

A Scientist-Friendly Approach to Software Testing

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Introduction

What are we talking about today?

- Automated software tests
 - Regularly re-run (by machine)
 - Evaluated objectively (by machine)
 - Expected to work on all user deployments
→ ANYONE can run & interpret
- Reproducible, deterministic results
 - We do not want a reproducibility crisis in scientific software

STATUS	RUN	COMMIT	BRANCH
✓	441	–	master
✓	1	–	PR-1555
✓	440	cc00c23	master
✓	3	–	PR-1542
✗	2	1e43ad3	PR-1542
✓	439	4156b8e	master
✓	1	–	PR-1553



Automated testing frameworks

- Discovers and runs test functions
- Can help ensure **test isolation**
- Let you **select subsets** of tests to run
- Reporting features (coverage, xml, ...)



A screenshot of a terminal window titled "brian@FlatTop: ~/sandbox/experimental-testing-exercises". The window shows the output of a pytest command: `pytest ./00/ -k midpoint -v`. The output indicates a test session starting on a platform with Python 3.11.0, pytest-8.3.3, and pluggy-1.5.0. It shows the collection of 10 items, with 5 deselected and 5 selected. The selected tests are `test_binary_search_soln.py::test_midpoint_even`, `test_binary_search_soln.py::test_midpoint_odd`, `test_binary_search_soln.py::test_midpoint_small`, `test_binary_search_soln.py::test_midpoint_same`, and `test_binary_search_soln.py::test_midpoint_massive`, all of which passed. A progress bar on the right shows the completion of the test session at 100%. The terminal concludes with `5 passed, 5 deselected in 0.01s`.

```
brian@FlatTop: ~/sandbox/experimental-testing-exercises
[brian@FlatTop experimental-testing-exercises on main [!]] $ pytest ./00/ -k midpoint -v
=====
test session starts =====
platform linux -- Python 3.11.0, pytest-8.3.3, pluggy-1.5.0 -- /home/brian/.miniforge3/envs/stan/bin/python3.11
cachedir: .pytest_cache
rootdir: /home/brian/sandbox/experimental-testing-exercises
plugins: order-1.3.0, anyio-4.6.0
collected 10 items / 5 deselected / 5 selected

00/test_binary_search_soln.py::test_midpoint_even PASSED
00/test_binary_search_soln.py::test_midpoint_odd PASSED
00/test_binary_search_soln.py::test_midpoint_small PASSED
00/test_binary_search_soln.py::test_midpoint_same PASSED
00/test_binary_search_soln.py::test_midpoint_massive PASSED

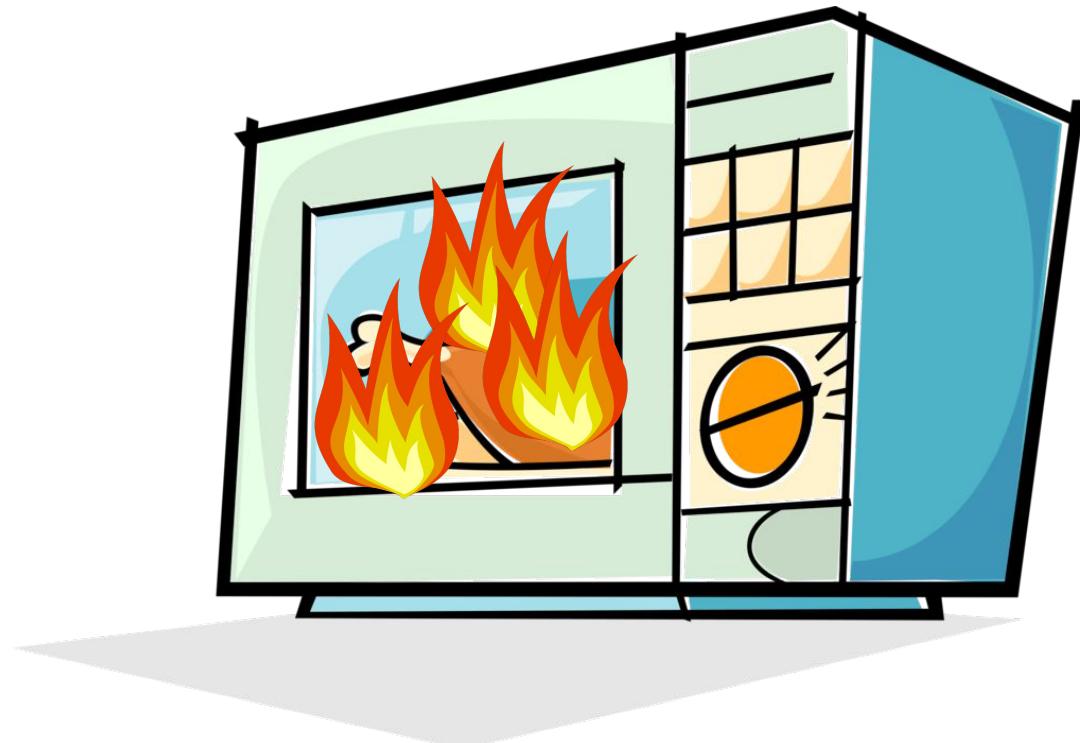
=====
5 passed, 5 deselected in 0.01s
[brian@FlatTop experimental-testing-exercises on main [!]] $
```

