

Intermediate Linux Course

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More Commandline Tools

Here is a quick list of useful commandline tools which will be used throughout the rest of the document. Many of these tools have quite extensive functionality and only a very limited part can be discussed here, so the reader is encouraged to read more about these using the links given in the in the links section...

1.1 Commandline Tools

1.1.1 GZIP

gzip is a compression/decompression tool.

```
Usage: gzip [options] file(s)
```

When used on a file (without any parameters) it will compress it and replace the file by a compressed version with the extension '.gz' attached:

```
# ls textfile*
  textfile
# gzip textfile
# ls textfile*
  textfile.gz
```

To revert this / to uncompress, use the parameter -d:

```
# ls textfile*
  textfile.gz
# gzip -d textfile
# ls textfile*
  textfile
```

Note: As a convenience, on most Linux systems, a shellscript named gunzip exists which simply calls gzip -d

1.1.2 TAR

tar (tape archive) is a tool to handle archives. Initially it was created to combine multiple files/directories to be written onto tape, it is now the standard tool to collect files for distribution or archiving.

tar stores the permissions of the files within an archive and also copies special files (such as symlinks etc.), which makes it an ideal tool for archiving... Usually tar is used in conjunction with a compression tool such as gzip to create a compressed archive:

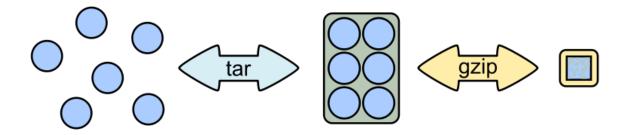


Fig. 1.1: source: Th0msn80 (Wikipedia)

The most common commandline switches are:

Option:	Effect:
-c	create an archive
-t	test an archive
-x	extract an archive
-z	use gzip compression
-f	filename filename of the archive

Note: Don't forget to specify the target filename. It needs to follow the -f parameter. Although you can combine options like such: tar -czf archive.tar the order matters, so tar -cfz archive.tar will *not* do what you want...

Creating an archive containing two files:

```
# tar -cf archive.tar textfile1 textfile2
```

Listing the contents of an archive:

```
# tar -tf archive.tar
textfile1
textfile2
```

Extracting an archive:

```
# tar -xf archive.tar
```

Creating and extracting a compressed archive containing two files:

```
# tar -czf archive.tar.gz textfile1 textfile2
# tar -xzf archive.tar.gz
```

Creating a backup (eg. before doing something dangerous?):

```
 \begin{tabular}{ll} \# tar -czf /folder/containing/the/BACKUP.tgz /folder/you/want/to/$$ $\hookrightarrow backup $$ \end{tabular}
```

1.1.3 GREP

grep finds lines matching a pattern in textfiles.

Usage: grep [options] pattern file(s)

```
# grep -i ensembl P04637.txt

DR Ensembl; ENST00000269305; ENSP00000269305; ENSG00000141510.
DR Ensembl; ENST00000359597; ENSP00000352610; ENSG00000141510.
DR Ensembl; ENST00000419024; ENSP00000402130; ENSG00000141510.
DR Ensembl; ENST00000420246; ENSP00000391127; ENSG00000141510.
DR Ensembl; ENST00000445888; ENSP00000391478; ENSG00000141510.
DR Ensembl; ENST00000455263; ENSP00000398846; ENSG00000141510.
```

Useful options:

Option:	Effect:
-V	Print lines that do not match
-i	Search case-insensitive
-1	List files with matching lines, not the lines itself
-L	List files without matches
-с	Print count of matching lines for each file

Count the number of fasta sequences (they start with a ">") in a file:

```
# grep -c '>' twoseqs.fasta
2
```

List all files containing the term "Ensembl":

```
# grep -l Ensembl *.txt
P04062.txt
P12931.txt
```

Search a file compressed with gzip using zgrep:

```
# zgrep -c '@M34567' IlluminaReads.fastq.gz 34956188
```

1.1.4 REV

rev is a tool that reverses lines of input.

