Best Practices for Reproducible Research Using Python

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Click here for Google Slides Link

Thanks: Joel Mathew

9/19/2019

ME = $\int_{2008}^{2019}$ ~~👨‍💻~~ dt

t

B.E. in Computer Science and Engineering
@ VTU, Belgaum, India (2008-2012)

exploratory
+ full stack!

Software Engineer
@ SimplyPhi, Bengaluru, India (2012-2015)

Big Data + ML +
Text Analytics...
Platform building.

Technical Co-Founder
@ Datoin, Bengaluru, India (2013-*)

M.S. in Computer Science
@ USC Viterbi School of Engineering (2015-2017)

Data
Science

Data Scientist *(Internship x 3 times)*
@ NASA Jet Propulsion Lab (2016-2017)

(Volunteer) **Committer** + **PMC Member**
@ Apache Software Foundation (2015-2017)

Research Assistant
@ USC Info Retrieval and Data Science (2016)

Mentor
@ Google Summer of Code (2017)

Research Programmer *(Current Role)*
@ USC Information Sciences Institute (2017-*)

Deep Learning +
NLProc research

Ph. D. in Computer Science *(In Progress)*
@ USC Viterbi School of Engineering (2018-*)

@thammegowda

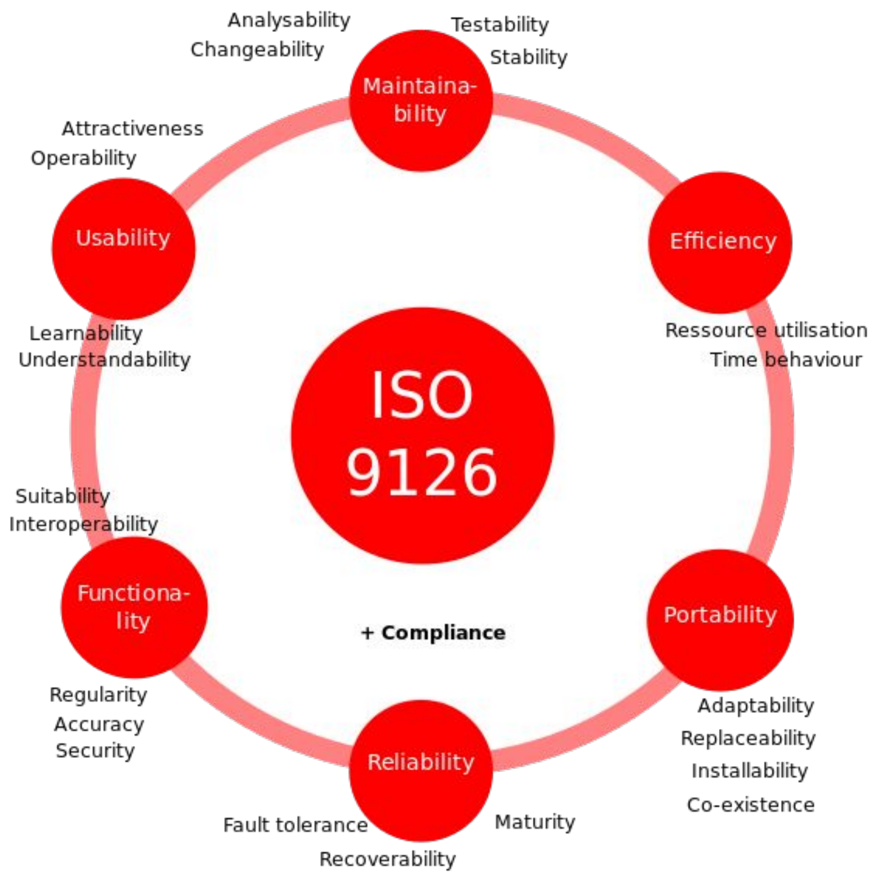
Overview

- Motivation
- Tools and Best Practices
- Portability and Reproducibility
- Readability of Python code
- Some more tools for productivity

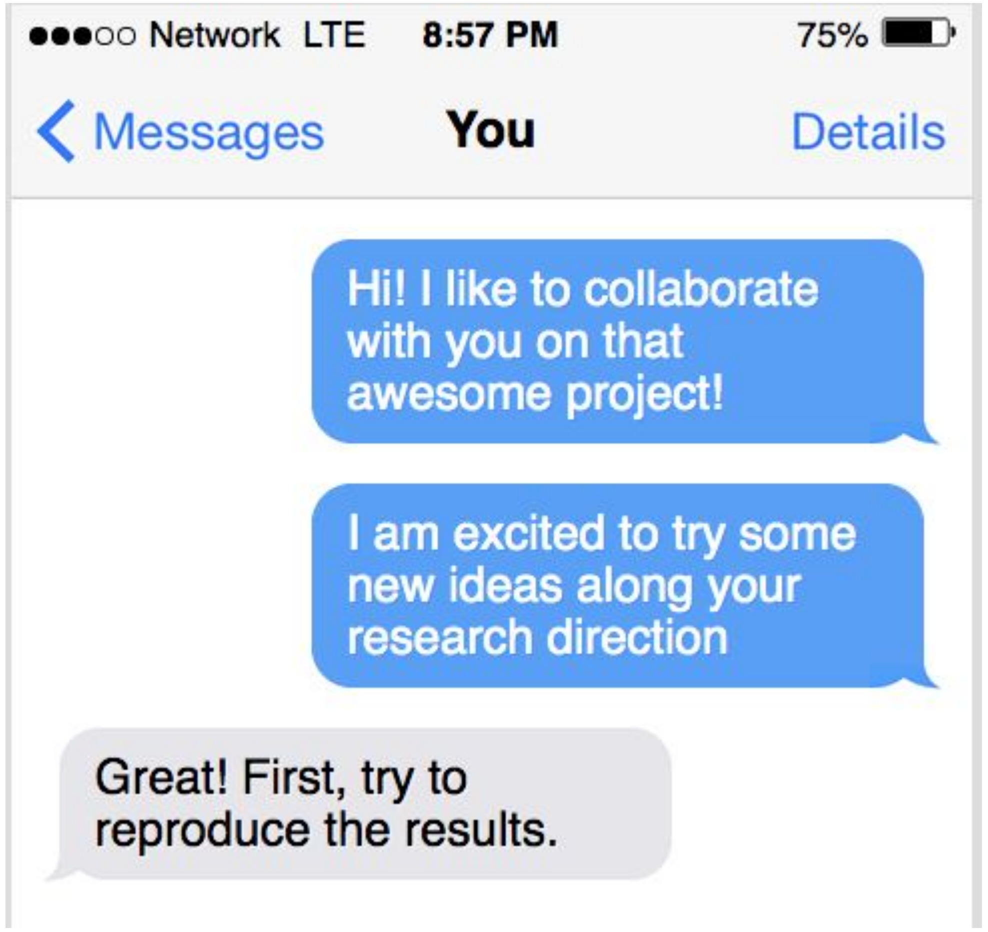
Motivation

- Tools and Practices that improve
  - Your **Productivity**
  - Your code's **Portability**
  - Your code's **Readability**

