Texas A&M University

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BIOL 689 Digital Biology

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Notes from the class and revision notes

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Abstract

Notes from my BIOL 689 Digital Biology class at Texas A&M University in the first summer session of 2014.

To be completed. . .

Revision History

Revision History:

1. Version 0.1, June 3, 2014. Initial copy of the report.
2. Version 0.2, June 23, 2014. Added material for the first lecture.
3. Version 0.3, June 23, 2014. Added material about computing (SSH, rsync, and Git) for the second lecture.
4. Version 0.X, June ???, 2014. Added BLAH and modified BLAH:
   (a)
5.

Contents

Chapter 1

Introuctory Material

Prof. Rodolfo Aramayo is my class instructor.
This is a UNIX-based class.

My username is db00XX. See the comments of this statement for my username.

Ricardo is my (lab) teaching assistant (TA).

Genome assembly is still an unsolved problem.

GitLab (from GitHub, Inc.) will be used for the first time in this class. Three concepts will be covered in the introduction: Wiki for the class, which contains the standard class information; the code repository that the Wiki uses; and the *Git* version control system.

The outline of the class (i.e., syllabus and class schedule) will be modified as the semester progresses.

On Thursday, June 5, 2014, we will cover genome analysis, gene models, and gene files. Next week, we will cover next generation DNA sequencing. We will also look at library construction methodology and techniques, and associated challenges. Next Thursday, we will also look at "small reads." We will write small scripts to process small data sets, and organize the pipeline (or design the algorithm) for the program/script. That is, design the control and data- flow graph of the algorithm. Furthermore, we will look at genome mapping, genome assembly, data display (i.e., data visualization), and transcriptome mapping and transcriptome assembly. Subsequently, we will be given data sets from the professor to carry out (machine) learning for pattern classification, and explore read archives (with unknown outputs).

Chapter 2

Software Engineering Basics

2.1 UNIX Basics

My TA, Ricardo, suggested using Guake (<http://en.wikipedia.org/wiki/Guake>) as a substitute for the common/normal `Terminal` application.

We will be using the `Terminal` to do a lot of our work in this class. Prof. Rodolfo Aramayo briefly talked about the history of UNIX and its derivatives, such as *Linux*, *BSD*, *Oracle/SUN Solaris*, and *Mac OS X*. UNIX was started at *Bell Labs*. He also talked about the UNIX philosophy.

We shall operate in the UNIX environment via text files. Everything (including directories) is a file in UNIX. Some files can be read visually (i.e., text files), while others (i.e., binary files) cannot.

The kernel is the heart of the operating system. The UNIX shell (accessed via applications, such as the `Terminal`) is an application that allows users to interact with the kernel indirectly.

Anatomy of UNIX commands: `command_name [options] [arguments]`. Double dashes for options of UNIX commands cannot be combined. However, for options for single dash lines, they can be combined.

The "`man`" page is the UNIX manual. To find documentation of a UNIX command, use the `man` command.

UNIX commands to learn:
1. alias: "alias ll"
2. apropos: "apropos copy" would search the UNIX "man" pages for the keyword "copy".
3. cat: conCATenate
4. cd
5. chmod: Change mode
6. clear
7. cp: cp –version
8. dir -l
9. date
10. du: "du -hd 0 ." list the size of the directory in KB, and "du -hd 1 ." list the size of the directory and its files. "df -h" indicates the size of the directory and its contents.

11. echo: "echo -e" refers to `echo` enhanced, which redirects the output in the UNIX pipeline to a file. *echo -e " 'date'" > tata1.* "echo $PATH"

12. file

13. history

14. info cp

15. less

16. ls [-al]

17. more

18. mkdir

19. mv

20. pwd

21. rm

22. rmdir

23. rsync:
    (a) An example of how the command can be used is: "rsync -v username@host:∼/path/to/file .". This commands copies the file at the specified path to the current working directory. The "-v" option runs the UNIX command in verbose mode.
    (b) Its "-vr" option runs the command recursively in verbose mode.
    (c) Prof. Aramayo mentioned something about an option that transfers files with automatic compression and decompression. Is this option "-a", or something else? Use the "tar" command to compress/uncompress files.

24. touch

25. tree

26. type: type zrio

27. whatis

28. which: which blastn

Use "tab" to autocomplete filenames and directory names. Avoid using spaces in filenames and directories to keep file and directory access simple.

Directory access: The "." file is the current working directory, and the ".." is the parent directory. A directory can also be called a folder. By using the `cd` command, I can return to my home directory.

You cannot undo operations in UNIX. Hence, save and backup files before performing removal operations in UNIX. There is also no "trash can" or "recycle bin".

