

Welcome to the 2022 M&M Short Course X-16

Data Analysis in Materials Science with



Presented by (a selection of) the HyperSpy developers/power users:

- Carter Francis
- Joshua Taillon

A decorative header featuring a repeating pattern of light blue and white hexagons, resembling a honeycomb or molecular structure, set against a dark blue background.

NIST Disclaimer

Certain commercial equipment, instruments, materials, vendors, and software are identified in this talk for example purposes and to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Some logistics before we get started...

- Each session will be led by one instructor, but throughout the day, the other instructor will be around to answer questions. Feel free to raise your hand at any time if you need individual assistance
- You (hopefully) should have already downloaded the tutorial files and installed HyperSpy. *If not:* We have USB drives with the data and installers pre-loaded that we can copy to your laptop
- Rules from the M&M organizers:
 - **Masks Required:** Masks are required indoors in the Oregon Convention Center, in alignment M&M 2022 attendance guidelines. M&M attendees will be required to wear masks as follows:
 - Speakers will be permitted to remove their masks when actively giving their presentations, if they wish
 - Attendees will be permitted to remove their masks briefly while actively eating or drinking at official M&M 2022 functions

Helpful Resources:

- Agenda and course materials: https://pages.nist.gov/hyperspy_tutorial
 - Also contains helpful links to Binder, resources, installation help, etc.
- Repository of notebook and data files (to download manually):
https://github.com/usnistgov/hyperspy_tutorial

A note about Binder:



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- You access a server owned by Binder via the web-browser, the code runs on their servers and displays back to you
- This makes it very easy to get familiar with Python/HyperSpy, but will not help you if you need to do your own analysis
 - Only pre-defined "templates" are available, and the server has limited resources
 - It may also be fairly slow depending on the connection speed between you and Binder's servers (conference Wifi is not known for its speed...)

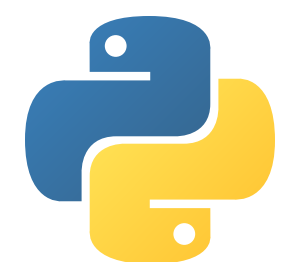
A decorative header featuring a repeating pattern of light blue and white hexagons, some of which are slightly offset to create a 3D effect.

Session 1: An Introduction to Python and HyperSpy:

The multi-dimensional data analysis toolbox

Josh Taillon

July 31, 2022



What is this "Python" that I've heard of?

What is  python[™] ?

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- High-level, *general purpose* programming language with "batteries included"
 - *i.e.*, it comes with enough features to do most basic programming tasks

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- Simple enough for quick scripts; featured enough for complex projects
- Used extensively on the web, in applications, and throughout science
- Syntax emphasizes readability and explicitness

A "Hello, World!" comparison:

Java:

```
public class HelloWorld {  
  
    public static void main(String[] args) {  
        System.out.println("Hello, World!");  
    }  
}
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A "Hello, World!" comparison:

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```

C++:

```
#include <iostream>  
using namespace std;  
  