1. Productivity FTW!
   a. Collaboration is necessary.
2. Readability and Portability
   a. For successful collaborations
   b. For the *Pride of Workmanship, Satisfaction*
   c. Karma: What you give, comes back to you



Don't worry, we are not going to ISO-9126 today!

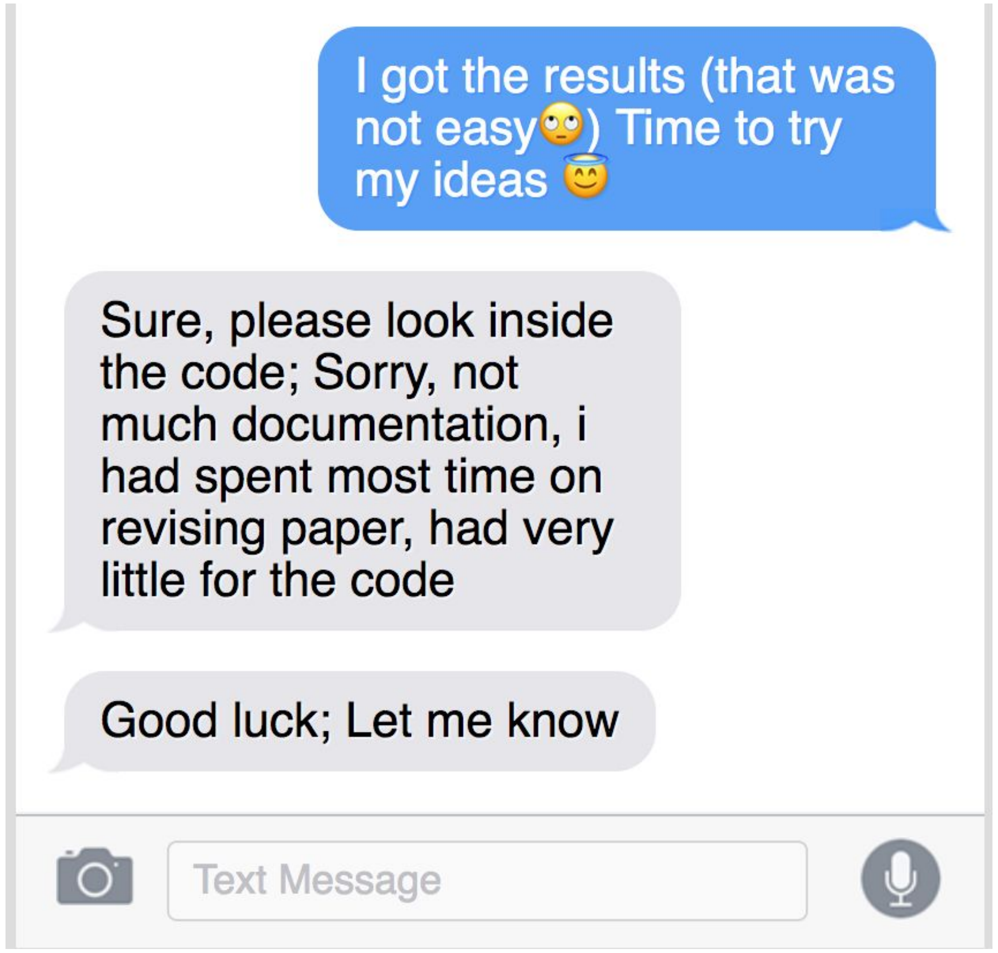

●●●○○ Network LTE 8:57 PM 75%

Messages You Details

Hi! I like to collaborate with you on that awesome project!

I am excited to try some new ideas along your research direction

Great! First, try to reproduce the results.


I got the results (that was not easy🙄) Time to try my ideas 😇

Sure, please look inside the code; Sorry, not much documentation, i had spent most time on revising paper, had very little for the code

Good luck; Let me know

Text Message

Benefits for You: Productivity

- What? Do more with less time.
- Why? Don't ruin after-hours, weekends, and sleep
- How? Use right/best **tools** and **practices**. They help:
  - Get tasks done faster and much faster: automate
  - Catch bugs ahead of time: have fewer bugs
  - **Collaborate**: others can help you, only if it's easy to step-in
  - Organize: make code easy to find and modify
- Which tools and what practices, precisely?
  - *<u>Some of them</u> will be covered in this talk*
  - *Maybe not covered entirely, they will be just pointed out*

Benefits for Others:

Portability

Facilitate your peers to easily run your code. As a black-box, without having to look inside.

⇒ **Reproducibility**

Readability

Use a (code) writing style that is easier for you and your peers to read and understand, without having to pull hairs out.

