Programming in Python, without messing it up

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You know Python. Great!

Now the real fun begins...

- ¿Reliable software?
- ¿Managing complexity?
- ¿Sustainable software development?


¿How to debug?
¿How to avoid bugs?


Oh no! I wrote
this code when I was 25.
This is going
to be a long night!
imgflip.com

Write code in style

- = rules for readability
- In general, adhere to PEP8
  https://www.python.org/dev/peps/pep-0008/
- Tools:
  - `pip install --user` **`pycodestyle`**
    Checks a subset of PEP8 rules
  - `pip install --user` **`pydocstyle`**
    Checks a subset of PEP257 (docstrings)
  - `pip install --user` **`pylint`**
    Checks subset of PEP8 and other things.
  - Cardboardlint => our wrapper for many checkers

Write transparent code

- **Single line of code = self-explaining**
  - Give variables, functions, … **sensible names**.
  - **Not too much** stuff in one line. No crazy one-liners.
- **Comments explain code** (implementation)
  - **English**, please.
  - Comment on **groups of lines**, rarely individual lines.
- **Docstrings explain usage of code** (API)
  - **Document** a function, class, module, …
  - **Describe** parameters, return values, exceptions & behavior

```
def fire_in_the_disco(msg):
    """Contributed by https://pythondev.slack.com/team/staticmethod
    This code was written for obfuscation contest.
    """
    reconstitute(msg,wwpd)
    try:
        f=type((lambda:(lambda:None for n in range(len(((((),((((),((((((((((
().next())
        u=(lambda:type((lambda:(lambda:None for n in
range(len(zip((((((((((((((((((((.func_code))()
        n=f(u(int(wwpd[4][1]),int(wwpd[7][1]),int(wwpd[6][1]),int(wwpd[9]
[1]),wwpd[2][1],
            (None,wwpd[10][1],wwpd[13][1],wwpd[11][1],wwpd[15][1]),(wwpd[20]
[1],wwpd[21][1]),
            (wwpd[16][1],wwpd[17][1],wwpd[18][1],wwpd[11][1],wwpd[19]
[1]),wwpd[22][1],wwpd[25][1],int(wwpd[4][1]),wwpd[0][1]),
            {wwpd[27][1]:__builtins__,wwpd[28][1]:wwpd[29][1]})
        c=partial(n, [x for x in map(lambda i:n(i),range(int(0xbeef)))])
        FIGHT = f(u(int(wwpd[4][1]),int(wwpd[4][1]),int(wwpd[5]
[1]),int(wwpd[9][1]),wwpd[3][1],
                (None, wwpd[23][1]), (wwpd[14][1],wwpd[24][1]),(wwpd[12]
[1],),wwpd[22][1],wwpd[26][1],int(wwpd[8][1]),wwpd[1][1]),
                {wwpd[14][1]:c,wwpd[24][1]:urlopen,wwpd[27]
[1]:__builtins__,wwpd[28][1]:wwpd[29][1]})
        FIGHT(msg)
    except:
        pass
```

```
def compute_surface_polygon(x, y):
    """Compute the surface area of a 2D polygon.

    Parameters
    ----------
    x : np.array
        X-coordinates of the polygon's corners.
    y : np.array
        Y-coordinates of the polygon's corners.

    Returns
    -------
    area : type of x and y
        The surface area of the polygon.

    """
    # Shoelace algorithm, Meister, 1769
    if len(x) != len(y):
        raise TypeError("Arguments x and y must have the same length.")
    if len(x) <= 2:
        return 0.0
    else:
        return abs( x[-1]*y[0] + np.dot(x[:-1], y[1:])
                    -x[0]*y[-1] - np.dot(x[1:], y[:-1]))/2
```

$$A = \frac{1}{2}\left| x_N y_1 - x_1 y_N + \sum_{i=1}^{N-1} x_i y_{i+1} - x_{i+1} y_i \right|$$