int main() {  
    cout << "Hello, World!" << endl;  
    return 0;  
}
```


A "Hello, World!" comparison:

Python:

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Matlab:

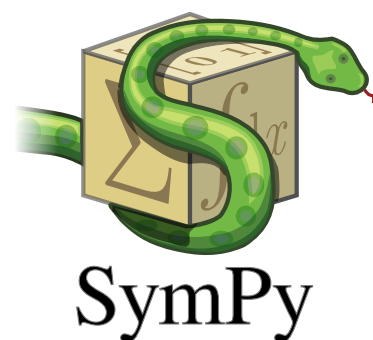
```
disp("Hello, World!")
```

Okay, but what does this have to do with science?

The "scientific Python" ecosystem provides almost any functionality you may need:



matplotlib

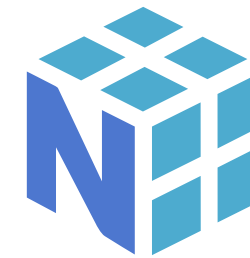


 **pandas**



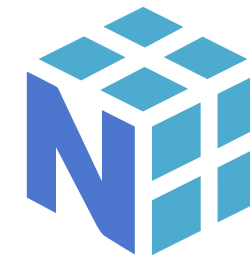
Linear algebra, optimization, machine learning...

- Numerical computing with `NumPy` (like what you would use Matlab for):



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- Signal processing, numerical integration, optimization, etc. with `SciPy`:



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- Machine learning with `scikit-learn` (and others):




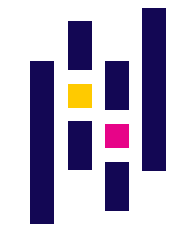
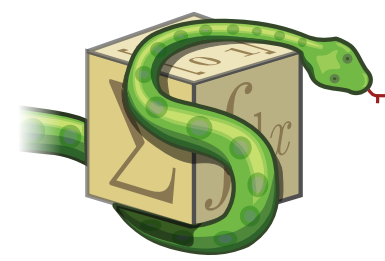
Visualization, statistics, computer algebra...

- Scientific visualization with matplotlib: *matplotlib*

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- Data frames/series and statistical analysis with pandas:  **pandas**

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- Symbolic computation with SymPy: 
SymPy

A better (?) way to create and publish your work

- Literate programming using a notebook interface with [Jupyter](#):



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- Creation of interactive computational analysis documents (not just scripts):
 - Facilitates reproducibility
 - Makes analyses more accessible (anyone can recreate your figure when they want!)

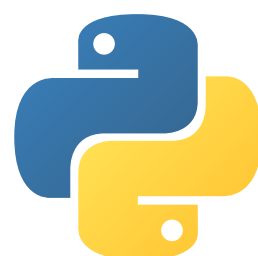
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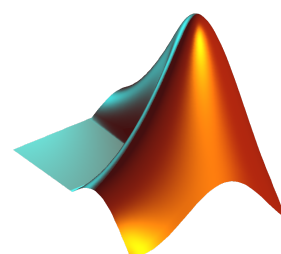
- Creation of interactive computational analysis documents (not just scripts):
 - Facilitates reproducibility
 - Makes analyses more accessible (anyone can recreate your figure when they want!)
- Easy to contribute back to the "open source" scientific ecosystem

Can't I just use Matlab?



End To End development to execution	Slightly more code required than Matlab to do same procedures
Vast array of open source scientific packages	Quality of third-party packages varies quite a bit
Great for general programming and application development	Package management (dependencies) can be difficult (getting easier with tools like conda)
Can be a “glue” language to connect R, C++, and others	IDE is not “built-in” like Matlab
Free (as in speech and as in beer)!	By default, some operations are slower

VS.



Scripts tend to be short due to high level of integration	Can not execute code; must be compiled into another language at runtime
Easy visualization and GUI development	Expensive! Must be licensed per-user (\$\$)
Well-tested and supported (commercial product)	Does not integrate well with other languages large projects are <i>extremely</i> difficult to manage
Built-in IDE and powerful debugger	Much functionality locked away in extra licensed packages (\$)
Multi-threading easier than in Python	Cannot develop stand-alone applications (must distribute Matlab runtime)

Adapted from: <https://towardsdatascience.com/r-vs-python-vs-matlab-vs-octave-c28cd059aa69>

File Exchange is good, but...

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[Get MATLAB](#)

File Exchange

File Exchange ▾ 🔍

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Trial software

Filter by Source

- ☐ Community 35,621
- ☐ MathWorks 260

Filter by Category

Using MATLAB

Language Fundamentals	879
Data Import and Analysis	1,056
Mathematics	1,391
Graphics	1,857
Programming	366
App Building	409
Software Development Tools	144
External Language Interfaces	431
Environment and Settings	119
Installation, Licensing, and Activation	10
Parallel Computing	135
Application Deployment	60
Report Generation	63

Applications

Science and Industry	3,280
Image Processing and Computer Vision	2,450
Data Analytics and Machine Learning	1,492