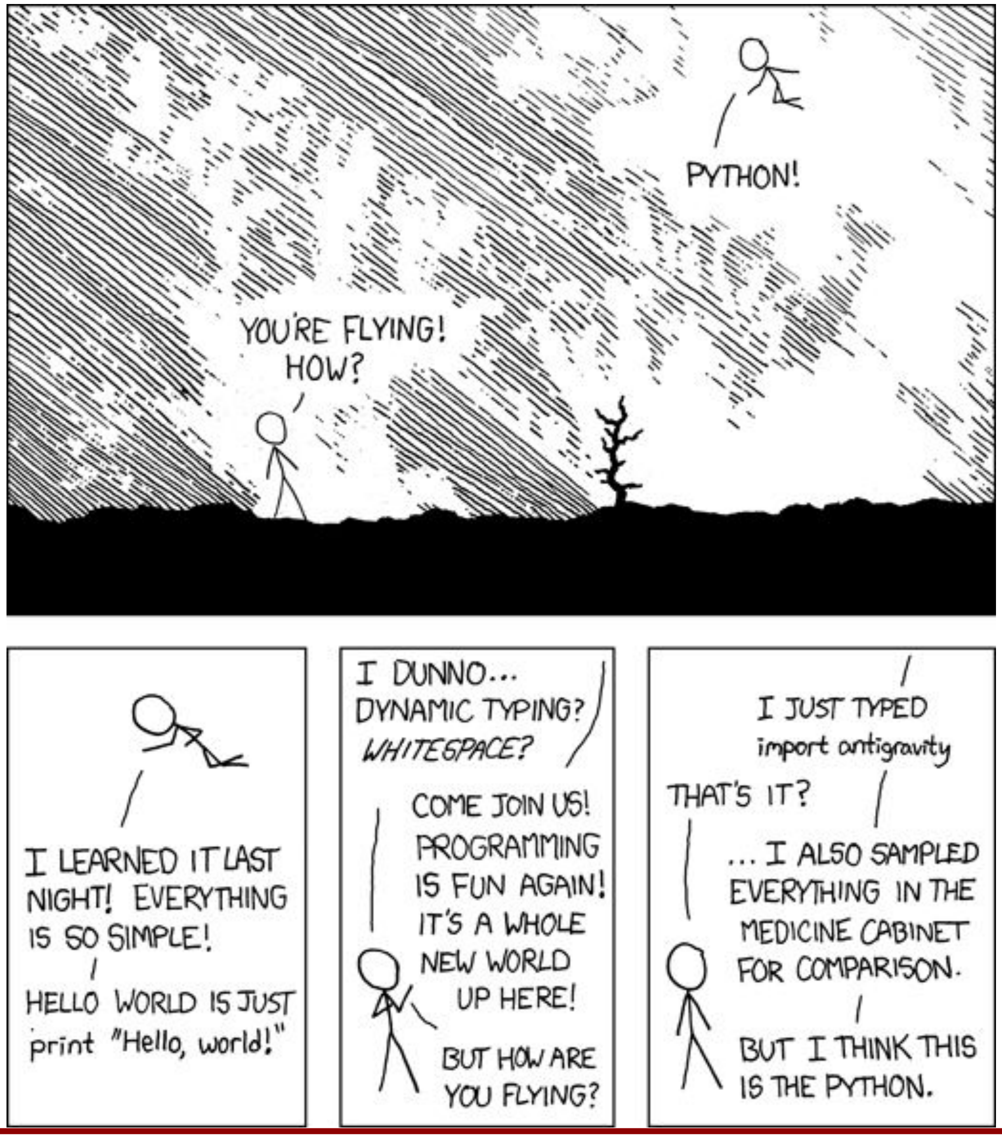
⇒ **Collaboration**

How to:

1. Use right tools
2. Use best practices

Python

- Still using Python 2.7? Please upgrade to 3.7+


YOU'RE FLYING! HOW?
PYTHON!
I LEARNED IT LAST NIGHT! EVERYTHING IS SO SIMPLE!
HELLO WORLD IS JUST print "Hello, world!"
I DUNNO... DYNAMIC TYPING? WHITESPACE?
COME JOIN US! PROGRAMMING IS FUN AGAIN! IT'S A WHOLE NEW WORLD UP HERE!
BUT HOW ARE YOU FLYING?
I JUST TYPED import antigravity
THAT'S IT?
... I ALSO SAMPLED EVERYTHING IN THE MEDICINE CABINET FOR COMPARISON.
BUT I THINK THIS IS THE PYTHON.

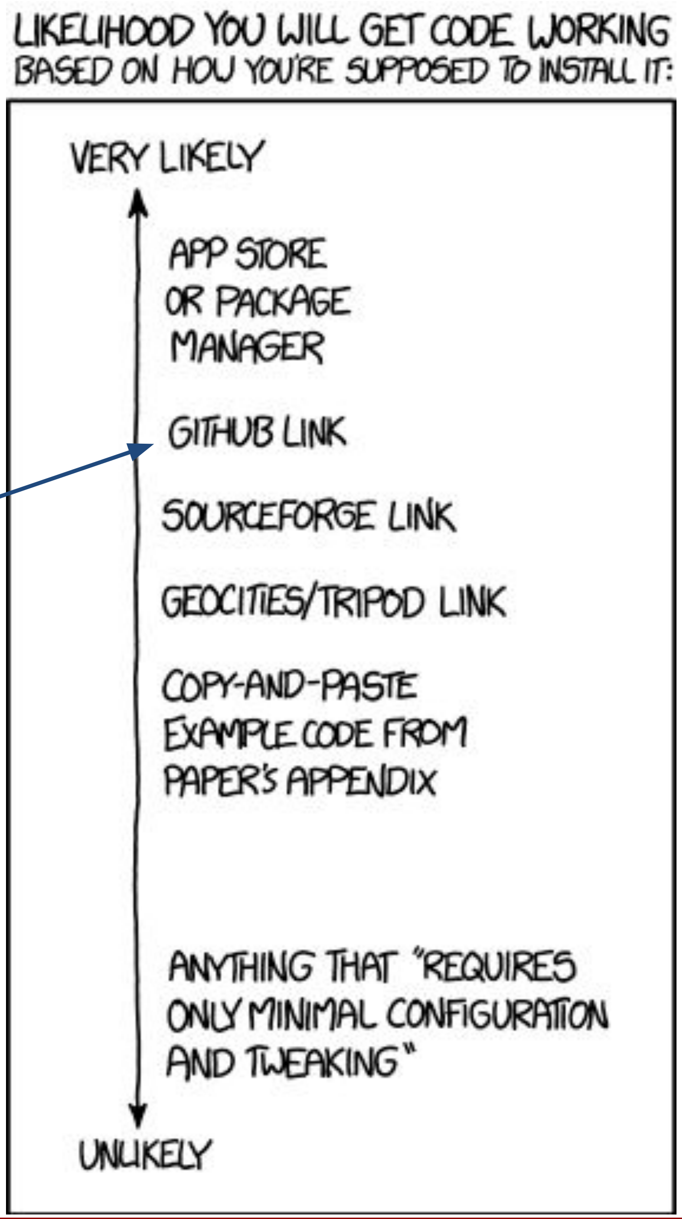
https://xkcd.com/353/

Python

- Portable code - for reproducibility
  - Python is portable, by default
  - Yet we come across code that is so hard to run 🤦‍♂️
- Readable code - for collaboration
  - Python is one of the easiest languages ever (👉 executable-pseudocode)
  - Yet we see cryptic, awkwardish, complicated code 🤦‍♂️