Write unit tests

- = function to validate another function
- Runs fast, easy to start
- Write tests first, certainly not months later.
- Write many!
- Think of corner cases
- Coverage analysis = check if code is tested

```
def check_single(x, y, area):
    np.testing.assert_almost_equal(compute_area_polygon(x, y), area)

def check_variants(x, y, area):
    x = np.asarray(x)
    y = np.asarray(y)
    check_single(x, y, area)
    check_single(x[::-1], y[::-1], area)
    check_single(x + 0.3, y - 0.5478, area)
    check_single(-2*x, 0.8*y, 1.6*area)
    xp = np.cos(0.3)*x - np.sin(0.3)*y
    yp = np.sin(0.3)*x + np.cos(0.3)*y
    check_single(xp, yp, area)

def test_compute_area_polygon():
    # Simple geometries
    check_single([0, 0, 1, 1], [0, 1, 1, 0], 1.0)
    check_single([0.0, 0.0, 2.0], [0.0, 1.0, 1.0], 1.0)
    check_single([-0.5, 2.5, 1.0, 0.0], [0.0, 0.0, 0.5, 0.5], 1.0)

    # Corner cases: flat, coinciding points, too short vectors
    check_single([0.0, 2.0, -1.0], [0.0, 2.0, -1.0], 0.0)
    check_single([0.0, 0.0, 2.0, 2.0], [0.0, 1.0, 1.0, 1.0], 1.0)
    check_single([], [], 0.0)
    check_single([1], [2], 0.0)
    check_single([2.0, 1.0], [0.0, 0.0], 0.0)
```

Live demo

```
# Plain, without coverage
nosetests -v meister.py

# With coverage analysis
nosetests -v meister.py \
    --with-coverage \
    --cover-html \
    --cover-package=meister
```