Signal Processing and Wireless Communications	2,271
Mathematics and Optimization	930
Control Systems	891
Robotics and Autonomous Systems	240
Hardware Interfacing and IoT	605
Games	503

Using Simulink

Simulink Fundamentals	435
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Most Recent

Benford's Law

A framework for Benford's Law conformity assessment.

2 Downloads ⓘ ⭐⭐⭐⭐☆

csearch

Fast C-MEX for Array Lookups and Masking

0 Downloads ⓘ ⭐⭐⭐☆☆

.c81-File-Parser

Parser for .c81 airfoil table files.

0 Downloads ⓘ ⭐⭐☆☆☆

castor-matlab

Matlab class to connect to castor API

0 Downloads ⓘ ⭐⭐☆☆☆

Schwarzschild black hole simulation

Simulation of observers moving and emitting light in a Schwarzschild spacetime, in either Schwarzschild

5 Downloads ⓘ ⭐⭐☆☆☆

Structure fields to variables

Code writing tool for importing/exporting workspace variables to or from a struct.

26 Downloads ⓘ ⭐⭐⭐⭐☆

Show All

Community Toolboxes

GUI Layout Toolbox

Layout manager for MATLAB graphical user interfaces

892 Downloads ⓘ ⭐⭐⭐⭐☆

Simulink Onramp

Learn the basics of how to create, edit, and simulate Simulink models through an interactive tutorial.

829 Downloads ⓘ ⭐⭐⭐⭐☆

Numerical Computing with MATLAB

Toolbox containing files and app from Numerical Computing with MATLAB

505 Downloads ⓘ ⭐⭐⭐⭐☆

PIVlab - particle image velocimetry (PIV) tool

Easy to use, GUI based tool to analyze, validate, postprocess, visualize and simulate PIV data.

391 Downloads ⓘ ⭐⭐⭐⭐☆

Feature Selection Library

Feature Selection Library (MATLAB Toolbox)

391 Downloads ⓘ ⭐⭐⭐⭐☆

"JSON": MATLAB

JSONlab: a toolbox to encode/decode JSON files

A toolbox to encode/decode JSON and UBJSON files in MATLAB/Octave

219 Downloads ⓘ ⭐⭐⭐⭐☆

Show All 1,144

Distributing code is simple in the Python community

(and integrated directly into Python tools)

-  **GitHub**: Community standard is to (at least) release code on GitHub (or similar service)

-  : Placing into the PyPI, the **Python Package Index** enables installing with simple:

- `pip install my-awesome-package`

-  : Anaconda enables multiple environments and complex dependency management

- `conda install my-awesome-package`

What does it mean to be "open source"?

“...something people can modify and share because its design is publicly accessible

— opensource.com

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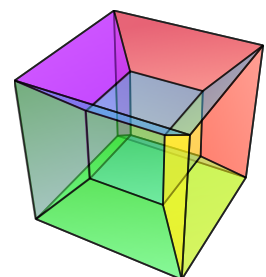
What about "open science"?

“...science must be done in an open, and reproducible fashion where all components of research are open

— [Marcus Hanwell \(also opensource.com\)](#)

Open-source and Python in the microscopy ecosystem:

General Purpose		Others	
HyperSpy	http://hyperspy.org/	AbTEM	https://abtem.readthedocs.io
Nion Swift	https://nionswift.readthedocs.io	HRTEMFringe Analyzer	https://github.com/ialxn/HRTEMFringeAnalyzer
pycroscopy	https://github.com/pycroscopy/pycroscopy	Atomap	https://atomap.org/
DigitalMicrograph	https://www.gatan.com/run-python-script	LumiSpy	https://lumispy.readthedocs.io/en/latest/
		Kikuchipy	https://kikuchipy.org
Pixelated STEM		Prismatic	https://prism-em.com/
pyXem	https://pyxem.github.io/pyxem-website/	tomopy	https://tomopy.readthedocs.io/en/latest/
py4DSTEM	https://py4dstem.readthedocs.io/	tomotools	https://github.com/usnistgov/tomotools
LiberTEM	https://libertem.github.io/LiberTEM/	tomviz	https://tomviz.org/
fpd	https://gitlab.com/fpdpy/fpd/		



What is HyperSpy, anyway?

What is



HyperSpy ?
multi-dimensional data analysis

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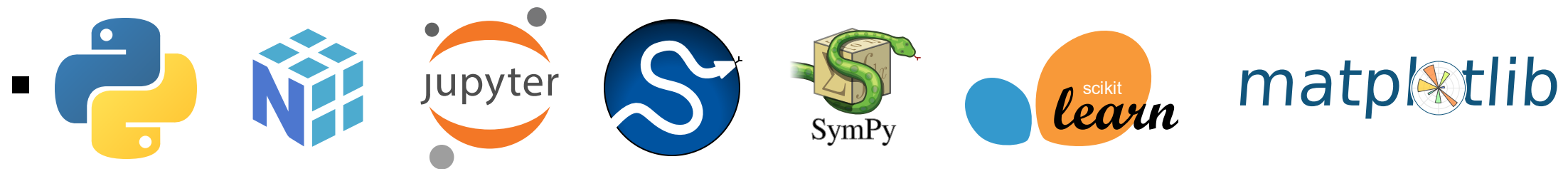
multi-dimensional data analysis

- Open-source Python library for interactive data analysis of multi-dimensional datasets

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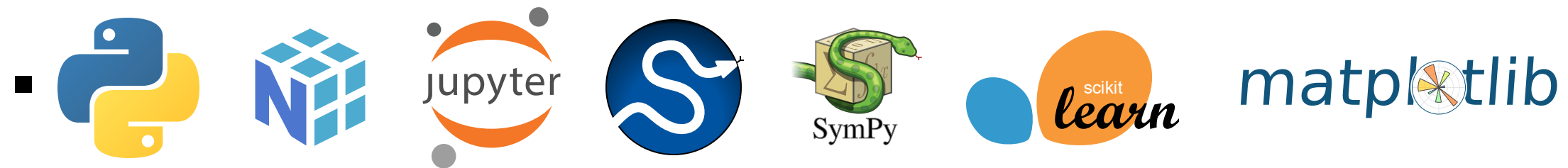
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What is HyperSpy ?

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- Leverages the Scientific Python ecosystem for much of its functionality:



- Accessed like any other Python library:

```
import numpy as np      ----->      import hyperspy.api as hs
```

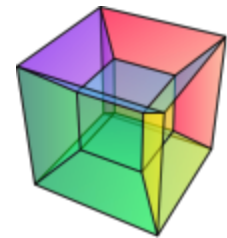
Why would you use



HyperSpy
multi-dimensional data analysis ?

- Makes it easy to operate on multi-dimensional arrays as you would a single spectrum (or image)

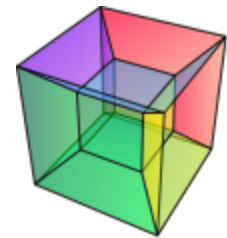
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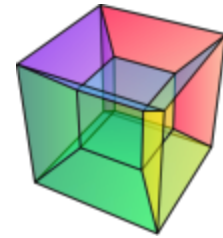
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- Use of Jupyter notebooks encourages reproducible and sharable analyses (FAIR data)

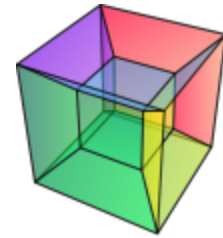
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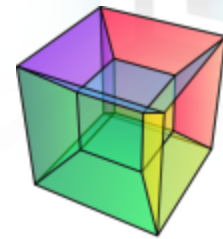


HyperSpy
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 - Provides facilities for easy access to proprietary software formats
 - EDS:
 - Background removal
 - Net intensity line map extraction
 - Quantification (k-factor, ζ -factors, ionization cross sections)

Why would you use

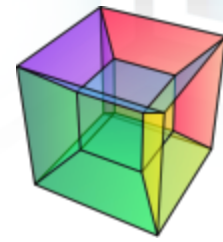


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 - EELS:
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 - Curve fitting for quantification (including ELNES)
 - All of Egerton's famous methods

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 - Curve fitting for quantification (including ELNES)
 - All of Egerton's famous methods
 - "Advanced" methods:
 - Multivariate statistical analysis
 - General curve fitting
 - Dimensionality reduction/signal separation

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- Thanks to `numpy` and other libraries, similar (or often better) performance than MATLAB

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- Originally called EELSLab:

Talk EELSLab: a Python toolbox for (hyper)spectroscopy data analysis

Presented by Francisco de la Peña in Poster and Demo Session 2011

Abstract

EELSLab: a Python toolbox for (hyper)spectroscopy data analysis

F. de la Peña^{1, 3, *}, M. Sarahan², S. Mazzucco^{4, 5}, L-F. Zagonel^{1, **}, M. Walls¹

1) Laboratoire de Physique des Solides, Bât. 510, Université Paris-Sud. 91405 Orsay Cedex

