

Best Practices

Scientific Programming with Python

Nicola Chiapolini

University of Zurich
Faculty of Science

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Introduction

- ▶ We write code regularly
- ▶ We have not been formally trained

Best Practices

- ▶ evolved from experience
- ▶ increase productivity
- ▶ decrease stress
- ▶ still evolve with tools and languages

Development Methodologies

- ▶ e.g. Agile Programming or Test Driven Development
- ▶ lots of buzzwords
- ▶ still many helpful ideas

Outline

Introduction

Style & Documentation

Special Statements

KIS(S) & DRY

Refactoring

Development Methodologies

Outline

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Coding Style

- ▶ readability counts (often more than brevity or speed)
- ▶ give things *intention revealing* names
 - ▶ For example: `numbers` instead of `n`
 - ▶ For example: `numbers` instead of `list_of_float_numbers`
 - ▶ See also: [Ottinger's Rules for Naming](#)

Example

```
def fun(n):  
    """ no comment """  
    r = 1  
    for i in n:  
        r *= i  
    return r
```

Coding Style

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 - ▶ For example: `numbers` instead of `list_of_float_numbers`
 - ▶ See also: [Ottinger's Rules for Naming](#)

Example

```
def my_product(numbers):  
    """ Compute the product of a sequence of numbers. """  
    total = 1  
    for item in numbers:  
        total *= item  
    return total
```

Formatting Code

- ▶ use coding conventions, e.g: [PEP-8](#)
- ▶ conventions specify
 - ▶ layout
 - ▶ white-space
 - ▶ comments
 - ▶ naming
 - ▶ ...
- ▶ OR use a consistent style (especially when collaborating)

Formatting Code: Tools

Checker

- ▶ `pylint` (e.g. `pylint my_product.py`)
- ▶ `pycodestyle` (e.g. `pycodestyle my_product.py`)
- ▶ `pydocstyle` (e.g. `pydocstyle my_product.py`)
- ▶ `flake8` (e.g. `flake8 my_product.py`)

Formatter

- ▶ `autopep8` (e.g. `autopep8 --in-place my_product.py`)
- ▶ `yapf3` (e.g. `yapf3 --in-place my_product.py`)
- ▶ `black` (e.g. `black my_product.py`)

Combined

- ▶ `ruff` (e.g. `ruff check my_product.py`)

Finding Bugs with Pylint

Example

```
def current_rotation(beta, iota, phi, sigma):  
    """ calculate current rotation """  
    return np.cos(beta)*np.cos(phi)*np.cos(sigma)  
    +np.sin(beta)*np.cos(phi)*np.sin(sigma)*np.cos(iota)  
    -np.sin(beta)*np.sin(phi)*np.sin(iota)
```

Finding Bugs with Pylint

Example

```
def current_rotation(beta, iota, phi, sigma):  
    """ calculate current rotation """  
    return np.cos(beta)*np.cos(phi)*np.cos(sigma)  
    +np.sin(beta)*np.cos(phi)*np.sin(sigma)*np.cos(iota)  
    -np.sin(beta)*np.sin(phi)*np.sin(iota)
```

```
[...]:7:4: W0101: Unreachable code (unreachable)  
[...]:7:4: W0106: Expression "+np[...]" is assigned to nothing [...]  
[...]:8:4: W0106: Expression "-np[...]" is assigned to nothing [...]
```

Documenting Code: Docstrings

Example

```
def my_product(numbers):  
    """ Compute the product of a sequence of numbers. """
```

- ▶ at least a single line
- ▶ also for yourself
- ▶ is on-line help too
- ▶ Document arguments and return objects, including types
- ▶ For complex algorithms, document every line, and include equations in docstring
- ▶ Use docstring conventions: [PEP257](#) and/or [numpy](#)

