Biol 366 – Introduction to Bioinformatics

Mini-project – 15%

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**Introduction**

For my mini-project I decided to learn the programming language python and set out to make a tool that determines the X, Y, Z coordinates and the temperature factor (B value) of any given PDB file.

Python is a clear and powerful object-oriented programming language that uses an elegant syntax, comes with a large standard library that supports common programing tasks such as connecting to webservers and is easily extended by adding new pre-made modules to help you.

In this assignment, I will be using a software called Enthought Canopy. Enthought Canopy is a comprehensive Python analysis environment that provides easy installation of the core scientific analytic and scientific python packages, creating a robust platform to develop on. I added in *modules* such as: *Numpy* 1.8.1-3, *Scipy* 0.15.1-1 and the most important *biopython* 1.65-1.

Numpy is an extension to pyton, adding support for large, multi-dimensional arrays and matrices, along with a large library of high-level mathematical functions to operate on these arrays.

Scipy is a python based ecosystem of open-source software for mathematics, science and engineering in particular. They are: NumPy, SciPy library, Matplotlib, IPython, Sympy, and pandas.

Biopython is a set of freely available tools, it is a distributed collaborative effort to develop python libraries and applications which address the needs of current and future work in bioinformatics. Unfortunately this tool is only available for computers that have 32 bits, thus we use Enthought Canopy to set up a virtual environment to write our code in.

PDB stand for the Protein Data Bank, the Protein Data bank is an archive of experimentally determined 3D structures of large biological molecules, including proteins and nucleic acids. The PDB archive is available at no cost to users and is updated weekly.

Each PDB file contains: PDB identifiers, date deposited, methods used, NMR simulation, compound molecule/keywords, PDB authors, primary literature references, other literature references, Sequence of DNA chain D, Sequence of protein chains, Heteroatom declarations, locations of where the author thinks the helices & beta sheets are, crystallographic information, Nucleic acid atom residue coordinates, Amino acid atom residue coordinates, heteroatom atom coordinates, water atom coordinates, and some odds and end information to wrap it all up.

Let’s break down what the script does and what does it all mean. In simple terms: the script written uses pre-made classes and modules to achieve our goal of determining the X, Y, Z coordinates and the Temperature factor (B-value­) from a PDB file.





















Code written in Python 3.4.1

This is what the code looks like with the sample input being the1C7D.pdb file in .ent format. The file is called pdb1c7d.ent and is located in \Bio\c7 folder.

# -\*- coding: utf-8 -\*-

**import** Bio

#first we import the Bio Module from BioPython

**from** Bio **import** PDB

pdb1 **=** PDB**.**PDBList**()**

pdb1**.**retrieve\_pdb\_file**(**"1C7D"**)**

parser **=** PDB**.**PDBParser**(**PERMISSIVE**=**1**)**

structure **=** parser**.**get\_structure**(**"1C7D"**,**r'C:\Users\Sameer\AppData\Local\Enthought\Canopy\User\Lib\site-packages\Bio\c7\pdb1c7d.ent'**)**

**print(**structure**)**

**for** model **in** structure**:**

**for** chain **in** model**:**

**for** residue **in** chain**:**

**for** atom **in** residue**:**

N **=** atom**.**get\_name**()**

I **=** atom**.**get\_id**()**

Y **=** atom**.**get\_coord**()**

V **=** atom**.**get\_vector**()**

O **=** atom**.**get\_occupancy**()**

B **=** atom**.**get\_bfactor**()**

**if** 10 **<** B **<** 50**:**

**print(**Y**,** B**)**

#print(dir(structure))

#print(dir(model))

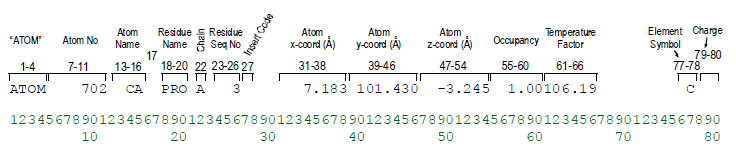
#print(dir(chain))

#print(dir(model))

#print(dir(residue))

#print(dir(atom))

The # means that they are just the comments and will not be interpreted by python. The last 6 lines are there for reference if one forgets the methods available to them for each of the classes.

What the raw PDB file looks like and the official coordinate file format

And this is what the output looks like when we run the code. Keep in mind, this is a very small bit of the output. The X, Y and Z coordinates are put into a vector format!.



**Definitions:**

**Argument:** A value provided to a function when the function is called. This value is assigned to the corresponding parameter in the function.

**Body:** The sequence of statements inside a function definition.

**Conditional statement:** A statement that controls the flow of execution depending on some condition.

**Condition:** The Boolean expression in a conditional statement that determines which branch is executed.

**Compound statement:** A statement that consists of a header and a body. The header ends with a Colon (:). The body is indented relative to the header.

**Class:** A user-defined type. A class definition creates a new class object.

**Class object:** An object that contains information about a user-defined type. The class object can be used to create instances of the type.

**Floating-point:** A type that represents numbers with fractional parts.

**Function:** A named sequence of statements that performs some useful operation. Functions may or may not take arguments and may or may not produce a result.

**Function object:** A value created by a function definition. The name of the function is a variable that refers to a function object

**Function call:** A statement that executes a function. It consists of the function name followed by an argument list.

**Loop:** A part of a program that can execute repeatedly.

**Module:** A file that contains a collection of related functions and other definitions.

Import statement: A statement that reads a module file and creates a module object.

**Module object**: A value created by an import statement that provides access to the values defined in a module.

**Method:** A function that is associated with an object and called using dot notation.

**Object:** Something a variable can refer to. For now, you can use “object” and “value” interchangeably.

**Object-oriented programming:** A style of programming in which data and the operations that manipulate it are organized into classes and methods.

**Parse:** To examine a program and analyze the syntactic structure.

**Print statement:** An instruction that causes the Python interpreter to display a value on the screen.

**Relational operator:** One of the operators that compares its operands: ==, !=, >, <, >=, and <=.

**Scrip**t: A program stored in a file (usually one that will be interpreted).

**Syntax:** The structure of a program.

**String:** A type that represents sequences of characters.

**Statement:** A section of code that represents a command or action. So far, the statements we have seen are assignments and print statements.

**Type:** A category of values. The types we have seen so far are integers (type int), floating-point numbers (type float), and strings (type str).

**Value:** One of the basic units of data, like a number or string, that a program manipulates.

**Variable:** A name that refers to a value.

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