

Advanced Python *for* Data Science

```
from functools import partial
from unittest import TestCase, main
from weakref import WeakKeyDictionary

from luigi import ExternalTask, Task

class Requires:
    def __call__(self, task):
        reqs = {}
        for cls in type(task).mro():
            for k, v in cls.__dict__.items():
                if isinstance(v, Requirement) and not k in reqs:
                    reqs[k] = v(task)
        return reqs

    def __get__(self, instance, owner):
        if instance is None:
            return self

        return partial(self, instance)
```

```
class Requirement:
    def __init__(self, req, **kwargs):
        self.req = req
        self.kwargs = kwargs
        self._names = WeakKeyDictionary()

    def __set_name__(self, owner, name):
        self._names[owner] = name

    def __get__(self, instance, owner):
        if instance is None:
            return self
        return self(instance)

    def __call__(self, task):
        return task.clone(self.req, **self.kwargs)

    def get_name(self, owner):
        return self._names[owner]
```

```
class RequirementTests(TestCase):
    def test_names(self):
        class DataTask(ExternalTask):
            pass

        class MyTask(Task):
            data = Requirement(DataTask)

        assert MyTask.data.get_name(MyTask) == 'data'
```

```
def test_inheritance(self):
    class DataTask(ExternalTask):
        pass

    class MyTask(Task):
        data = Requirement(DataTask)
        requires = Requires()

    class ChildClass(MyTask):
        in2 = Requirement(DataTask)
```

Scott Gorlin, Ph.D.

Advanced Python for Data Science

Scott Gorlin

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This is a [Leanpub](#) book. Leanpub empowers authors and publishers with the Lean Publishing process. [Lean Publishing](#) is the act of publishing an in-progress ebook using lightweight tools and many iterations to get reader feedback, pivot until you have the right book and build traction once you do.

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Preface

Introduction

What is this book?

Today, most people enter the world of Data Science through the buzz and allure of “AI.” We tackle Kaggle challenges, voraciously consume Stack Overflow, and eat, live, and breathe through the Jupyter Notebook. Python, along with its “killer app” of Machine Learning, has done nothing short of revolutionize the way we “do data science,” and the world is a more interesting place because of it!

The Big Cloud providers, and many open source tools, have done wonders to democratize this technology. But, ‘easy access’ to high technology comes with a cost - we can easily go too far, rely too much on the tools we have today, and forget how to build the tools we need to truly transform our individual projects.

Most of the time, your impact as a Data Scientist is limited by your ability to enact your ideas - not by the ideas themselves. You can train a model on ‘clean’ data using Scikit Learn or FastAI, or run an ANOVA, in a notebook. Enacting that idea means getting to the data in the first place. It means knowing how to store it. It means processing your data at scale. It means running your processing script, reliably, every day on fresh data. It means testing that script. It means collaborating on that script with a coworker - or 10 - as the project scales. It means curating a library and building tools to solve the same problem for 5 new projects. It means packaging a model up for distribution - sharing with another data scientist, or deploying it as a service.

It means changing the way you think about problems by adopting new paradigms that accelerate you - and your work - across your organization. It means ***building an approach*** to data science within the broader python ecosystem.

This book is about python, and how to be an effective python programmer, as a Data Scientist. We learn the advanced python skills we need to accelerate you, and solve the real, daily problems you face in your DS role.

Who is it for?

The ideal reader has at least 1 year of active daily python use and is ready to learn more. You should be comfortable writing functions, classes, and reading source code. You should not be confused about basic syntax, data types, etc, and when you see something you don’t understand, you should be comfortable reading the docs or source code yourself. You should know how to import a package or module. You should know how to define a class. You should know how to look up python syntax and how to answer questions about python. You should be comfortable reading the source code for

packages you work with, rather than reverting to StackOverflow for every question. You should know how to debug an error message - if you are not used to reading and interpreting errors, launching a line-by-line debugger, you should get comfortable breaking and debugging code before you dive into a book like this.

Often, I get feedback from students who find this material too challenging - “it’s like sitting down to a piano lesson and learning how to tune a piano” and “it’s like showing up for an intro to Russian class only to learn the class is taught in Russian.” These, in fact, are very appropriate descriptions - as an **advanced** subject, this book is written in native python, and we learn exactly when and how to tune python for advanced, but very common, needs. It is extremely technical, and earns the advanced designation. I only hope you will find the material valuable.

What will you learn?

