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Welcome to the BPS Blog. Our blog provides the unique opportunity to share with the biophysics community worldwide BPS-related news, updates, and biophysic interdisciplinary nature of biophysics provides the opportunity for biologists, physicists, chemists, bioengineers, and others to collaborate and push scientific disco back often for the latest news and updates.

Science in python: tools for faster, better biophysics



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I came to this conference with the goal of showcasing new or underappreciated developments in so particular open source projects. From the conversations I've had with folks who use some of the toruse or develop, it occurred to me that there are also many robust **general-purpose** software tools i today that are not widely used by people in our field. Somehow these tools haven't penetrated the bubble, at least not to the degree they almost certainly could.

I'd like to introduce three tools that you may have heard of, but perhaps haven't used or aren't sure they could fill in your day-to-day research. Incidentally all of these are Python packages. Being Pyth means a few things (to quote 'S' Software Carpentry (http://software-carpentry.org/)):

- 1. it's free, well-documented, and runs almost everywhere;
- 2. it has a large (and growing) user base among scientists; and
- 3. experience shows that it's easier for novices to pick up than most other languages.

If you're new to Python, or just want to brush up, a good place to start is the Software Carpentry introductory Python lesson (http://swcarpentry.github.io/py inflammation/).

Using pandas for slicing and dicing datasets

If you've ever used a statistical analysis environment like R, you've probably used a **dataframe**. If not, you've almost certainly used a spreadsheet program, in wl laid out (hopefully) in a well-structured way in terms of columns and rows. A dataframe is a set of columns giving observations aligned on a single index, which i column of names, dates, or anything convenient to uniquely identify rows.

☐ pandas (http://pandas.pydata.org/) provides a DataFrame object for use with Python, which when loaded with data from a ☐ common data format (http://pandas.pydata.org/pandas-docs/stable/io.html) allows you to easily obtain ☐ descriptive statistics (http://pandas.pydata.org/pandas.pydata.org/pandas.pydata.org/pandas.pydata.org/pandas-docs/stable/visualization.html#visualization), and dive into de relationships within your data through ☐ groupby's on column values (http://pandas.pydata.org/pandas-docs/stable/groupby.html).

pandas is built on top of the robust numpy library, so operations on even millions of rows are quick and fit into memory well. For datasets that are larger than you memory, there are new libraries such as **dask (http://dask.pydata.org/)** that build on the same ideas **pandas** functions on.

Science jazz with the Jupyter Notebook

A pain point when writing code to analyze data is that often the context of a scientific finding is removed from the work that produced it. Plots are in a folder over is in a folder over there, and meanwhile the insights into what these things mean might live in a paper notebook on the other side of the desk.

It doesn't have to be this way. The Day Jupyter Project (http://jupyter.org/) provides a notebook-style environment for writing and executing code, producing plots expressive notes about what this all means in a single place.

(/login?returnurl=/blog/science-inThe Jupyter Notebook makes it easy to spend the affernoon taking a dataset and exploring it from any (or every) angle you desire, all the while keeping a record purphop tools—for-faster-better—you've done and what motivated—. (Patengalican Cales Better) which was a purphop to the prophop of the prop

Machine learning with scikit-learn Membership & Communities (https://www.blophysics.org/membership-communities)

As data becomes an embarrassment of riches and insights harder to discern, it can sometimes take a clever dimensionality reduction or two to get going. 🗷 sci

(http://scikit-learn.org/stable/) is a Python library that gives robust and fast implementations of many common classification, regression, clustering, and dimens (hetings & Events (https://www.biophysics.org/publications) Publications (https://www.biophysics.org/publications) reduction algorithms with a common interface. This last bit is important, because it makes trying out different algorithms pretty painless, and once you've learn

idea of using one algorithm you can just as easily use any other. T

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he documentation is also extensive, with references, and it's written in such a way that it's often helpful in choosing what algorithms may be most appropriate f data you'll be applying them to.

