Python for Data Science and Materials Science

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Overview

Preliminaries

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- In this lecture, we will provide an overview of the Python programming language.
- This will form the basis for your first lab on materials data wrangling in Python.
- Very quick overview of chapters 1-4 of the Python Data Science Handbook[1] + materials science libraries.
- Content is targeted at giving a complete beginner to Python and the scientific python stack enough background to get started.
- This lecture is extremely heavy on practical demos and examples. Please bring your laptop so that you can follow along.
- *Coding is best learned by attempting to solve a practical problem.* The goal of this lecture is not to comprehensively cover all the libraries (which would be impossible in a one-quarter course).

Python

Introduction to Python

- General-purpose, high-level programming language
- Design emphasizes code readability
- Supports multiple programming paradigms (OOP, imperative, functional, procedural)
- Dynamically typed, automatic memory management and large standard library
- Available on almost all platforms

Python vs other languages

- Java

```java
public class Hello {
    public static void main(String[] args) {
        System.out.println("Hello World!");
    }
}
```

- Python

```python
print("Hello world")
```

Python Version

- We will be using Python 3.10+.
- Options for this course:
    - Install python on your laptop - faster, not-reliant on internet connection, most modern version of Python possible.
    - Google Colab - Online Python notebooks. No installation required. But Python version and installed libraries may lag the latest versions (sometimes by years).

Installing Python

- Regardless of whether your OS comes with Python, it is recommended that you install your own version of python using a package manager (e.g., the Anaconda distribution, uv, poetry, etc.).
- For the Anaconda distribution, you have two options:

Miniconda	Minimal installation of Python interpreter itself + conda command-line tool. conda is essentially a package manager. Link
Anaconda	Miniconda + several scientific packages such as scipy, numpy, etc. Several GB in size. Link

- Recommendation: Use miniconda to keep bloat to a minimum.

Basics of Python

- Dynamically typed, i.e., no need for variable declaration.

```python
x = 1  # integer
y = 2.0  # float
my_string = "Hello world"  # string
my_list = [1, 2, 3, "a"]  # list
my_dict = {"a": 1, "b": 2, "c": 3}  # dict
```

- Other than some basic operations and functions, most other functions are in packages and modules and must be *imported* prior to use.

```python
import math

z = math.sin(3.14159)  # Gives ~0
```

- Please go through official Python tutorial.

Virtual environments

- Isolated environment for Python projects, i.e., each env has its own Python and packages. Both conda and python3 itself comes with the ability to create virtual environments.
  ```
  conda create --name nanox81 python=3.10
  conda activate nanox81
  ```
- To start over, you can remove the environment:
  ```
  conda remove --name nanox81 --all
  ```
- You can also create reproducible environments from a file.
  ```
  conda env create -f nanox81_env.yml
  ```
- Example nanox81_env.yml file given in the NANOx81RGithub repo.

Installing packages using conda

- We will get into the details of the specific packages later.

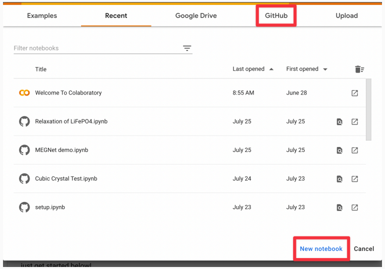
```
# Scientific python stack
conda install numpy scipy matplotlib seaborn jupyter
# Data Science tools
conda install pandas scikit-learn tensorflow
# Materials science library
conda install --channel conda-forge pymatgen
```

- To update a package, use:

```
conda update numpy
```

Google Colab Demo

- URL: `https://colab.research.google.com`
- Start a new blank notebook or download one from Github.



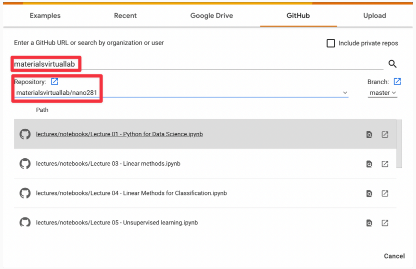
Examples | Recent | Google Drive | GitHub | Upload

Filter notebooks

	Title	Last opened	First opened
	Welcome To Colaboratory	8:55 AM	June 28
	Relaxation of LiFePO4.ipynb	July 25	July 25
	MEGNet demo.ipynb	July 25	July 25
	Cubic Crystal Test.ipynb	July 24	July 23
	setup.ipynb	July 23	July 23

New notebook   Cancel

just get started below!



