Introduction to Python, Unix and Version Control for Chemists

Getting Started

This course is run entirely from the Microsoft Azure notebook platform. To access all the relevant course files follow this link: https://notebooks.azure.com/s-a-munday/projects/software-course and enter your institution details to log in.

Once you have logged in, you need to clone the repository by pressing the ‘clone’ button circled in red.

A screenshot of a computer

Description automatically generated

A pop-up window will appear asking you to name the clone and to set the security settings. Once done, confirm that you want to create the clone by pressing the clone button in the bottom corner.

The notebooks can then be run via the Microsoft Azure service. To do this, choose the notebook that you wish by ticking the box next to its name and then click ‘Run on Free Compute’.

You can also download the notebooks and edit them in your preferred editor if you wish.

A screenshot of a cell phone

Description automatically generated

You are now all set to start the course!

What is Azure

Azure Notebooks is a free service that allows you to start programming in Python in the cloud with no installation needed. This makes it perfect for an introductory course.

Although the Python aspect of this course can be run remotely in the cloud with Azure Notebooks, Module 1 contains a guide for setting up Python on your own computer. This will be important for when you carry out your own Python projects.

Module Overview

The contents of each module are found within their respective folders.

**Module 0** repeats these instructions.

**Module 1** contains the installation and instructions for Python and Anaconda. The Python section of this course can be run directly on the Azure platform, however it is important to get your own Python distribution as you may want to build your own environment for any. future work you do.

**Module 2** covers the basic of Python with a few short simple questions at the end of each section.

**Module 3** covers some popular Python libraries and how best to use them.

**Module 4** introduces the software carpentry side of the course. It covers basic bash, terminal use and version control.

**Module 5** contains a cheminformatics case study