Usage: rev file

rev can take input from STDIN as well as from a file, which can be useful if you need to reverse the output of a process.

You can combine rev with the cut tool, to capture the last columns in a file, without first needing to know the total number of columns.

Note the double use of rev in the example above - the output of the cut command must be reversed to restore the original orientation of the input file.

1.1.5 FMT

fmt is used to control the format of text input.

```
Usage: fmt [options] file(s)
```

By using fmt you can control the width and alignment of lines of text, while maintaining the larger structural elements such as paragraph breaks and indentation.

The most powerful use case when working with files containing data, is to convert a vector of values into a single column:

```
# echo "sample1 sample2 sample3 sample4 sample5" | fmt 1
  sample1
  sample2
  sample3
  sample4
  sample5
```

1.1.6 XARGS

xargs can be used to provide file contents or output of one command as arguments to the next.

```
Usage: xargs [options] [ tool [options] [arguments] ]
```

By default, xargs passes the strings given to it onto the echo command.

```
# cat motifs.txt
KPLGVALTNRFGEDADERID
RPIGPEIQNRFGENAEERIP
```

```
RSVATQVFNRFGDDTESKLP

# cat motifs.txt | xargs

KPLGVALTNRFGEDADERID RPIGPEIQNRFGENAEERIP RSVATQVFNRFGDDTESKLP
```

In this way we can achieve the reverse of the row vector -> column operation performed in the fmt example above. But xargs can be used for much more powerful things than only echoing command output. By providing an argument to xargs we can specify the tool/command that we want xargs to pass the strings to as arguments.

Use xargs in combination with the find command, allowing you to operate on multiple files across multiple locations at once. For example, to search for the word 'protein' in all .txt files underneath the 'Documents' directory, we could use the approach below:

```
# find ~/Documents -name '*.txt' | xargs grep 'protein'
DNA.txt:living organisms and many viruses. Along with RNA ...
DNA.txt:within proteins. The code is read by copying stret...
DNA.txt:chromatin proteins such as histones compact and or...
DNA.txt:structures guide the interactions between DNA and ...
P04062.txt:RT "Identification and quantification of N-li...
```

Similarly, we can use xargs and find to quickly delete multiple files spread throughout the filesystem.

```
# find /tmp -name '*.tmp' | xargs rm
```

Take care whenever you use commands like rm and mv that overwrite/remove files permamently. Helpfully, xargs provides an option -p that will prompt the user before executing commands.

```
# find / -size +5GB | xargs -p rm
rm /home/toby/alignments/giant_alignment.bam? y
```

This is a good way of sweeping your filesystem to find the largest files and then choosing

whether to remove them. You could employ a similar approach with xargs to compress these large files.

If you need to control where exactly the strings passed to xargs are placed in the command that it subsequently calls, use the -I option:

```
# find /home/toby/alignments -name "*.fasta" | xargs -I OLDFASTA mv⊔ →OLDFASTA OLDFASTA.old
```

Useful options:

Option:	Effect:	
-n INT	pass INT strings as arguments to each invocation of tool	
-0	use NULL as separator (good for handling strings/filenames containing	
	spaces)	
-t	echo commands to STDERR as they are executed	
-p	prompt with command before execution	
-I	specify placeholder name for arg	
STRING		

1.1.7 SED

sed is a Stream EDitor, it modifies text (text can be a file or a pipe) on the fly.

