Jupyter Data Science Workflow, Remastered

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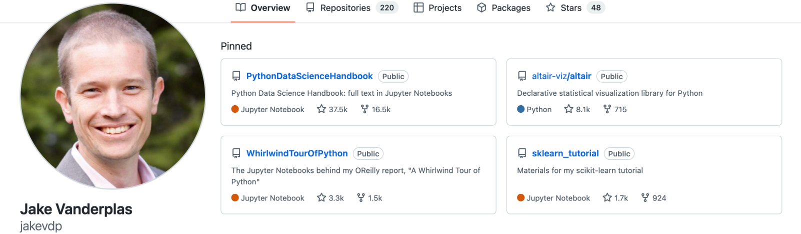
20-Feb-2023

Jupyter Workflow

In this session we will revisit the classic workflow by Jake Vanderplas Reproducible Data Analysis in Jupyter.



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PythonDataScienceHandbook Public
Python Data Science Handbook: full text in Jupyter Notebooks
● Jupyter Notebook ☆ 37.5k 16.5k

altair-viz/altair Public
Declarative statistical visualization library for Python
● Python ☆ 8.1k 715

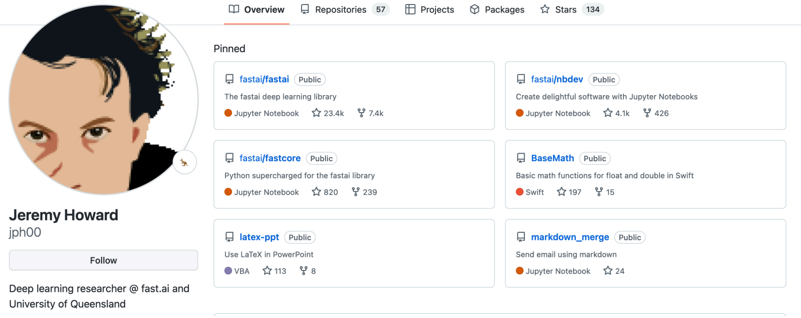
WhirlwindTourOfPython Public
The Jupyter Notebooks behind my OReilly report, "A Whirlwind Tour of Python"
● Jupyter Notebook ☆ 3.3k 1.5k

sklearn_tutorial Public
Materials for my scikit-learn tutorial
● Jupyter Notebook ☆ 1.7k 924

Jake Vanderplas
jakevdp

Nbdev

Nbdev is a notebook-driven development platform. With nbdev, you get documentation, tests, continuous integration, and packaging.



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Jeremy Howard
jph00

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Deep learning researcher @ fast.ai and University of Queensland

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fastai/fastai Public The fastai deep learning library ● Jupyter Notebook ☆ 23.4k 7.4k	fastai/nbdev Public Create delightful software with Jupyter Notebooks ● Jupyter Notebook ☆ 4.1k 426
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Agenda

- Hands-on Walkthrough

Extras

- Notebook Best Practices
- Qmd Documents
- RenderScripts
- Git-Friendly Jupyter
- Blogging
- Pre-Commit Hooks
- Documentation Only Sites
- Modular nbdev
- Nbdev plugins

Hands-on Walkthrough

Live coding.
What could possibly go wrong? :)

Code repo

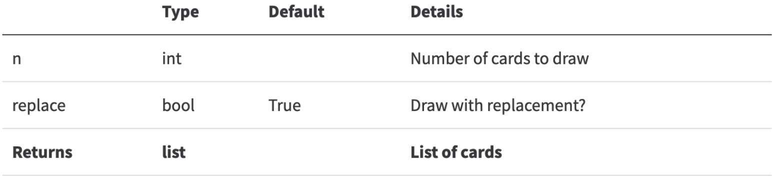
Notebook Best Practices

Document parameters with docments

With docments, this function:

```
def draw_n(n:int, # Number of cards to draw
           replace:bool=True # Draw with replacement?
          )->list: # List of cards
    "Draw `n` cards."
```