2) SuperSTEM, STFC Daresbury Laboratories. Keckwick Lane, Warrington WA4 4AD – UK

3) CEA-LETI, MINATEC 17, avenue des Martyrs, 38054 GRENOBLE Cedex 9 – France

4) Center for Nanoscale Science and Technology, National Institute of Science and Technology, 100 Bureau Drive, Gaithersburg, MD 20899-6203, USA

5) Institute for Research in Electronics and Applied Physics (Bldg. 223), Paint Branch Drive, University of Maryland, College Park, MD 20742-3511, USA

* Current address: department of Materials Science and Metallurgy, University of Cambridge. Pembroke Street, Cambridge, CB2 3QZ – UK

** Current address: Associação Brasileira de Tecnologia de Luz Sincrotron, Laboratório de Microscopia Eletrônica.13083-970 - Campinas, SP – Brasil

Modern scientific instruments from several disciplines now yield multidimensional spectroscopic data. As an example, a modern transmission electron microscope (TEM) can acquire spectral data from sub-atomic volumes that ultimately could reveal the position and nature of each atom of a material [1]. However, such datasets are usually quite large and difficult to work with.

EELSLab [2] has been developed as a tool to facilitate hyperspectral data analysis. Originally it was intended for TEM data analysis, but it has been successfully used in other domains. Specifically, it provides easy access to multidimensional curve fitting, peak analysis and machine learning algorithms, as well as a viewing framework for navigating data and reading and writing capabilities for several popular hyperspectral formats.

This talk will discuss how Python has been used to implement these features, with demonstrations of applications to both spatially-resolved spectroscopic data (so-called spectrum images) [3] and to structural analysis of atomic resolution image stacks [4]. The blend of intuitiveness, power, and availability of high-quality scientific libraries that Python offers has allowed the creation of a simple, natural tool that scientists from many disciplines can both use and easily extend into new scientific domains.