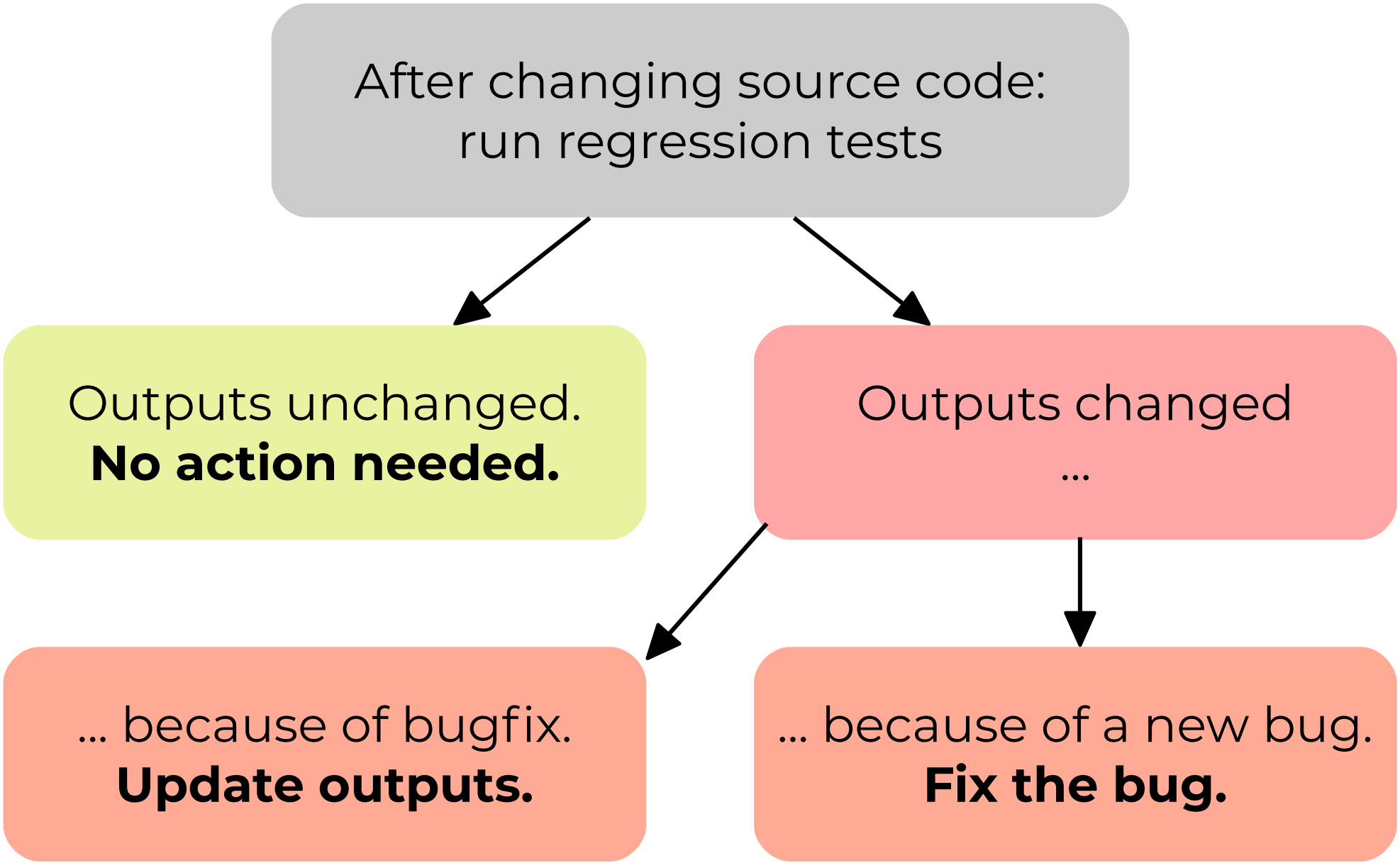
Write regression tests

- = tests for entire program
- Slower than unit tests
- Test whether program changes behavior.

Pairs of input and output
for every feature of your program

test1.in	test1.out
test2.in	test2.out
test3.in	test3.out
test4.in	test4.out
...	...

Regression test workflow



Hands-on: the Kabsch algorithm

1. Write the function signature & docstring.
2. Write one unit test.
3. Implement the Kabsch algorithm.
4. Write more unit tests.
5. Perform coverage analysis.
6. Corner cases?
7. Review your neighbour's code.

~~¿How to write complex software?~~
¿How to hide complexity?

Use built-in packages

Ideal for reducing code:

- **argparse**
  command-line argument parser
- **collections** (namedtuple)
  beyond lists and dicts
- **glob** & **fnmatch**
  UNIX-style pattern matching: `"foo*_???.txt"`
- **JSON**
  simple data representation, very widely used.
- **YAML**
  JSON generalization,
  better suited for humans

Live demo

```
from collections import namedtuple
Point = namedtuple('Point', ['x', 'y'])
p = Point(11, y=22)
p[0] + p[1]
x, y = p
x, y
p.x + p.y
p
p._replace(x=100)

Point = namedtuple('Point', ['x', 'y'], verbose=True)
```

Use third-party packages

Scientific computing, besides the usual (NumPy, SciPy, MatplotLib, pandas):

- **H5Py:** binary cross-platform array file format
- **Cython:** Python C++ interface
- **Scikit-learn:** (old-school) machine learning & statistics
- **RDkit:** cheminformatics
- **Sympy:** symbolic calculus
- **Dask:** parallel workflows
- **AutoGrad:** algorithmic differentiation
- **Numba:** just-in-time compiler for Python
- **Mars:** parallel Numpy

Split code into modules

```python
# foo.py
def add(a, b):
    return a+b
```

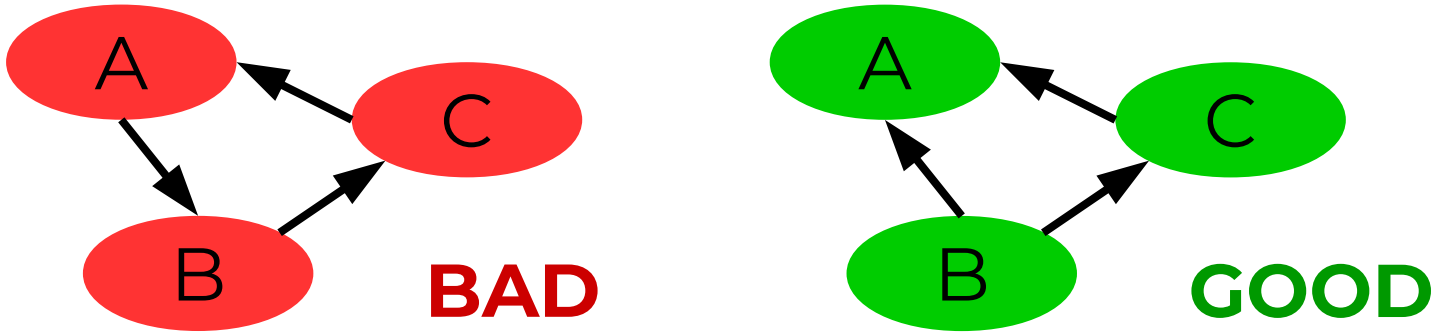
```python
# bar.py
import foo
print(foo.add(1, 2))

from foo import add
print(add(1, 2))

from foo import *
```

Make *modular* modules

1. **No cyclic dependencies** between modules.
   You use a module ⇒ module does not use you.