...would include the following table as part of its documentation:



	Type	Default	Details
n	int		Number of cards to draw
replace	bool	True	Draw with replacement?
Returns	**list**		**List of cards**

Notebook Best Practices

Code examples as tests by adding assertions

fastcore.test provides a set of light wrappers around assert for better notebook tests (for example, they print both objects on error if they differ).
Here's an example using `fastcore.test.test_eq`:

```
def inc(x): return x + 1
test_eq(inc(3), 4)
```

Notebook Best Practices

Document error-cases as tests

Nbdev recommends documenting errors with actual failing code using fastcore.test.test_fail. For example:

```
def divide(x, y): return x / y
test_fail(lambda: divide(1, 0), contains="division by zero'
```

Qmd documents

Qmd documents are Markdown documents, but with extra functionality provided by Quarto and Pandoc.
For example images arranged into layouts.

```
::: {layout-ncol=3}
![Jupyter](jupyter.jpg){width=50px fig-align="left"}

![Vscode](vscode.jpg){width=50px fig-align="left"}

![Git](git.jpg){width=50px fig-align="left"}
:::
```

Figure 1: Jupyter

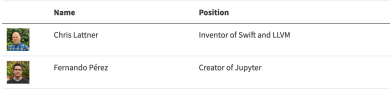
Figure 2: Vscode

Figure 3: Git

RenderScripts

RenderScripts are just like regular Python scripts. These scripts are run when your site is rendered.

For example to produce below table from a python list, the following script is used:



	Name	Position
	Chris Lattner	Inventor of Swift and LLVM
	Fernando Pérez	Creator of Jupyter

```
testimonials = [
    ('chris-lattner.png', 'Chris Lattner', 'Inventor of Sw
    ('fernando-pérez.jpeg', 'Fernando Pérez', 'Creator of 
]

print(qmd.tbl_row(['','Name','Position']))
print(qmd.tbl_sep([1,3,4]))
for fname,name,position in testimonials:
    print(qmd.tbl_row([im(fname, 60), name, position]))
```

Git-Friendly Jupyter

Jupyter notebooks don't work with version control by default. Nbdev provides a set of hooks which enable git-friendly Jupyter notebooks in any git repo.

nbdev provides three hooks to ease Jupyter-git integration.

- nbdev_merge on merging notebooks with git, that automatically fixes conflicting outputs and metadata
- nbdev_clean on saving notebooks in Jupyter, to automatically clean unwanted metadata and outputs from your notebooks
- nbdev_trust after merging notebooks with git, to trust a repo once-off, and all notebooks and changes thereafter

Blogging

Nbdev uses Quarto for blogging via Jupyter Notebooks. Although nbdev is not required to blog with notebooks, it will add some functionality (testing, exporting, adding blog to nbdev project website)

Pre-Commit Hooks

Nbdev provides hooks for the pre-commit framework to catch and fix uncleaned and unexported notebooks, locally, without having to wait for continuous integration pipelines to run:

1. pre-commit runs each hook on your staged changes
2. If a hook changes files pre-commit stops the commit, leaving those changes as unstaged
3. You can now stage those changes and make any edits required to get pre-commit to pass
4. Redo the git commit, and if it succeeds, your commit will be created.

Documentation Only Sites

Nbdev can be used for the purposes of documenting existing code. For example, you can use the following features of nbdev without creating a python package:

- Custom nbdev directives such as #|hide_line.
- Testing with nbdev_test.
- Automated entity linking with doclinks.
- Rendering API documentation with docments and show_doc.

Modular nbdev

You can use various nbdev tools separately:

- Document existing code with `show_doc`
- Testing notebooks with `nbdev_test`
- Export code to modules with `nb_export`
- Jupyter-git integration
- Python packaging, utlities for easy packaging on PyPI, conda, and GitHub

Nbdev plugins

With nbdev, it's possible to customize and extend it further beyond the standard capabilities.