Scientific testing means treating tests as . . .

- **controlled experiments** that
- each **confirm one specific property** or **invariant** of
- the **code artifact** you are publishing

Test result must depend on **your code – a small part of your code – and nothing but your code**

Test your oven with a thermometer, not a turkey.

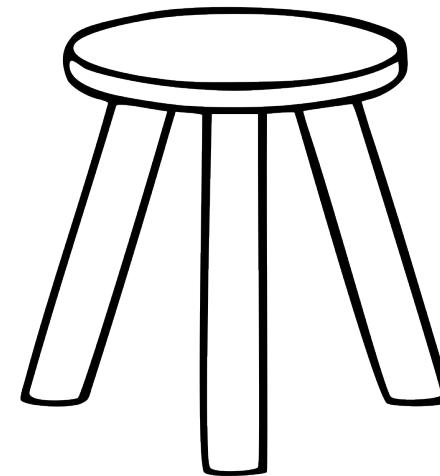


Scientific testing can

- Show **correctness** of our implementation
- **Localize** sources of error
- Increase confidence during **future code changes**
- **Document** code expectations/design choices

Three pillars of test suites

- Fast
- Trustworthy
- Specific



Honorable mention: maintainable
Implicit requirement: independent

What you need to follow along today

- https://github.com/flatironinstitute/sciware/tree/main/42_ScientificTesting
- If you're using Python, we recommend installing pytest
- If you want to use C++, we will provide links to the Compiler Explorer



Anatomy of a test

What makes a test?

To do a test, you must:

- Set up the preconditions for the behavior you're testing
- Call the code whose behavior you're testing
- Compare the actual result with the expected result

Mnemonic is “arrange, act, assert”

...but the greatest of these is **assert**



```
assert Frob().bar is not None
```

Assertion libraries

- You've only tested what you've **asserted**
- Good tools help you **zero in on discrepancies**
 - Expressive comparisons, error handlers, etc. let you make more precise assertions
- **Hypothesis testing tools** can help turn invariants into assertions automatically
- Gold/expect/cram testing can help ensure reliable output (but may be brittle)

```

1 #include <gtest/gtest.h>
2
3 TEST(fp, equality) {
4     EXPECT_EQ(0.1 + 0.2, 0.3);
5 }
6
7 TEST(fp, better_equality){
8     EXPECT_FLOAT_EQ(0.1 + 0.2, 0.3);
9 }
```

```
[-----] 2 tests from fp
[ RUN      ] fp.equality
/app/example.cpp:4: Failure
Expected equality of these values:
 0.1 + 0.2
    Which is: 0.3000000000000004
 0.3

[ FAILED  ] fp.equality (0 ms)
[ RUN      ] fp.better_equality
[      OK ] fp.better_equality (0 ms)
```

Let's look at some tests

Follow along at

https://github.com/flatironinstitute/sciware/tree/main/42_ScientificTesting

Folder 'binary_search'

Goals for tests

One test, one property

- Every test should test a specific, explicitly stated property of the code
- It should pass if, and only if, that property holds

Yes, this will lead to lots of tests!

This is not a problem so long as you keep them all fast.

Controlled experiments

- Success or failure should depend **only** on the property under test
- Any **other** factors should be set to known values
- Systems not under test should be **omitted**
 - by use of fakes/stubs/mocks, monkey-patching, etc.

Only test your code

- A useful test must **call the implementation**
 - It's common to write a slow/naive version of an algorithm for testing, but make sure you're comparing that to the *real* one at some point!
- There's little point to testing library code

Three varieties of bad tests

Those that...

- Never fail (tautological, or fail to assert anything)
- Never pass (or: fail if you breathe on them)
- Might fail or pass on the same inputs

Also fishy: tests that take a huge amount of work to achieve control

Assumptions and invariants

What to assert?