Portable code for Reproducibility

Start here and move up

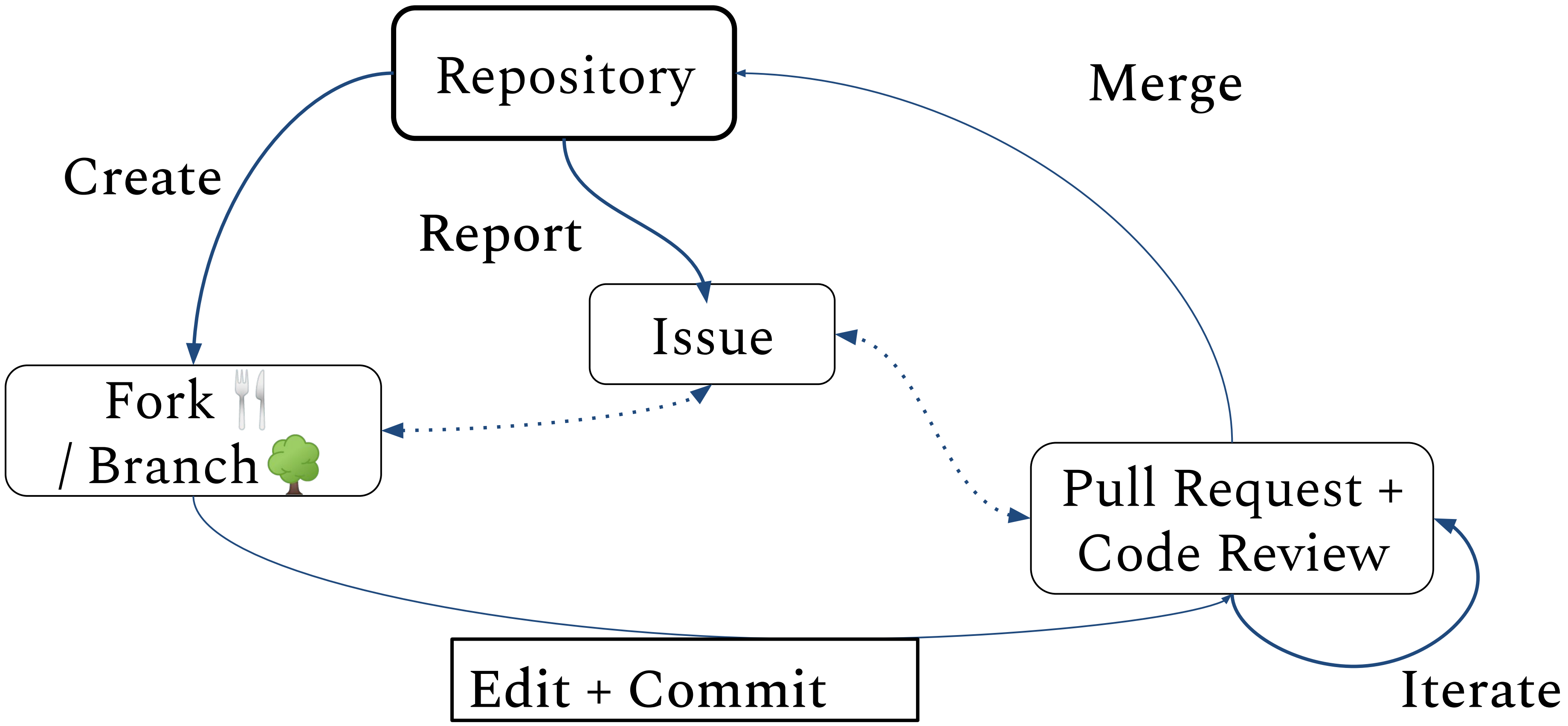

LIKELIHOOD YOU WILL GET CODE WORKING BASED ON HOW YOU'RE SUPPOSED TO INSTALL IT:
VERY LIKELY
APP STORE OR PACKAGE MANAGER
GITHUB LINK
SOURCEFORGE LINK
GEOCITIES/TRIPOD LINK
COPY-AND-PASTE EXAMPLE CODE FROM PAPER'S APPENDIX
ANYTHING THAT "REQUIRES ONLY MINIMAL CONFIGURATION AND TWEAKING"
UNLIKELY

https://xkcd.com/1742/

Setting up a Project

- Create a git repository
  - Need version control/backup: *use git*
  - Multiple features/ideas/fixes in parallel: *use git*
  - Multiple people contribute code in parallel: *use git*
  - …
- **GitHub** is a goto place for hosting git repos
  - ***GitLab** is popular too*
- Many useful tools to improve productivity
  - Issues and Discussion threads
  - Pull Requests and Code Reviews
  - Wikis