Usage: sed command file,

The most common usecases are:

Usecase	Command:
Substitute TEXT by REPLACEMENT:	s/TEXT/REPLACEMENT/
Transliterate the characters x a, and y b:	y/xy/ab/
Print lines containing PATTERN:	/PATTERN/p
Delete lines containing PATTERN:	/PATTERN/d

```
# echo "This is text." | sed 's/text/replaced stuff/'
This is replaced stuff.
```

By default, text substitution are performed only once per line. You need to add a trailing 'g' option, to make the substitution 'global' ('s/TEXT/REPLACEMENT/g'), meaning all occurrences in a line are substituted (not just the first in each line). Note the difference:

```
# echo "ACCAAGCATTGGAGGAATATCGTAGGTAAA" | sed 's/A/_/'
   _CCAAGCATTGGAGGAATATCGTAGGTAAA
# echo "ACCAAGCATTGGAGGAATATCGTAGGTAAA" | sed 's/A/_/g'
   _CC__GC_TTGG_GG__T_TCGT_GGT___
```

You can use transliteration to replace all instances of a character with another character. For example, to switch Thymidines to Uridines in a sequence:

```
# echo "AGTGGCTAAGTCCCTTTAATCAGG" | sed 'y/T/U/'
AGUGGCUAAGTCCCUUUAAUCAGG
```

In the pattern specified in the sed command, each character in the first set is replaced with the character in the equivalent position in the second set. For example, to get the reverse transcript of a DNA sequence:

```
# echo "AGTGGCTAAGTCCCTTTAATCAGG" | sed 'y/ACGT/UGCA/'
UCACCGAUUCAGGGAAAUUAGUCC
```

This is the complementary sequence, but we wanted the reverse complement, so we need to use the Linux command rev to reverse the output of the sed command:

```
# echo "AGTGGCTAAGTCCCTTTAATCAGG" | sed 'y/ACGT/UGCA/' | rev
CCUGAUUAAAGGGACUUAGCCACU
```

When used on a file, sed prints the file to standard output, replacing text as it goes along:

```
# echo "This is text" > textfile
# echo "This is even more text" >> textfile
# sed 's/text/stuff/' textfile
This is stuff
This is even more stuff
```

sed can also be used to print certain lines (not replacing text) that match a pattern. For this you leave out the leading 's' and just provide a pattern: '/PATTERN/p'. The trailing letter determines, what sed should do with the text that matches the pattern ('p': print, 'd': delete)

```
# sed '/more/p' textfile
This is text
This is even more text
This is even more text
```

As sed by default prints each line, you see the line that matched the pattern, printed twice. Use option '-n' to suppress default printing of lines.

```
# sed -n '/more/p' textfile
This is even more text
```

Delete lines matching the pattern:

```
# sed '/more/d' textfile
This is text
```

Multiple sed statements can be applied to the same input stream by prepending each by option '-e' (edit):

```
# sed -e 's/text/good stuff/' -e 's/This/That/' textfile
That is good stuff
That is even more good stuff
```

Normally, sed prints the text from a file to standard output. But you can also edit files in place. Be careful - this will change the file! The '-i' (in-place editing) won't print the output. As a safety measure, this option will ask for an extension that will be used to rename the

original file to. For instance, the following option '-i.bak' will edit the file and rename the original file to textfile.bak:

```
# sed -i.bak 's/text/stuff/' textfile
# cat textfile
This is stuff
This is even more stuff
# cat textfile.bak
This is text
This is even more text
```

1.1.8 AWK

awk is more than just a command, it is a complete text processing language (the name is an acronym of the author's names). Each line of the input (file or pipe) is treated as a record and is broken into fields. Generally, awk commands are of the form:

```
awk condition { action }
```

where:

- condition is typically an expression
- action is a series of commands

If no condition is given, the action is applied to each line, otherwise just to the lines that match the condition.

```
# awk '{print}' textfile
This is text
This is even more text

# awk '/more/ {print}' textfile
This is even more text
```

awk reads each line of input and automatically splits the line into columns. These columns can be addressed via \$1, \$2 and so on (\$0 represents the whole line). So an easy way to print or rearrange columns of text is:

```
# echo "Bob likes Sue" | awk '{print $3, $2, $1}'
Sue likes Bob

# echo "Master Obi-Wan has lost a planet" | awk '{print $4,$5,$6,
→$1,$2,$3}'
lost a planet Master Obi-Wan has
```

awk splits text by default on whitespace (spaces or tabs), which might not be ideal in all situations. To change the field separator (FS), use option '-F' (remember to quote the field separator):

```
# echo "field1, field2, field2" | awk -F',' '{print $2, $1}'
field2 field1
```