Example Docstring

```
def my_product(numbers):  
    """ Compute the product of a sequence of numbers.  
  
    Parameters  
    -----  
    numbers : sequence  
        list of numbers to multiply  
  
    Returns  
    -----  
    product : number  
        the final product  
  
    Raises  
    -----  
    TypeError  
        if argument is not a sequence or sequence contains  
        types that can't be multiplied  
    """
```

DEMO

Documenting Your Project

- ▶ tools generate website from docstrings
 - ▶ [pydoc](#)
 - ▶ [sphinx](#)
 - ▶ [Overview List](#)
- ▶ when project gets bigger
 - ▶ how-to
 - ▶ FAQ
 - ▶ quick-start

The screenshot shows a web browser displaying a Sphinx-generated documentation page. The page title is "my_product_docstring module". Below the title, the function signature is shown: `my_product_docstring.my_product(numbers)`. The description states: "Compute the product of a sequence of numbers." The parameters section lists: **Parameters:** `numbers` : sequence, with a description "list of numbers to multiply". The returns section lists: **Returns:** `product` : number, with a description "the final product". The raises section lists: **Raises:** `TypeError`, with a description "if argument is not a sequence or sequence contains types that can't be multiplied". On the right side, there is a sidebar with a "This Page" button, a "Show Source" link, and a "Quick search" section with an input field and a "Go" button. The footer of the page includes the text "test 0 documentation" and "modules | index" on the left, and "© Copyright 2016, nc. Created using Sphinx 1.3.6." on the right.

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import

- ▶ Don't use the *star import*: `from module import *`
 - ▶ not obvious what you need
 - ▶ modules may overwrite each other
 - ▶ Where does this function come from?
 - ▶ will import *everything* in a module
 - ▶ ...unless you have a very good reason: e.g. `pylab`, `interactive`
- ▶ Put all imports at the beginning of the file...
- ▶ ...unless you have a very good reason

Example

```
import my_product as mp
mp.my_product([1,2,3])

from my_product import my_product
my_product([1,2,3])
```

import: Pitfalls

Python evaluates the imported code at import time.

```
""" Bad Things happen here. """

def append_one(list_=[]):
    """ Do not use mutable default values """
    list_.append(1)
    return list_

def default_arg(bad=1 / 0):
    """ Do not trigger exceptions in keyword-arguments """
    return bad

def constants():
    """ This can not be imported in Python < 3.6 """
    return 9999999 ** 9999999
```

DEMO

Exceptions

- ▶ use try, except and raise
- ▶ often better than if (e.g. IndexError)

Example

```
try:
    my_product(1, 2, 3)
except TypeError as e:
    raise TypeError("'my_product' expects a sequence") from e
```

- ▶ don't use *special* return values:
1, 0, False, None
- ▶ Fail early, fail often
- ▶ use built-in Exceptions

assert

- ▶ Not intended for checks needed in production.

Example

```
def withdraw(balance, amount):  
    assert balance > amount, "Balance too small"  
    return balance - amount  
  
print(withdraw(50, 100))
```

running: python3 withdraw.py

```
Traceback (most recent call last):  
  [...]  
    assert balance > amount, "Balance too small"  
           ~~~~~  
AssertionError: Balance too small
```

assert

- ▶ Not intended for checks needed in production.

Example

```
def withdraw(balance, amount):  
    assert balance > amount, "Balance too small"  
    return balance - amount  
  
print(withdraw(50, 100))
```

running: `python3 -0 withdraw.py`

assert

- ▶ Not intended for checks needed in production.

