing

This isn't a topic we will discuss in much detail but is worth mentioning as the jargon here can be another factor that is intimidating. In fact there are entire websites (http://softwaretestingfundamentals.com) dedicated to explaining the different types of testing. Ultimately, however there are only a few types of testing that we need to worry about.

Unit Testing

The main type of testing kind we will be dealing with in this course. Unit testing refers to taking a component of a program and testing it in isolation. Generally this means testing an individual class or function. This is part of the reason that testing encourages more modular and sustainable code development. You're encouraged to write your code into functionally independent components that can be easily unit tested.

Functional Testing

Unlike unit testing that focuses on independent parts of the system, functional testing checks the compliance of the system overall against a defined set of criteria. In other words does the software as a whole do what it's supposed to do?

Regression Testing

This refers to the practice of running previously written tests whenever a new change is introduced to the code. This is good to do even when making seemingly insignificant changes. Carrying out regression testing allows you to remain confident that your code is functioning as expected even as it grows in complexity and capability.

Testing Done Right

It's important to be clear about what software tests are able to provide and what they can't. Unfortunately it isn't possible to write tests that completely guarantee that your code is bug free or provides a one hundred percent faithful implementation of a particular model. In fact it's perfectly possible to write an impressive looking collection of tests that have very little value at all. What should be the aim therefore when developing software tests?

In practice this is difficult to define universally but one useful mantra is that good tests ***thoroughly exercise critical code***. One way to achieve this is to design test examples of increasing complexity that cover the most general case the unit should encounter. Also try to consider examples of special or edge cases that your function needs to handle especially.

A useful quantitative metric to consider is **test coverage**. Using additional tools it is possible to determine, on a line-by-line basis, the proportion of a codebase that is being exercised by its tests. This can be useful to ensure, for instance, that all logical branching points within the code are being used by the test inputs.

Testing and Coverage

Consider the following Python function:

Python

```
def recursive_fibonacci(n):
    """Return the n'th number of the fibonacci sequence"""
    if n <= 1:
        return n
    else:
        return recursive_fibonacci(n - 1) + recursive_fibonacci(n - 2)
```

Try to think up some test cases of increasing complexity, there are four distinct cases worth considering. What input value would you use for each case and what output value would you expect? Which lines of code will be exercised by each test case? How many cases would be required to reach 100% coverage?

For convenience, some initial terms from the Fibonacci sequence are given below:
0, 1, 1, 2, 3, 5, 8, 13, 21

Solution

Case 1 - Use either 0 or 1 as input

Correct output: Same as input
Coverage: First section of if-block
Reason: This represents the simplest possible test for the function. The value of this test is that it exercises only the special case tested for by the if-block.

Case 2 - Use a value > 1 as input

Correct output: Appropriate value from the Fibonacci sequence
Coverage: All of the code
Reason: This is a more fully fledged case that is representative of the majority of the possible range of input values for the function. It covers not only the special case represented by the first if-block but the general case where recursion is invoked.

Case 3 - Use a negative value as input

Correct output: Depends…
Coverage: First section of if-block
Reason: This represents the case of a possible input to the function that is outside of its intended usage. At the moment the function will just return the input value, but whether this is the correct behaviour depends on the wider context in which it will be used. It might be better for this type of input value to cause an error to be raised however. The value of this test case is that it encourages you to think about this scenario and what the behaviour should be. It also demonstrates to others that you've considered this scenario and the function behaviour is as intended.

Case 4 - Use a non-integer input e.g. 3.5

Correct output: Depends…
Coverage: Whole function
Reason: This is similar to case 3, but may not arise in more strongly typed languages. What should the function do here? Work as is? Raise an error? Round to the nearest integer?

Summary

The importance of automated testing for software development is difficult to overstate. As testing on some level is always carried out there is relatively low cost in formalising the process and much to be gained. The rest of this course will focus on how to carry out unit testing.

