Research Computing

Xinyu Zhong
Queens' College

November 16, 2023

Contents

Abstract

Abstract of this course

1 Terminal Command lines

Navigation ls pwd cd

Ownership chomd, chown, cumask

Search grep find

Modify touch mv rm, mkdir, rmdir

Read cat more less

Wildcards globbing (files) regexp -(text)

Help **man**

Convenience tab, up error, down arrow to go through commands

File manipulation file, tar, zip, unzip, diff, cut

- **tar** -czf (c:create, z:zip f:file)
- **tar** -xf (x: extract)
- **tar** vs **zip**, tar creates smaller zipped files, can only zip and unzip all the files together
- **diff** tells you what has changed
- **diff** Git uses a bunch of diff files to keep track of the file changes for version control

Redirection STDIN - (CMD) = STDOUT + STUDERR ¿
¿¿
¡
—

1.1 Shell

BASH = Bourne-Again Shell, it is a type of shell, like ksh csh tcsh and zsh Bash is tha complete programming languague
U can use ./complile to run the commands You can define you own commands using alias that runs a python or c++ files

2 Maintenance

We are going to discuess documentation, modularity, prototyping

2.1 Documentation

A __init__.py file in the package
Enforce a certain style for such as i, j, k, underscores etc.

3 Robustness of confidence

3.1 I/O

3.1.1 Storing parameters

Store your constant in a file for development

3.1.2 Error Trapping

Use **try, except, else** blocks

3.2 Debugging

Use **%debug** magic command

3.3 Unit Testing/Testing led developement

Write test files.
Have the habit of write test files before developement

3.3.1 Continuous Integration

Works with Github built-in functions to run tests every time a new change is pushed

4 Optimisation

4.1 Timing Operations