2. Modules should have a **minimal API**.
3. Modules should have a well-defined **purpose**, which can be **summarized in 1 sentence**.

Idiomatic Python

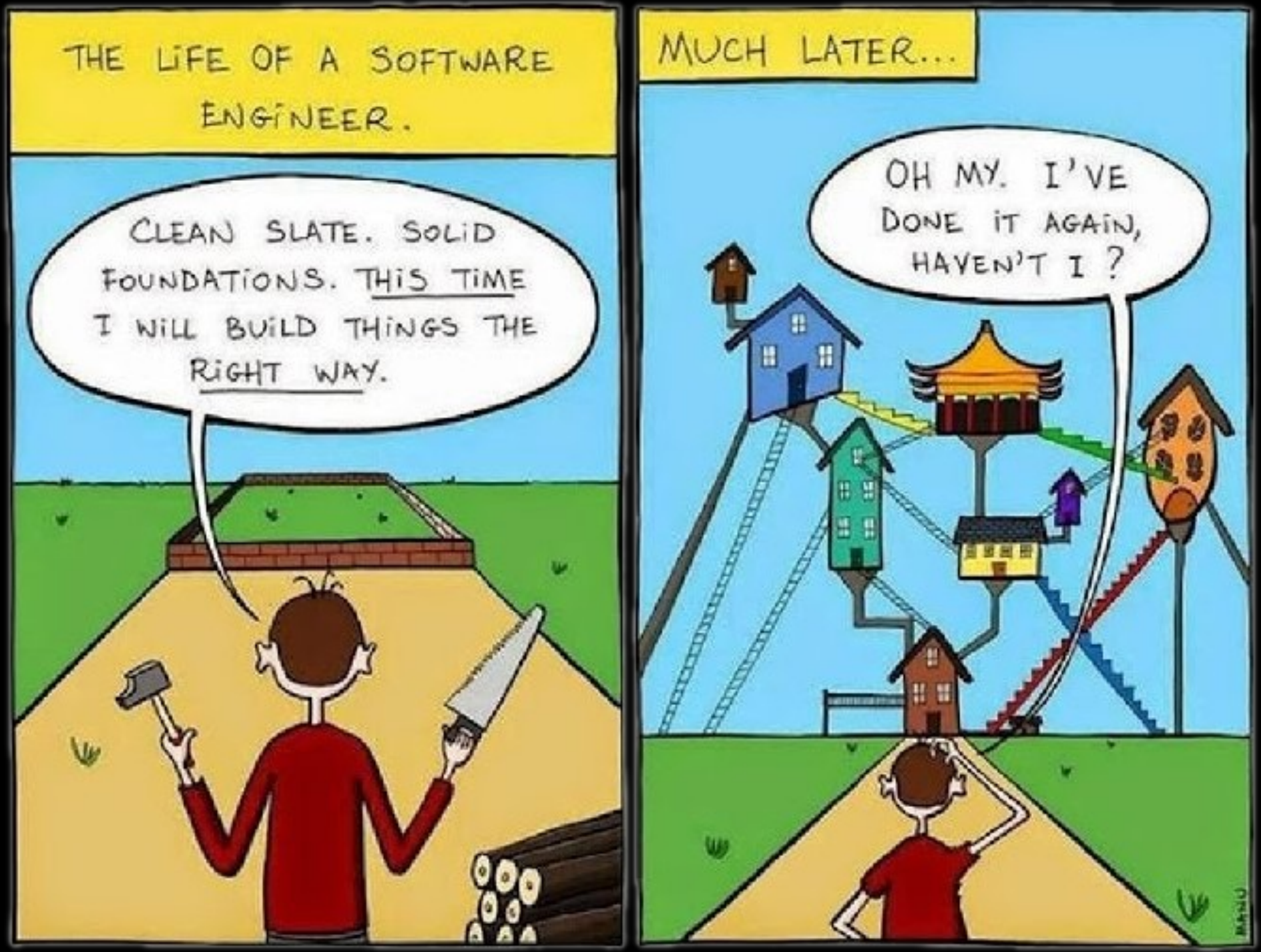
```
# Pythonic code, use context manager ("with") and enumerate:
with open("somefile.txt") as fh:
    for counter, line in enumerate(fh):
        print(counter, " ", line[: -1])

# C++ish code:
fh = None
try:
    fh = open("somefile.txt")
    counter = 0
    line = fh.readline()
    while len(line) > 0:
        print(counter, " ", line[:-1])
        counter += 1
        line = fh.readline()
finally:
    if fh is not None:
        fh.close()
```

