Software Carpentry

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Based on a talk by Pietro Berkes

Scientific Programming

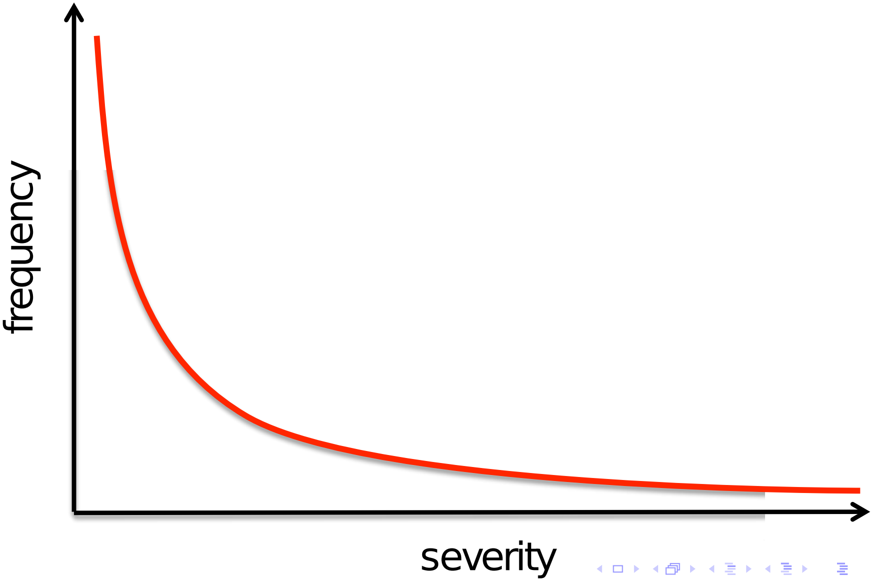
Goal

- 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

‹ Prev | Table of Contents | Next ›

NEWS OF THE WEEK

SCIENTIFIC PUBLISHING

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

Greg Miller

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.)

The Scientist » News & Opinion » Daily News

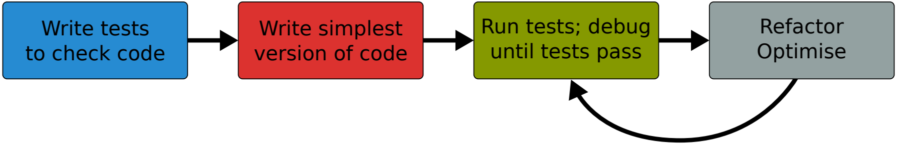
PLoS journal retracts phylogenetics paper

Computational Biology journal pulls paper about estimating the accuracy of phylogenetic trees, in what colleagues deem an exemplary process

By Graciela Flores | June 18, 2007

PLoS Computational Biology is retracting a paper published in March that claimed that metrics used to measure the accuracy of phylogenetic trees don't work. Senior author Barry Hall from the Bellingham Research Institute in Bellingham, Washington requested the retraction after a colleague noticed a discrepancy, the fault of a software bug that upended the paper's conclusion. "We are retracting the paper because the conclusion that we came to was completely wrong," Hall told *The Scientist*. "We found no correlation between clade confidence and phylogenetic tree accuracy, but

Outline



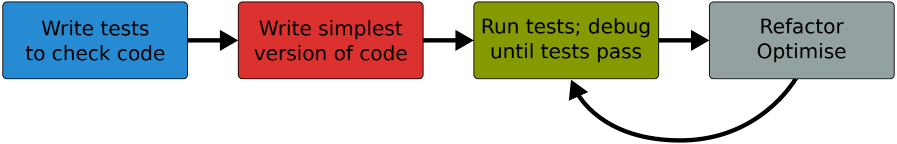
unittest
doctest
coverage

pdb

timeit
cProfile
runsnake

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

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

An Example

```
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

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

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

An Example

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

```
ERROR: test_remove_array (__main__.RemoveTest)
--------------------------------------------------------------
Traceback (most recent call last):
  File "list_tests.py", line 19, in test_remove_array
    lrm.remove(l, x)
  File ".../examples/list_removal.py", line 3, in remove
    thelist.remove(entry)
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

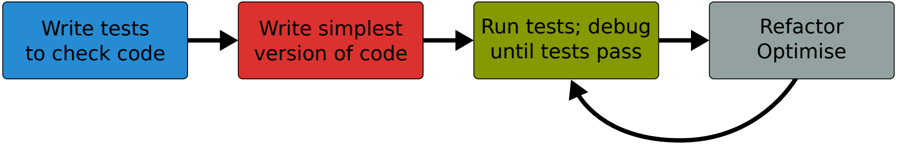
Start Testing

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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unittest

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

Alternatives

- nosetests (often used just to run unittests)
- py.test

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)
```

```
python test_module.py
```

Option 2 Execute all tests in one file

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

Option 3 Discover all tests in all submodules

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

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
```

