Introduction to programming for astronomers (fall 2015)

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Chapter 1

Introduction

In astronomy, and outside of it, programming is becoming an increasingly important skill. The general availability of lots of compute power creates new opportunities for astronomy. There are three general areas in astronomy where computers play an increasingly important role. First, the latest generations of observatories produce high data rates that at times need to be searched in real time for interesting signals. Second, there is a move to more open data sharing and public archiving of observational data, which creates opportunities for data mining. Third the availability of massive amounts of computational power allows increasingly detailed astrophysical simulations to be performed.

1.1 Basic Linux and Coding for Astronomy & Astrophysics

The aim of the course *Basic Linux and Coding for AA (5214BLCF3Y)* is to to get you up and running in Linux with some basic knowledge of its command line interface and teach you the basics of programming. This course will use the Python programming language (more specifically Python 2.7 which, despite Python 3 being available, is still the most prevalent in research). Python was chosen for its relatively straightforward syntax, its free availability, the wide range of libraries in its "eco system". For the fields physics and astronomy in particular, Python provides a large number of libraries for scientific computing and is displacing packages like IDL¹ and Matlab².

The Linux part of our course will teach you some of the backgrounds and commands that you will need to be productive. More specifically:

- You should attain basic knowledge of the UNIX/Linux file system layout and the use of permissions on UNIX/Linux to control file access.
- · You should be able to access the command line (we will be using the BASH shell throughout this course).
- You should be able to manage running processes on a Linux system, to start or stop programs and to find out which processes are running.
- · You should be able to navigate the UNIX/Linux file system and find files and programs.
- · You should be able to manipulate text files through the command line and search for specific content.

The programming part of this course aims to teach you the basics of programming in general and programming in Python in particular. Because of the limited extent of this course, we will focus our attention on a practical subset of the Python language — and test whether you attain working knowledge of that subset. Specifically:

You should be able to design and implement a properly structured Python program written in the standard
Python style. You will also learn to properly document you program, use proper variable and function
naming, how to modularize you program using functions, and how to make your program reusable.

¹http://www.exelisvis.com/ProductsServices/IDL.aspx

²http://www.mathworks.com/products/matlab,

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- · You should be able to read and write simple text data files.
- · You should be able create basic plots using Matplotlib.
- You should be familiar with Numpy and Scipy and be able to use these libraries to implement simple scientific
 calculations efficiently.

A further more general goal is that you develop problem solving skills using programming tools.

- Learn how to find help when programming. That includes how to read the documentation available with Python and its libraries, and which resources are available on-line.
- Develop the skills to, when presented with new data files, inspect that data, create plots and write small tools to work with them.

1.2 Conventions

This reader uses a number of typographical conventions differentiate normal text, programming code snippets, commands you enter and program output. In running text you may come across monospaced examples or names. When these examples are underlined, <u>like this</u>, they are (partial) commands or snippets you may enter. When programs require key presses that are not really commands (not followed by an enter), they are type set as for instance or control + z if two keys must be pressed at the same time. Program output and names of programs are typeset like this. Examples of shell usage, interactive Python sessions and Python source code are below. First a shell session:

```
Gretchen:~ thijscoenen$ cd coolstuff/
Gretchen:coolstuff thijscoenen$ ls
Whatever alice.txt blah.txt hello noperm
Gretchen:coolstuff thijscoenen$ head alice.txt
ALICE'S ADVENTURES IN WONDERLAND

Lewis Carroll

CHAPTER I. Down the Rabbit-Hole

Alice was beginning to get very tired of sitting by her sister on the bank, and of having nothing to do: once or twice she had peeped into the book her sister was reading, but it had no pictures or conversations in Gretchen:coolstuff thijscoenen$
```

The second example is an interactive Python session:

```
>>> l = range(10)
>>> print l[:5]
[0, 1, 2, 3, 4]
>>> 1 / 0
Traceback (most recent call last):
   File "<stdin>", line 1, in <module>
ZeroDivisionError: integer division or modulo by zero
>>>
```

Here the prompt >>> is followed on the same line by some Python code and followed by some output from that command on the following line(s). The last example is Python source code:

```
#!/usr/env/bin python
'''
Print a custom greeting.
'''

def say_hello(person):
    print 'Hello {}'.format(person)

if __name__ == '__main__':
    say_hello('Jan Janssen')
```

1.3 Contents of this reader

This reader consists of 3 parts. The first part explains the basics of the Linux command line, the basics of Python and some libraries useful for scientific computing. The second part contains a number of assignments that will be used during the tutorials. Finally, the third part (the appendix) contains some extra background information.

Part I

Reading

Chapter 2

Linux and its Command Line

In this chapter I will quickly introduce you to the very basics of using Linux through its command line interface. After a little history of Linux and operating systems like it, I will explain how you get access to the command line and go over some of the commands you will need. This chapter can be skipped safely if you are already familiar with the Linux command line. The examples in this chapter use the so called Bourne Again Shell (BASH). This shell comes standard with many flavors of Linux or UNIX.

2.1 UNIX and Linux

UNIX is an operating system developed in the early 1970s at AT&T Bell Labs. Unlike some of its contemporaries UNIX was designed as a multi user system from the start, it used a hierarchical file system (see 2.1.2) and consisted of many small programs that could be combined to perform complex operations. UNIX became popular in academia, where UNIX like systems are still used. In the early 1990s Linus Torvalds developed a new UNIX like operating system that he could run on his own PC. This operating system became known as Linux and, while initially developed by volunteers and hobbyists, it was soon picked up by businesses. Nowadays a large fraction of Linux' development is done by very large computer companies like Google, IBM and Samsung. Apple's Mac OS X is another popular UNIX version.

Today Linux is used on computers ranging from mobile phones (e.g. Google's Android) to the largest super computer clusters. It furthermore runs a large fraction of the Internet's infrastructure (e.g. routers and web servers). Because UNIX was developed before graphical displays became generally available, its earliest interfaces were all text driven. Although graphical user interfaces are available for UNIX and Linux nowadays the textual interface persists. This textual user interface is also called a *command line* interface and on UNIX is provided through a so-called *shell*. Several different shells are available, but this chapter will only explain the basics of the Bourne Again Shell (BASH).

