### Test, Debug, Profile

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Based on a talk by Pietro Berkes



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Test

Debug

# Scientific Programming

#### Goal

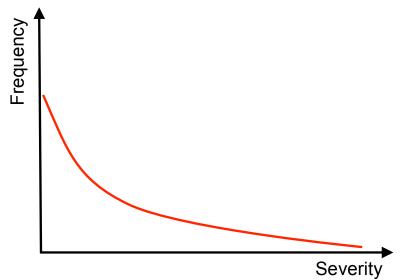
Introduction

- allow exploring many different approaches
- allow frequent changes and adjustments
- produce correct and reproducible results

#### Requirements

- bugs most be noticed
- code can be modify easily
- others can run code too
- scientist's time is used optimally

### Effect of Software Errors



### Effect of Software Errors: Retractions

Science 22 December 2006: Vol. 314 no. 5807 pp. 1856-1857 DOI: 10.1126/science.314.5807.1856

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NEWS OF THE WEEK

#### SCIENTIFIC PUBLISHING

#### A Scientist's Nightmare: Software Problem Leads to Five Retractions

#### Greg Miller

Introduction

Due to an error caused by a homemade data-analysis program, on page 1875, Geoffrey Chang and his colleagues retract three Science papers and report that two papers in other journals also contain erroneous structures. (Read more.)

#### Retraction Watch

Error in one line of code sinks cancer study

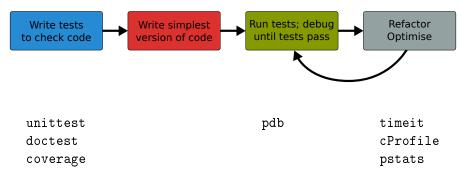




Authors of a 2016 cancer paper have retracted it after finding an error in one line of code in the program used to calculate some of the results.

Test

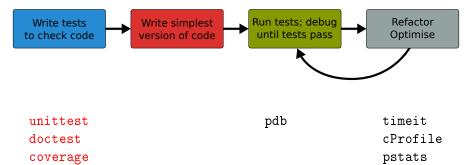
### **Outline**



- standard python tools
- ipython magic commands
- mostly command line

Test

### **Outline**



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### **Testing**

#### Something you do anyway.

- run code and see if it crashes
- check if output makes sense
- run code with trivial input
- **.** . . .

## Formal Testing

- important part of modern software development
- unittest and integration tests
- tests written in parallel with code
- tests run frequently/automatically
- generate reports and statistics

```
[...]
replace predefined histogram ... ok
add a legend; change line color of last histogram to red ... ok
put title and axis labels ... ok

Ran 18 tests in 5.118s

OK
GoodBye!
```

### **Benefits**

- only way to trust your code
- faster development
  - know where your bugs are
  - fixing bugs will not (re)introduce others
  - change code with out worrying about consistency
- encourages better code
- provides example/documentation

```
FAIL: test_result (test_fibonacci.FiboTest)
test 7th fibonacci number
Traceback (most recent call last):
  File "test_fibonacci.py", line 18, in test_result
    self.assertEqual(result, expect)
AssertionError: 21 != 13
```

### An Example

Introduction

```
def remove(thelist, entry):
    """ remove entry object from list """
    for idx, item in enumerate(thelist):
        if entry is item:
            del thelist[idx]
            break
    else:
        raise ValueError("Entry not in the list")
```

Assume we find this code in an old library of ours.

### An Example

Introduction

```
def remove(thelist, entry):
    """ remove entry object from list """
    thelist.remove(entry)
```

We prefer to keep it simple! Everything fine, right?

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# An Example

```
def remove(thelist, entry):
    """ remove entry object from list """
    thelist.remove(entry)
```

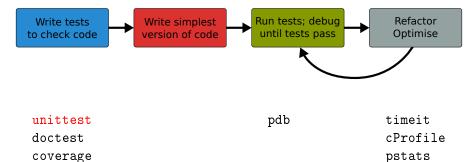
### Start Testing

Introduction

At the beginning, testing feels weird:

- 1. It's obvious that this code works
- 2. The tests are longer than the code
- 3. The test code is a duplicate of the real code
- → it might take a while to get used to testing, but it will pay off quiet rapidly.