See also:
https://docs.python.org/3.0/howto/doanddont.html

Before going into detail:

- OOP is sometimes over-rated. (Java)
- OOP does not solve all your problems.
- Keep it simple.
- Python does not support all OOP concepts. Hooray!


THE LIFE OF A SOFTWARE ENGINEER.
CLEAN SLATE. SOLID FOUNDATIONS. THIS TIME I WILL BUILD THINGS THE RIGHT WAY.
MUCH LATER...
OH MY. I'VE DONE IT AGAIN, HAVEN'T I ?

- Next to built-in types (int, list, str, ...), you can define more general "**objects**" with **attributes** and a **behavior**.

Live demo

- Classes can "**inherit**" from other classes, and add & override attributes & methods.

Live demo

"Polymorphism" justifies inheritance.

= Difference in behavior with the same API

Object-oriented programming (OOP)

Benefits

- Related elements (data and code) are also nearby in source.
- Higher-level programming, in terms of objects
- Polymorphism can reduce many "if" statements.

Limitations

- Methods are essentially unary operators.

Pitfalls

- Too many classes.
- Too complex inheritance diagrams. Use composition where possible.
- Too many methods.

Free functions

- = method “degraded” to a function.
  See https://www.youtube.com/watch?v=nWJHhtmWYcY
- Goal: keep classes simple & easy to understand
- When to write a free function?
  - Attributes are not modified (directly).
  - Algorithms that "work with" objects
  - Binary (or higher) operators.
  - When a class becomes too complicated.