2.1.1 Users and Permissions

Because UNIX was designed as a multi user operating system, it has a notion of users. Associated with every user are a level of access to the operating system. The so-called root user has full access to a UNIX system while the other users have more restricted access. On your own computer you will likely be able to log in as root while on shared computers you will only have access to your own files. Do note that even if you can log in as root, it is absolutely a bad idea to do so for day-to-day work. Since the root is all-powerful, a mistake while logged in as root can be much worse than a mistake while logged in as an ordinary user. Furthermore the software that you use may contain flaws or security problems that become a problem when that software (running as root) has full access to the computer. Furthermore each user is also assigned to a group of users that have the same system privileges.

UNIX controls access to files and directories based on ownership and so-called *permissions*. Each file and directory on a UNIX system has an *owner* (one of the users on that system) and permissions. UNIX has three permissions: *read*, *write* and *execute*. Read permission is needed to be able to view the contents of that file. Write permission is needed on directories to create files in that directory. For files write permission is needed to change or erase them. Execute permission is needed on directories to be able to view their contents and on files to execute them.

Permission may also be set at the *group* level or for all *other* users with access to a computer system (see Section 2.2.12).

2.1.2 The File System

UNIX uses a hierarchical file system meaning that directories in it can be arbitrarily nested. Each directory can contain files or sub directories — the former directory is also referred to as *parent* while the latter are referred to as *children*. The directory hierarchy is a tree with the directory at the base of that tree referred to as *root*, denoted as *f.*. When specifying locations, or *paths*, in a file system two different notations may be used. *Absolute paths*, on the one hand, describe the location of a file or directory in absolute terms, i.e. without reference to some other location on the file system. *Relative paths*, on the other hand, specify a location in the file system relative to some other location in the file system (usually the current location of the user). Absolute paths start at the root, i.e. they start with /, while relative paths do not.

Because a UNIX system may be shared between many users, each user has his or her own directory to store files in. This special directory is called a *home directory*. Home directories can be found in /home on Linux systems and in /Users for Mac OS X systems. E.g. my user (thijscoenen) has the home directory /Users/thijscoenen on a Mac OS X system and /home/thijscoenen on a Linux system.

The UNIX(-like) operating systems have very specific file system layouts, with some directories assigned to programs or even parts of the operating system itself. Most directories that reside directly in the root directory are in fact system directories and as a normal user you will rarely need access to them. Below, as an example, the contents of my Mac OS X machine's root directory none of which is part of my own files or directories¹

Gretchen:coolstuff thijscoenen\$ ls /						
Αį	oplications	System	cores	mach_kernel	tmp	
De	eveloper	Users	dev	net	usr	
L:	ibrary	Volumes	etc	private	var	
Ne	etwork	bin	home	sbin		
G	Gretchen:coolstuff thijscoenen\$					

UNIX also allows so-called *hidden files* that are normally invisible. Any filename or directory name that starts with a dot will be hidden. Hidden files are generally used for settings or for those files that a user does not need access to directly (only through some program). E.g. the settings for the BASH shell are kept in a file called .bash_profile or .bashrc in your home directory.

2.2 The Command Line

2.2.1 Accessing the Shell

The command line interface, provided by a shell program, is generally accessible through a terminal emulator program. The name terminal derives from the simple computers (terminals) that were used in the past to access large shared computer systems. When you start a terminal emulator you are generally dropped into your home directory. On Mac OS X you can use the "Terminal" program, while on a Linux systems with KDE you use "Konsole", on Linux systems with Gnome "GNOME Terminal" and on Linux systems with Unity the program is also called "Terminal". This chapter will only explain the basics of the BASH shell as it is standard on many Linux systems and on all recent versions of Mac OS X.

2.2.2 Navigating the File System

Assuming you have access to the command line, you will be presented with a so called prompt. What the prompt looks like depends on the version of UNIX or Linux you are using and how it was configured. In my case the command prompt looks like²:

 $^{^{1}} The\ example\ shows\ some\ directories\ that\ are\ Mac\ OS\ X\ specific:\ Applications,\ Developer,\ Library,\ Network,\ System\ and\ Volumes.$

²What your prompt looks like exactly depends on the settings of your shell and is a matter of taste. My computer shows computername:directory username\$, with Gretchen being the name of my computer.



Figure 2.1: A screenshot showing Mac OS X's built-in Terminal program. This program allows you to access the underlying BASH shell on Mac OS X.

Gretchen:~ thijscoenen\$

You can issue your commands by typing them followed by a press of the return key. One of the first things you may ask yourself, is where am I? Usually when you start a new command line session you will be dropped off in your user's home directory. To find out where in the file system you are you use the pwd (print working directory) command. The following example shows you what the output looks like for me:

```
Gretchen:~ thijscoenen$ pwd
/Users/thijscoenen
Gretchen:~ thijscoenen$
```

The home directory in these examples has a subdirectory called coolstuff that we will access. To change directories to the coolstuff directory use the cd (change directory) command. In the following example a pwd command issued as well to show we have actually changed directory:

```
Gretchen:~ thijscoenen$ cd coolstuff
Gretchen:coolstuff thijscoenen$ pwd
/Users/thijscoenen/coolstuff
Gretchen:coolstuff thijscoenen$
```

The eagle eyed among you may have noticed the $\tilde{}$ (tilde) appearing in the shell session examples. This is shorthand for your home directory, and your shell will expand it to your full home directory. You can use the tilde in commands to shorten them. To return to your home directory use the \underline{cd} $\tilde{}$ command.