Microsoft Excel has a maximum limit of 65,000 rows in the spreadsheet. Hence, this limits the amount of information that I can process with Microsoft Excel. To process more data, such as GBs or TBs of data, I need other software applications or develop my own computer program.

Symbolic links in UNIX are like shortcuts or aliases in Windows. An example of creating a symbolic link is: "ln -s ../01/test01".

The human genome has been decoded into a file about 7 TB.

The colon ":" serves as a dummy placeholder to remove the contents of a file; ": > filename"

Standard output stream, `stdout`, is described along with exit signals of UNIX processes. Standard error output stream will write to the standard error output file. UNIX redirection for standard output and error streams are described.

Use *tree* to show contents of a directory as a tree.

Discussed UNIX path redirection, pipelining of UNIX commands, and separate execution of UNIX commands (using the semicolon ";" symbol).

Covered special/escape characters to use tabs and newlines to print information.

Covered information on how to go to the "home" directory. "~" refers to the home directory.

Covered absolute paths and relative paths in UNIX.

Detailed explanation of the "ls" command. It indicates when the file has been created/modified. It also indicates the size of the file in bytes. It also indicates the username ("db0015") and the group ("student") that I belong to. Permissions to access files are determined by the group that I belong to. File permissions are indicated for read, write, and execute. They are set for individual users, groups, and everybody with access to the computer network/system. File types are indicated for directories ("d"), regular/normal files ("-"), and symbolic links ("l").

Most files have the file permissions set as 755.

Discussed how to create aliases in UNIX.

Configure my UNIX environment with the ".bashrc" (or ".bash_profile") file.

The `.profile` is used by `shell`, and is equivalent to `.bashrc` for Bash.

GUI-based *Galaxy* is used for this class.

Regarding file transfer, avoid unencrypted file transfer that can be accessed by others. People can listen or snoop on the packet transmission of files, and find out what you are doing. An aside: Email service providers, such as Google, transmit emails between their servers without encryption.

There are many applications for downloading files from the Internet. The applications `curl` and *wget* are more common for downloading files.

The UNIX command `ifconfig` gives you information about computer networking for your computer or computing account (if you are connected to a remote computer).

Further references in my research database about UNIX include the following: [1, 5–7, 9–16, 18–21].

2.1.1 SSH Basics

`SSH` is an application that allows me to connect securely to another computer that is connected to the same computer network, or to the Internet. It uses encryption for network connection, including file

transfer between computers in the same network, or between different networks. Its various levels of encryption correspond to various levels of simplicity in the encryption.

The actual/real `SSH` application requires paid subscription. However, its open source variant is FREE!!!

SSH key generation creates a pair of private and public keys. Keep the private key private to myself (only). Allow others to have the public key, so that a valid authentication of myself can be made.

`rsync` is an application for file copying and synchronization between different computer accounts. It does not copy all files in your directory, but copy modifications to existing files and copies only new files. It transfers files in compressed format. That is, it transfer files between different computers by synchronizing them via delta modifications. This is because copying entire directories of huge files take a lot of time. Hence, use `rsync` to carry out file transfer to save time. `rsync` uses the public key of SSH (from SSH key generation) to connect the local machine to the remote machine. For example, I can create the authentication file (SSH public key) and transfer the public key to the remote machine.

2.1.2 Shell Scripting Basics

To review the basics of UNIX shell script, see my internship report (and associated material) for my internship at the Institute of Microelectronics, Singapore [8].

2.1.2.1 Related Issues

Download data to group directory on "Geiger", so that I do not corrupt the local machine.

Use "tree" to find out the directory structure of the specified directory.

For class on June 17, 2014, clone the repository from Prof. Aramayo, https://geiger.tamu.edu/gitlab/raramayo/digitalbiology_project_summer2014. Work on this directory to practise the UNIX sub-lesson for today.

2.1.3 Version Control (Or Revision Control)

Revision control is also known as version control or source control. It is an aspect of software configuration management (SCM). For this class, `Git` [2–4, 17, 22] will be our revision control tool.

`git status` tells me the status of my `Git` repository. `git diff` tells me the difference between different commits/stages of my repository. Watch videos about `Git` to learn more about `Git`, via hyperlinks provided on the class Wiki. Also, read "`Git` in the Trenches."

While adding files to my `Git` repository, use the `Markdown` language to provide some structure to the presentation of information for my project repository. Save files in the `Markdown` language as `filename.md`. `Markdown` is a document markup language, just like LaTeX, HTML, and XML.

2.2   Other Computing Issues

Launch system monitor to track how much CPU time are processes taking.

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