Hands-on: polygon & regular polygon

1. Write polygon class and add features:

• compute_area and compute_perimeter

• rotate, scale and translate

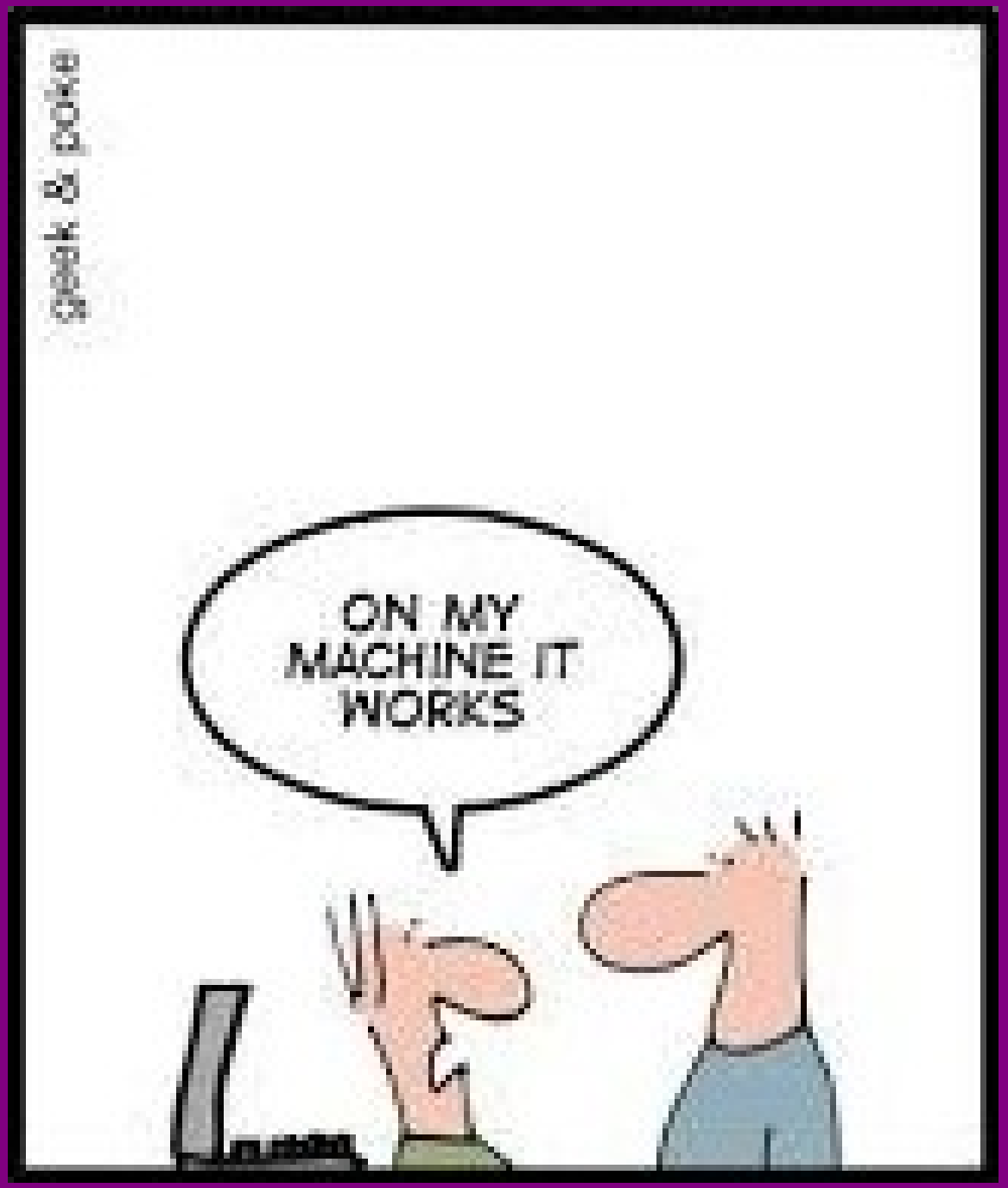
• regular polygon

Select the “best” patterns: inheritance or composition, method or function.

2. Minimization of perimeter/area ratio

- Implement function for ratio with 1 argument: x & y arrays concatenated.
  Add regularization term, 1e-6*(1−area)**2.
- Implement gradient with autograd.
- Minimize with scipy.optimize.fmin_lbfgs_b.


geek & poke
YESTERDAY IT WORKED


geek & poke
ON MY MACHINE IT WORKS

Even if you don't collaborate...

Long-term maintenance

≈

Collaboration with your future self

More than *avoiding bugs* & *hiding complexity*.

Semantic versioning

https://semver.org/

Given a version number MAJOR.MINOR.PATCH, increment the:

- **MAJOR** version when you make incompatible API changes,
- **MINOR** version when you add functionality in a backwards-compatible manner, and
- **PATCH** version when you make backwards-compatible bug fixes.

Version Control System (VCS)

= records history of all changes in source code

Why?

Collaboration

- Merging: combine changes from different persons.
- Review code before merging.
- When was a bug introduced (bisection)
- Blame people for their ugly code. :)