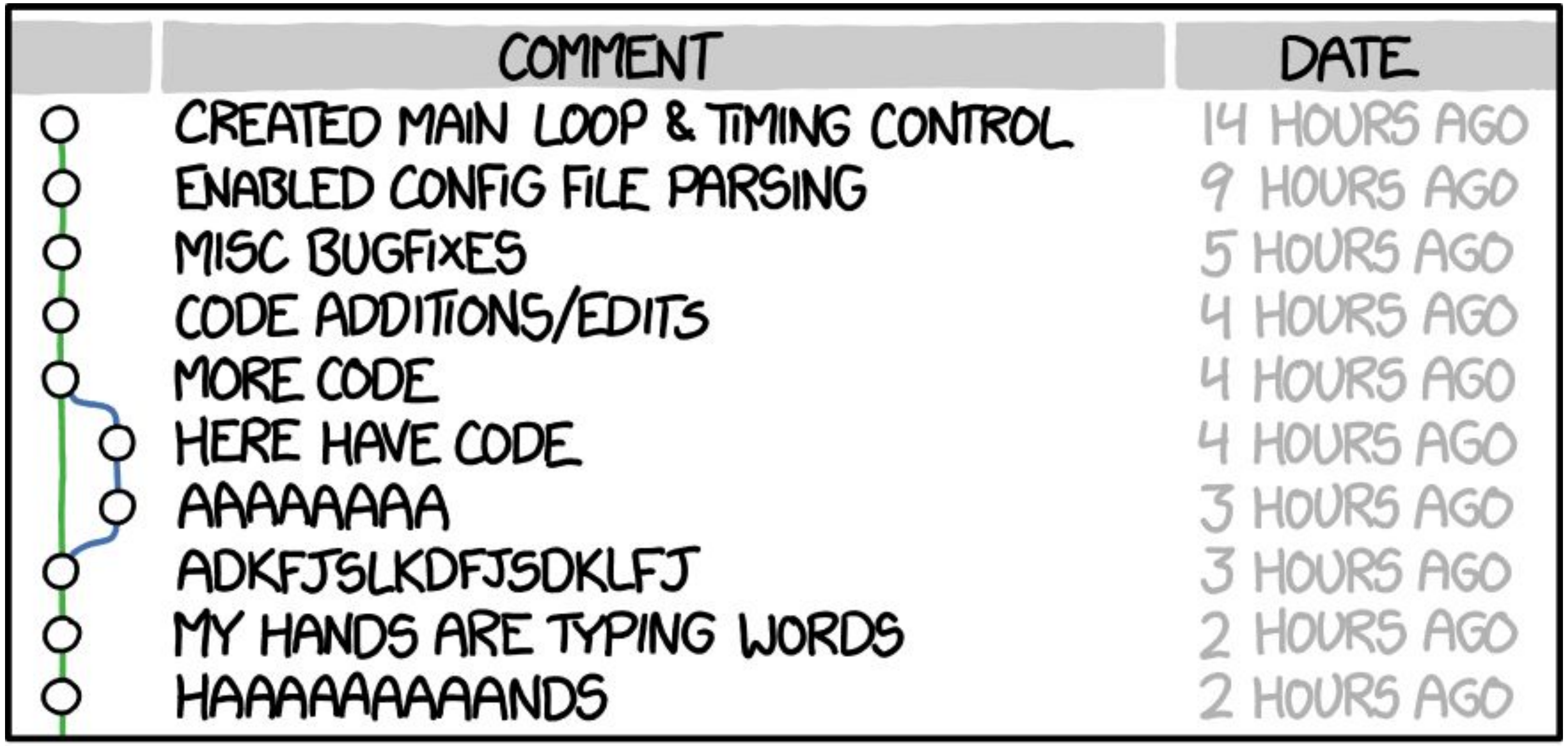
GitHub Workflow



Checklist

- ✓ Create Github/Gitlab account (if you don't already have one)
- ✓ Create a repository for your project. Decide private / public
- ✓ Add collaborators
- ✓ Create a README file *(more details on this soon)*
- ✓ git clone ✓ git pull
- ✓ git add ✓ git commit
- ✓ git push
- ✓ git branch ✓ git checkout
- ✓ Github Pull Request ✓ Code Reviews

Git commit messages in long run



COMMENT	DATE
CREATED MAIN LOOP & TIMING CONTROL	14 HOURS AGO
ENABLED CONFIG FILE PARSING	9 HOURS AGO
MISC BUGFIXES	5 HOURS AGO
CODE ADDITIONS/EDITS	4 HOURS AGO
MORE CODE	4 HOURS AGO
HERE HAVE CODE	4 HOURS AGO
AAAAAAAA	3 HOURS AGO
ADKFJSLKDFJSDKLFJ	3 HOURS AGO
MY HANDS ARE TYPING WORDS	2 HOURS AGO
HAAAAAAAANDS	2 HOURS AGO

AS A PROJECT DRAGS ON, MY GIT COMMIT MESSAGES GET LESS AND LESS INFORMATIVE.

https://xkcd.com/1296/

git DOs and DON'Ts

- ✓ DO: Write meaningful and truthful commit messages
- ✓ DO: Use branches for working in parallel
  - ✓ DO: Always keep the branches up-to date synchronized
  - ✓ DO: Keep **master** branch in working condition
- ✓ DO: One commit per sub task: [[Small $\xrightarrow{\text{<balance>}}$ Big]]

- ⛔ DON'T: commit generated files
  - such as compiler generated, outputs, and log files
  - binary files that change often
- ⛔ DON'T: commit unwanted files
- ⛔ DON'T: commit a huge batch of changes at once

Write a README

- Description: what is this code for?
- Markdown or richer format; sections with headings
- How to install?
- Where are the settings? Incase we need to change any
- A quick example of how to run/use the code is must
- A detailed tutorial will be nicer
- License → Should have a separate discussion on this topic
- Contributors and Acknowledgement
- How to report issues? → use Github/Gitlab issues

Installing Dependencies

- **`brew apt yum conda pip`** …. or give a **`docker`** image
- Recommend: cross-platform tools: **pip** and **conda**
  - 👉 **pip** and **conda** work together; you need both

pip

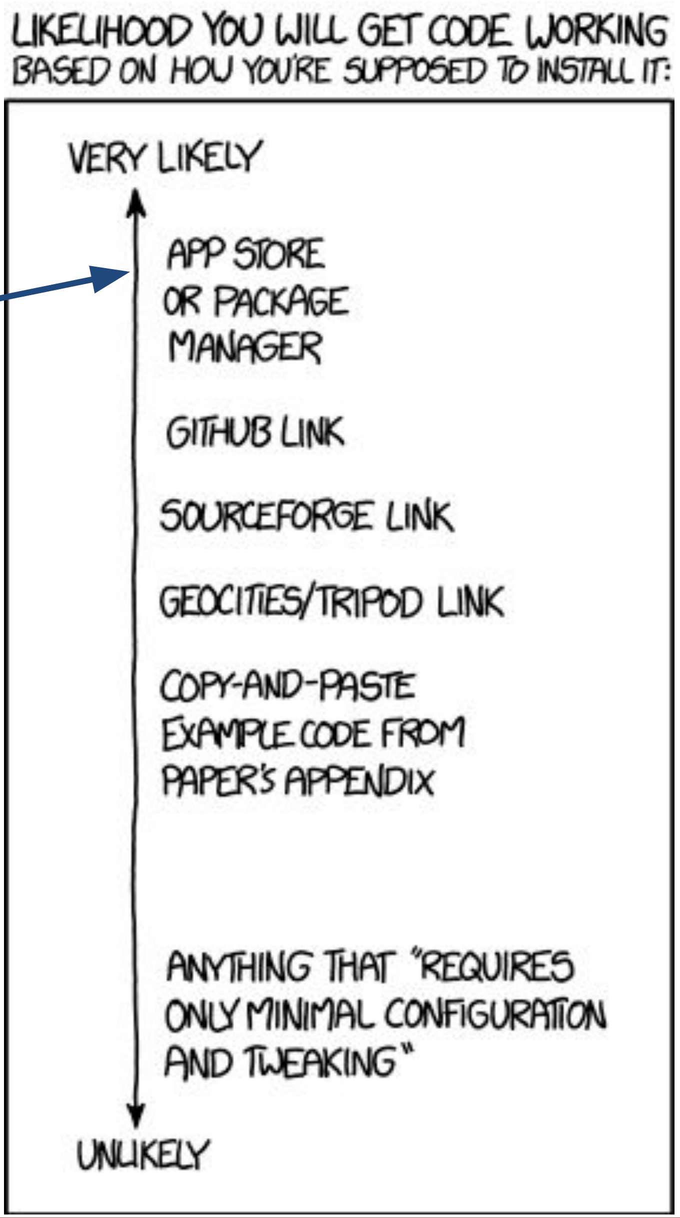
- https://pypi.org/
- `pip install <name>`
- `pip install <name>==<version>`
- List down all the libs and versions in `requirements.txt`
  - One `<name>==<version>` per line
- `pip install -r /path/to/requirements.txt`
- 👉 DON'T forget the version numbers

