

Introduction to Scientific Computing: A Crash Course

Presented by Travis J Lawrence and Dana L Carper

Quantitative and Systems Biology

University of California, Merced

Worksheet 1_2

1. Using your package manager that was installed prior to coming to this workshop (homebrew, on mac), Install python3

a. What command did you use?

b. If you use a package manager do you need to worry about installing dependencies yourself?

c. How can you test to see if python3 was installed correctly? (hint try a command)

2. Python has a package management system, pip (pip3 if python3) that allows for easy installing of python software packages.

a. Use pip (or pip3) to install biopython

b. What command did you use

c. How can you check to see if biopython is installed?

3. Now use your package manager to install git (used for github)

a. What command did you use?

b. How can you test to see if git is installed?

4. We are now going to use git to clone a repository from github. The program we want to get is called HISAT2 which is an alignment program.

a. Who owns the github for HISAT2?

b. Along the right side of the page you should see a green button that says clone or download. When you click on it, it provides a web address what is it?

c. Using the command line and the web address you got in part b, clone the HISAT2 repository, what command did you use?

d. This repository was cloned to wherever you are currently in the terminal, what command do you use to check where you are? What command do you use to check if the HISAT2 folder is there?

5. We are going to be getting the program HMMER: biosequence analysis using profile hidden Markov models

a. Find the program, what is the web address for the program?

b. Download the file, the file is a tar.gz which is a compression type, to uncompress it use the following command:

```
$ tar -xvzf hmmer-3.1b2.macosx-intel.tar.gz
```

what was created when you ran this command?

c. This programs requires you to compile it from source code, Why might you want to compile software from its source code?

d. What are the steps for compiling and installing software?

e. First look at the contents of the folder that was created in part b, take a screen shot of the contents. Now run the first step in compiling software, what command did you use? What file was created from this step? (hint compare contents before and after)

f. Continue on and complete the installation, how can you test to make sure the program was installed?

6. We are now going to install the program HISAT2 which we obtained in question 4.

a. Navigate to the folder that was created when you cloned the git, what command did you use?

b. This is a slightly different installation then we did in question 7, even though both are from source code, why? (Hint look at the contents of the folder)

c. What command do you need to run to install this program?

d. After running the command in part C, you get files that are executable (meaning they are usable by the computer to run the program), what do you need to do to add these tools to your path?

e. Finish installing the program and check to see if it has been installed, what did you do to check for the installation?

7. We are going to install a program called FAST: Analysis of Sequences Toolbox for use in future worksheets.

a. Find the github page for this program, who is the owner of the github?

b. What is the easiest way to install the FAST toolbox, as stated by the authors?

c. Install FAST using the CPAN method following the commands on the github page, type one of the commands from the program to check to see if it is installed