What does the coolstuff directory actually contain? To get a listing of the contents of a directory you can use the ls command. This command takes many options but the easiest way of using it is as follows:

```
Gretchen:coolstuff thijscoenen$ ls alice.txt hello noperm Gretchen:coolstuff thijscoenen$
```

Hidden files on UNIX systems have names that start with a dot. There are two special directories that are always present in every directory, the single dot and double dot directories. The former . is shorthand for the current directory and the latter . . is shorthand for the parent directory. By passing the $\underline{\ }$ a option to 1s you make hidden files visible.

```
Gretchen:coolstuff thijscoenen$ ls -a
. . . alice.txt hello noperm
Gretchen:coolstuff thijscoenen$ cd ..
Gretchen:~ thijscoenen$ pwd
/Users/thijscoenen
Gretchen:~ thijscoenen$
```

The 1s command has many options, but several are worthy of mention. First, the <u>-1</u> option will list the directory contents with one file or directory per line and also show the size (in bytes) and permissions for each entry. Second, the <u>-h</u> option will show the file sizes in human readable format (so not in bytes for large files, see below for an example).

```
Gretchen:coolstuff thijscoenen$ ls -l
total 312
-rw-r--r-- 1 thijscoenen staff 147731 22 jul 23:27 alice.txt
-rwxr--r-- 1 thijscoenen staff 43 7 aug 18:02 hello
-rw-r--r-- 1 thijscoenen staff 50 11 aug 14:35 noperm
Gretchen:coolstuff thijscoenen$ ls -lh
total 312
-rw-r--r-- 1 thijscoenen staff 144K 22 jul 23:27 alice.txt
-rwxr--r-- 1 thijscoenen staff 43B 7 aug 18:02 hello
-rw-r--r-- 1 thijscoenen staff 50B 11 aug 14:35 noperm
Gretchen:coolstuff thijscoenen$
```

Another nice command is <u>ls -lrt</u> which will list all files and sorted by the time of last access (oldest to newest). This is handy when you want to find the most recently accessed file in a directory as it will be at the end of the ls output.

The ls command can furthermore be used to list the content of a specific directory. Using the previous example I can list the contents of the coolstuff directory from my home directory using the command Ls coolstuff. When you want to recursively list the contents of some directory you can use the Ls -R command. It shows the content of the current directory, the content of the subdirectories and the content of the subdirectories of each sub directory etc. Because this command produces a lot of output I suggest you try it for yourself.

2.2.3 Running Programs

The shell can only start programs it can find, and the directories where the shell will look for programs are listed in an environment variable (see Section 2.2.13 for an explanation) called \$PATH. For programs that are on the \$PATH, i.e. in one of the directories listed by the \$PATH variable, you can just type their name and press enter (even if the program is in a different directory than you are). The programs 1s and cd are on the \$PATH (on my system they actually reside in the /bin directory). When you try to run a non-existent program or a program that your shell cannot locate, you will see an error like the following:

```
Gretchen:coolstuff thijscoenen$ ls
alice.txt hello noperm
Gretchen:coolstuff thijscoenen$ nosuchthing
-bash: nosuchthing: command not found
Gretchen:coolstuff thijscoenen$
```

This will even happen for programs present in the same directory as you — unless that directory happens to be on the \$PATH. To remedy this problem, prepend the program name with __/ (this tells your shell to look in the current directory).

```
Gretchen:coolstuff thijscoenen$ hello
-bash: hello: command not found
Gretchen:coolstuff thijscoenen$ ./hello
Hello world!
Gretchen:coolstuff thijscoenen$
```

You may not have sufficient permissions to run just any program on UNIX. To check whether you have permissions to run the program you can just attempt to run it, your shell will report an error if you have insufficient permissions.

```
Gretchen:coolstuff thijscoenen$ ./noperm
-bash: ./noperm: Permission denied
Gretchen:coolstuff thijscoenen$
```

All the previous examples were for programs that run for a short time, if you have long running programs you may want to continue issuing new commands without waiting for some program to finish. You could just start a second (or third etc.) terminal and continue issuing commands in that new terminal. The BASH shell however allows you to start programs in the background so that it is possible to keep issuing commands in that same shell. To start a program in the background just add a space and ampersand $\underline{}$ to the command. You can move a program from the background to the foreground with the fg command:

```
Gretchen:background-demonstration thijscoenen$ ls
runs-1-minute
Gretchen:background-demonstration thijscoenen$ ./runs-1-minute &
[1] 55868
Gretchen:background-demonstration thijscoenen$ pwd
/Users/thijscoenen/background-demonstration
Gretchen:background-demonstration thijscoenen$ fg
./runs-1-minute
One minute passed
Gretchen:background-demonstration thijscoenen$
```

As you can see in the example above a number is shown in the shell after the program was started using the $\underline{\underline{\&}}$. This number is the process number of the program just started, in Section 2.2.7 these process numbers will be explained. If you started a program in the foreground, but want to move it to the background you first suspend the program and then move it to the background. Suspend the program by pressing $\underline{\texttt{Control}} + \underline{\texttt{Z}}$ and then move it to the background by issuing the bg command.

In this example you can see that the <code>Control</code> + <code>Z</code> key presses are shown in the shell as ^Z. It is also possible to terminate a program running in the shell by pressing <code>Control</code> + <code>C</code>. Some programs may not react to an attempt to terminate it this way and you may have to resort to the kill command described below in Section 2.2.7.

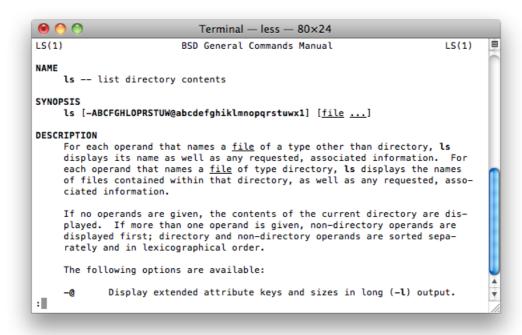


Figure 2.2: The man documentation viewer showing part of the documentation for ls.

2.2.4 Getting Help

While this reader will get you started using Linux it cannot possibly explain all features of BASH or all programs available by default on a UNIX machine. Fortunately a large amount of documentation is available, some of it accessible directly from the command line and some of it on line. Most command line programs have simple built in help that is usually displayed when no options are specified on the command line or through options as -?, -h or --help.

While many programs provide some simple documentation about themselves UNIX provides a standard command line documentation viewer called man. To get help about a specific program just type the command man program-name, where you should replace program-name with the program that you want help for. Figure 2.2 shows the help for 1s (accessed by typing man 1s). The documentation can be navigated using the up and down arrows, to move up and down by a line, and space to jump a full page. The documentation can also be searched by typing a forward slash of followed by the word you are looking for and then return. When there are several matches for a search you can jump to the next match by pressing (or in reverse with N). The viewer can be quit by typing a q. More information about navigating in man can be accessed by pressing while it is running. The documentation available through man are also called "man pages". Some software will be documented using info, try running that like you would man in case no man pages are available (because the documentation may be written in info format).