conda

- Download and install miniconda
  https://docs.conda.io/en/latest/miniconda.html
- Suggestion: *one conda environment per project*
- **`conda create -n <myenv> python=3.7`**
- **`conda activate <myenv>`**
- **`conda env create -f environment.yml`**

- **`conda`** can do more than managing python environments
  - It can install system libraries ***without needing sudo***

Going up here



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Code as a Package

- Create a **`setup.py`**, with requirements
- It's easy! Copy-paste a template and modify
- Installation: **`pip install .`**
  - Development installation: **`pip install --editable .`**
- Ready to give it to the world for free, release to **PyPI**
  Simple tutorial: https://github.com/thammegowda/awkg/blob/master/HowToRelease.md
  Detailed tutorial: https://twine.readthedocs.io/en/latest/
- If you don't want to **`pip`**, create a **`setup.sh`** script
- If data needs to be downloaded, write **`get-data.sh`** script

Example setup.py

```python
from setuptools import setup
from pathlib import Path
import awkg # import own package

long_description = Path('README.md').read_text(encoding='utf-8')
setup(name='awkg',   version=awkg.__version__,
   packages=['awkg'],  # for a single .py file, use py_modules=[]
   description=awkg.__description__, long_description=long_description,
   long_description_content_type='text/markdown',
   license='GNU General Public License v3 (GPLv3)',
   classifiers=classifiers, python_requires='>=3.6',
   url='https://github.com/thammegowda/awkg',
   platforms=['any'],
   author='Thamme Gowda',
   entry_points={'console_scripts': ['awkg=awkg:AWKG.main'],})
```

DON'T write hard local paths

- DONT: hard code local paths

- DO: Use an environment variable
- DO: Make everything relative to it

- Example:

```
$<project>_HOME/data
$<project>_HOME/conf
$<project>_HOME/bin
$<project>_HOME/libs
```

Image Credit: Reddit

All Configs at One Place

- DON'T spread the configs all over your project code
- DO keep all configs at one place.
- DO create a config for experiment for reproducibility

Format of config file:

- **`config.py`**
- **`config.ini`**
- **`config.xml`** : old school! hard to read/manipulate in python☹️
- **`config.json`** : almost usable, but doesn't support comments
- **`config.yml`** : 🤟 Use **`ruamel.yaml`** to preserve comments
- **`config.jsonnet`** : https://jsonnet.org/

Good Use of Existing Env. Variables

- $HOME variable
- What if commands were already in PATH?
  - No need to set full path to the command binary
- What if the python code was already in PYTHONPATH?
  - No need for set full path
  - just "`from my_script import my_func`"
- **`conda`** environment can do that for you!
- Try not to invent too many new variables

Improving Readability of Python Code

Follow Python Conventions

- Python community didn't start with a set of conventions
  Developers used whatever conventions they liked
  No conventions were also okay.
- Conventions have evolved, and became **PEP8 or PEP-0008**
  https://www.python.org/dev/peps/pep-0008/
- Use an IDE: such as **pycharm**
  - Watch out the red and yellow lines

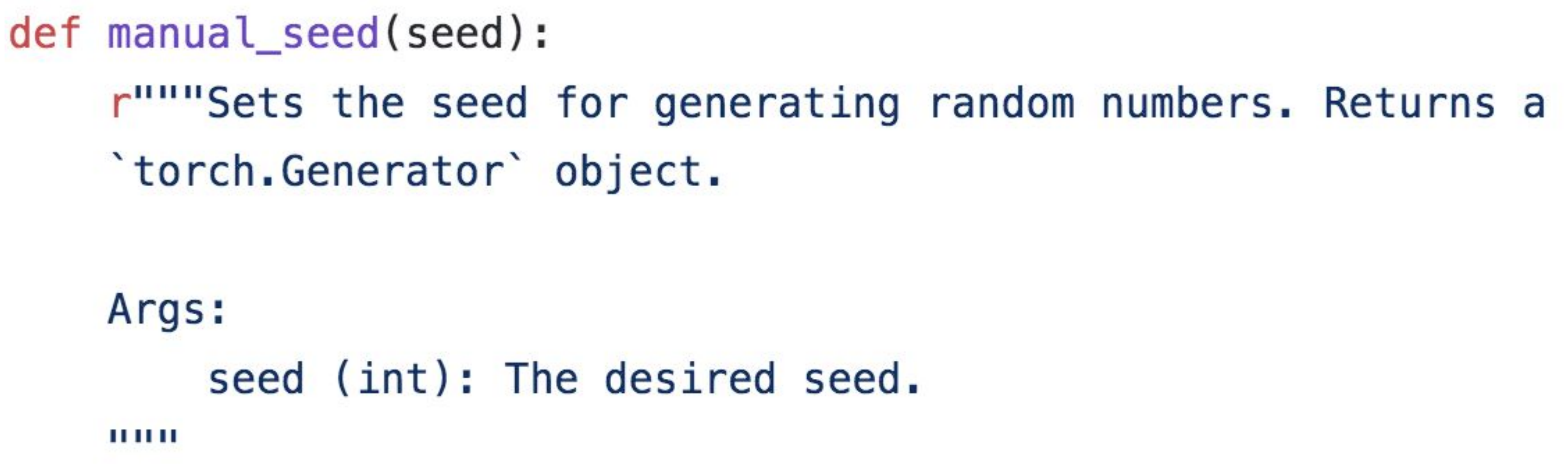
PEP8: Naming Conventions

- `ClassName`
- `method_name()`   not `dontUseMixedCase()`
- `variable_name`   not `dontUseMixedCase`
- `_internals_one_underscore`
- `__two_underscores__` such as `__init__()`
- `CONSTANTS_ARE_CAPS`
- `dontUseMixedCase`, unless already used and it's too late
- `Dont_Do_This_Either`