Note two things here: First, the field separator is not printed, and second, if you want to have space between the output fields, you actually need to separate them by a comma or they will be concatenated together...

```
# echo "field1,field2,field2" | awk -F',' '{print $1 $2 $3}'
field1field2field3
```

You can also combine the pattern matching and the column selection techniques, in this example we'll print only the third column of the lines matching the pattern 'PDBsum' (case sensitive):

```
$ awk '/PDBsum/ {print $3}' P12931.txt
1A07;
1A08;
1A09;
1A1A;
...
```

awk really is powerful in filtering out columns, you can for instance print only certain columns of certain lines. Here we print the third column of those lines where the second column is 'PDBsum':

```
# awk '$2=="PDBsum;" {print $3}' P12931.txt
1A07;
1A08;
1A09;
1A1A;
...
```

Note the double equal signs "==" to check for equality and note the quotes around "PDB-sum;". If you want to match a field, but not exactly, you can use ' \sim ' instead of '==':

```
# awk '$4~"sum" {print $3}' P12931.txt
1A07;
1A08;
1A1A;
...
```

1.2 I/O Redirection

Three IO "channels" are available by default:

- Standard input (STDIN, Number: 0): The input for your program, normally your keyboard but can be an other program (when using pipes or IO redirection)
- **Standard output (STDOUT, Number: 1)**: Where your program writes its regular output to. Normally your terminal
- Standard error (STDERR, Number: 2): Where your programs normally write their error message to. Normally your terminal

Input, output and error messages can be redirected from their default "targets" to others. If using the file descriptor numbers (0, 1, 2) in redirections, then there must be no whitespace between the numbers and the redirection operators.

Hint: Redirect to /dev/null to discard the output of any command

Write the output of *cmd* into *afile*. This will **overwrite** *afile*:

```
$ cmd > afile
```

Write the output of *cmd* into *afile*. This will **append** to *afile*:

```
$ cmd >> afile
```

Discard the output of cmd

```
$ cmd > /dev/null
```

Write the output of *cmd* into *afile* (overwriting *afile*!) and write STDERR to the same place:

```
$ cmd > afile 2>&1
```

Append the output and error messages of cmd to afile:

```
$ cmd >> afile 2>&1
```

Same as above:

```
$ cmd > afile 2> afile
```

Append the output of *cmd* to *afile* and discard error messages:

```
$ cmd >> afile 2>/dev/null
```

Three times the same: Discard output and error messages completely:

```
$ cmd > /dev/null 2>&1
$ cmd > /dev/null 2>/dev/null
$ cmd >& /dev/null
```

Use output of *cmd*2 as standard input for *cmd*1:

```
$ cmd1 < cmd2
```

See also

• Bash One-Liners Explained, Part III: All about redirections ¹

¹ http://www.catonmat.net/blog/bash-one-liners-explained-part-three

- Bash Redirections Cheat Sheet ²
- Redirection Tutorial ³

1.3 Variables

The shell knows two types of variables: "Local" *shell* variables and "global" exported *environment* variables. By convention, environment variables are written in uppercase letters.

Shell variables are **only available to the current shell** and not inherited when you start another shell or script from the commandline. Consequently, these variables will not be available for your shellscripts.

Environment variables are passed on to shells and scripts started from your current shell.

1.3.1 Setting, Exporting and Removing Variables

Variables are set (created) by simply assigning them a value

```
$ MYVAR=something
$
```

Note: There must be no whitespace surrounding the equal sign!