Key Points

- Testing is the standard approach to software quality assurance
- Testing helps to ensure that code performs its intended function: well-tested code is likely to be more reliable, correct and malleable
- Good tests thoroughly exercise critical code
- Code without any tests should arouse suspicion, but it is entirely possible to write a comprehensive but practically worthless test suite
- Testing can contribute to performance, security and long-term stability as the size of the codebase and its network of contributors grows
- Testing can ensure that software has been installed correctly, is portable to new platforms, and is compatible with new versions of its dependencies
- In the context of research software, testing can be used to validate code i.e. ensure that it faithfully implements scientific theory
- Unit (e.g. a function); Functional (e.g. a library); and Regression, (e.g. a bug) are three commonly used types of tests
- Test coverage can provide a coarse- or fine-grained metric of comprehensiveness, which often provides a signal of code quality
- Automated testing is another such signal: it lowers friction; ensures that breakage is identified sooner and isn't released; and implies that machine-readable instructions exist for building and code and running the tests
- Testing ultimately contributes to sustainability i.e. that software is (and remains) fit for purpose as its functionality and/or contributor-base grows, and its dependencies and/or runtime environments change

‹ (../l1-06-design_patterns/index.html)

› (../l2-02-testing_

(../l2-01-testing_overview/index.html) Essential Software Engineering for Researchers (../) (../)

Writing unit tests

Overview

Teaching: 40 min
Exercises: 60 min
Questions

- What is a unit test?
- How do I write and run unit tests?
- How can I avoid test duplication and ensure isolation?
- How can I run tests automatically and measure their coverage?

Objectives

- Implement effective unit tests using pytest
- Execute tests in Visual Studio Code
- Explain the issues relating to non-deterministic code
- Implement fixtures and test parametrisation using pytest decorators
- Configure git hooks and pytest-coverage
- Apply best-practices when setting up a new Python project
- Recognise analogous tools for other programming languages
- Apply testing to Jupyter notebooks

Introduction

Unit testing validates, in isolation, functionally independent components of a program.

In this lesson we'll demonstrate how to write and execute unit tests for a simple scientific code.

This involves making some technical decisions…

Test frameworks

We'll use pytest (https://docs.pytest.org/en/latest/) as our test framework. It's powerful but also user friendly.

For comparison: testing using `assert` statements:

Python

```
from temperature import to_fahrenheit

assert to_fahrenheit(30) == 86
```

Testing using the built-in `unittest` library:

Python

```
from temperature import to_fahrenheit
import unittest

class TestTemperature(unittest.TestCase):
    def test_to_farenheit(self):
        self.assertEqual(to_fahrenheit(30), 86)
```

Testing using `pytest`:

Python

```
from temperature import to_fahrenheit

def test_answer():
    assert to_fahrenheit(30) == 86
```

Why use a test framework?

- Avoid reinventing the wheel - frameworks such as pytest provide lots of convenient features (some of which we'll see shortly)

- Standardisation leads to better tooling, easier onboarding etc

Projects that use pytest:

- numpy (https://github.com/numpy/numpy/blob/master/README.md) (example (https://github.com/numpy/numpy/blob/master/numpy/core/tests/test_umath.py#L220))
- pandas (https://github.com/pandas-dev/pandas)
- SciPy (https://github.com/scipy/scipy)
- Devito (https://github.com/devitocodes/devito/blob/master/README.md) (tests (https://github.com/devitocodes/devito/tree/master/tests))

📌 Learning by example

Reading the test suites of mature projects is a good way to learn about testing methodologies and frameworks

Code editors

We've chosen Visual Studio Code (https://code.visualstudio.com/) as our editor. It's free, open source, cross-platform and has excellent Python (and pytest) support. It also has built-in Git integration, can be used to edit files on remote systems (e.g. HPC), and handles Jupyter notebooks (plus many more formats).