On line there are several good resources for help with UNIX problems, that can be very helpful because the man pages are quite technical and at times hard to read. The very basic UNIX commands tend to have Wikipedia pages with examples. Stack overflow, a community site about programming problems (see http://stackoverflow.com), can be helpful as can be the related Stack Exchange site about UNIX and Linux (see http://unix.stackexchange.com). A nice site that can explain some shell commands is Explain Shell (see http://explainshell.com), it allows you to cut and paste a command and it then shows you an explaination of it. The Linux Documentation Project (see http://www.tldp.org) is also useful. A note about using Google to find documentation on the Internet: not everything you find will be correct so refrain from just copying whatever you find!

2.2.5 Copying, Moving and Removing Files

To copy files, or directories use the cp command. The general shape of the command is <u>cp source destination</u>. If the source is a file and the destination is also a filename the contents of source will be copied over the destination file. If destination does not exist yet source will be copied to a file with the specified destination as name. If destination is a directory the source file will be copied to it. If the source is a directory itself the copying will fail (these examples use cat to show file contents):

```
Gretchen:cp-demonstration thijscoenen$ ls -l
drwxr-xr-x 2 thijscoenen staff 68 21 aug 22:40 directory_a
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file_a.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file_b.txt
Gretchen:cp-demonstration thijscoenen$ cat file_a.txt
This is file A.
Gretchen:cp-demonstration thijscoenen$ cat file_b.txt
This is file B.
Gretchen:cp-demonstration thijscoenen$ cp file_a.txt file_c.txt
Gretchen:cp-demonstration thijscoenen$ ls -l
drwxr-xr-x 2 thijscoenen staff 68 21 aug 22:40 directory_a
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file_a.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file b.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:41 file c.txt
Gretchen:cp-demonstration thijscoenen$ cat file c.txt
Gretchen:cp-demonstration thijscoenen$ cp file a.txt file b.txt
Gretchen:cp-demonstration thijscoenen$ cat file b.txt
This is file A.
Gretchen:cp-demonstration thijscoenen$ cp file a.txt directory a/
Gretchen:cp-demonstration thijscoenen$ ls directory a/
Gretchen:cp-demonstration thijscoenen$ cp directory a whatever
cp: directory a is a directory (not copied).
Gretchen:cp-demonstration thijscoenen$
To copy a directory and all it contains use the <u>-r</u> option of cp:
Gretchen:cp-demonstration thijscoenen$ cp -r directory_a/ whatever
Gretchen:cp-demonstration thijscoenen$ ls whatever/
file a.txt
Gretchen:cp-demonstration thijscoenen$
```

To just move a file to a different filename or location use the mv command. Simple use of mv takes the shape mv source destination. If source is a file and destination does not exist yet source will be moved there (after this operation source will cease to exist). If destination does exist, and is a file, it will be overwritten. If destination is a directory the file source will be moved to that directory. If source itself is a directory it will be moved to destination, with similar rules:

```
Gretchen:cp-demonstration thijscoenen$ ls -l
total 24
drwxr-xr-x 3 thijscoenen staff 102 21 aug 22:42 directory_a
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file_a.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:42 file_b.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:41 file_c.txt
```

```
drwxr-xr-x 3 thijscoenen staff 102 21 aug 22:45 whatever Gretchen:cp-demonstration thijscoenen$ mv file_a.txt file_b.txt Gretchen:cp-demonstration thijscoenen$ ls -l total 16 drwxr-xr-x 3 thijscoenen staff 102 21 aug 22:42 directory_a -rw-r--r- 1 thijscoenen staff 16 21 aug 22:40 file_b.txt -rw-r--r- 1 thijscoenen staff 16 21 aug 22:41 file_c.txt drwxr-xr-x 3 thijscoenen staff 102 21 aug 22:45 whatever Gretchen:cp-demonstration thijscoenen$ mv whatever directory_a/Gretchen:cp-demonstration thijscoenen$ ls -l total 16 drwxr-xr-x 4 thijscoenen staff 136 21 aug 22:40 file_b.txt -rw-r--r- 1 thijscoenen staff 16 21 aug 22:40 file_b.txt fre-r--r- 1 thijscoenen staff 16 21 aug 22:41 file_c.txt Gretchen:cp-demonstration thijscoenen$ mv directory_a/ file_b.txt mv: rename directory_a/ to file_b.txt: Not a directory Gretchen:cp-demonstration thijscoenen$
```

As you can see trying to move a directory to an existing file will fail.

Removing files is done with the rm command. Generally you just use the <u>rm somefile</u> command. If somefile is a directory this will fail because only *empty* directories are removed with <u>rmdir</u>.

```
Gretchen:cp-demonstration thijscoenen$ ls -l
total 16
drwxr-xr-x 4 thijscoenen staff 136 21 aug 22:57 directory_a
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:40 file_b.txt
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:41 file_c.txt
Gretchen:cp-demonstration thijscoenen$ rm file_b.txt
Gretchen:cp-demonstration thijscoenen$ ls -l
total 8
drwxr-xr-x 4 thijscoenen staff 136 21 aug 22:57 directory_a
-rw-r--r-- 1 thijscoenen staff 16 21 aug 22:41 file_c.txt
Gretchen:cp-demonstration thijscoenen$ rm directory_a/
rm: directory_a/: is a directory
Gretchen:cp-demonstration thijscoenen$ rmdir directory_a/
rmdir: directory_a/: Directory not empty
Gretchen:cp-demonstration thijscoenen$
```

If you want to remove a directory and all its content (whether files or sub directories) you can use the $\underline{\mathsf{rm}} \ \mathsf{-rf} \ *$. Note though that this is a very dangerous command, if not the "most dangerous command ever"³, as it will recursively (the -r option) remove everything (matched by the * "glob pattern") and skip any questions (the -f option). For more information on glob patterns see Section 2.2.9. Note that $\underline{\mathsf{rm}} \ \mathsf{-rf} \ *$ cannot be undone!

2.2.6 Creating Directories

Because in the previous section it was shown how to remove directories you may ask yourself how you create them in the first place. UNIX has the mkdir command for that. You can create a directory with the command mkdir somedirectory where some directory is the name of the directory to be created. It is also possible to create several directories in one go by listing their names after mkdir separated with spaces. If you have to create a directory inside of several that is possible using the command mkdir -p followed the full path you want to create.

```
Gretchen:mkdir-examples thijscoenen$ ls
Gretchen:mkdir-examples thijscoenen$ mkdir dir1 dir2 dir3
```

³According to one of my proofreading colleagues.