To create an environment variable, export is used. You can either export while assigning a value or in a separate step. Both of the following procedures are equivalent:

```
1. $ export MYGLOBALVAR="something else" $
```

```
2. $ MYGLOBALVAR="something else" $ export MYGLOBALVAR $
```

Note: There is no \$ in front of the variable: To reference the variable itself (not its content) the name is used without \$

Variables are removed with unset:

```
$ unset MYVAR
$
```

1.3. Variables

² http://www.catonmat.net/blog/bash-redirections-cheat-sheet

³ http://wiki.bash-hackers.org/howto/redirection_tutorial

Note: Assigning a variable an empty value (i.e. MYVAR=) will *not* remove it but simply set its value to the empty string!

1.3.2 Listing Variables

You can list all your current environment variables with env and all shell variables with set. The list of shell variables will also contain all environment variables

```
$ set | more
BASH=/bin/bash
BASH_ARGC=()
BASH_VERSION='4.1.2(1)-release'
COLORS=/etc/DIR_COLORS.256color
COLUMNS=181
...
$
```

1.3.3 Variable Inheritance

Only environment variables will be available in shells and scripts started from your current shell. However in shell commands run in subshells (i.e. commands run within round brackets) also local (shell) variables of your current shell are available.

Examples

Consider the following small shellscript "vartest.sh':

```
#!/bin/sh
echo $MYLOCALVAR
echo $MYGLOBALVAR
echo ----
```

We will use it in the following examples to illustrate the various variable inheritances:

1. Set the variables and run the script i.e. in a new shell:

```
$ export MYGLOBALVAR="I am global"
$ MYLOCALVAR="I am local"
$ ./vartest.sh
I am global
-----
$
```

2. "source" the script, i.e. run it within your current shell:

```
$ source ./vartest.sh
I am local
I am global
```

```
$
```

3. Access the variables in a subshell:

```
$ (echo $MYGLOBALVAR; echo $MYLOCALVAR)
I am global
I am local
$
```

1.4 Tips and Tricks

1.4.1 Quoting

In programming it is often necessary to "glue together" certain words. Usually, a program or the shell splits sentences by whitespace (space or tabulators) and treats each word individually. In order to tell the computer that certain words belong together, you need to "quote" them, using either single (') or double (") quotes. The difference between these two is generally that within double quotes, variables will be expanded, while everything within single quotes is treated as string literal. When setting a variable, it doesn't matter which quotes you use:

```
# MYVAR=This is set
  -bash: is: command not found

# MYVAR='This is set'
# echo $MYVAR
  This is set
# MYVAR="This is set"
# echo $MYVAR
  This is set
```

However, it does matter, when using (expanding) the variable: Double quotes:

```
# export MYVAR=123
# echo "the variable is $MYVAR"
the variable is 123
# echo "the variable is set" | sed "s/set/$MYVAR/"
the variable is 123
```

Single quotes:

```
# export MYVAR=123
# echo 'the variable is $MYVAR'
the variable is $MYVAR
# echo "the variable is set" | sed 's/set/$MYVAR/'
the variable is $MYVAR
```

Weird things can happen when parsing data/text that contains quote characters:

```
# MYVAR='Don't worry. It's ok.'; echo $MYVAR
>
# you need to press Ctrl-C to abort
# MYVAR="Don't worry. It's ok."; echo $MYVAR
Don't worry. It's ok.
```

Expanding and Escaping

You already learned how to expand a variable such that its value is used instead of its name:

```
# export MYVAR=123
# echo "the variable is $MYVAR"
the variable is 123
```

"Escaping" a variable is the opposite, ensuring that the literal variable name is used instead of its value:

```
# export MYVAR=123
# echo "the \$MYVAR variable is $MYVAR"
the $MYVAR variable is 123
```

Note: The "escape character" is usually the backslash "\".

