Creative Jupyter

Tools for literate computing, exploration, collaboration.

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About Me

- Software Developer, Leipzig (DE), Data Engineer, github.com/miku
- Part-time: Author, Trainer

Personal History

- IPython REPL for daily work (API exploration, data digging, ...)
- Jupyter for Python courses
- Jupyter for semi-ad-hoc analysis
- Collected material for book on Jupyter, but still long way to go ...
- Regular exposure to data related problems

Creativity in Context

- have material available
- have tools available
- progress and trial and error
- comments and collaboration

Programming Context

Translated to programming and data context:

- (1) materials (data)
- (2) tools, exploration (languages, libraries, extensions)
- (3) experiments, allow for failure (version control)
- (4) comments and sharing (packaging, sharing, reproducibility)

Literate programming

- original paper from Knuth (1984)
- similar but different idea: write one document, generate executable and documentation from the same source
- alternative names: literate computing, interactive computing

(1) Materials

- What data you want to access?
- How do you access data in notebooks?

(1) Materials

Example data access scenarios:

A company wants to run **business analysis** across data from different databases (articles, customers, ...) or other systems (search, API)

Exploratory analysis of weather data in **scientific context**.

Data **journalism**.

(1) Material

Options to make raw data available:

- download file and put it the repo (e.g. under data folder)
- have a download.sh script fetching larger data sets
- expose obj.load() or obj.load_data() functions on dataset helpers
- factor out an adapter library, that will allow to access data quickly

(1) Material

Options for other artifacts; e.g. ML toolkits (sklearn, tensorflow.datasets, keras, pytorch) include utilities for varied formats (tarball, npz, ...).

```
In [3]: _ = cifar10.load_data()
Downloading data from https://www.cs.toronto.edu/~kriz/cifar-10-python.tar.gz
In [4]: from keras.datasets import reuters
In [5]: x = reuters.load_data()
Downloading data from https://s3.amazonaws.com/text-datasets/reuters.npz
```

(1) Material Example

Example:

Performance evaluation of various search systems: catalog frontends, search APIs. Wrote small wrapper library (about 600 SLOC), exposing objects with a common interface (e.g. a search method, taking a query string, returning results and metadata from 3 kinds of systems).

Quick generation of input data on the fly, then open up questions:

- Performance
- Query result overlaps and similarity
- ...

(1) Material Example

```
In [13]: stimes = [(q, ubl.search(q).get('took')) for q in tqdm.tqdm(queries)]
                            | 26/26 [02:03<00:00, 4.74s/it]
In [14]: df = pd.DataFrame(stimes, columns=["query", "took"])
          df.set index("query", drop=True, inplace=True)
          df.plot(kind='barh', figsize=(8, 11), grid=True)
Out[14]: <matplotlib.axes. subplots.AxesSubplot at 0x7fa6cc140fd0>
                                                             München, 1938
                                                                                                                                 took took
                                                             München 1938
                                                                    1938
                                                 Just a list of the common words
                                                           Jupyter Notebooks
              Jupyter Notebooks-a publishing format for reproducible computational workflows.
                                                       we call it Voight-Kampff
                                                            we call it Voight
                                                                 we call it
                                                                   we call
```

(1) Material Example

Advantages:

- data access module independent of notebook (e.g. usable in IPython or any other script)
- notebooks are readable documents (broader audience), no extra report needed
- adjustable

(1) Material

Generic ways to package data:

- data package, spec
- json stat

Data dissemination is not the business of a few anymore. Even though the JSON-stat format can be the perfect companion for the open data initiatives of National Statistical Offices, it is suitable for all kinds of data disseminators because it has been designed with simplicity in mind.

(1) Material Demo

- Making data accessible quickly.
- Example: demos/Accessing JSON Stat.ipynb

(2) Tools

For most things, you will need an external library. Basic Python practices apply, among them: try to isolate your environment:

- documentation
- reproducibility

(2) Tools

Can be as simple as a watermark, a Jupyter magic % extension to timestamp a notebook along with SW and HW information.

```
%watermark

2016-01-29T22:55:57

CPython 3.5.1
IPython 4.0.3

compiler : GCC 4.2.1 (Apple Inc. build 5577)
system : Darwin
release : 15.3.0
machine : x86_64
processor : i386
CPU cores : 4
interpreter: 64bit
```

(2) Tools

Make it simple to go from a repo to a notebook locally.

When using a virtual environment.

Setup.

```
$ python -m ipykernel install --user --name=myenv
Installed kernelspec myenv in $HOME/.local/share/jupyter/kernels/myenv
```

Teardown.

\$ jupyter kernelspec uninstall myenv

(3) Experiments

Although notebooks are in a textual format (JSON), they are hard to version control, since there is some state associated with the execution.

(3) Experiments

There are tools to work around that, e.g. Notedown and Jupytext.

- Notedown, write markdown and convert to a notebook
- Jupytext, associate Markdown file with Notebook and sync them
- nbstripout, clean output cells

(3) Notedown

- convert between various formats (markdown, Rmd, ipynb)
- works, albeit maybe less maintained, with some forks, e.g. knitty
- demo

(3) Jupytext

- bidirectional
- uses the contents API
- allows to create plaintext workflows, using Python, Markdown and a few other formats
- programmatic access
- demo, conversion, programmatic access

(3) nbstripout

- strips output cell
- can be part a pre-commit hook
- demo

(4) Colaboration

- Run a server and use token to share a workspace (e.g. in a container)
- Run JupyterHub -- TLJH (1-100 users, support for ARM, WIP)

(4) The littlest JupyterHub (TLJH)

- 1-100 users
- runs on Ubuntu 18.04

(4) Binder

Turn a Git repo into a collection of interactive notebooks.

Have a repository full of Jupyter notebooks? With Binder, open those notebooks in an executable environment, making your code immediately reproducible by anyone, anywhere.

(4) Turn notebooks into containers

repo2docker

repo2docker can build a reproducible computational environment for any repository that follows The Reproducible Execution Environment Specification.

It looks for a various configuration files.

demo, generation of a Dockerfile

(4) Install as Cloud Native application

Kubeflow

What is Kubeflow? The Kubeflow project is dedicated to making deployments of machine learning (ML) workflows on Kubernetes simple, portable and scalable.

Enabling easier **notebook sharing** across the organization. Users can create notebook containers or pods directly in the cluster, rather than locally on their workstations.

- Jupyter notebooks as experimental setup
- Data volumes can be mounted
- Tries to model end-to-end workflow, up to e.g. ML model serving

(4) Export to various formats

Export Notebooks as slides, PDF and other formats with nbconvert.

• demo: PDF export

(4) Platforms

- bringing data and people together
- hide operational complexity, e.g. preparation of datasets, clusters

Examples:

- An internal data science platform based on Spark and Jupyter (blog)
- Quantopian Notebooks (https://www.quantopian.com/notebooks/survey)

A hosted research environment with flexible data access, custom plotting, and post-hoc analysis on backtest and live trading results in an IPython Notebook.

Wrap up

- Jupyter Notebooks work standalone and have many extension points
- Both data integration and reproducibility features are getting better
- Formats available for version control
- Platforms emerge, domain-specific tasks, cloud and on premise

Thanks