📌 Demonstration of pytest + VS Code + coverage

- Test discovery, status indicators and ability to run tests inline
- Code navigation ("Go to Definition")
- The Test perspective and Test Output
- Maximising coverage (`assert recursive_fibonacci(7) == 13`)
- Test-driven development: adding and fixing a new test (`test_negative_number`)

A tour of pytest

Checking for exceptions

If a function invocation is expected to throw an exception it can be wrapped with a pytest `raises` block:

Python

```
def test_non_numeric_input():
    with pytest.raises(TypeError):
        recursive_fibonacci("foo")
```

Parametrisation

Similar test invocations can be grouped together to avoid repetition. Note how the parameters are named, and "injected" by pytest into the test function at runtime:

Python

```
@pytest.mark.parametrize("number,expected", [(0, 0), (1, 1), (2, 1), (3, 2)])
def test_initial_numbers(number, expected):
    assert recursive_fibonacci(number) == expected
```

This corresponds to running the *same* test with *different* parameters, and is our first example of a pytest decorator (`@pytest`). Decorators (https://realpython.com/primer-on-python-decorators/) are a special syntax used in Python to modify the behaviour of the function, without modifying the code of the function itself.

Skipping tests and ignoring failures

Sometimes it is useful to skip tests (conditionally or otherwise), or ignore failures (for example if you're in the middle of refactoring some code).

This can be achieved using other `@pytest.mark` annotations e.g.

Python

```
@pytest.mark.skipif(sys.platform == "win32", reason="does not run on windows")
def test_linux_only_features():
    ...

@pytest.mark.xfail
def test_unimplemented_code():
    ...
```

📌 Refactoring

Code refactoring (https://en.wikipedia.org/wiki/Code_refactoring) is “the process of restructuring existing computer code without changing its external behavior” and is often required to make code more amenable to testing.

Fixtures

If multiple tests require access to the same data, or a resource that is expensive to initialise, then it can be provided via a fixture. These can be cached by modifying the scope of the fixture. See this example from Devito:

Python

```
@pytest.fixture
def grid(shape=(11, 11)):
    return Grid(shape=shape)

def test_forward(grid):
    grid.data[0, :] = 1.
    ...

def test_backward(grid):
    grid.data[-1, :] = 7.
    ...
```

This corresponds to providing the *same* parameters to *different* tests.

Tolerances

It’s common for scientific codes to perform estimation by simulation or other means. pytest can check for approximate equality:

Python

```
def test_approximate_pi():
    assert 22/7 == pytest.approx(math.pi, abs=1e-2)
```

📌 Random numbers

If your simulation or approximation technique depends on random numbers then consistently seeding your generator can help with testing. See `random.seed()` (https://docs.python.org/3/library/random.html#random.seed) for an example or the pytest-randomly (https://github.com/pytest-dev/pytest-randomly) plugin for a more comprehensive solution.

doctest

pytest has automatic integration with the Python’s standard doctest (https://docs.python.org/3/library/doctest.html) module when invoked with the `--doctest-modules` argument. This is a nice way to provide examples of how to use a library, via interactive examples in docstrings (https://realpython.com/documenting-python-code/#documenting-your-python-code-base-using-docstrings):

Python

```
def recursive_fibonacci(n):
    """Return the nth number of the fibonacci sequence

    >>> recursive_fibonacci(7)
    13
    """
    return n if n <=1 else recursive_fibonacci(n - 1) + recursive_fibonacci(n - 2)
```

Hands-on unit testing

Getting started

Setting up our editor

1. If you haven't already, see the setup guide (../setup) for instructions on how to install Visual Studio Code and conda.
2. Download and extract this zip file (https://github.com/ImperialCollegeLondon/diffusion/archive/master.zip). If using an ICT managed PC please be sure to do this in your user area on the C: drive i.e. `C:\Users\your_username`
   - *Note that files placed here are not persistent so you must remember to take a copy before logging out*
3. In Visual Studio Code go to **File > Open Folder…** and find the files you just extracted.
4. If you see an alert "This workspace has extension recommendations." click **Install All** and then switch back to the **Explorer** perspective by clicking the top icon on the left-hand toolbar
5. Open Anaconda Prompt (Windows), or a terminal (Mac or Linux) and run:

   Bash

   ```
   conda env create --file "path_to_environment.yml"
   ```

   The `path_to_environment.yml` can be obtained by right-clicking the file name in the left pane of Visual Studio Code and choosing "Copy Path". Be sure to include the quotation marks. Right click on the command line interface to paste.
6. **Important**: After the environment has been created go to **View > Command Palette** in VS Code, start typing "Python: Select interpreter" and hit enter. From the list select your newly created environment "diffusion"

Running the tests

1. Open `test_diffusion.py`
2. You should now be able to click on **Run Test** above the `test_heat()` function and see a warning symbol appear, indicating that the test is currently failing. You may have to wait a moment for **Run Test** to appear.
3. Switch to the **Test** perspective by clicking on the flask icon on the left-hand toolbar. From here you can **Run All Tests**, and **Show Test Output** to view the coverage report (see Lesson 1 (../l2-01-testing_overview/) for more on coverage)
4. **Important**: If you aren't able to run the test then please ask a demonstrator for help. It is essential for the next exercise.

Introduction to your challenge

You have inherited some buggy code from a previous member of your research group: it has a unit test but it is currently failing. Your job is to refactor the code and write some extra tests in order to identify the problem, fix the code and make it more robust.

The code solves the heat equation, also known as the "Hello World" of Scientific Computing (https://github.com/betterscientificsoftware/hello-heat-equation). It models transient heat conduction in a metal rod i.e. it describes the temperature at a distance from one end of the rod at a given time, according to some initial and boundary temperatures and the thermal diffusivity of the material:

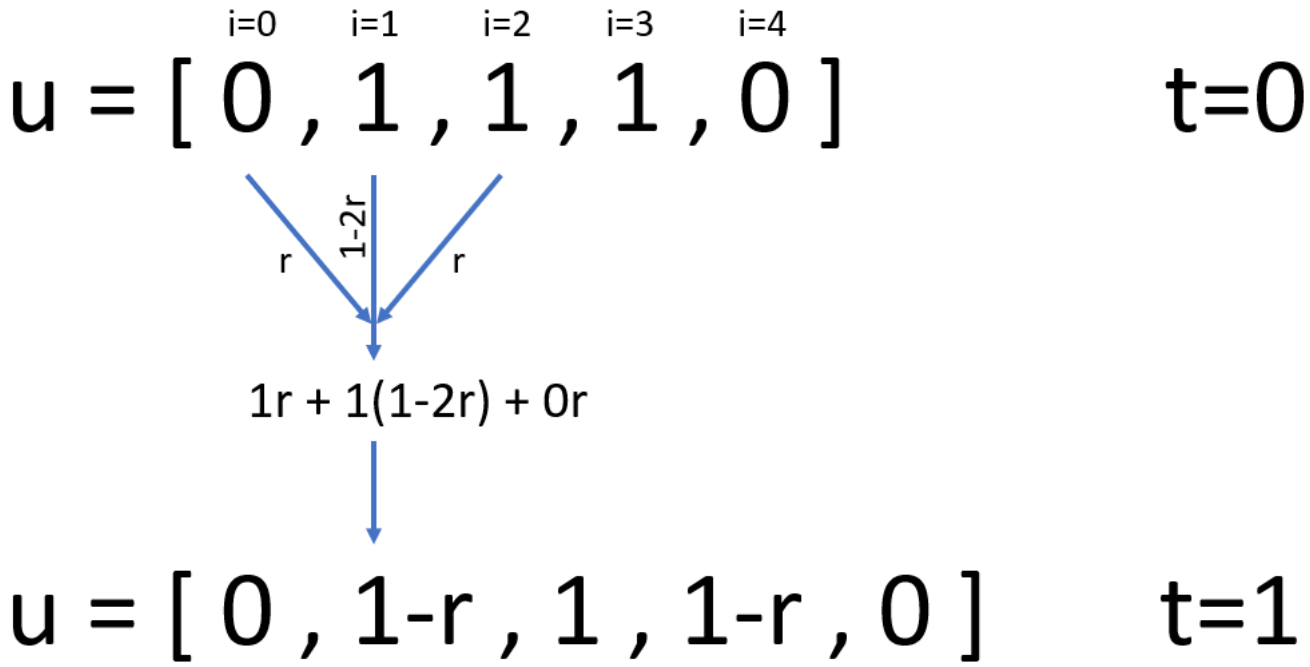
The function `heat()` in `diffusion.py` attempts to implement a **step-wise numerical approximation** via a finite difference method (https://en.wikipedia.org/wiki/Finite_difference_method):