Examples | Recent | Google Drive | GitHub | Upload

Enter a GitHub URL or search by organization or user   Include private repos

materialsvirtuallab

Repository: materialsvirtuallab/nano281   Branch: master

Path

lectures/notebooks/Lecture 01 - Python for Data Science.ipynb
lectures/notebooks/Lecture 03 - Linear methods.ipynb
lectures/notebooks/Lecture 04 - Linear Methods for Classification.ipynb
lectures/notebooks/Lecture 05 - Unsupervised learning.ipynb

Cancel

- Most of the data science packages we will be using are pre-installed.
- To install a missing package (e.g., pymatgen), run the following in the first cell:

```
! pip install pymatgen
```

Scientific Python

Scientific Python Packages

jupyter	Software for interactive computing
Numpy	Fundamental package for numerical computation. Defines array and matrix types and basic operations on them.
Scipy	Efficient numerical routines such as routines for numerical integration and optimization.
pandas	High-performance, easy to use data structures.
scikit-learn	Tools for predictive data analysis.
TensorFlow	Library for developing and training ML models.
PyTorch	Library for developing and training ML models.
matplotlib	De facto plotting library
seaborn	Statistical data visualization

Brief note on coverage

- In the following slides, we will provide a brief background on all these packages, with a heavy focus on actual demos.
- It should be noted that it is not possible to comprehensively the extensive functionality of these packages in this course.
- Focus will be on modules and methods that pertain to the data science problem we are solving. You are expected to navigate the relevant documentation pages of each package (plus a generous amount of googling) to identify the appropriate module or method for what you need to do.
- numpy and scipy are the backbone for many of the other packages such as pandas and scikit-learn. You need to understand the basics of numpy arrays and how to perform various simple linear algebra operations. In most instances, the actual data science package (scikit-learn) will be the one you interact with most.

Jupyter notebook

- We will primarily be using Jupyter for its notebook application, though it is capable of a lot more. (Google Colab is similar.)
- Jupyter Notebook is an open-source web application to create and share documents that contain code, equations, visualizations and narrative text, etc.
- All lecture examples will be done in Jupyter notebooks. You will also be submitting notebooks (ipynb files) as your lab reports.
- Document: link
- Running a jupyter notebook:

```
jupyter notebook
```

- The notebook server will be running at http://localhost:8888 (typically).

Jupyter notebook, contd.

- Things you can do in a notebook:
    - Run code in a cell with ‘shift+return‘ - helpful things include tab completion, magic functions (e.g., ?, ! and % are the key ones to know, especially ?).
    - Write text/narrative - set cell to markdown mode and write markdown.
    - Make plots.
- Very useful for quick code prototyping and data analysis.

Numpy

- Implements the array and matrix objects.
- Underlying implementation is in C, and hence extremely efficient.
- Vectorization of operations, as opposed to loops, is key to efficiency.
- Recommend that you focus on the array object and ignore the matrix object.
- Note that standard operations such as +, -, * and / for np.arrays are element-wise. For matrix multiplications, use special numpy functions, e.g., numpy.dot or the new @ operator available in Python 3.7 and above.
- For those of you who are familiar with Matlab, it helps to read the Numpy for Matlab users doc.
- Documentation: link

Numpy examples

```
import numpy as np

x = np.array([[1, 2, 3], [4, 7, 6], [9, 4, 2]])
y = np.array([1.5, 0.5, 3])
x * x
# array([[ 1,  4,  9],
#         [16, 49, 36],
#         [81, 16,  4]])
np.dot(x, x)
# array([[36, 28, 21],
#         [86, 81, 66],
#         [43, 54, 55]])
np.linalg.inv(x)
# array([[ 0.16949153, -0.13559322,  0.15254237],
#         [-0.77966102,  0.42372881, -0.10169492],
#         [ 0.79661017, -0.23728814,  0.01694915]])
```

Scipy

- Efficient numerical routines for numerical integration, interpolation, optimization, linear algebra, and statistics, etc.
- scipy.linalg is a superset of numpy.linalg, and is always compiled with BLAS/LAPACK. So use scipy.linalg.
- Dependency for most other packages you will be using.

```python
from scipy import stats  # Statistics package

dist = stats.norm(0, 1)  # Gaussian distribution
print(dist.cdf(1.96))
# Result: 0.9750021048517795
from scipy import constants  # Physical constants

print(constants.e)
# Result: 1.6021766208e-19
```

- Documentation: link
- Scipy lectures (very useful resource): link

Pandas

- Data analysis library
- Data structures designed for working with relational or labeled data
- Two main data types:

Series	1D labeled homogeneously-typed array
DataFrame	2D labeled, size-mutable tabular structure with potentially heterogeneously-typed column

- It is helpful to think of DataFrame as essentially a Python object representing the contents of a table, e.g. such as what you would have in Excel spreadsheet. This is similar to the dataframe in R.
- Please go through the Pandas Guide.