1.4.2 Keyboard Shortcuts

When getting comfortable with working on the command line, it can be helpful to learn some tricks that can save you time, better manage your session, and help you to avoid annoying errors due to typos.

Tab-Completion: A Reminder

You're probably already aware of tab-completion, where you push the TAB key to complete the name of a command, file, directory, etc. This is a huge time-saver and great tool for preventing the accidental inclusion of errors.

Move Quickly Through the Command Line

As well as tab-completion, you might be aware of CTRL-A to jump the cursor to the beginning of a line, and CTRL+E to jump to the end. On most systems, using the arrow keys while holding down the alt key will jump left or right by one word (or word-like string) at a time.

When editing a line, CTRL-W can be used to delete left from the current cursor position to the next beginning of a word. CTRL+U will delete left from the current cursor position to the beginning of the line.

Searchable Command History

You're probably aware of the command history, and that you can use the up and down arrow keys to scroll back and forth throughout that history. You can also use CTRL+R to search that command history. If you type CTRL+R and then the beginning of a command, you will see the most recent command in the history that matches that pattern (anywhere in the command). You can hit CTRL+R again to scroll backwards through the matches.

Job Management

Use CTRL+C to abort the current process, and CTRL+D to close the current shell.

If you don't want to abort, you might instead want to use CTRL+Z to suspend the current process. You can resume the most recently-suspended job with fg, to run it in the 'foreground' of the shell, or bg to run it in the 'background'. In the shell, a command running in the foreground is a job that will prevent the user from executing further commands until the job has finished. A job running in the background will continue to run while the user can carry on using the shell prompt to execute other commands. On a related note: to put a job in the background when you execute it, just add "&" to the end of the command.

If you have multiple jobs running/suspended at one time, you can view a list of these processes and their current status with jobs:

As mentioned before, you can restart the most recently-suspended job with fg or bg. To restart another job in the list, you can refer to it with %1 for job number 1 in the list (sleep 100 in the example above), %2 for job 2, and so on. If, instead of restarting a job, you want to kill a suspended process, you can use the kill command and specify the job afterwards:

```
# jobs
[1]+ Stopped sleep 100
[2]- Running sleep 250 &
# kill %2
[2]- Terminated: 15 sleep 250
```

The jobs list contains details of all running or stopped tasks that were initiated within the current session. If you try to leave a session with exit while you still have a job running or suspended, you will receive a warning message. (Note that this is one of the rare occasions where the command line interface will ask you if you're sure before doing something that could be potentially bad for you.) Use exit a second time and the session will end, killing any remaining jobs as it does so.

1.4. Tips and Tricks

Commandline Exercises

2.1 TAR & GZIP

- 1. Use gzip to compress the file P12931.txt
- 2. Decompress the resulting file P12931.txt.gz (revert previous command)
- 3. Use tar to create an archive containing all fasta files in the current directory into an archive called "fastafiles.tar"
- 4. Use gzip to compress the archive "fastafiles.tar"
- 5. How can you achieve the two previous steps "using tar to create archive" and "gzip the archive" in one command?
- 6. Test (list the contents of) the compressed archive "fastafiles.tar.gz"
- 7. Download the compressed PDB file for entry 1Y57 from rcsb.org (eg. wget "http://www.rcsb.org/pdb/files/1Y57.pdb.gz") and decompress it.

2.2 GREP

- 1. Which of the DNA files ENST0* contains "TATATCTAA" as part of the sequence?
- 2. List only the names of the DNA files ENST0* that contain "CAACAAA" as part of the sequence.
- 3. Considering the previous example, would you consider grep a suitable tool to perform motif searches? Why not? Try to find the pattern "CAACAAA" by manual inspection of the first three lines of each sequence.
- 4. Count the number of ATOMs in the file 1Y57.pdb.
- 5. Does this number agree with the annotated number of atoms? The PDB file has a comment which tells you how many atoms there are annotated in this file. This comment can be found by searching for the term "protein atoms" (use quotes and case insensitive search here!).