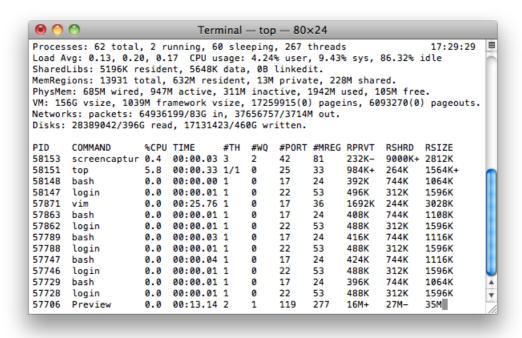


Figure 2.3: This screenshot shows top running on a Mac OS X system.

```
Gretchen:mkdir-examples thijscoenen$ ls
dir1 dir2 dir3
Gretchen:mkdir-examples thijscoenen$ ls -l
total 0
drwxr-xr-x 2 thijscoenen staff 68 21 aug 23:28 dir1
drwxr-xr-x 2 thijscoenen staff 68 21 aug 23:28 dir2
drwxr-xr-x 2 thijscoenen staff 68 21 aug 23:28 dir3
Gretchen:mkdir-examples thijscoenen$ mkdir -p container/subdir/subdir/whatever
Gretchen:mkdir-examples thijscoenen$ cd container/subdir/subdir/whatever
Gretchen:whatever thijscoenen$ pwd
/Users/thijscoenen/mkdir-examples/container/subdir/subdir/whatever
Gretchen:whatever thijscoenen$
```

2.2.7 Listing and Killing Processes

On UNIX each running program consists of one or sometimes more processes that are identified by *process numbers* often abbreviated to PID. To get an idea of the running programs use the <u>top</u> command. This will show you a continually updating list of running processes, sortable by for instance memory use or processor use. When your computer is stuck it is quite often possible to find the offending program by looking through the most active processes in top. As with man you can exit top by pressing <u>p</u>. Figure 2.3 shows a screenshot of top. You can get a list of the currently running processes using the ps command, which unlike top will not continually update - it is like an ls for processes. Run without options ps only shows the processes running in the current shell while you can get a list of all processes running in all shells for a certain user using <u>ps -u username</u> (with username replaced with relevant username). For example, while logged in on a LOFAR⁴ compute node as coenen:

⁴The Low Frequency Array, a large radio telescope array operating at low radio frequencies that has its core in the Netherlands.

```
      coenen@locus048:~$
      ps

      PID
      TTY
      TIME
      CMD

      14099
      pts/2
      00:0:0:00
      bash

      15518
      pts/2
      00:0:0:00
      ps

      coenen@locus048:~$
      ps -u coenen
      coenen

      PID
      TTY
      TIME
      CMD

      14098
      ?
      00:0:00
      sshd

      14099
      pts/2
      00:00:00
      sshd

      15229
      ?
      00:00:00
      bash

      15230
      pts/3
      00:00:00
      top

      15522
      pts/3
      00:00:00
      top

      15522
      pts/2
      00:00:00:00
      ps

      coenen@locus048:~$
```

Another useful option to ps is <u>-A</u> which will select all processes, also not necessarily running in a terminal. The process numbers can be used to terminate unresponsive programs or those that are otherwise stuck. The kill command allows you to terminate processes by process number:

Some processes may still not terminate, you can then send them a stronger message using the -9 (KILL) signal. E.g. to kill process 101 using the KILL signal: kill -9 101.

2.2.8 Dealing with Text Files

You will inevitably have to work with text files, because, among other reasons, programming source code are text files, many of UNIX's settings are in small text files in your home directory and quite a few scientific data sets are encoded in text files. Luckily UNIX has many tools to work with text files from the command line. The first command is cat which will show the contents of a text file in your terminal. Since cat does not paginate, this will likely cause your terminal to scroll. In the following example I look at the contents of the hello file (which is a Python script and therefore text):

```
Gretchen:coolstuff thijscoenen$ ls
Whatever alice.txt hello noperm
Gretchen:coolstuff thijscoenen$ cat hello
#!/usr/bin/env python
print "Hello world!"
Gretchen:coolstuff thijscoenen$
```

If the file you are working with is large, then using cat to look at its content is inconvenient. By using the more or less commands you will be presented with a so-called pager that allows you to view and move around in the text file without scrolling. The less command allows you to move in both directions through the file using the up and down arrow keys. You can search for words by pressing a forward slash [] followed by the word you are looking for and then enter. If there are several matches you can move between them using [] (or [N] for the reverse direction). Help is accessible by pressing [] and you can quit less by pressing []. This is very similar to the man works because it actually uses less to show the actual man page (visible in the title bar of the window in Figure 2.2).

If you are only interested in a quick peek at the contents of some text file, you can use the head or tail commands to, respectively, look at the first few lines or last few lines of a text file. Similarly if you want to find out the number of words or lines in a file the wc (word count) command is useful, without options it shows the number of lines, the number of words and the number of bytes in the file.

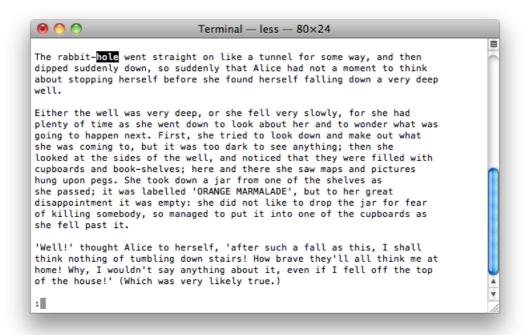


Figure 2.4: The less program showing a text file, you can move through the file using the arrow keys.

```
Gretchen:coolstuff thijscoenen$ head alice.txt
ALICE'S ADVENTURES IN WONDERLAND

Lewis Carroll

CHAPTER I. Down the Rabbit-Hole

Alice was beginning to get very tired of sitting by her sister on the bank, and of having nothing to do: once or twice she had peeped into the book her sister was reading, but it had no pictures or conversations in Gretchen:coolstuff thijscoenen$

Gretchen:coolstuff thijscoenen$ wc alice.txt

3335 26444 147731 alice.txt

Gretchen:coolstuff thijscoenen$ wc -l alice.txt

3335 alice.txt

Gretchen:coolstuff thijscoenen$
```

The last example (the \underline{wc} -1 alice.txt command) shows you how to count only the number of lines in a file. A oft used file format to encode tabular data is a so called Comma Separated Values (CSV) file (white space or tab separation are also used frequently). The lines in these files generally correspond to one data point, you can thus get a quick feel for the size of the data set by using \underline{wc} -1 on that file.