Congratulations on starting this journey - it is tough, but I promise it will be rewarding. Roughly speaking we will cover 4 main themes in this book, learning advanced Python syntax and tools in the context of solving real-world Data Science problems. The themes are:

Workflows

How to test, deploy, share, merge, version, review, and iterate on your code. We will look at build systems - pipenv, conda, poetry - versioning tools, templating with cookiecutter, how to work with git, and more.

Skeletons

The bones upon which we build projects. These frameworks give us new perspectives and approaches - how to build ETL’s with Airflow and Luigi, how to structure and train a model with MLOps tools, how to compose new frameworks and build repeatable tools using context managers, decorators, and descriptors.

Data

How to store, process, search in the context of big data and small, row based or columnar, using parquet or SQL, scaling with tools like Dask

Algorithms

The universal CS concepts that help many projects, including hashing, memoization techniques, JIT and static compilation, visualization, data sketching, and more

I hope this whet’s your appetite, and you join me and your fellow scientists on this journey.

The state of the book

This book originated as slides and lecture notes I developed while teaching CSCI E-29, Advanced Python for Data Science, at Harvard Extension School. Currently, the book contains light transformation of those notes from slide into prose, which leaves a lot of opportunity to improve and flesh out the text. After all the notes are transcribed, diagrams reformatted for the book medium, etc, I will come back to rewrite the text as needed for textbook form.

An introduction to Advanced Python

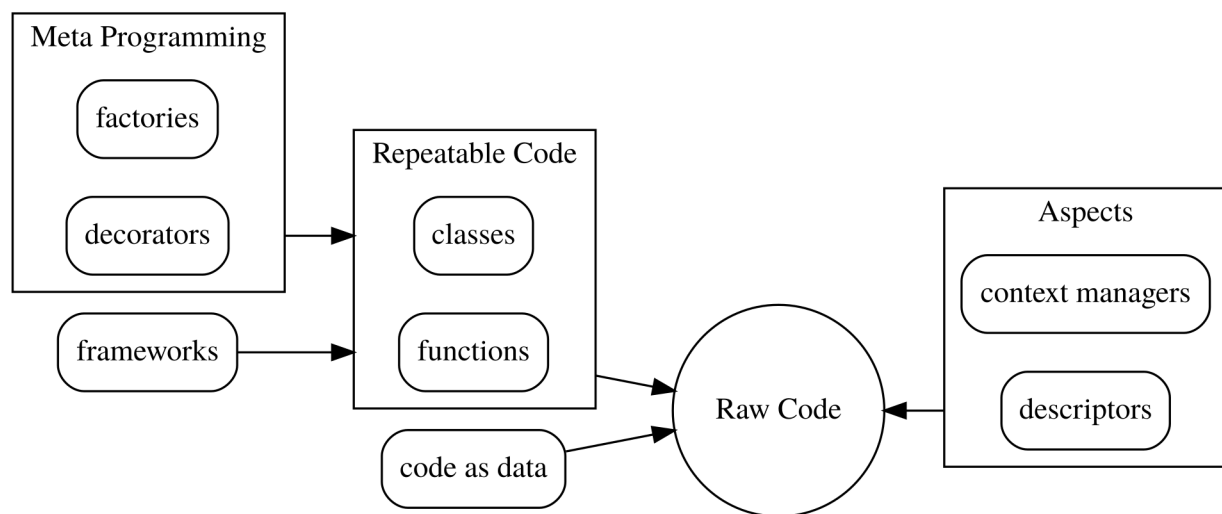
What is *Advanced* Python?

... is it an awesome notebook?

... or knowing every function?

... and writing faster code?

It's about higher levels



It's about the science

Columnar & Sparse Representations

Probabilistic Data Structures

Parallel & Distributed Algorithms

It's about repeatability

A manual install

```
pip install numpy
ipython
```

- No env
- No data flow

Minimally repeatable

```
pip install -r reqs.txt
python script.py in.csv
```

- Minimal reqs
- Implicit flow

A fully repeatable process

```
pipenv install
make output.parquet
```

- Frozen env
- Explicit flow

... and standards/enforcement

Why learn “best practices” if you can *build* them?