Access to all versions

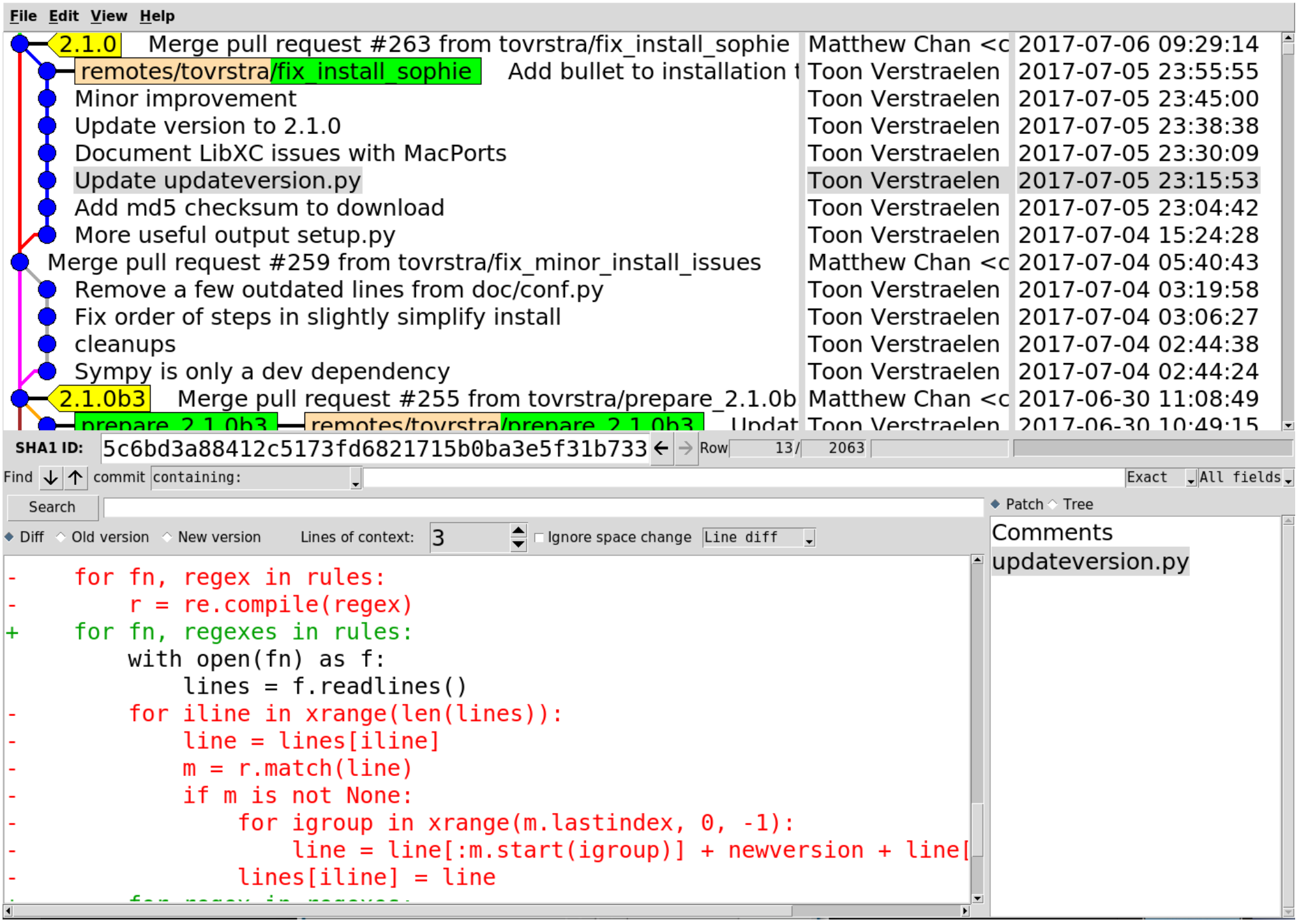
Backup

A patch (file)

```
diff --git a/horton/grid/cext.pyx b/horton/grid/cext.pyx
index e4615275..47c607fc 100644
--- a/horton/grid/cext.pyx
+++ b/horton/grid/cext.pyx
@@ -55,7 +55,7 @@
     'PowerExtrapolation', 'PotentialExtrapolation', 'tridiagsym_solve',
     'CubicSpline', 'compute_cubic_spline_int_weights',
     # evaluate
-    'index_wrap', 'eval_spline_grid', 'eval_decomposition_grid',
+    'eval_spline_grid', 'eval_decomposition_grid',
     # ode2
     'hermite_overlap2', 'hermite_overlap3', 'hermite_node',
     'hermite_product2', 'build_ode2',
@@ -477,10 +477,6 @@


-def index_wrap(long i, long high):
-    return evaluate.index_wrap(i, high)
-
-
 def eval_spline_grid(CubicSpline spline not None,
                      np.ndarray[double, ndim=1] center not None,
                      np.ndarray[double, ndim=1] output not None,
```

Patch, Commit, Branch, Review, Merge, Release



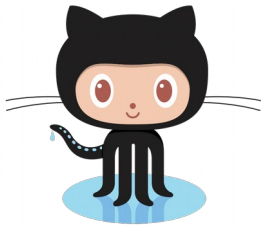
Git & Github

Git = probably the best VCS software

https://git-scm.com/

- Steep learning curve, but worth it.
- Lots of online tutorials.

Github = Git hosting



https://github.com/

- Hosts git repositories
- Extra's: issue tracker, pull requests, web hosting

Continuous integration (CI)

= automatically analyze every commit on Github:

- Unit tests + coverage analysis
- Coding style (pylint, pycodestyle, ...)
- Test package build & install
- ...