So far we have only treated looking through files, not editing or creating them. Many different text editors are available on UNIX, spanning the gamut from editors that run in your terminal and use arcane commands to more modern text editors with a graphical user interface. Note though that in this context modern does not always mean more efficient! The choice of editor is personal and there is not enough space in this reader to explain how to use

them all. Instead, I have added a chapter to the appendix that lists some good text editors (see Appendix C). For now I will just mention that you will want a text editor that is focused on programmers as they allow you to work more efficiently.

To search a file for a certain piece of text you can use the grep command. To find out on which lines the Cheshire cat appears in the text we use \underline{grep} with the $\underline{-n}$ option to print line numbers and $\underline{-i}$ option to perform case insensitive matches:

```
Gretchen:coolstuff thijscoenen$ grep -ni "Cheshire" alice.txt

1313:'It's a Cheshire cat,' said the Duchess, 'and that's why. Pig!'

1319:'I didn't know that Cheshire cats always grinned; in fact, I didn't know

1433:was a little startled by seeing the Cheshire Cat sitting on a bough of a

1440:'Cheshire Puss,' she began, rather timidly, as she did not at all know

2068:'It's the Cheshire Cat: now I shall have somebody to talk to.'

2100:'It's a friend of mine--a Cheshire Cat,' said Alice: 'allow me to

2144:When she got back to the Cheshire Cat, she was surprised to find guite a
```

If you want more context to each match use the $\underline{-B}$ option to specify how many lines *before* a match should also be printed and $\underline{-A}$ for the number of lines *after* a match (output truncated after the first two matches to save space):

```
Gretchen:coolstuff thijscoenen$ grep -B 1 -A 2 -i "Cheshire" alice.txt

'It's a Cheshire cat,' said the Duchess, 'and that's why. Pig!'

She said the last word with such sudden violence that Alice quite
--

'I didn't know that Cheshire cats always grinned; in fact, I didn't know that cats COULD grin.'
```

Each match is separated by a line with two dashes --. If you are only interested in knowing whether a file contains a match you can use the -1 option to print the filename in stead of the matching text:

```
Gretchen:coolstuff thijscoenen$ grep -li "Cheshire" *.txt
alice.txt
Gretchen:coolstuff thijscoenen$
```

grep is a very powerful tool that can also match patterns, it is useful to read through the man pages to see what more it can do for you.

2.2.9 Glob Patterns

The BASH shell supports filename expansion, that is it will expand special wildcard symbols and match them to filenames. This is also called *globbing*, and the pattern that is matched *glob pattern*. I will first explain the parts that make up a glob pattern, then show you how you use them with BASH.

- * Matches any text in filename.
- ? Matches zero or one unspecified character.
- [ABC] Allow one character from a specified set of characters to be matched, in this case the characters A, B and C make up that set. Will match a single character only, not ABC.
- [0-9] Will match a number in the range 0 through 9.
- [a-z] Match any lower case character in the range a through z.

- [a-z] Match any upper case character in the range A through Z.
- [A-Za-z] Match any upper case character in the range A through Z or any lower case character in the range a through z.
 - \ Escape character, use this if you should match one of the characters that have a special meaning in a glob pattern. E.g. if you want to match the *, your glob pattern should include * so that the * itself matched and not expanded.
 - ! This will negate a pattern. E.g. if you want to match anything not a lower case character use ![a-z].

Glob pattern can then be used in combination with other programs, what follows is a simple example that shows how 1s can be combined with some glob patterns to look for some specific files.

```
Gretchen:glob-demonstration thijscoenen$ ls
         604.txt
101.txt
                                       ABC.txt
123.txt
                   709.dat
                                       ABC123.txt
Gretchen:glob-demonstration thijscoenen$ ls [0-9]*
101.txt 123.txt 604.txt 709.dat
Gretchen:glob-demonstration thijscoenen$ ls [!0-9]*
            ABC123.txt
Gretchen:glob-demonstration thijscoenen$ ls [5-9]*
604.txt 709.dat
Gretchen:glob-demonstration thijscoenen$ ls *dat
Gretchen:glob-demonstration thijscoenen$ ls 1[2468]*
123.txt
Gretchen:glob-demonstration thijscoenen$
```

2.2.10 Finding Files

A common problem is, how do I find some specific file? The naive approach, use 1s and move around the file system until you find what you were looking for, is time consuming and . Beyond the glob patterns that your shell provides (see Section 2.2.9) the UNIX find command is useful. With find you can look through a directory hierarchy for filenames matching a certain pattern or certain properties. You can then run some commands for each file that was found. At its simplest you can use find to look for a certain file called needle.txt in this example:

```
Gretchen:find thijscoenen$ find . -name "needle.txt"
./haystack/hay/hay/needle.txt
./haystack/straw/needle.txt
Gretchen:find thijscoenen$
```

As you can see two files were found, but what if we know that the file we need contains the word gold? It turns out you can run other programs on each found file using the -exec option of find. In the following example grep is used to check whether a match contains gold:

```
Gretchen:find thijscoenen$ find . -name "needle.txt" -exec grep -li "gold" {} \;
./haystack/straw/needle.txt
Gretchen:find thijscoenen$
```

2.2.11 gzip and tar

To conserve disk space it is sometimes a good idea to pack files more densely, there are several tools to do so. If you have used Windows so called zip files may be familiar. Although utilities to handle zip files exist (zip and unzip) on UNIX, you are more likely to come across .gz or .bz2 files. Below I give examples of how to deflate and reinflate a file using gzip, note that I use a so-called pipe | and grep to only show filenames containing alice. Pipes are a way of sending output from one program to another, which are explained in Section 2.2.14. The following example shows that the Alice in Wonderland story can be packed to only about 36 % of its original size:

```
Gretchen:coolstuff thijscoenen$ ls -l | grep alice
-rw-r--r-- 1 thijscoenen staff 147731 22 jul 23:27 alice.txt
Gretchen:coolstuff thijscoenen$ gzip alice.txt
Gretchen:coolstuff thijscoenen$ ls -l | grep alice
-rw-r--r-- 1 thijscoenen staff 53596 22 jul 23:27 alice.txt.gz
Gretchen:coolstuff thijscoenen$ gunzip alice.txt.gz
Gretchen:coolstuff thijscoenen$ ls -l | grep alice
-rw-r--r-- 1 thijscoenen staff 147731 22 jul 23:27 alice.txt
Gretchen:coolstuff thijscoenen$
```

The bzip2 and bunzip2 programs work similarly and may achieve a slightly higher compression than gzip, but the latter is used more often.

