WalkerLabs Code Summer Workshop

Syllabus and Schedule

Last Updated: July 12, 2023

Day 1 - Best Practices

Lead	Mark
TA	Kaushalya

An introduction to programming as a field, best practices, thinking like a computer, quality control, optimisation, and coding environments. **Goals** for the day include setting up a GitHub account, installation and use of a simple jupyter notebook, basic understanding of pseudocode and algorithm development.

Day 2 - Python Basics

Lead	Tim
TA	Kaushalya

Introduction to the Python programming language, including error handing, file input/output, library imports, and system interactions. **Goals** for the day include reading and writing a text file, importing and using common python libraries, addressing errors in code, and interacting with the operating system.

Day 3 - Python Functions

Lead	Tim
TA	Vishaka

Learning about functions in python, including passing arguments, returning values, wrappers and decorators, and global variables. **Goals** for the day include an understanding of how functions work as part of a larger program, how variables and functions interact, and how functions may be modified by other functions.

Day 4 - Python Classes

Lead	Tim
TA	Vishaka

Advanced python classes, focused on object-oriented programming and the use of classes for storage and manipulation of large and complex data sets, as well as the concept of inheritance between classes. **Goals** for the day include an understanding of how classes work in python, how inheritance can make use of existing classes for new ones, and how data is stored, modified, and retrieved in classes.

Day 5 - Python Modules

Lead	Mark
TA	

Advanced python modules, including overall structure of a module, internal interactions with classes and functions. Includes in-depth introduction to common python libraries like Numpy, Pandas, Matplotlib, and RDKit. Also includes basic unit tests for python. **Goals** for the day include understanding how modules work in python as well as basic skills with several common python libraries.

Day 6 - C++ Introduction

Lead   Morgan
TA   Mark

An introduction to the basics of C++, including compilation of code, sections of source code, input/output, variable handling, and file/system interactions. **Goals** for the day include being able to write, compile, and execute a simple C++ program that interacts with the user, performs mathematical functions, or reads and writes a file.

Day 7 - C++ Functions

Lead   Mark
TA

C++ Functions including declarations vs. definitions, pass-by-reference vs. pass-by-value, arguments and returns, datatypes, and more. **Goals** for the day include a basic understanding of how functions exist and operate inside a C++ program and how variables interact with functions in different forms.

Day 8 - C++ Classes

Lead   Mark
TA

C++ classes including constructors, destructors, public vs. private, variables, and functions. **Goals** for the day include an understanding of how C++ classes operate within the larger program, including proper creation and destruction with respect to memory management and program execution.

Day 9 - Introduction to Machine Learning

Lead   Solomon
TA   Morgan

We will use Andrew White's *Deep Learning for Molecules and Materials* and information from the MolSSI Machine Learning workshop to become acquainted with basic principles of machine learning.

Day 10 - Large Language Models and Chemoinformatics

Lead   Morgan
TA   Solomon

Introduction to large language models and chemoinformatics.