Each of these examples represents a design decision - and best practice - wrapped up in code

```
with atomic_write('output.csv') as f:
    df.to_csv(f)
```

```
mlflow.sklearn.save_model(model, "my_model")
```

```
with submit_pset('Pset 0') as quiz_submission:
    quiz_submission.answer_submission_questions(...)
```

It's about collaboration

- Workflows that facilitate development
- Code that is consistent and self-documenting
- Units of work that build on each other seamlessly

It's about the ecosystem

The modern Data Scientist leverages a broader ecosystem of tools than anyone else in the history of man

Python is a *glue* language, and is popular because it is the *best interface* to all of these tools

We will *embrace* the ecosystem, rather than have you work in a sandbox

It's about the deliverable

Your output is not enough; *show your work*.

It's about you

You are the most valuable asset, and usually the bottleneck. Python gives you wings.

Tech Requirements

Prerequisites

You should already know Python! This book assumes *fluency* in basic to intermediate python syntax.

You should know how to use libraries, functions, classes, and basics of python packaging!

You should be familiar with numpy, scipy, and pandas



There are many good tutorials to brush up, eg from [Software Carpentry](#)¹:

- [Python](#)²
- [Python Modules and Packages](#)³
- [Python Testing](#)⁴
- [Make and Makefiles](#)⁵
- [git](#)⁶

Students have the most difficulty understanding python packages vs modules vs scripts, how to build and configure their environments, and set up repositories and cloud accounts. Make sure you are comfortable with the basic daily tools (the things used in real life that they don't teach you in Python 101) and can debug and communicate problems effectively.

¹<https://software-carpentry.org/lessons/>

²<http://swcarpentry.github.io/python-novice-inflammation/>

³<https://docs.python.org/3/tutorial/modules.html>

⁴<http://carpentries-incubator.github.io/python-testing/>

⁵<https://swcarpentry.github.io/make-novice/>

⁶<http://swcarpentry.github.io/git-novice/>

Python 3.8

This book will target 3.8.

The focus of this book is *python*. New versions bring new features, but we are focused on a much bigger picture - what makes python *python*, not what you can do with any new feature.

The vast majority of things you can and should do as an advanced Python programmer are achievable in any version, pending library support, perhaps with minor syntax variations. We are chasing the forest here, not the trees.

IDE

Pick one that helps with:

- *Debugging!*
- Source code/doc lookups
- Syntax checks, autocomplete, runtime config...

If you have never line-by-line debugged a program before, this is the place to start!

This is your chance to learn to debug!

Debugging provides most of what you want from Jupyter, but much, much better experience:

- Jump to source
- Line-by-line stepping
- Stack inspection
- ...

... not Jupyter!

You should *not* be using Jupyter Notebooks for this course!

You will get the impression that I hate Jupyter. That is not true.

It's great for EDA, but lacks *repeatability, composeability, and cooperativity*.

Use the right tool for the right job. Jupyter is not the right tool for Advanced Python!

Documentation

You need to document and comment your code!

Pick one of:

- [Google Docstring](#)⁷
- [Numpy](#)⁸
- [SphinxReST](#)⁹

```
def fetch_bigtable_rows(big_table):
    """Fetches rows from a Bigtable

    More notes...

    Args:
        big_table: A Bigtable Table
        ...

    Returns:
        A dict...

    """
```

Black

<https://black.readthedocs.io/en/stable/>

Why spend time formatting code?

Code format is about more than just style. Everyone has different aesthetics, but we would not spend much time discussing it if it were merely preferences.

When code is merged or committed, we see deltas regardless if the change is functional or stylistic. Adopting an automatic, strict style minimizes the latter. If your code is always formatted consistently, you can easily merge work from another branch without seeing or dealing with distracting stylistic deltas. It helps you collaborate.

Plus, it removes the mental energy of learning or conforming to a style. Just auto format all the time!

This is an example of how we don't learn or set a 'best practice;' rather, we pick a framework that automates or enforces the practice for us.

Helpful Themes

Typing

Python doesn't require types, but you shouldn't forget them!

⁷<https://github.com/google/styleguide/blob/gh-pages/pyguide.md#38-comments-and-docstrings>

⁸<https://numpydoc.readthedocs.io/en/latest/>

⁹<http://www.sphinx-doc.org/>

The following all ‘safely’ handle a basic lookup, but make different decisions about the type and content of the default value

```
ENCODING = {
    1: 'one',
    2: 'two',
}

def encode(x: int) -> str:
    # Preserves type, but is a new 'magic' value
    return ENCODING.get(x, 'none')

def encode(x: int) -> Union[str, None]:
    # Standard tombstone value, but
    # may cause problems eg encode(9).upper()
    return ENCODING.get(x, None)

def encode(x: int) -> str:
    # Preserve type and boolean eg 'if encode(x)'
    return ENCODING.get(x, '')
```

Functions should operate on an expected data type, and return an expected type.