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Plug in

The scientific Python ecosystem is mature and vibrant, with the scientific community standing as the beneficiary of its advances. With the explosion of "data sci career path in industry, the Python community has stepped up to the plate to build the tools that lead to better and faster insights. The biophysics community c this too, but only if it is willing to try new tools with the potential to change the day-to-day grind of scientific research for the better.

-David Dotson

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The scope of science is relatively increased and pec researching.

Science Theory

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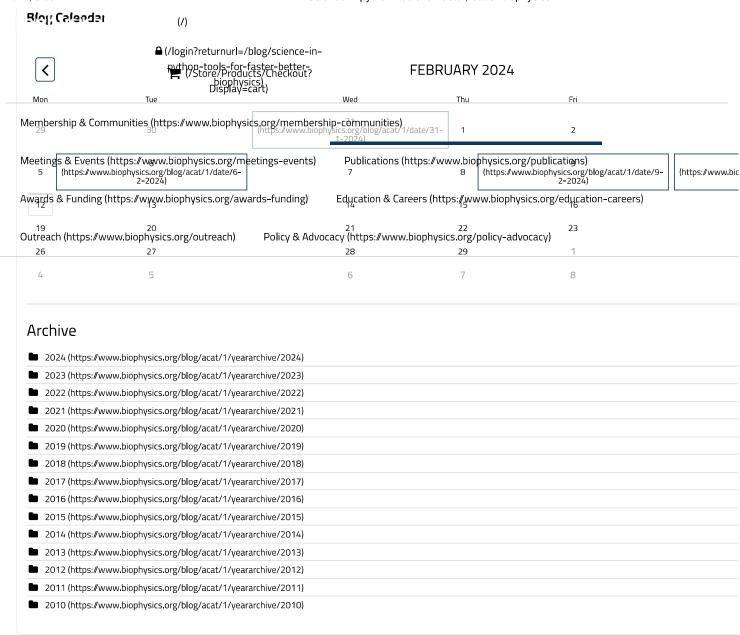
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SAHELI MITRA: (https://www.biophysics.org/mybps?userId=11571) A must read.

3/19/2020 8:24:40 AM

Coronavirus Structure, Vaccine and Therapy Development (https://www.biophysics.org/blog/coronavirus-structure-vaccine-and-therapy-development#c214)



Brennan Weaver: (https://www.biophysics.org/mybps?userId=13518) Pretty nice read. I wish I could have written something about Pi. It's my 2nd favorite num Also, I don't think Pi is as mysterious as everyone thinks it is. It's just a number with a lot of personalities. And I do believe there is a last digit.
4/14/2019 4:19:21 PM

▶ Pi Is Encoded in the Patterns of Life (https://www.biophysics.org/blog/pi-is-encoded-in-the-patterns-of-life#c211)



Harel Weinstein: (https://www.biophysics.org/mybps?userld=576) Just perused the article "From Dynamics to Membrane Organization- Experimental Breakth Occasion a "Modeling Manifesto" in the August 21 issue. While the Perspective is intriguing, the sheer Chutzpah of writing a "manifesto" about a field with lists of "demands" based on experiments that in many cases are more limited in scope or reality than any physics-based model, is quite astoundin artificial membrane slabs, nor "live cells" imaged under conditions in which cells have a shabby life that doesn't last long (how much of this is due to the mistreatment of the membrane proteins?) share established behaviors that must be matched or else.... No experiment, computational or using imaging mimic reality, only to probe it based on models and assumptions that can be falsified.

As to the role of the cytoskeleton, what does this tell us about the membrane itself, or the behavior of membrane proteins as individual molecules in the with the membrane? And since this unrelated scaffold differs greatly between cells, what is the "correct matching standard"? All models are wrong, so (computational, or on the stage of a microscope) are useful, but in my opinion, self-critical, humble, and rigorous scientific reasoning are preferable to a order to foster progress.

8/21/2018 3:48:33 PM

In Search of...Protein Interaction Partners (https://www.biophysics.org/blog/in-search-ofprotein-interaction-partners#c204)

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