When you download software or data you will come across so-called tarballs, which are files that can encapsulate many separate files or even directory full hierarchies. The name tarball derives from the tar utility that can create or unpack them. The name tar itself derives from tape archive (archiving to tape was and still is cheaper than archiving to disk). The example that follows shows how you create (-c option) a tarball that is compressed using gzip (-z option) how you can list its contents (-t option) and how you can extract it again (-x option):

```
Gretchen:coolstuff thijscoenen$ ls
              alice.txt hello
Whatever
                                                    noperm
Gretchen:coolstuff thijscoenen$ tar -czf cool.tar.gz *
Gretchen:coolstuff thijscoenen$ tar -tzf cool.tar.gz
Whatever
alice.txt
hello
Gretchen:coolstuff thijscoenen$ rm Whatever alice.txt noperm hello
Gretchen:coolstuff thijscoenen$ ls
cool.tar.gz
Gretchen:coolstuff thijscoenen$ tar -xzf cool.tar.gz
Gretchen:coolstuff thijscoenen$ ls
Whatever cool.tar.gz
                                noperm
alice.txt
              hello
Gretchen:coolstuff thijscoenen$ rm cool.tar.gz
Gretchen:coolstuff thijscoenen$
```

Note that some tarballs are compressed using bzip2 in which case you can use the -j option in stead of -z.

2.2.12 Permissions Continued

In Section 2.1.1 users and their permissions were introduced. UNIX has several commands that let you manage file permissions and ownership. UNIX also allows a user to temporarily acquire more privileges. We will start by demonstrating how file permissions can be changed. The owner of a file and a user with root privileges can change its permissions. The first step is to check the permissions, run for example <u>ls -l</u> to get a file listing that shows the permissions in the first column of the output.

```
Gretchen:chmod-demo thijscoenen$ ls -l
total 16
-rw-r--r-- 1 thijscoenen staff 68 27 aug 22:02 demo.py
----r--- 1 thijscoenen staff 15 27 aug 22:00 nopriv.txt
drwxr-xr-x 2 thijscoenen staff 68 27 aug 22:12 subdir
```

The first column can be further split, taking demo.py as an example we get the file type -, owner permissions rw-, group permissions r-- and finally the permissions for everyone else r--. The file type can be: - for a file, d for a directory and 1 for a "symbolic link". In our example we are dealing with a normal file. The user permissions are listed in the order read, write and execute using the abbreviations rwx. If a permission is not granted the permission will be replaced with a dash. In our example the owner of the file has read and write permissions but no execute permissions: rw-. The group permissions in the example are only read permissions: r--. All other users are also only able to read the file: r--. The second column in the output of <u>ls -l</u> is not interesting for our current purposes, but the third is: it shows the owner of the file. In this case that user is thijscoenen. The following column shows the group that the file is assigned to, in this case the group staff. The next column shows the file size in bytes, followed by a column that shows the last time the file was changed. The last column shows the actual file or directory name. To change the permissions of the user, group and all other users the file owner (or a sufficiently privileged user like root) can use <u>chmod</u>. This command takes as options a string like <u>ugo+rwx</u> that specifies which user should gain or lose which permissions and finally as arguments the files for which the permissions should be changed. The options should be read as: the owner, the group and all others (ugo), gain (+) the permissions to read, write and execute (rwx). If we want to make the demo.py file executable for its owner, the following command will do the trick:

```
Gretchen:chmod-demo thijscoenen$ chmod u+x demo.py
Gretchen:chmod-demo thijscoenen$ ls -l
total 16
-rwxr--r-- 1 thijscoenen staff 82 27 aug 22:29 demo.py
----r--- 1 thijscoenen staff 15 27 aug 22:00 nopriv.txt
drwxr-xr-x 2 thijscoenen staff 68 27 aug 22:12 subdir
Gretchen:chmod-demo thijscoenen$
```

If we want to disallow other users to see what is in the subdir directory we can remove (-) the execute permissions on that directory for its group and all other users:

```
Gretchen:chmod-demo thijscoenen$ chmod go-x subdir/
Gretchen:chmod-demo thijscoenen$ ls -l
total 16
-rwxr--r-- 1 thijscoenen staff 82 27 aug 22:29 demo.py
----r--- 1 thijscoenen staff 15 27 aug 22:00 nopriv.txt
drwxr--r-- 2 thijscoenen staff 68 27 aug 22:12 subdir
Gretchen:chmod-demo thijscoenen$
```

You can also specify several files by just typing their names or by using the appropriate glob patterns. To recursively change the permissions of some directory hierarchy use the <u>-R</u> option, for example to change the permissions on subdir and everything it contains to be completely open to everyone: chmod-Rugo=rwx subdir. In this last command we use = to just set the permissions. Old examples explaining chmod may show numerical permissions, but they are not necessary to manage the permissions and will not be treated here.

To change the owner of a file use the <a href="https://en.py

```
Gretchen:chmod-demo thijscoenen$ chown root:staff demo.py chown: demo.py: Operation not permitted
Gretchen:chmod-demo thijscoenen$ sudo chown root:staff demo.py
Password:
Gretchen:chmod-demo thijscoenen$ ls -l
total 16
```

```
-rwxr--r-- 1 root staff 82 27 aug 22:29 demo.py
----r-- 1 thijscoenen staff 15 27 aug 22:00 nopriv.txt
drwxrwxrwx 2 thijscoenen staff 68 27 aug 22:12 subdir
```

As you can see there is a small hitch, the user thijscoenen cannot change the ownership to root and group staff, because that user is not privileged enough. The second time chmod is preceded with sudo, which means execute the command that follows as a super user (root on most systems). To prove that you in fact are allowed to acquire root privileges you are asked to enter the password that belongs to that user. After acquiring the privileges chown to root becomes possible. While this example is a bit silly sudo is very important when installing software. A lot of software is installed system wide and that means somewhere in the system directories of UNIX. Those directories are not writable for normal user, a problem that is solved with sudo. Note: if you are using a university computer you will most likely not have the ability to use sudo, because most system administrators will not give out root privileges to just anyone — on your own Mac or Linux machine that should be no problem.