Example

```
def withdraw(balance, amount):  
    assert balance > amount, "Balance too small"  
    return balance - amount  
  
print(withdraw(50, 100))
```

running: python3 -0 withdraw.py

-50

mypy: Type Hints and Static Checking

- ensures variables and functions are used correctly

Example

```
def factorial(n):  
    res = 1  
    for i in range(1,n+1):  
        res *= i  
    return res  
  
def concat(str1, str2):  
    return str1+str2  
  
n = 4.  
res = factorial(n)  
concat(f"{n}! = ", res)
```

mypy: Execute with Python

python3 factorial.py

```
Traceback (most recent call last):
  File ".../factorial_nohint.py", line 26, in <module>
    res = factorial(n)
          ~~~~~
  File ".../factorial_nohint.py", line 3, in factorial
    for i in range(1,n+1):
                  ~~~~~
TypeError: 'float' object cannot be interpreted as an integer
```

- ▶ `n` must be integer
- ▶ once fixed, we get the next error: `str2` must be string

mypy: Adding Type Hints

- ▶ can add type info to variables and function definitions

Example

```
def factorial(n: int) -> int:
    res = 1
    for i in range(1,n+1):
        res *= i
    return res

def concat(str1: str, str2: str) -> str:
    return str1+str2

n = 4.
res = factorial(n)
concat(f"{n}! = ", res)
```

mypy: Check with mypy

```
python3 -m mypy factorial.py
```

```
factorial.py:15: error: Argument 1 to "factorial" has incompatible type "float"; expected "int" [arg-type]
factorial.py:16: error: Argument 2 to "concat" has incompatible type "int"; expected "str" [arg-type]
Found 2 errors in 1 file (checked 1 source file)
```

- ▶ spots both problems
- ▶ must be run separately (ideally automatically)

mypy: Summary

Cons

- ▶ additional work for programmer
- ▶ defining correct types can be tricky
([type hints cheat sheet](#))
- ▶ code gets more verbose and maybe confusing

Pros

- ▶ prevent a lot of possible bugs
- ▶ valuable even if not all code covered

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Keep it Simple (Stupid) – KIS(S) Principle

Keep it Simple

Debugging is twice as hard as writing the code in the first place.
Therefore, if you write the code as cleverly as possible,
you are, by definition, not smart enough to debug it.

– Brian W. Kernighan

Don't Repeat Yourself (DRY)

- ▶ No copy & paste!
- ▶ Not just lines of code, but knowledge of all sorts
- ▶ Do not express the same piece of knowledge in two places. . .
- ▶ . . . or you will have to update it everywhere
- ▶ It is not a question of *if* this may fail, but *when*

Don't Repeat Yourself (DRY): Types

Example

- ▶ Copy-and-paste a snippet, instead of refactoring it into a function
 - ▶ Repeated implementation of utility methods
 - ▶ because you don't remember
 - ▶ because you don't know the libraries
 - `numpy.prod([1,2,3])`
 - ▶ because developers don't talk to each other
 - ▶ Version number in source code, website, readme, package filename
- ▶ If you detect duplication: refactor!

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- ▶ re-organise your code without changing its functionality
- ▶ rethink earlier design decisions
- ▶ break large code blocks apart
- ▶ rename and restructure code
- ▶ will improve the readability and modularity
- ▶ will usually reduce the lines of code

Common Refactoring Operations

- ▶ Rename class/method/module/package/function
- ▶ Move class/method/module/package/function
- ▶ Encapsulate code in method/function
- ▶ Change method/function signature
- ▶ Organise imports (remove unused and sort)
- ▶ Always refactor one step at a time, and ensure code still works
 - ▶ version control
 - ▶ unit tests

Refactoring Example

```
def product_minus_sum(numbers):  
    """ Subtract sum of numbers from product of numbers. """  
    total = 0  
    for item in numbers:  
        total += item  
    total2 = 1  
    for item in numbers:  
        total2 *= item  
    return total - total2
```

- ▶ split into functions
- ▶ use libraries/built-ins
- ▶ fix bug

Refactoring Example

```
from my_math import my_product, my_sum

def product_minus_sum(numbers):
    """ Subtract sum of numbers from product of numbers. """
    sum_value = my_sum(numbers)
    product_value = my_product(numbers)
    return sum_value - product_value
```