2.3 REV

1. By combining rev with the cut tool, print the last word of each line in DNA.txt. Make sure that the words are readable when they are printed out.

2.4 XARGS

- 1. Use xargs to print the first line of the files listed in to_be_previewed.txt
- 2. Create a copy of each of these files by passing the lines in to_be_copied.txt two-at-a-time to cp
- 3. A better way to back up these files might be to keep the original names while copying them. Make another copy of each file listed in to_be_previewed.txt, adding ".backup" onto the end of each filename. (Hint: remember the "-I" option!)
- 4. ADVANCED: we've made a bit of a mess now, and it's time to clean up. Make a new directory called 'garbage', which you will move all these new files into it by combining the find tool with xargs and mv. Use find to find all files in the current directory that were last modified less than ten minutes ago, and xargs with mv to change their location. BE CAREFUL! ..Hint:: you'll need to check out the options available for find, and you might consider using the "-p" option with xargs to help avoid accidentally deleting something that you might regret!) Once you've moved the files, check the contents of the 'garbage' directory and, if you're sure that you don't want any of those files anymore, delete them and the directory.

2.5 SED

- 1. Use sed to print only those lines that contain "version" in the files P05480.txt and P04062.txt
- 2. Use sed to change the text "sequence version 3" to "sequence version 4" in the files P05480.txt and P04062.txt (without actually changing the files, just printing)
- 3. Use sed to update the text "sequence version 3" to "sequence version 4" in the files P05480.txt and P04062.txt (this time, make the changes directly in the files)
- 4. Replace (transliterate) all occurrences of "r" by "l" and "l" by "r" (at the same time) in the file PROTEINS.txt (so that "structural" becomes "stluctular")

2.6 AWK

- 1. Use awk to print only those lines that contain "version" in the files P12931.txt and P05480.txt and think about how this procedure is different to sed.
- 2. For all FASTA files that begin with "P" ("P*.fasta") print only the second item of the header (split on "|") eg. for ">sp|P12931|SRC_HUMAN Proto-oncogene", print only "P12931"

- 3. The file "P12931.csv" contains phosphorylation sites the in pro-"P12931.csv" P12931. (If file not exist, the use wget http://phospho.elm.eu.org/byAccession/P12931.csv to download it).
 - (a) Column three of this file lists the amino acid position of the phosphorylation site. You are only interested in position 17 of the protein. Try to use "grep" to filter out all these lines containing "17".
 - (b) Now use awk to show all lines containing "17".
 - (c) Next try to show only those lines where column three equals 17 (Hint: The file is semicolon-separated...).
 - (d) Finally print the PMIDs (column 6) of all lines that contain "17" in column 3.

2.7 Quoting and Escaping

- 1. Familiarize yourself with quoting and escaping.
 - 1. Run the following commands to see the difference between single and double quotes when expanding variables:

```
$ echo "$HOSTNAME"
...
$ echo '$HOSTNAME'
```

2. Next, use ssh to login to a different machine to run the same command there, again using both quoting methods:

```
$ ssh pc-atcteach01 'echo $HOSTNAME'
...
$ ssh pc-atcteach01 "echo $HOSTNAME"
```

2. Closely inspect the results; is that what you were expecting? Discuss this with your neighbour.

Basic Shell Scripting

3.1 What is a Script?

A script is nothing else than a number of shell command place together in a file. The simplest script is maybe just a complex oneliner that you don't want to type each time again. More complex scripts are seasoned with control elements (conditions and loops) which allow for a sophisticated command flow. scripts might allow for configuration and customization, thus allowing one script to be flexibly used in several different environments. Whatever you do in a script, you can also do on the commandline. This is also the first way to test your scripts step by step!

3.2 Script Naming and Organization

It is good practice - though not technically required - to give your scripts an extension which specifies their type. I.e. ".sh" for Bourne Shell and Bourne Again Shell scripts, ".csh" for C-Shell scripts. Sometimes ".bash" for Bourne Again Shell scripts is used.