Advantages?

docstrings and comments

- **DO**: add docstrings, atleast to the public functions
- Example:



```
def manual_seed(seed):
    r"""Sets the seed for generating random numbers. Returns a
    `torch.Generator` object.

    Args:
        seed (int): The desired seed.
    """
```

Caution: Complexity Increases Over Time

If the code becomes too complex over the time, *please refactor code*

- Line length: Used to be 80; Can go upto 120 chars now
- Number of lines in function: [Not too many]
- How many arguments to functions: [Not too many]
- How many code files in a directory: [Not too many]
  - Use namespaces/packages: and of course use meaningful names
- Too much Dead Code? Consider removing it!
  - Dead code: commented out source code
  - Don't worry, git has everything saved for you (if you had committed it)

CLI with argparse

DONT: Directly manipulate **sys.argv**

```
foo = sys.argv[1]
bar = sys.argv[2]
```

DO: Use **argparse**

```
parser = argparse.ArgumentParser(description='Description of your program')
parser.add_argument('-f','--foo', help='Description for foo argument', required=True)
parser.add_argument('-b','--bar', help='Description for bar argument', required=True)
args = vars(parser.parse_args())
```

Integrations via subprocess?

- **DON'T** write everything under **`__main__`** block
  - Only luck we have with this is call via **subprocess**
  - Often no need for launching frequent external processes
- Setup PYTHONPATH properly,
  "**`from myscript import method`**"; call "**`method(args)`**"
- You can pass complex data structures in memory
- It's nicer that way than subprocess
  - No unnecessary work like writing and reading files
  - No unnecessary CLI arg parsing and disk IO

Are too many args bad? Example

Example from tensorflow/tensor2tensor:

```
y = common_attention.multihead_attention(
   common_layers.layer_preprocess(
       x, hparams, layer_collection=layer_collection),
   None,
   decoder_self_attention_bias,
   hparams.attention_key_channels or hparams.hidden_size,
   hparams.attention_value_channels or hparams.hidden_size,
   hparams.hidden_size,
   hparams.num_heads,
   hparams.attention_dropout,
   attention_type=hparams.self_attention_type,
   max_relative_position=hparams.max_relative_position,
   heads_share_relative_embedding=(
      hparams.heads_share_relative_embedding),
   add_relative_to_values=hparams.add_relative_to_values,
   save_weights_to=save_weights_to,
   cache=layer_cache,
make_image_summary =make_image_summary,
dropout_broadcast_dims =attention_dropout_broadcast_dims,
max_length=hparams.get("max_length"),
decode_loop_step =decode_loop_step,
vars_3d=hparams.get("attention_variables_3d" ),
activation_dtype =hparams.get("activation_dtype" , "float32"),
weight_dtype =hparams.get("weight_dtype" , "float32"),
layer_collection =layer_collection,
recurrent_memory =recurrent_memory,
chunk_number =chunk_number,
hard_attention_k =hparams.get("hard_attention_k" , 0),
gumbel_noise_weight =hparams.get("gumbel_noise_weight" , 0.0),
max_area_width =max_area_width,
max_area_height =max_area_height,
memory_height =memory_height,
area_key_mode =hparams.get("area_key_mode" , "none"),
area_value_mode =hparams.get("area_value_mode" , "none"),
training=(hparams.get("mode",
 tf.estimator.ModeKeys. TRAIN)
==tf.estimator.ModeKeys. TRAIN))
```

Too many args: Redesigned

```
class MultiHeadedAttention(nn.Module):
   def __init__(self, n_heads, hid_size, dropout=0.1):
      …
   def forward(self, query, key, value, mask=None):
     …
```

Usage:

```
multi_attn = MultiHeadedAttention(n_heads, hid_size, dropout=dropout)
attn_val = multi_attn(query, key, value, mask))
```

Use Logger

Use logger with proper levels

```
import logging as log
log.basicConfig(level=log.INFO)

log.debug("Building Index...")
log.info("Index is valid")

log.warning("Index is invalid")
log.error("Index is invalid; exiting")
```

Level	**Numeric value**
CRITICAL	50
ERROR	40
WARNING	30
INFO	20
DEBUG	10
NOTSET	0

New Features

- typing: 3.5+
- f-strings aka literal strings : 3.6+
- pathlib : 3.4+
- dataclasses: 3.7+

typing

- Typed code is easier to understand and debug than non typed
- DO: Annotate public function args with types

```
def word_count(input):
   # bad arg name; what is this input thing? too broad

def word_count(sentences):
   # good argument name, but how do sentences?

from typing import List, Dict
def word_count(sentences: List[List[str]]) -> Dict[str, int]:
   # Nice huh ?
```

docstring with typing

BEFORE

```
def manual_seed(seed):
    r"""Sets the seed for generating random numbers. Returns a
    `torch.Generator` object.
    Args:
        seed (int): The desired seed.
    """
```

AFTER

```
def manual_seed(seed: int) -> torch.Generator:
    r"""Sets the seed for generating random numbers.
    Args:
        seed: The desired seed.
    """
```