TestCase.assertRaises

- most convenient with context managers

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

- Important: use most specific exception class

```
with self.assertRaises(IOError):           # error
    file(1, 'r')

with self.assertRaises(Exception):
    file(1, 'r')                           # pass

""" a TypeError is raised, as file needs string or buffer """
```

TestCase.assertMoreThings

```
assertGreater(a, b)
assertLess(a, b)

assertRegexpMatches(text, regexp)

assertIn(value, sequence)

assertIsNone(value)

assertIsInstance(my_object, class)

assertItemsEqual(actual, expected)

assertDictContainsSubset(subset, full)
```

complete list at
https://docs.python.org/2/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

```
class SpecialCases(unittest.TestCase):
    def test_numpy(self):
        a = numpy.array([1, 2])
        b = numpy.array([1, 2])
        self.assertEqual(a, b)
```

```
===========================================================
ERROR: test_numpy (__main__.SpecialCases)
-----------------------------------------------------------
Traceback (most recent call last):
  [..]
ValueError: The truth value of an array with more than one
element is ambiguous. Use a.any() or a.all()
```

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?

What does a good test look like?

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

What does a good test look like? – Example

```
import unittest

class LowerTestCase(unittest.TestCase):

    def test_lower(self):
        # given
        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: Loops

```
import unittest

class LowerTestCase(unittest.TestCase):

    def test_lower(self):
        # given
        # Each test case is a tuple (input, expected)
        test_cases = [('HeLlO wOrld', 'hello world'),
                      ('hi', 'hi'),
                      ('123 ([?', '123 ([?'),
                      ('', '')]
        for string, expected in test_cases:
            # when
            output = string.lower()
            # then
            self.assertEqual(output, expected)
```

Reduce Overhead: 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
```

What is special for scientific code?

often deterministic test cases very limited/impossible

Numerical Fuzzing

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

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

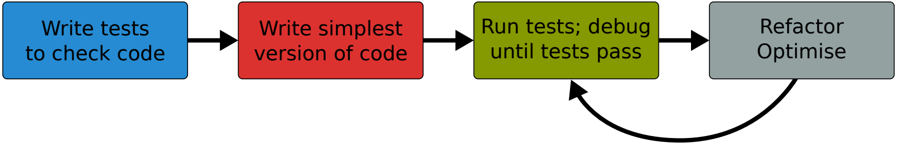
- choose next feature
- write test(s) for feature
- write simplest code

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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doctest

- poor man's unittest
- ensure docstrings are up-to-date

```python
def add(a,b):
    """ add two numbers

    Example
    -------
    >>> add(40,2)
    42

    """
    return a+b
```

```
python -m doctest [-v] my_doctest.py

Trying:
    add(40,2)
Expecting:
    42
ok
1 items had no tests:
    my_doctest
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

```
python -m coverage run test_file.py
python -m coverage report [-m]
```

- not in standard library
  get from http://nedbatchelder.com/code/coverage/

DEMO

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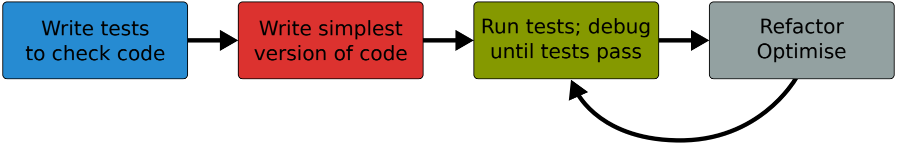

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Debugging

- 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

- enter at start of file

```
python -m pdb myscript.py
```

- enter at statement/function

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

- enter at point in code

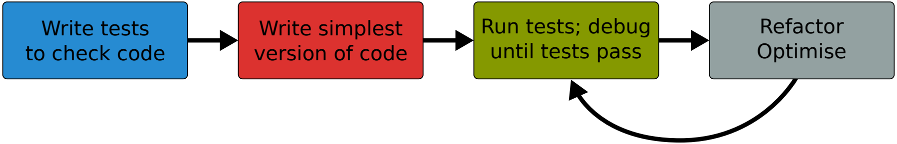
```
# some code here
# the debugger starts here
import pdb; pdb.set_trace()
# rest of the code
```

- from ipython

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

DEMO

Outline



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Optimising

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

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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)
10000000 loops, best of 3: 139 ns per loop

In [3]: %timeit a**2
10000000 loops, best of 3: 72.3 ns per loop
```

cProfile & RunSnake

Profiling identify where most time is spent
cProfile standard python module for profiling
RunSnake graphic tool to show profiling data

- run cProfile

```
python -m cProfile [-o myscript.prof] myscript.py
```

- analyse output from shell

```
import pstat
p = pstat.Stats("myscirpt.prof")
p.sort_stats(sort_order)
p.print_stats()
```

- or with RunSnake

```
runsnake myscript.prof
```

DEMO

Final Thoughts

- 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