$$u_i^{t+1} = ru_{i+1}^t + (1-2r)u_i^t + ru_{i-1}^t$$

This relates the temperature `u` at a specific location `i` and time point `t` to the temperature at the previous time point and neighbouring locations. `r` is defined as follows, where `α` is the thermal diffusivity:

$$r = \frac{\alpha \Delta t}{\Delta x^2}$$

We approach this problem by representing `u` as a Python list. Elements within the list correspond to positions along the rod, `i=0` is the first element, `i=1` is the second and so on. In order to increment `t` we update `u` in a loop. Each iteration, according to the finite difference equation above, we calculate values for the new elements of `u`.



The `test_heat()` function in `test_diffusion.py` compares this *approximation* with the *exact* (analytical) solution for the boundary conditions (i.e. the temperature of the end being fixed at zero). The test is correct but failing - indicating that there is a bug in the code.

Testing (and fixing!) the code

Work by yourself or with a partner on these test-driven development tasks. Don't hesitate to ask a demonstrator if you get stuck!

Separation of concerns

First we'll refactor the code, increasing its modularity. We'll extract the code that performs a single time step into a new function that can be verified in isolation via a new unit test:

1. In `diffusion.py` move the logic that updates `u` within the loop in the `heat()` function to a new top-level function:

Python

```
def step(u, dx, dt, alpha):
    ...
```

Hint: the loop in `heat()` should now look like this:

Python

```
for _ in range(nt - 1):
    u = step(u, dx, dt, alpha)
```

2. Run the existing test to ensure that it executes without any Python errors. It should still fail.
3. Add a test for our new `step()` function:

Python

```
def test_step():
    assert step(...) == ...
```

It should call `step()` with suitable values for `u` (the temperatures at time `t`), `dx`, `dt` and `alpha`. It should `assert` that the resulting temperatures (i.e. at time `t+1`) match those suggested by the equation above. Use `approx` if necessary. _Hint: `step([0, 1, 1, 0], 0.04, 0.02, 0.01)` is a suitable invocation. These values will give `r=0.125`. It will return a list of the form `[0, ?, ?, 0]`. You'll need to calculate the missing values manually using the equation in order to compare the expected and actual values.

4. Assuming that this test fails, fix it by changing the code in the `step()` function to match the equation - correcting the original bug. Once you've done this all the tests should pass.

Solution 1

Now we'll add some further tests to ensure the code is more suitable for publication.

Testing for exceptions

We want the `step()` function to raise (https://docs.python.org/3/tutorial/errors.html#raising-exceptions) an Exception (https://docs.python.org/3/tutorial/errors.html#exceptions) when the following stability condition (https://en.wikipedia.org/wiki/Von_Neumann_stability_analysis) *isn't* met:

$$r \leq \frac{1}{2}$$

Add a new test `test_step_unstable`, similar to `test_step` but that invokes `step` with an `alpha` equal to `0.1` and expects an `Exception` to be raised. Check that this test fails before making it pass by modifying `diffusion.py` to raise an `Exception` appropriately.

Solution 2

Adding parametrisation

Parametrise `test_heat()` to ensure the approximation is valid for some other combinations of `L` and `tmax` (ensuring that the stability condition remains true).

Solution 3

After completing these two steps check the coverage of your tests via the Test Output panel - it should be 100%.