2.2.13 Environment Variables

Some of the settings of your BASH shell are put in so-called *environment variables*. A *variable* is a name (or an identifier) associated with some stored value that can be changed. We already came across an environment variable called \$PATH, its value is a list of directories that are searched for executables. The BASH <u>echo</u> \$PATH command will echo (show) the value of the variable \$PATH, the \$ is needed to signify that the following name is a variable (the example below shows what goes wrong without the \$):

```
Gretchen:~ thijscoenen$ echo $PATH
/Library/Frameworks/Python.framework/Versions/2.7/bin:/usr/bin:/usr/sbin:/sbin:/usr/local/bin:
/usr/texbin:/usr/X11/bin
Gretchen:~ thijscoenen$ echo PATH
PATH
Gretchen:~ thijscoenen$
```

As you can see \$PATH contains multiple directories separated with a colon:. When you change \$PATH you should know that the directories are searched for a executable program in the same order as they are specified in \$PATH. To set a variable to a certain value use the export command, e.g. to set \$GREETING to Good morning use the following command:

```
Gretchen:~ thijscoenen$ export GREETING="Good morning"
Gretchen:~ thijscoenen$ echo $GREETING
Good morning
Gretchen:~ thijscoenen$
```

This variable will be defined as long as your BASH session exists. If you are running several BASH sessions, the variable will only be defined for that one session where it was defined. To define a variable for all future BASH session you should edit the settings file for your BASH sessions. This file is probably called <code>.bashrc</code> (Linux) or <code>.bash_profile</code> (Mac OS X) in your home directory. Be careful editing these files, getting it wrong may make your shell inoperable.

If you want to know which environment variables are defined in your shell and what their values are you can use \underline{env} . Running this command will result in a list of environment variables and their values. Because this is a long list I suggest you run this command on your own computer.

2.2.14 UNIX Pipes

So far we have treated a number of simple commands and utilities available on the command line. The power of the UNIX command line partially derives from the ability to connect different commands. The output of one program can be sent to another program using a so-called pipe. A pipe is signified with the | character. E.g. to use grep to look for a file called .bash_profile in my home directory:

```
Gretchen:~ thijscoenen$ ls -la | grep ".bash_profile"
-rw-r--r-- 1 thijscoenen staff 573 22 jul 23:38 .bash_profile
Gretchen:~ thijscoenen$
```

This may be a very simple example but the principle generalizes easily. The next example shows how you can search through a directory with some type of pulsar data files, looking for the dispersion measure, sorting by dispersion measure and then looking at only the first 10 lines:

```
Gretchen:00000143 thijscoenen$ ls *.inf | wc -l
Gretchen:00000143 thijscoenen$ cat *.inf | grep "Dispe" | sort -n -k 6 | head -n 10
Dispersion measure (cm-3 pc)
                                   = 2.6
Dispersion measure (cm-3 pc)
                                     = 2.65
Dispersion measure (cm-3 pc)
Dispersion measure (cm-3 pc)
                                     = 2.75
Dispersion measure (cm-3 pc)
Dispersion measure (cm-3 pc)
Dispersion measure (cm-3 pc)
Dispersion measure (cm-3 pc)
                                     = 2.95
Dispersion measure (cm-3 pc)
Dispersion measure (cm-3 pc)
                                     = 3.05
Gretchen: 00000143 thijscoenen$
```

Understanding how you can combine different UNIX command line utilities can help you automate boring tasks. This document is not about BASH programming so I will stop here now.

2.2.15 Output Redirects

The output of programs that shows up in your shell was written to "standard out" or "standard error" (a program should use the former for normal output while the latter can be used for errors or warnings). If you want these messages in a text file, you could copy the text from your shell into a text editor and save a file, but that is a lot of work. In stead you can just redirect standard out to a text file with a > sign:

```
Gretchen:coolstuff thijscoenen$ ls -l > blah.txt

Gretchen:coolstuff thijscoenen$ cat blah.txt

total 312

-rw-r--r-- 1 thijscoenen staff 0 15 aug 16:35 Whatever
-rw-r--r-- 1 thijscoenen staff 147731 22 jul 23:27 alice.txt
-rw-r--r-- 1 thijscoenen staff 0 28 aug 01:31 blah.txt
-rwxr--r-- 1 thijscoenen staff 43 7 aug 18:02 hello
-rw-r--r-- 1 thijscoenen staff 50 11 aug 14:35 noperm

Gretchen:coolstuff thijscoenen$
```

If you want to capture both standard out and standard error in a file you can add $\underline{2-61}$ to the end of the redirect

```
Gretchen:~ thijscoenen$ python divide_by_zero.py
Hi I'll divide by zero!
The result is
Traceback (most recent call last):
   File "divide_by_zero.py", line 2, in <module>
        print "The result is", 1/0
ZeroDivisionError: integer division or modulo by zero
Gretchen:~ thijscoenen$ python divide_by_zero.py > output1.txt
Traceback (most recent call last):
   File "divide_by_zero.py", line 2, in <module>
```

```
print "The result is", 1/0
ZeroDivisionError: integer division or modulo by zero
Gretchen:~ thijscoenen$ cat output1.txt
Hi I'll divide by zero!
The result is
Gretchen:~ thijscoenen$ python divide_by_zero.py > output2.txt 2>&1
Gretchen:~ thijscoenen$ cat output2.txt
Hi I'll divide by zero!
The result is
Traceback (most recent call last):
   File "divide_by_zero.py", line 2, in <module>
        print "The result is", 1/0
ZeroDivisionError: integer division or modulo by zero
Gretchen:~ thijscoenen$
```

In this example you can see that Python sends the text associated with an ZeroDivisionError to standard error and the rest of the messages to standard out. The file output1.txt only contains the text that went to standard out, while the file output2.txt contains both the text for standard out and standard error. In case you do not want to overwrite an existing file, but append to the new output to it replace the \geq with \geq .