Very neat, involved setup, **use cookiecutter**.

https://travis-ci.org/

Example: https://github.com/theochem/grid/pull/4

Write user documentation

README.md

- Links to other documentation
- Quick install instructions
- Contact & License information

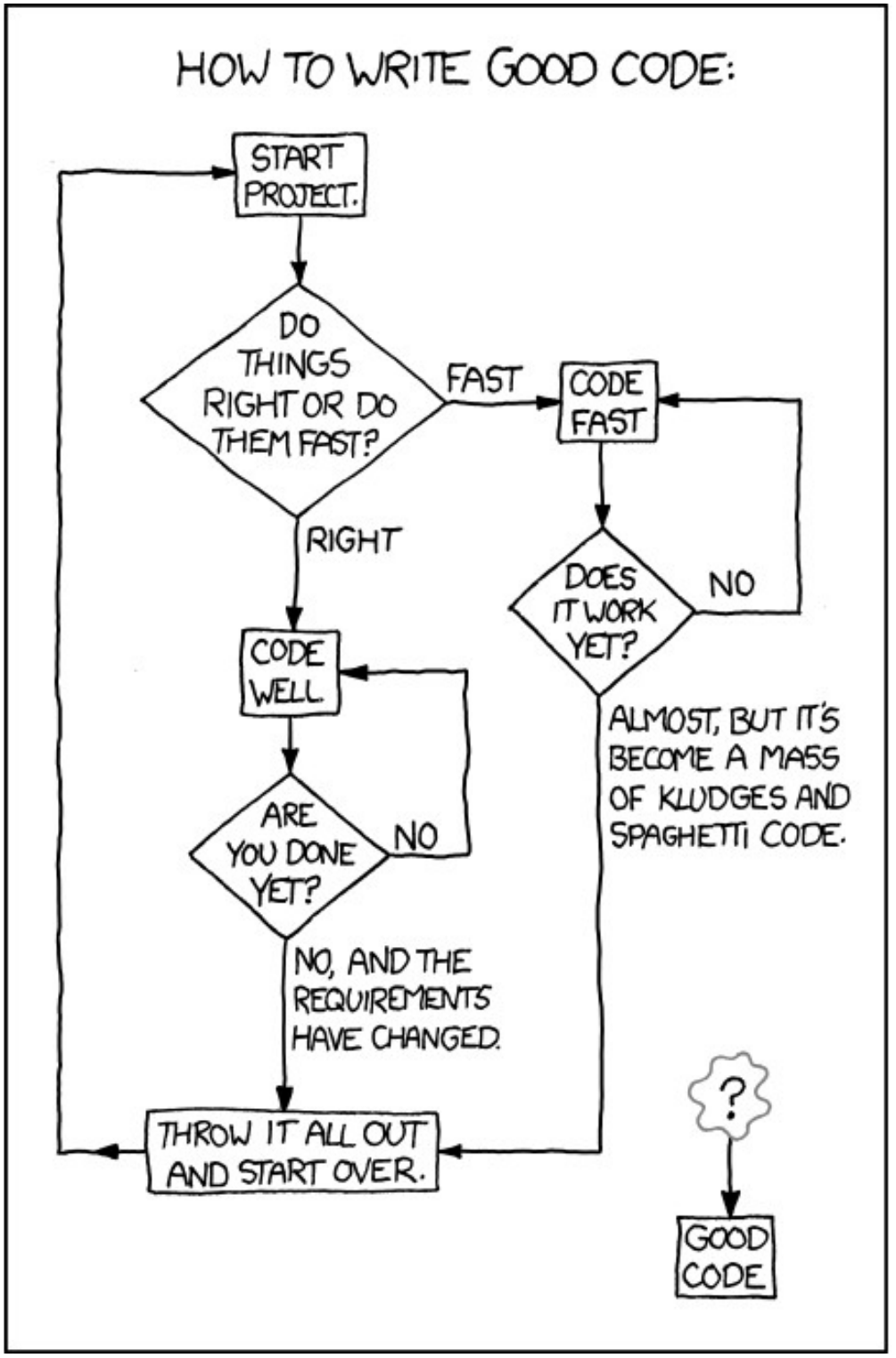
Website (use Sphinx; http://www.sphinx-doc.org)

- Background
- Tutorials
- API reference

Assignment: fix a simple bug

Fix Scipy documentation:

https://github.com/scipy/scipy/issues/7168



SCRUM

Keep it simple.