The full, final versions of diffusion.py (https://github.com/ImperialCollegeLondon/diffusion/blob/develop/diffusion.py) and test_diffusion.py (https://github.com/ImperialCollegeLondon/diffusion/blob/develop/test_diffusion.py) are available on GitHub.

Bonus task(s)

- Write a doctest-compatible docstring for `step()` or `heat()`
- Write at least one test for our currently untested `linspace()` function
  - *Hint: you may find inspiration in numpy's test cases (https://github.com/numpy/numpy/blob/021163b5e2293286b26d22bdae51305da634e74d/numpy/core/tests/test_function_base.py#L222), but bear in mind that its version of linspace (https://docs.scipy.org/doc/numpy/reference/generated/numpy.linspace.html) is more capable than ours.*

Advanced topics

More pytest plugins

- `pytest-benchmark` (https://pytest-benchmark.readthedocs.io/en/stable/) provides a fixture that can transparently measure *and track* performance while running your tests:

Python

```
def test_fibonacci(benchmark):
    result = benchmark(fibonacci, 7)
    assert result == 13
```

📌 pytest-benchmark example

Demonstration of performance regression via recursive and formulaic approaches to Fibonacci calculation (output (https://imperiallondon.sharepoint.com/sites/RSE/Shared%20Documents/Graduate%20School%20RSE%20course/Supplementary%20teaching%20material/Essential%2
02%20pytest-benchmark%20output.png))

- `pytest-notebook` (https://pytest-notebook.readthedocs.io/en/latest/) can check for regressions in your Jupyter notebooks (see also Jupyter CI (https://github.com/mwoodbri/jupyter-ci))
- Hypothesis (https://hypothesis.readthedocs.io/en/latest/) provides property-based testing, which is useful for verifying edge cases):

Python

```
from fibonacci import recursive_fibonacci
from hypothesis import given, strategies

@given(strategies.integers())
def test_recursive_fibonacci(n):
    phi = (5 ** 0.5 + 1) / 2
    assert recursive_fibonacci(n) == int((phi ** n - -phi ** -n) / 5 ** 0.5)
```

Taking testing further

Testing in other languages

- We've discussed tools and approaches for Python but analogues exist for other languages
- We (the RCS) have had success with:
  - C++: Catch2 (https://github.com/catchorg/Catch2)
  - Fortran: pFUnit (https://github.com/Goddard-Fortran-Ecosystem/pFUnit)
  - R: testthat (https://github.com/r-lib/testthat)
- See the Software Sustainability Institute's Build and Test Examples (https://github.com/softwaresaved/build_and_test_examples) for many more

Further resources

- `ImperialCollegeLondon/pytest_template_application` (https://github.com/ImperialCollegeLondon/pytest_template_application)
- A tried-and-tested workflow for software quality assurance (https://doi.org/10.5281/zenodo.1409199) (repo (https://gitlab.com/mwoodbri/rse18))
- Using Git to Code, Collaborate and Share (https://www.imperial.ac.uk/study/pg/graduate-school/students/doctoral/professional-development/research-computing-data-science/courses/git-to-code-callobrate-share/)
- RCS courses (https://wiki.imperial.ac.uk/display/HPC/Courses) and clinics (https://www.imperial.ac.uk/admin-services/ict/self-service/research-support/rcs/support/attend-a-clinic/)
- Research Software Community (https://www.imperial.ac.uk/computational-methods/rse/)

Key Points

- Testing is not only standard practice in mainstream software engineering, it also provides distinct benefits for any non-trivial research software
- pytest is a powerful testing framework, with more functionality than Python's built-in features while still catering for simple use cases
- Testing with VS Code is straightforward and encourages good habits (writing tests as you code, and simplifying test-driven development)
- It is important to have a set-up you can use for every project - so that it becomes as routine in your workflow as version control itself
- pytest has a myriad of extensions that are worthy of mention such as Jupyter, benchmark, Hypothesis etc
- Adding unit tests can verify the correctness of software and improve its structure: isolating logical distinct code for testing often involves untangling complex structures

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