Profile

Test, Debug, Profile

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June 7, 2016

Based on a talk by Pietro Berkes



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Scientific Programming

Goal

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

Requirements

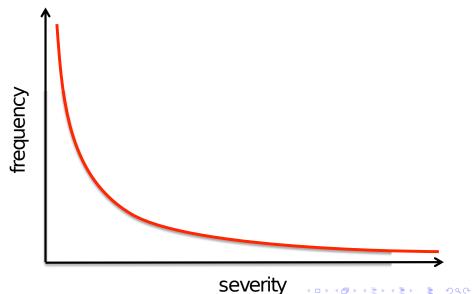
- bugs most be noticed
- code can be modify easily
- others can run code too
- scientist's time is used optimally

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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

Due to an error caused by a homemade data-analysis program, on page <u>1875</u>, 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

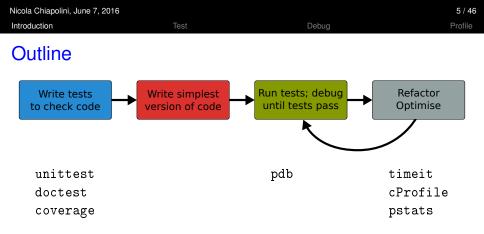
PLoS journal retracts phylogenetics paper

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

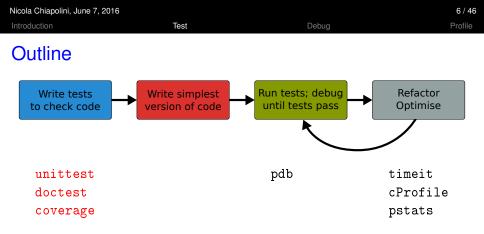
By Graciela Flores | June 18, 2007



PLoS Comparational Biology is refracting a page published in March that claimed that merics used to measure the accuracy of physicinetic trees don't voice. Series author Earny affait from the Bellingham Research Institute is 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 urong. Hait and Ta's Softents'. We bound no constellato thetwen clade confidence and physiogenetic tree accuracy, but



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



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Something you do anyway.

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

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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

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

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An Ex	ample		
def	<pre>remove(thelist, entry): """ remove entry object from list for idx. item in enumerate(thelis</pre>		

```
""" 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.

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An Exa	mple		
	emove(thelist, entry): "" remove entry object from l	ist """	

thelist.remove(entry)

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

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An Ex	ample			
def	<pre>remove(thelist, er """ remove entry of thelist.remove(entry)</pre>	object from list ""	"	
ERR	DR: test_remove_arm	ray (mainRemov	eTest)	
	ceback (most recent ile "list_tests.py" lrm.remove(l, x)	t call last): ", line 19, in test	_remove_array	
Val	thelist.remove(ent 1eError: The truth	list_removal.py", l try) value of an array v Use a.any() or a.a	with more than one	
	0	v		

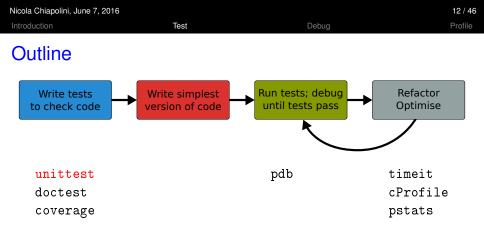
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Start Testing

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.



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

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()
```

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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 	
<pre>assertTrue('Hi'.islower())</pre>	# fail
<pre>assertFalse('Hi'.islower())</pre>	# pass
Check equality assertEqual(2+1, 3) """ assertEqual can compare all sorts assertEqual([2]+[1], [2, 1])	<pre># pass of objects """ # pass</pre>

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)

assertIsNone(value)

```
assertIsInstance(my_object, class)
```

```
assertCountEqual(actual, expected)
```

complete list at https://docs.python.org/3/library/unittest.html

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TestCase.assertNotSomething

Most of the ${\tt assert}$ methods have a ${\tt Not}$ 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
```

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Example

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

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Strategies for Testing

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

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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 = 'HeLl0 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):
    # 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:
        # 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):
    # 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:
        with self.subTest(config = string):
            # when
            output = string.lower()
            # then
            self.assertEqual(output, expected)
```

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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):
```

```
Qclassmethoddef setUpClass(self):# called at start of TestCasedef setUp(self):# called before each testdef 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 (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

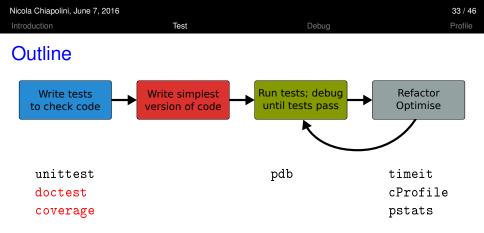
- choose next feature
- write test(s) for feature
- write simplest code

Benefits

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

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

Nicola Chia Introductio	apolini, June 7, 2016 n		84 / 46 rofile
doct	est		
	poor man's unittes ensure docstrings		
def	add(a,b): """ add two number	python3 -m doctest [-v] my_doctest.p	у
	Example	Trying: add(40,2) Expecting:	
	>>> add(40,2) 42	42 ok	
		1 items had no tests: my_doctest	
	return a+b	<pre>1 items passed all tests: 1 tests in my_doctest.add 1 tests in 2 items. 1 passed and 0 failed. Test passed.</pre>	୬୯୯

Code Coverage

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

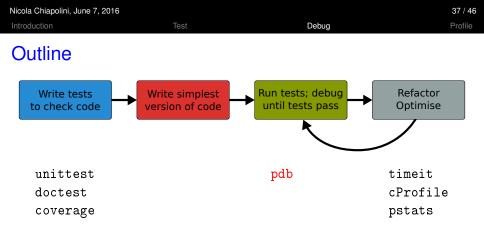
coverage.py

- python script
- produces text and HTML reports

```
python3 -m coverage run test_file.py
python3 -m coverage report [-m]
```

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

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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

```
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

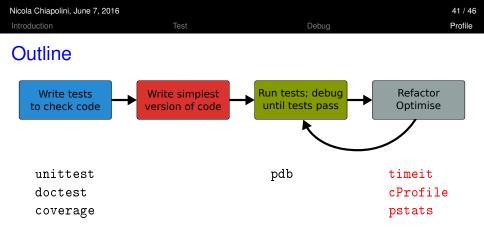
%pdb	#	enter	pdb	on exc	ception
%debug	#	enter	pdb	after	exception

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

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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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Optimising

- 1. don't rush into optimisation
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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 & Pstats

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

run cProfile

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

different options for graphical displays, but no standard yet

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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