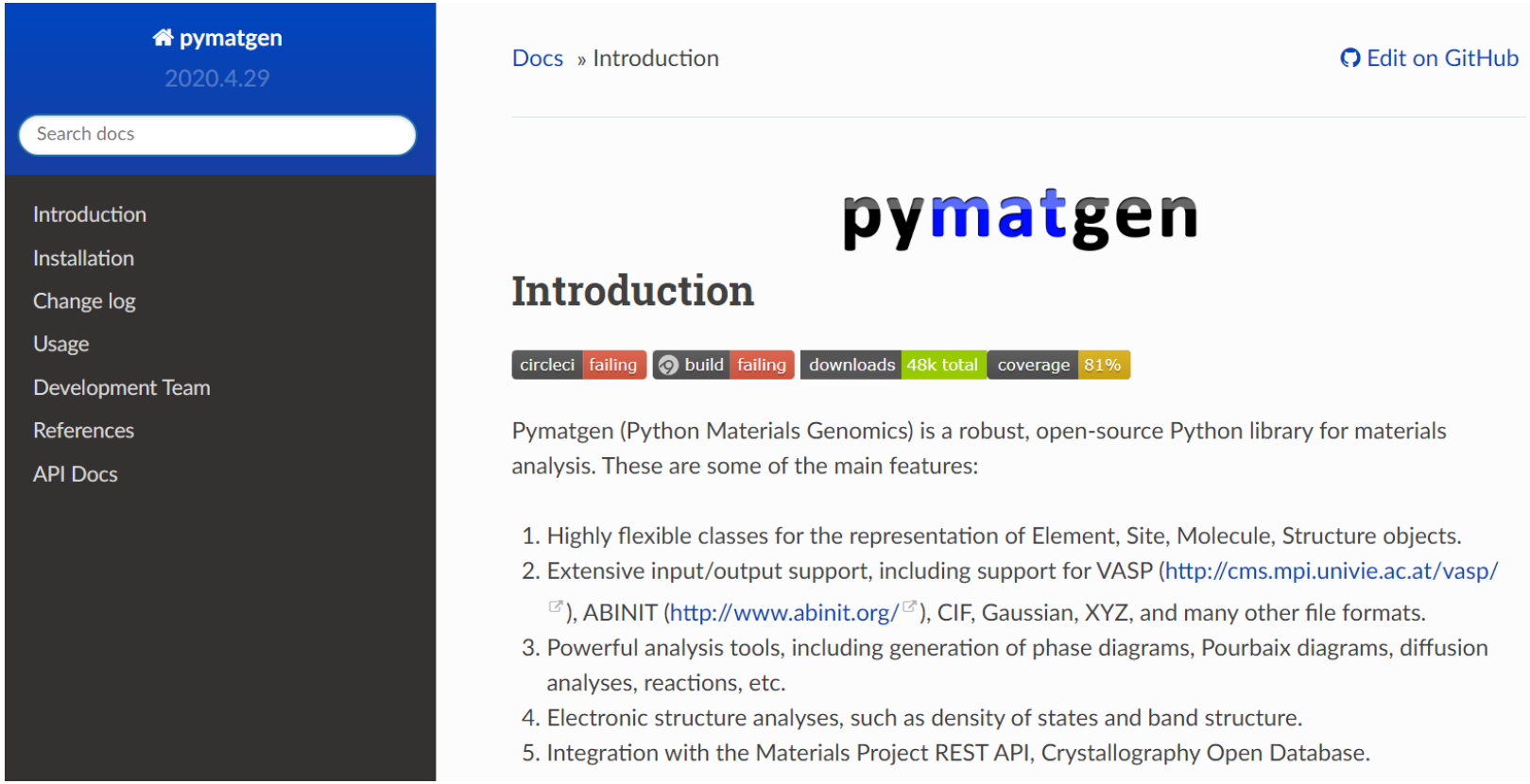
MSE1065: Lab 5

Case study #3: Crystal structure prediction through Logistic Regression

Learning objectives for this lab

- Utilize Logistic regression model to predict the crystal structure
- Learn to utilize materials database and python utility, **pymatgen**

Source



Data availability:

https://pymatgen.org/

Dataset

- Downloaded from pymatgen: https://pymatgen.org/
- Inputs
  - Number of features 18
  - Features in clude Atomic mass, Ionic radius, Lattice constant, Young's Modulus etc.
- Output
  - Crystal structure – FCC, BCC, HCP

What will you accomplish in the lab?

- In this lab, we will implement different logistic regression models on the dataset provided
- We will be using SKLearn's LogisticRegression class to fit classification models and compute mean misclassification error.
- We will extend our model by including regularization using SKLearn
- In the last section, we will implement feature selection under Logistic regression by using 'L-1' penalty term

Lab notebook

jupyter Lab5_LogRegression Last Checkpoint: Yesterday at 1:54 PM (autosaved)

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Lab - 5 Logistic Regression

In this lab, we are going to perform classification of elements as 'FCC', 'BCC','HCP', given their elemental attributes. The attributes or input features to our model include atomic mass, electronegativity, ionic radius etc.

Detailed list is provided below

In [43]:
```
element_attributes = ["atomic_number", "atomic_volume", "boiling_point", "en_ghosh",  "evaporation_heat", "heat_of_forma
                      "lattice_constant", "melting_point", "specific_heat","atomic_mass", "atomic_radius",
                       "electrical_resistivity","molar_volume", "bulk_modulus", "youngs_modulus",
                      "average_ionic_radius", "density_of_solid", "coefficient_of_linear_thermal_expansion"]
```

In [44]:
```
# import libraries
import numpy as np
import pandas as pd
```

The data for 47 element is provided in the file 'inputX.csv' and corresponding structure values are provided in 'origSt.csv'. Load the csv files into appropriate data frames

In [45]:
```
inputX = np.loadtxt(open("inputX.csv", "rb"), delimiter=",")#pd.read_csv('inputX.csv')
```

In [46]:
```
outY = np.loadtxt(open("origSt.csv", "rb"),dtype='str',delimiter=",") #pd.read_csv('origSt.csv')
```