References

[1] Sandra Van Aert et al., « Three-dimensional atomic imaging of crystalline nanoparticles », *Nature* 470, n°. 7334 (17th of February, 2011): 374-377.

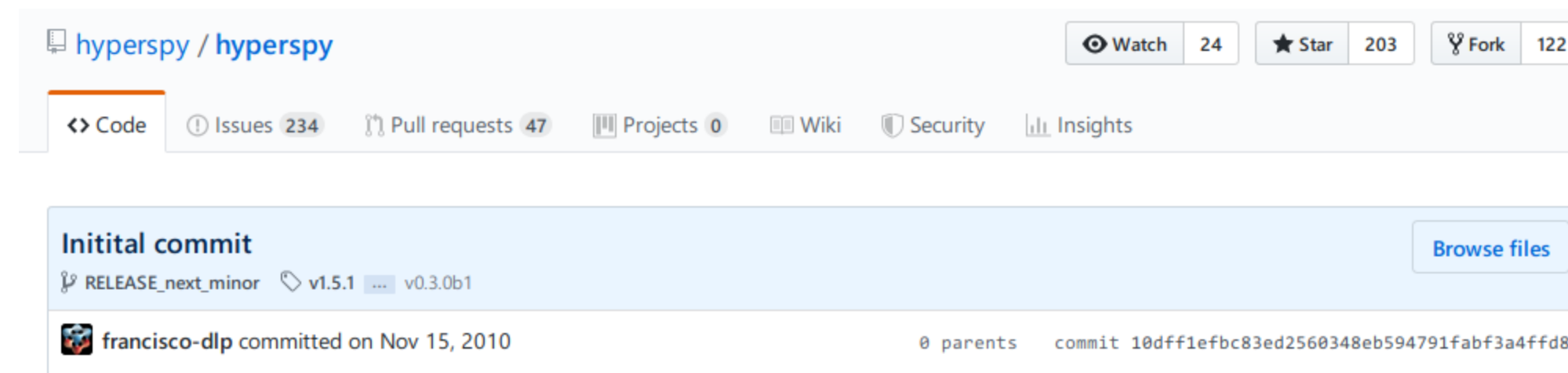
[2] <http://www.eelslab.org>

[3] R. Arenal et al., « Extending the analysis of EELS spectrum-imaging data, from elemental to bond mapping in complex nanostructures », *Ultramicroscopy* 109, n°. 1 (December 2008): 32-38.

[4] Michael C. Sarahan et al., « Point defect characterization in HAADF-STEM images using multivariate statistical analysis », *Ultramicroscopy* 111, n°. 3 (February 2011): 251-257.

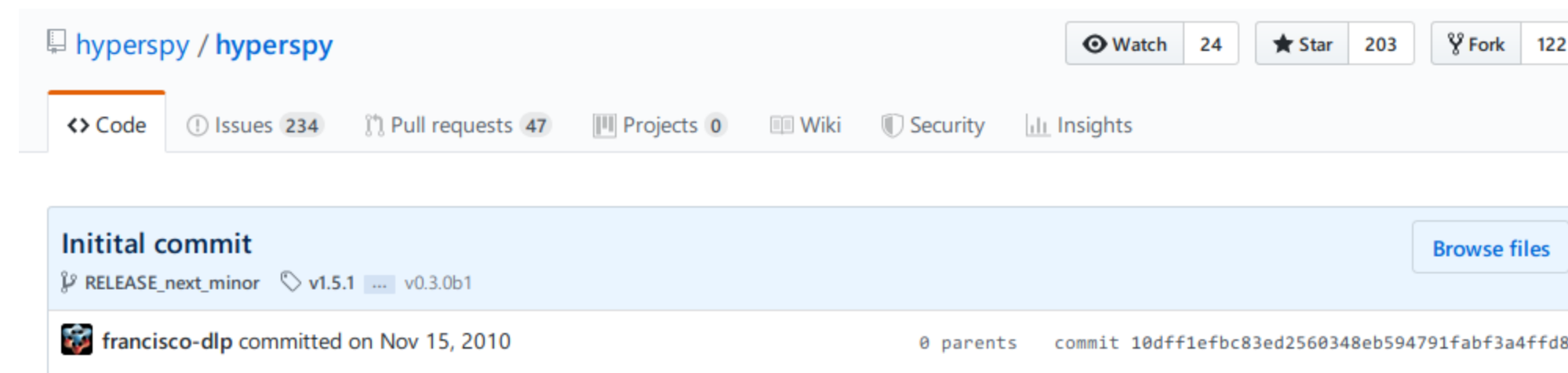
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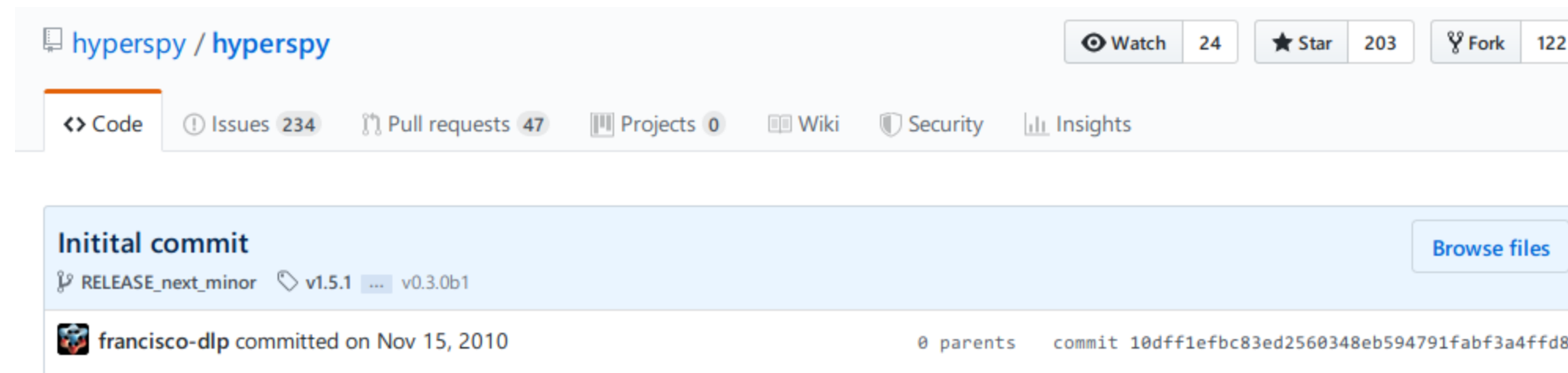
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- Renamed to HyperSpy in 2011
- Now... over 850 citations, 46 releases, 59 contributors, used in (at least) 115 other Github projects, and rapidly growing!

Design philosophy of HyperSpy

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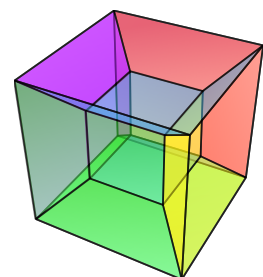
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- Data storage is in an open hierarchical format (HDF5)
 - Saves all metadata by default (including most processing steps)
- Analysis typically done via reproducible notebooks
- Feature development is completely open-source ([GPLv3](#))



Welcome to the community!

The power of community

- One of the *best* parts of HyperSpy is the community that surrounds it (personal opinion)

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- This software is made by researchers, for researchers
- HyperSpy is built from collaboration:
 - By collaborating, we advance faster and avoid reinventing the wheel

How to get help?

- HyperSpy website (www.hyperspy.org):



[Home](#) · [Download](#) · [Documentation](#) · [Demos](#) · [News](#) · [Support](#) · [Citing](#) · [Credits](#)

HyperSpy: multi-dimensional data analysis toolbox