Universal invariants: confirming expectations

- Results of a (deterministic) computation
- Correct logical branch was taken
- Error states are handled appropriately
- Does your code ‘do nothing’ correctly?

By making assumptions **explicit**, tests act as a kind of documentation

What to assert?

System invariants: interactions with external systems

- Did the file actually get written?
- Database call was correct?
- Handled unexpected response from system?

Requires **experimental control** (e.g. through fakes) and **test isolation**

What to assert?

Scientific invariants: domain-specific results

- Is energy conserved?
- Are results properly normalized?
- Do lists have the right length/shape, loops have right iterations, etc

Consider using **unrealistic inputs**

Test implementation, not methods

Implementation correctness is orthogonal to scientific correctness.

- Right result \neq correct code
 - evaluated by summary statistic?
 - error tolerance too loose?
- Wrong result \neq incorrect code
 - Newtonian simulator, relativistic problem

This is exactly why you need controls!

More code examples

https://github.com/flatironinstitute/sciware/tree/main/42_ScientificTesting
Folder ‘file_writer’

Gaining control

What is a control?

Removing influence of variables not under investigation

- In software tests, avoiding calls to code not under test
- Interpreted languages (Python): *mocking libraries*
- Compiled languages (C++): need to use *dependency injection*

Replace calls to outside libraries/expensive functions with observable substitutes

Why use controls?

- External resources (e.g. data downloads)
 - Unreliable (in uninteresting ways)
 - Costly to use for repeated testing
- Other parts of your code (e.g. file writing, computations)
 - Introduce stochasticity
 - Require cleanup
 - Slow
- Generating errors/rare states reliably

Consider: should it actually be user-facing?

Mocking in Python

`unittest.mock`

- `Mock` object
 - Replaces any functions or objects with minimal config
 - Can set function return values, side effects, errors thrown etc.
 - Tracks any calls made & what values were passed
- `patch` function
 - Replaces arbitrary code with `Mock` object
 - works as function decorator or context manager
 - syntax is idiosyncratic

Fakes in C++

Compiled: can't replace code arbitrarily

- Dependency injection
 - Replace hard-coded calls with function parameters or templates
 - Use a controlled implementation for testing
 - Exposes flexibility for actual users of code too
- This can get messy if taken too far, it's common to provide an overload with defaults for the user

These techniques can also be applied in interpreted languages!

Experimenting on a
world you shape

The envy of every experimentalist

- You create the very world you experiment upon!
- Reshape interfaces to something more convenient
- Or keep the interface but update the implementation
- Use testability as a guide to writing better code

Tests: beyond pass and fail

Code that's difficult to test is often also difficult to...

- Understand and reason about
- Explain and document
- Maintain & extend
- Actually use

Listen to your pain.

Signs that things need to change

- Lots of setup/fakes/mocks needed to achieve experimental control
- Cleanup required after calling ordinary functions
- Tests need a lot of logic to match the right case
- Difficult to state the expected result of an operation
- Things work with fakes but not with real values

Responding to common issues

- *Control is hard* → the units are too big/too ambitious
- *Frequent cleanup* → isolate code with external effects
- *Test contains logic* → separate control-flow and operational code
- *Hard to describe results* → code unit is too ambitious
- *Test passes with fakes only* → Poor interface documentation; ought to have many more tests

Final code examples

https://github.com/flatironinstitute/sciware/tree/main/42_ScientificTesting
Folders ‘histogram’ and ‘obfuscated’

Conclusion

Tests are experiments

They should be:

- Controlled
- Focused
- Repeatable

You have an advantage

- You usually control the system you're experimenting on
- Testability is highly correlated with other measures of code quality

Thank you



SURVEY



Appendix: Helpful tools

Tools to help with testing

Coverage reporting



- Visual tool to see what definitely hasn't been tested
- Cannot say what you **meaningfully asserted**, only what you called
- **Not** a progress bar (despite appearances)
- Particularly useful for checking conditional branches

```
102
103 const loadSamplingOptsFromString = (
104   data: ProjectDataModel,
105   json: string,
106   clearExisting: boolean = false,
107 ): ProjectDataModel => {
108   const newSampling = parseSamplingOpts(json);
109   const newSamplingOptsMember = clearExisting
110     ? { ...newSampling }
111     : { ...data.samplingOpts, ...newSampling };
112   return { ...data, samplingOpts: newSamplingOptsMember };
113 };
```