Pandas demo

- For this demo, we will utilize data that has been published by the MAterials Simulation Toolkit - Machine Learning (MAST-ML) on figshare.

```python
import pandas as pd

url = "https://ndownloader.figshare.com/files/13007075"
# Reads in the data as a pandas DataFrame.
data = pd.read_csv(url)

# Extracting a column as a Series.
form_e = data["E_raw (eV)"]

# Summary statistics
data.describe()
```

scikit-learn & TensorFlow & PyTorch

- Packages for machine learning.
- To some extent, scikit-learn, TensorFlow (TF) and PyTorch overlap in functionality.
- For the purposes of this course, we will use mainly scikit-learn for ML and will briefly touch on TF/PyTorch for neural networks.
- We will defer all specific code examples for scikit-learn until we go through specific types of ML models, e.g., linear regression, kernel regression, etc. Having the theory background of the ML methods will make it easier to understand the code usage and implementations.
- Instead, we will provide an overview of the high-level API design of scikit-learn.

Scikit-learn Model API

- All ML models inherit from BaseEstimator and various mix-in classes with standardized method names.

```
model = Model(**params)  # Init a model with parameters.
model.get_params()  # Get model parameters.
model.set_params(**params)  # Set model parameters
model.fit(X, y)  # Fit the model with a dataset
model.score(X, y)  # Provides the score for the dataset.
model.predict(X)  # Make a prediction using fitted model.
```

- Note that the params and score depends on the specifics of the ML model type.

Matplotlib and Seaborn

- Matplotlib is the de facto library for generating all kinds of plots and many other plotting engines (including seaborn) are built on top of it
- seaborn is a extremely helpful package for statistical data visualization. Works very well with Pandas DataFrame.

```python
import matplotlib.pyplot as plt
# Plot two variables x and y with 'x' as markers and solid lines.
plt.plot(x, y, "x-")
# Use circles as markers and dashed lines instead.
plt.plot(x, y, "o--")

import seaborn as sns
# Plot the distribution of x.
sns.histplot(x)
# Scatter plot using columns from DataFrame
sns.scatterplot(x="Melting point", y="Modulus", data=materials)
```

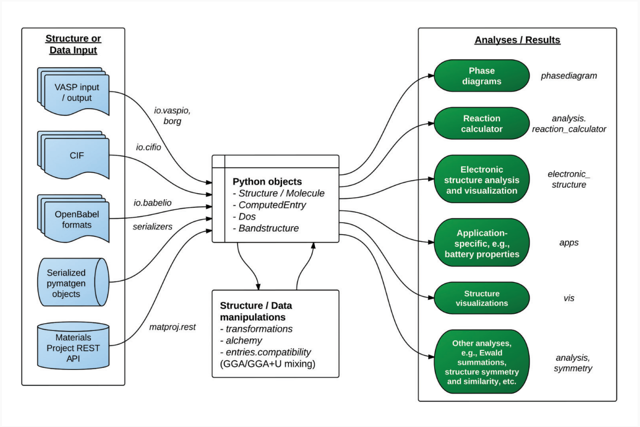
- Seaborn gallery contains may visual examples with source code.

Materials analysis

Python Materials Genomics (pymatgen)

- Core materials analysis powering the Materials Project.[2]
- Defines core extensible Python objects for materials data representation.
- Provides a robust and well-documented set of structure and thermodynamic analysis tools relevant to many applications.
- Establishes an open platform for researchers to collaboratively develop sophisticated analyses of materials data.
- High-level methods to access the Materials Project API.[3] (particularly useful for this course).

Overview of capabilities



Accessing the Materials API

- Accessed using the pymatgen.ext.matproj.MPRester class.
- Please review the https://api.materialsproject.org.

```python
from pymatgen.ext.matproj import MPRester

# Change "<APIKEY>" to the API key obtained from MP.
with MPRester("<APIKEY>") as mpr:
    data = mpr.summary.search(
        formula=["Fe2O3"],
        fields=["formula_pretty", "formation_energy_per_atom", "band_gap"],
    )

print(data)
import pandas as pd

df = pd.DataFrame(data)  # Convert to DataFrame
```

Bibliography i

- Jake VanderPlas.
  Python Data Science Handbook: Essential Tools for Working with Data.
  O'Reilly Media, Sebastopol, CA, 1 edition edition, December 2016.

- Shyue Ping Ong, William Davidson Richards, Anubhav Jain, Geoffroy Hautier, Michael Kocher, Shreyas Cholia, Dan Gunter, Vincent L. Chevrier, Kristin A. Persson, and Gerbrand Ceder.
  Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis.
  Computational Materials Science, 68:314–319, February 2013.

Bibliography ii

Shyue Ping Ong, Shreyas Cholia, Anubhav Jain, Miriam Brafman, Dan Gunter, Gerbrand Ceder, and Kristin a. Persson.
The Materials Application Programming Interface (API): A simple, flexible and efficient API for materials data based on REpresentational State Transfer (REST) principles.
Computational Materials Science, 97:209–215, February 2015.

The End