HyperSpy is an open source Python library which provides tools to facilitate the interactive data analysis of multi-dimensional datasets that can be described as multi-dimensional arrays of a given signal (e.g. a 2D array of spectra a.k.a spectrum image).

HyperSpy aims at making it easy and natural to apply analytical procedures that operate on an individual signal to multi-dimensional arrays, as well as providing easy access to analytical tools that exploit the multi-dimensionality of the dataset.

Its modular structure makes it easy to add features to analyze different kinds of signals.

Highlights

- Two families of named and scaled axes: *signal* and *navigation*.
- Visualization tools for multi-dimensional spectra and images.
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VERSIONS

Stable

1.5.1

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Development

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[Documentation](#)

SUPPORT

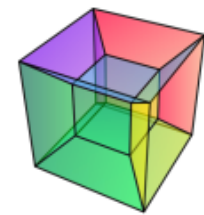
[Issue tracker](#)

[Mailing list](#)

[Gitter chat](#)

How to get help?

- HyperSpy website (www.hyperspy.org):



HyperSpy
multi-dimensional data analysis

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HyperSpy: multi-dimensional data analysis toolbox

HyperSpy is an open source Python library which provides tools to facilitate the interactive data analysis of multi-dimensional datasets that can be described as multi-dimensional arrays of a given signal (e.g. a 2D array of spectra a.k.a spectrum image).

HyperSpy aims at making it easy and natural to apply analytical procedures that operate on an individual signal to multi-dimensional arrays, as well as providing easy access to analytical tools that exploit the multi-dimensionality of the dataset.

Its modular structure makes it easy to add features to analyze different kinds of signals.

Highlights

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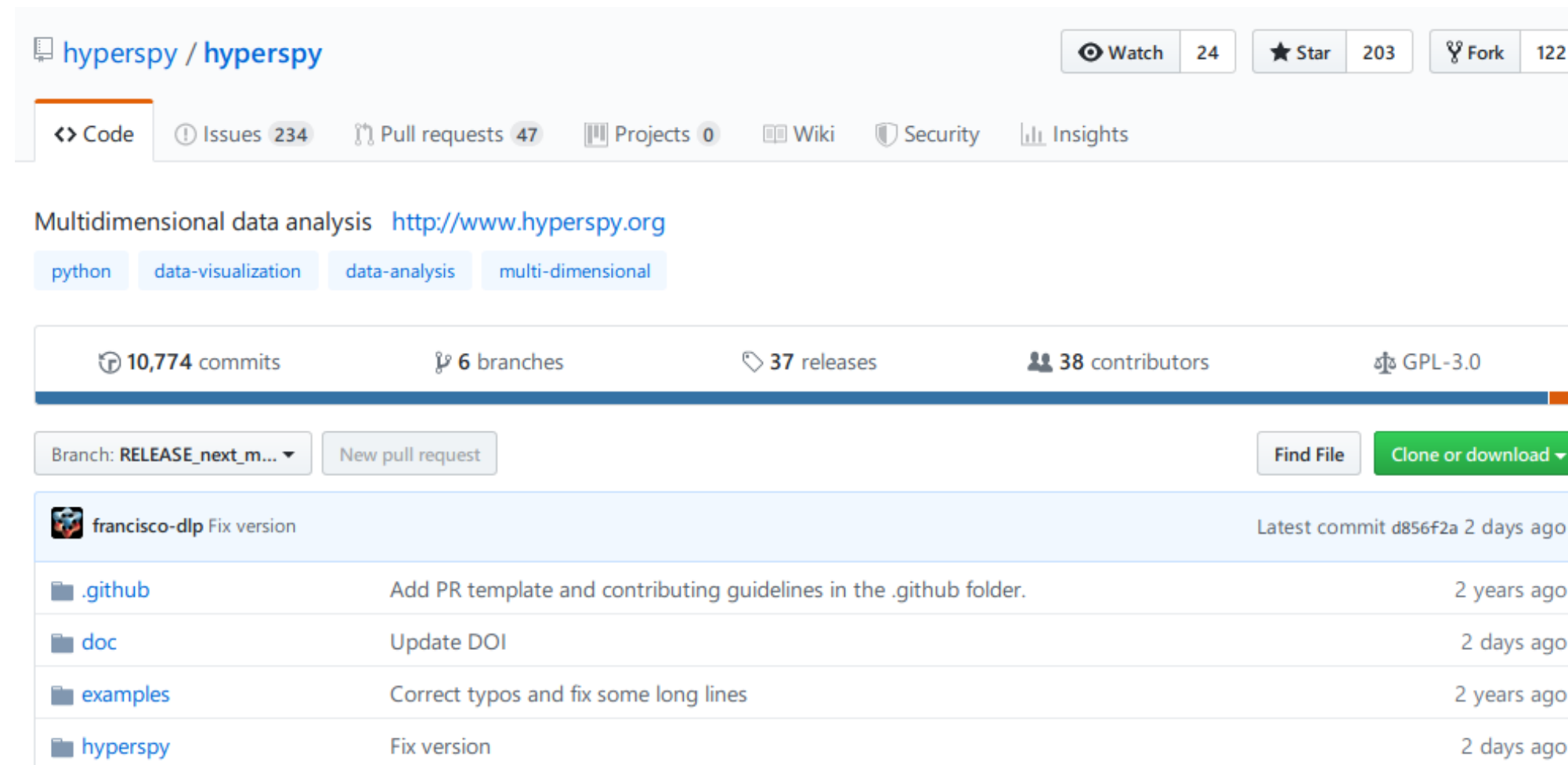
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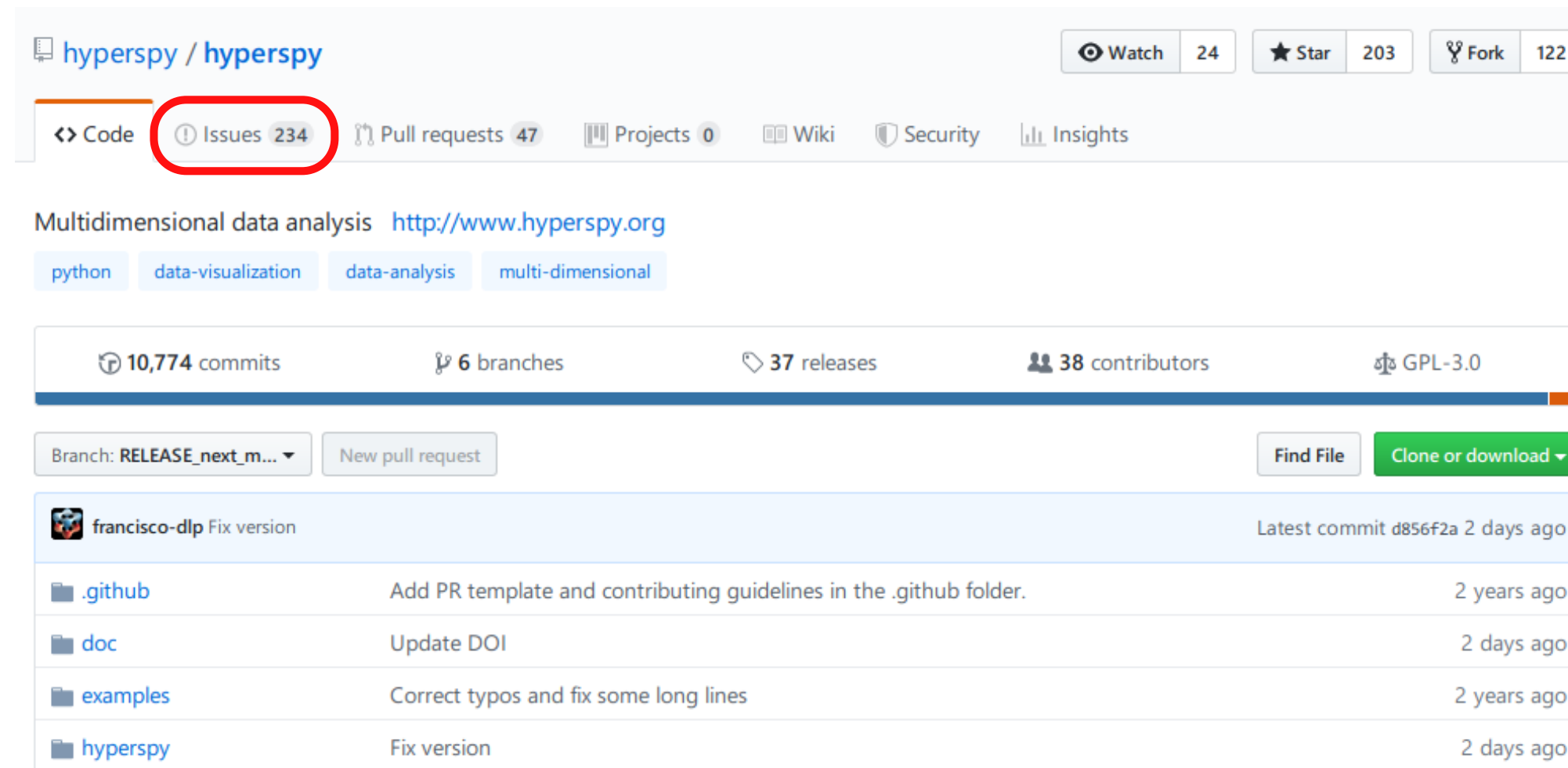


