Python for Materials Data Science

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Overview

Preliminaries

- In this lecture, we will provide a brief overview of the Python programming language for data science.
- 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

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 3 or 2?

- We will be using Python 3.7+.
- Modern version of Python that has been around since 2008 and is now the de facto standard from Jan 1 2020 - most major software packages are stopping support for Python 2 henceforth.

Installing Python

- Regardless of whether your OS comes with Python, it is recommended that you install your own version of python using the Anaconda distribution.
- Two versions:

  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.

```
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.

```
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 nano281 python=3.7
conda activate nano281
```

- Please use Python 3.7 as some of the packages are not yet available for Python 3.8.
- To start over, you can remove the environment:

```
conda remove --name nano281 --all
```

- You can also create reproducible environments from a file.

```
conda env create -f nano281_env.yml
```

- Example nano281_env.yml file given in the nano281 Github 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
```

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.
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 most of these packages have an extensive suite of functionality and it is not possible to comprehensively go through them in this course.
- Focus will be on modules and methods that pertain to the data science problem we are solving. You are expected to learn 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 ensure you 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.
- 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 (highly recommend that you put "%matplotlib inline" near the start of your notebook to display graphs inline).
- 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
- 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.

```
>>> from scipy import stats  # Statistics package
>>> dist = stats.norm(0, 1)  # Gaussian distribution
>>> dist.cdf(1.96)
0.9750021048517795
>>> from scipy import constants  # Physical constants
>>> constants.e
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 10 minute guide to pandas.

Pandas demo

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

```
from io import StringIO
import pandas as pd
import requests

# Get the raw text of the data directly from the figshare url.
url = "https://ndownloader.figshare.com/files/13007075"
raw = requests.get(url).text
# Then reads in the data as a pandas DataFrame.
data = pd.read_csv(StringIO(raw))

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

# Summary statistics
data.describe()
```

scikit-learn & TensorFlow

- Packages for machine learning.
- To some extent, scikit-learn and TensorFlow (TF) overlap in functionality.
- For the purposes of this course, we will use mainly scikit-learn for ML and will briefly touch on TF for neural networks.
- We will defer all specific code examples for scikit-learn and TF 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

- Plotting libraries.
- 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.

```
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.distplot(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.

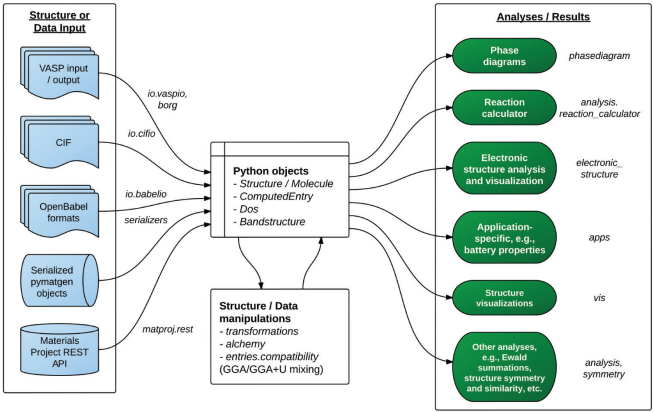
Materials Analysis

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.
- While there are many convenience methods to query for crystal structures and other object types, the most powerful and useful method for data analysis is the MPRester's query method.
- This method has to be used in conjunction with the Materials API documentation available at https://github.com/materialsproject/mapidoc.

```
from pymatgen.ext.matproj import MPRester
# Change "<APIKEY>" to the API key obtained from MP.
mpr = MPRester("<APIKEY>")
data = mpr.query(criteria={"pretty_formula": "Al2O3"},
                 properties=["final_energy", "band_gap"])
print(data)
import pandas as pd
df = pd.DataFrame(data)   # Convert to DataFrame
```

Bibliography

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The End