- ▶ split into functions
- ▶ use libraries/built-ins
- ▶ fix bug

Refactoring Example

```
from numpy import prod, sum

def product_minus_sum(numbers):
    """ Subtract sum of numbers from product of numbers. """
    sum_value = sum(numbers)
    product_value = prod(numbers)
    return sum_value - product_value
```

- ▶ split into functions
- ▶ use libraries/built-ins
- ▶ fix bug

Refactoring Example

```
from numpy import prod, sum

def product_minus_sum(numbers):
    """ Subtract sum of numbers from product of numbers. """
    sum_value = sum(numbers)
    product_value = prod(numbers)
    return product_value - sum_value
```

- ▶ split into functions
- ▶ use libraries/built-ins
- ▶ fix bug

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What is a Development Methodology?

Consists of:

- ▶ process used for development
- ▶ tools to support this process

Help answer questions like:

- ▶ How far ahead should I plan?
- ▶ What should I prioritise?
- ▶ When do I write tests and documentation?

Right methodology depends on scenario.

What is a Development Methodology?

Consists of:

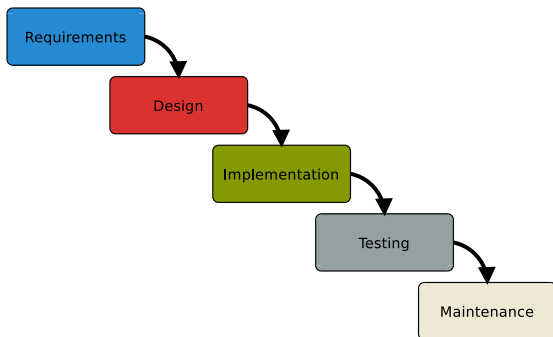
- ▶ process used for development
- ▶ tools to support this process

Help answer questions like:

- ▶ How far ahead should I plan?
- ▶ What should I prioritise?
- ▶ When do I write tests and documentation?

Right methodology depends on scenario.

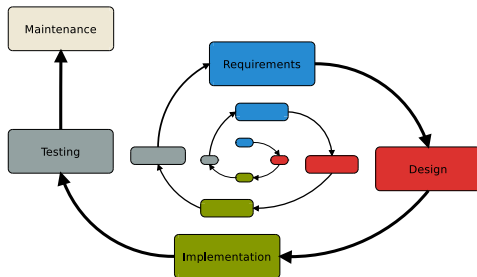
The Waterfall Model, Royce 1970



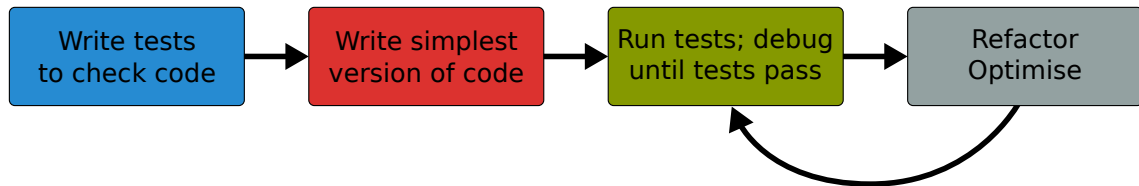
- ▶ sequential
- ▶ from manufacturing and construction

Agile Methods (late 90's)

- ▶ minimal planning, small development iterations
- ▶ frequent input from environment
- ▶ very adaptive, since nothing is set in stone



Test Driven Development (TDD)



- ▶ Define unit tests first!
- ▶ Develop one unit at a time!
- ▶ more tomorrow

An Almost Unrelated Note: Using VirtualEnv

The Problem

- ▶ different tools need different versions of a module
- ▶ your Linux distribution does not include a module

The Solution: virtualenv

- ▶ initialize folder `school_venv` to store modules of this project

```
python -m venv --system-site-packages ~/school_venv
```
- ▶ update the search-paths to include folders in `~/school_venv`

```
. ~/school_venv/bin/activate
```
- ▶ run your code or install libraries with `pip`
- ▶ undo changes to search-paths

```
deactivate
```