The screenshot shows the GitHub repository for HyperSpy. At the top, the repository name 'hyperspy / hyperspy' is displayed. To the right, there are buttons for 'Watch' (24), 'Star' (203), and 'Fork' (122). Below this, a navigation bar includes links for 'Code', 'Issues' (234), 'Pull requests' (47), 'Projects' (0), 'Wiki', 'Security', and 'Insights'. The repository description is 'Multidimensional data analysis' with a link to 'http://www.hyperspy.org'. Below the description are tags: 'python', 'data-visualization', 'data-analysis', and 'multi-dimensional'. A statistics bar shows '10,774 commits', '6 branches', '37 releases', '38 contributors', and 'GPL-3.0' license. Below this, there are buttons for 'Branch: RELEASE_next_m...', 'New pull request', 'Find File', and 'Clone or download'. The main content area shows a list of recent commits by user 'francisco-dlp'. The latest commit is 'Fix version' with hash 'd856f2a' from 2 days ago. Other commits include 'Add PR template and contributing guidelines in the .github folder.' (2 years ago), 'Update DOI' (2 days ago), and 'Correct typos and fix some long lines' (2 years ago).

Commit Hash	Message	Time
d856f2a	Fix version	2 days ago
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hyperspy / hyperspy

Watch 24 Star 203 Fork 122

Code Issues 234 Pull requests 47 Projects 0 Wiki Security Insights

Multidimensional data analysis <http://www.hyperspy.org>

python data-visualization data-analysis multi-dimensional

10,774 commits 6 branches 37 releases 38 contributors GPL-3.0

Branch: RELEASE_next_m... New pull request Find File Clone or download

francisco-dlp Fix version	Latest commit d856f2a 2 days ago
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- Developer guide (if you're into that sort of thing):
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Anyone can make HyperSpy better!

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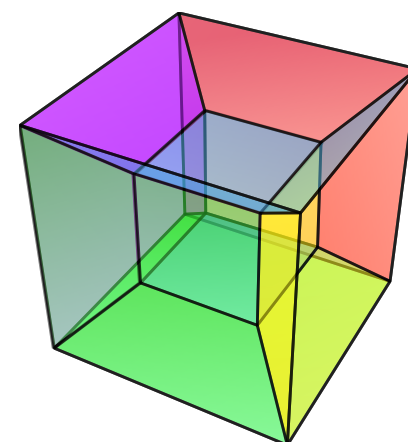
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- StackOverflow for general programming/Python questions: <https://stackoverflow.com/>



Thank you!

Any questions?

joshua.taillon@nist.gov