If this changes depending on the arguments, mass confusion will follow.

Strive for consistent, self-explanatory argument and return types

Never ever ever:

```
def sqrt(x: float) -> Union[float, str]:
    if x < 0:
        return 'invalid'
    return x**0.5
```

Typing (Overkill): Let your IDE and common sense do the heavy lifting

Good practices in the past are not *as* necessary today; see: [Hungarian Notation](https://en.wikipedia.org/wiki/Hungarian_notation)¹⁰.

¹⁰https://en.wikipedia.org/wiki/Hungarian_notation

```
def float_square_root(float_x: float) -> float:
    assert isinstance(float_x, float)
    return x**0.5
```

Encoding the type of a function into the name ... is brain damaged - the compiler knows the types anyway ... and it only confuses the programmer.

– Linus Torvalds

Cardinality & Ownership

Try to isolate and shrink the responsibility of your code

Smaller, isolated functions are easier to test and easier to reuse in new situations.

```
def process(df: DataFrame) -> DataFrame:
    # Hard codes column name and iteration method
    for i, x in enumerate(df['col']):
        df['col'].iloc[i] = x + 1
    return df
```

```
>>> df = process(df)
```

```
def process(vec: List) -> List:
    # Hard codes iteration method
    return [x + 1 for x in vec]
```

```
>>> df['col'] = process(df['col'])
```

```
def process(x: float) -> float:
    # Operates on a unit
    return x + 1
```

```
>>> df['col'].apply(process)
>>> process(df['col']) # If vectorizable
>>> process(3)
```

One cognitive burden when reading or designing DS code is the cardinality of your data - are you processing a single element, or a bunch of them?

Strive to make it clear whether your function is designed to work on elemental data (eg, a single primitive) or a collection (eg, an iterable, a series/dataframe, numpy array, etc).

In general, write code to operate on data primitives - this is much easier to test, a better assumption for how a function should work, and more likely that you can plug it in to other parts of your code. It also allows you to use other mechanisms for applying the same thing to the container, eg using `pandas .apply`, or `map` objects.

The big exception to this is if you need numpy vectorization for speed, and your function cannot be naively applied to a scalar vs a numpy array in the same way (eg, you need to access properties of the vector to perform the calculation).

Code as Data

Try to write every program as an operation on data.

Here is ‘good’ code:

```
print('one')
print('two')
```

But this code is ‘better’:

```
for arg in ['one', 'two']:
    print(arg)
```

And this is better still:

```
def map(func, seq):
    for el in seq:
        func(el)

map(print, ['one', 'two'])
```

Code-as-data, flow-based, object-oriented, and other higher-level programming concepts will be major focus areas in this book.

Readings

Now

- [Code Climate Workflow](https://docs.codeclimate.com/docs/workflow)¹¹
- [Continuous Integration](https://www.martinfowler.com/articles/continuousIntegration.html)¹²

¹¹<https://docs.codeclimate.com/docs/workflow>

¹²<https://www.martinfowler.com/articles/continuousIntegration.html>

- A Successful Git Branching Model¹³
- GitHub Flow vs Git Flow¹⁴
- Test Driven Dev for Data Science¹⁵
- CI for Data Science¹⁶
- I Don't Like Notebooks¹⁷

Soon

- Pipfile vs Setup.py¹⁸
- Freezing Python's Dependency Hell in 2018¹⁹
- API First Data Science²⁰

Reference

- Python Modules and Packages²¹

¹³<https://nvie.com/posts/a-successful-git-branching-model/>

¹⁴<http://scottchacon.com/2011/08/31/github-flow.html>

¹⁵<http://engineering.pivotal.io/post/test-driven-development-for-data-science/>

¹⁶<http://engineering.pivotal.io/post/continuous-integration-for-data-science/>

¹⁷<https://www.youtube.com/watch?v=7jiPeIFXb6U>

¹⁸<https://pipenv.readthedocs.io/en/latest/advanced/#pipfile-vs-setuptools>

¹⁹<https://tech.instacart.com/freezing-pythons-dependency-hell-in-2018-f1076d625241>

²⁰<http://engineering.pivotal.io/post/api-first-for-data-science/>

²¹<https://docs.python.org/3/tutorial/modules.html>

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Continuous science

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