#### **Outline**



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- mostly command line



#### unittest

Introduction

- library for unittests
- part of standard python
- at the level of other modern tools

#### **Alternatives**

- nosetests
- pytest

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### Anatomy of a TestCase

```
import unittest
class DemoTests(unittest.TestCase):
   def test_boolean(self):
        """ tests start with 'test' """
        self.assertTrue(True)
        self.assertFalse(False)
   def test_add(self):
        """ docstring can be printed """
        self.assertEqual(2+1, 3)
if name == " main ":
    """ execute all tests in module """
   unittest.main()
```

### Summary on Anatomy

#### **Test Cases**

- are subclass of unittest. TestCase
- group test units

#### **Test Units**

- methods, whose names start with test
- should cover one aspect
- check behaviour with "assertions"
- rise exception if assertion fails

### **Running Tests**

#### Option 1 execute all test units in all test cases of this file

```
if __name__ == "__main__":
    unittest.main(verbosity=1)
python3 test_module.py
```

#### Option 2 Execute all tests in one file

```
python3 -m unittest [-v] test_module
```

#### Option 3 Discover all tests in all submodules

```
python3 -m unittest discover [-v]
```

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# TestCase.assertSomething

check boolean value

```
assertTrue('Hi'.islower()) # fail
assertFalse('Hi'.islower()) # pass
```

check equality

```
assertEqual(2+1, 3)  # pass
""" assertEqual can compare all sorts of objects """
assertEqual([2]+[1], [2, 1])  # pass
```

check numbers are close

```
from math import sqrt, pi
assertAlmostEqual(sqrt(2), 1.414, places=3) # pass
""" values are rounded, not truncated """
assertAlmostEqual(pi, 3.141, 3) # fail
assertAlmostEqual(pi, 3.142, 3) # pass
```

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#### TestCase.assertRaises

most convenient with context managers

```
with self.assertRaises(ErrorType):
    do_something()
    do_some_more()
```

Important: use most specific exception class

```
bad_file = "inexistent"
with self.assertRaises(FileNotFoundError):  # raises NameError
    open(bad_fil, 'r')
with self.assertRaises(Exception):
    open(bad_fil, 'r')  # pass
```

# TestCase.assertMoreThings

```
assertGreater(a, b)
assertLess(a, b)
assertRegex(text, regexp)
assertIn(value, sequence)
assert IsNone (value)
assertIsInstance(my_object, class)
assertCountEqual(actual, expected)
```

#### complete list at

https://docs.python.org/3/library/unittest.html

### TestCase.assertNotSomething

#### Most of the assert methods have a Not version

```
assertEqual
assertNotEqual
```

assertAlmostEqual assertNotAlmostEqual

assertIsNone assertIsNotNone

### Testing with numpy

#### numpy arrays have to be compared elementwise

### numpy.testing

defines appropriate function

```
numpy.testing.assert_array_equal(x, y)
numpy.testing.assert_array_almost_equal(x, y, decimal=6)
```

use numpy functions for more complex tests

```
numpy.all(x)  # True if all elements of x are true
numpy.any(x)  # True if any of the elements of x is true
numpy.allclose(x, y)  # True if element-wise close
```

### Example

```
""" test that all elements of x are between 0 and 1 """
assertTrue(all(logical_and(x > 0.0, x < 1.0))
```

### Strategies for Testing

- What does a good test look like?
- What should I test?
- What is special for scientific code?

- Given put system in right state
  - create objects, initialise parameters, . . .
  - define expected result
- When action(s) of the test
  - one or two lines of code
- Then compare result with expectation
  - set of assertions

```
import unittest
class LowerTestCase(unittest.TestCase):
   def test_lower(self):
        # qiven
        string = 'HeLlO wOrld'
        expected = 'hello world'
        # when
        result = string.lower()
        # then
        self.assertEqual(result,expected)
```

### What should I test?

simple, general case

```
string = 'HeLlO wOrld'
```

corner cases

```
string = ''
string = 'hello'
string = '1+2=3'
```

often involves design decisions

- any exception you raise explicitly
- any special behaviour you rely on

### Reduce Overhead 1: Loops

```
import unittest
class LowerTestCase(unittest.TestCase):
   def test_lower(self):
        # qiven
        # Each test case is a tuple (input, expected)
        test_cases = [('HeLlO wOrld', 'hello world'),
                      ('hi', 'hi'),
                      ('123 ([?', '123 ([?'),
                      ('', '')
        for string, expected in test_cases:
            # run several subtests
            # when
            output = string.lower()
            # then
            self.assertEqual(output, expected)
```

### Reduce Overhead 1: Subtests

```
import unittest
class LowerTestCase(unittest.TestCase):
   def test_lower(self):
        # qiven
        # Each test case is a tuple (input, expected)
        test_cases = [('HeLlO wOrld', 'hello world'),
                      ('hi', 'hi'),
                      ('123 ([?', '123 ([?'),
                      ('', '')
        for string, expected in test_cases:
            with self.subTest(config = string):
                # when
                output = string.lower()
                # then
                self.assertEqual(output, expected)
```

### Reduce Overhead 2: Fixtures

- allow to use same setup/cleanup for several tests
- useful to
  - create data set at runtime
  - load data from file or database
  - create mock objects
- available for test case as well as test unit.

```
class FixureTestCase(unittest.TestCase):
   @classmethod
   def setUpClass(self):
                              # called at start of TestCase
   def setUp(self):
                              # called before each test
   def tearDown(self):
                              # called at end of each test
```

often deterministic test cases very limited/impossible

### Numerical Fuzzing

- generate random input (print random seed)
- still need to know what to expect

#### Know What You Expect

- generate data from model
- add noise to known solutions
- test general routine with specific ones
- test optimised algorithm with brute-force approach