Useful tools and libs

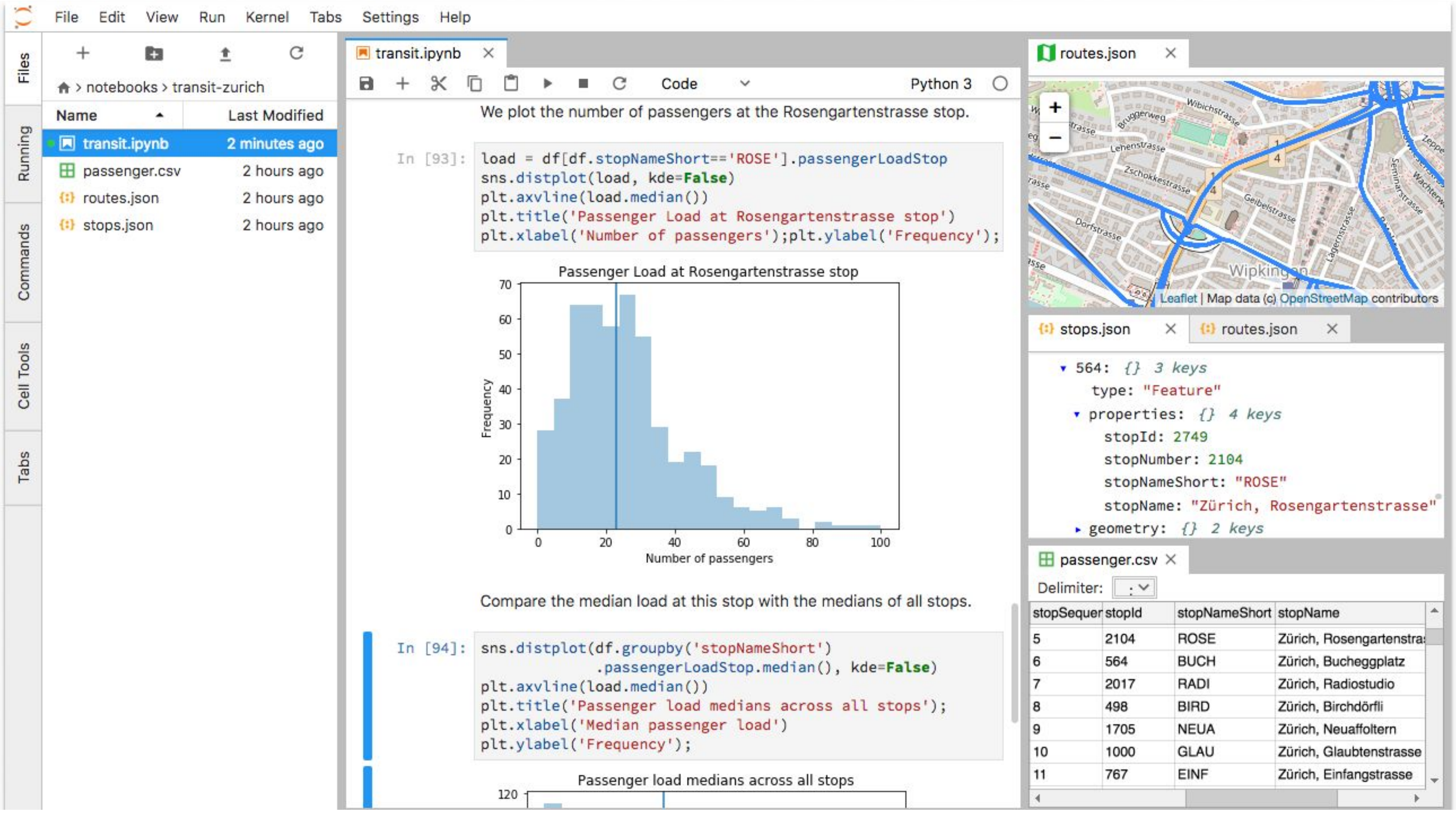
`jq`

- XML ? Use JSON
  - **`json.load(...)`** and **`json.dump(...)`**
- Too many JSON Documents? Use JSONLines
  - http://jsonlines.org/
- **`jq`** is awesome https://stedolan.github.io/jq/

Text Editor vs Notebook vs IDE

- Text Editors: vim/emacs/sublime/atom/brackets …
  - vim/emacs for tweaking on remote servers via ssh
- Prototype: Jupyter lab (jupyter notebook)
  - **`pip install jupyterlab`**
  - Google Colab : https://colab.research.google.com
- Production: Use an IDE
  - PyCharm is awesome https://www.jetbrains.com/pycharm/
  - Pay attention to yellow and red underlines marked by your IDE

jupyter lab



Name	Last Modified
transit.ipynb	2 minutes ago
passenger.csv	2 hours ago
routes.json	2 hours ago
stops.json	2 hours ago

We plot the number of passengers at the Rosengartenstrasse stop.

```
In [93]: load = df[df.stopNameShort=='ROSE'].passengerLoadStop
         sns.distplot(load, kde=False)
         plt.axvline(load.median())
         plt.title('Passenger Load at Rosengartenstrasse stop')
         plt.xlabel('Number of passengers');plt.ylabel('Frequency');
```

Compare the median load at this stop with the medians of all stops.

```
In [94]: sns.distplot(df.groupby('stopNameShort')
                      .passengerLoadStop.median(), kde=False)
         plt.axvline(load.median())
         plt.title('Passenger load medians across all stops');
         plt.xlabel('Median passenger load')
         plt.ylabel('Frequency');
```

```
▾ 564: {} 3 keys
    type: "Feature"
  ▾ properties: {} 4 keys
      stopId: 2749
      stopNumber: 2104
      stopNameShort: "ROSE"
      stopName: "Zürich, Rosengartenstrasse"
  ▸ geometry: {} 2 keys
```

stopSequer	stopId	stopNameShort	stopName
5	2104	ROSE	Zürich, Rosengartenstra
6	564	BUCH	Zürich, Bucheggplatz
7	2017	RADI	Zürich, Radiostudio
8	498	BIRD	Zürich, Birchdörfli
9	1705	NEUA	Zürich, Neuaffoltern
10	1000	GLAU	Zürich, Glaubtenstrasse
11	767	EINF	Zürich, Einfangstrasse

More python libs

- `numpy` and `matplotlib`
- `pandas`
- ML modeling:
  - Pytorch
  - Tensorflow 2.0 with Keras
  - sklearn
- HTTP / REST API:
  - client: `requests`
  - server: `flask`
- Web data:
  - XPATH (`lxml`)
  - `scrapy`

Try not to reinvent these libs;
instead take full advantage

CLI Tools

Don’t reinvent these:

- `grep`
- `sed`
- `cut; paste`
- `awk`
- `sort; uniq`
- `jq; yq`

Don’t reinvent these, seriously:

- `parallel`
- `rsync`
- `ssh`

Discussion / Thank You