### Test Driven Development (TDD)

#### **Tests First**

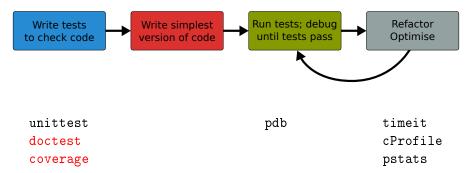
- choose next feature
- write test(s) for feature
- write simplest code

#### **Benefits**

- forced to think about design before coding
- code is decoupled and easier to maintain
- you will notice bugs

### **DEMO**

### **Outline**



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- ipython magic commands
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#### doctest

poor man's unittest

Nicola Chiapolini, September 5, 2017

ensure docstrings are up-to-date

```
def add(a,b):
                                  python3 -m doctest [-v] my_doctest.py
    """ add two numbers
                                  Trying:
    Example
                                      add(40,2)
                                  Expecting:
    >>> add(40,2)
                                      42
    42
                                  ok
                                  1 items had no tests:
    11 11 11
                                      my_doctest
    return a+b
                                  1 items passed all tests:
                                     1 tests in my_doctest.add
                                  1 tests in 2 items.
                                  1 passed and 0 failed.
                                  Test passed.
```

# Code Coverage

- it's easy to leave part untested
  - features activated by keyword
  - code to handle exception
- coverage tools track the lines executed

#### coverage.py

- python script
- produces text and HTML reports

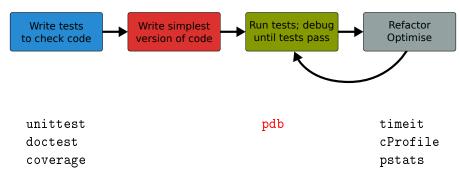
```
python3 -m coverage run test_file.py
python3 -m coverage report [-m] [--omit="/usr*"]
```

 not in standard library get from http://coverage.readthedocs.io/en/latest/

## **DEMO**

Test

## **Outline**



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- use tests to avoid bugs and limit "search space"
- avoid print statements
- use debugger

## pdb – the Python debugger

- command line based
- opens an interactive shell
- allows to
  - stop execution anywhere in your code
  - execute code step by step
  - examine and change variables
  - examine call stack

# **Entering pdb**

Introduction

enter at start of file

```
python3 -m pdb myscript.py
```

enter at statement/function

```
import pdb
# your code here
pdb.run(expression_string)
```

enter at point in code

```
# some code here
# the debugger starts here
import pdb; pdb.set_trace()
# rest of the code
```

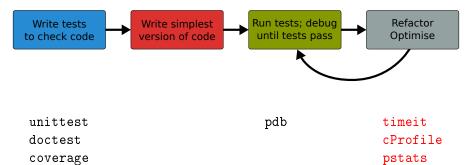
from ipython

```
%pdb # enter pdb on exception
%debug # enter pdb after exception
```

Debug

# **DEMO**

## **Outline**



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Introduction

- 1. don't rush into optimisation
- 2. identify time-consuming parts of code
- 3. only optimise those parts
- 4. keep running tests
- 5. stop as soon as possible

Introduction

# 1. don't rush into optimisation

- 2. identify time-consuming parts of code
- 3. only optimise those parts
- 4. keep running tests
- 5. stop as soon as possible

Introduction Test Debug Profile

#### timeit

- precise timing for function/expression
- test different versions of a code block
- easiest with ipython's magic command

```
a**2 Or pow(a,2)?
In [1]: a = 43563
In [2]: %timeit pow(a,2)
100000000 loops, best of 3: 268 ns per loop
In [3]: %timeit a**2
100000000 loops, best of 3: 209 ns per loop
```

### cProfile & Pstats

Nicola Chiapolini, September 5, 2017

Profiling identify where most time is spent cProfile standard python module for profiling pstats tool to look at profiling data

run cProfile

```
python3 -m cProfile [-s cumtime] myscript.py
python3 -m cProfile [-o myscript.prof] myscript.py
```

analyse output from shell

```
python3 -m pstats myscript.prof
stats # print statistics
sort # change sort order
callers # print callers
callees # print callees
```

### Non-Standard Tools

pyprof2calltree and kcachegrind: open cProfile output in GUI

```
python3 -m cProfile -o myscript.prof myscript.py
. ~/venv/bin/activate # on school laptops activate venv
pyprof2calltree -i myscript.prof -k
```

pprofile: line-granularity profiler

```
pprofile3 myscript.py

pprofile3 -f callgrind -o myscript.prof myscript.py
kcachegrind myscript.prof
```

line\_profiler: original line-granularity profiler (needs code change)

## **DEMO**

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## **Final Thoughts**

Introduction

- testing, debugging and profiling can help you a lot
- using the right tools makes life a lot easier
- python comes with good tools included
- it's as easy as it gets there are no excuses