We recommend to either store all scripts in one location (e.g. ~/bin) and add this location to your \$PATH variable (see *Variables* (page 11)) or to store the scripts together with the files that are processed by the script.

Hint: If you use scripts to process data, then the scripts should probably be archived together with the data files!

3.3 Running a Script

There are basically three ways to run a script, regardless of the language in which the script is written:

1. where the location to your script is not in your \$PATH variable, then you have to specify the full path to the script:

```
$ /here/is/my/script.sh
[...]
$
```

2. where the location to the script is in the \$PATH variable, then you can simply type its name:

```
$ script.sh
[...]
$
```

In both situations, the script will need to have execute permissions to be run. If for some reason you can only read but not execute the script, then it can still be run in the following way:

3. by specifying the interpreter (i.e. the program required to run the script). For shellscripts this is the appropriate shell). The full path (relative or absolute) to the script has to be provided in this case, no matter whether the script location is already contained in \$PATH or not:

```
$ /bin/sh /here/is/my/script.sh
[...]
$
```

3.3.1 Basic Structure of a Shellscript

Shellscripts have the following general structure:

- A line starting with "#!" which defines the interpreter. This line is called the *shebang line* and must be the first line in a script.
- A section where the configuration takes place, e.g. paths, options and commands are defined and it is made sure, that all prerequisites are met.
- A section where the actual processing is done. This includes error handling.
- A controlled exit sequence, which includes cleaning up all temporary files and returning a sensible exit status.

This is merely a recommendation to keep your scripts well structured. None of these sections are mandatory.

3.3.2 Readability and Documentation

Make your script easily readable. Use comments and whitespace and avoid super compact but hard to understand commandlines. Always take into account that not only the shell, but also human beings will probably have to read and understand your script. (see *Breaking up long lines* (page 36)) Even if your script is very simple - document it! This helps others understand what you did, but - most importantly - it helps you remember what you did, when you have to reuse the script in the future.

Documentation is done either by writing comments into the script or by creating a special documentation file (README.txt or similar). Documenting in the script can be done in several ways:

• A preamble in the script, outlining the purpose, parameters and variables of the script as well as some information about authorship and perhaps changes.

• Within the script as blocks of text or "End of line" comments.

To write comments, use the hash sign ("#"). Everything after a "#" is ignored when executing a script.

3.3.3 Anatomy of a Shellscript

Let's have a look at the following script, breaking it down into individual parts. First, the full script:

```
#!/bin/sh
                                                               Shebang line
                                                               Preamble with a short
# myscript.sh
                                                               description, usage
# General purpose script for extracting Glycine # occurrences in a datafile.
                                                               information, authorship etc.
                                                               etc.
# Usage: myscript.sh datafile
# Exit values: 1: No datafile given or file
                     doesn't exist
                 2: No Glycine found
# Author: Me, myself and I
# Date: Heidelberg, December 12., 2012
# --- Configuration ---
                                                               Configuration
GREPCMD=/bin/grep
DATAFILE=$1
# --- Check prerequisites ---
                                                               Checking prerequisites and
# first check for $1
                                                               sane environment
if [ -z $DATAFILE ]
  echo "No datafile given" 1>&2 # print on STDERR echo "USAGE: $0 datafile"
  exit 1
# then check if the file exists
if [ ! -f $DATAFILE ]
  echo "Datafile $DATAFILE does not exist!" 1>&2
  exit 1
# --- Now processing---
$GREPCMD -q Glycine $DATAFILE # Where is Glycine?
                                                               This is what you actually
                                                               wanted to do
# --- Exit ---
if [ $? -eq 0 ]
                                                               Ensure a valid and
                                                               meaningful exit status
then
  exit 0
else
  exit 2
fi
```

You can see from this example, that very often the actual computation is only a small part of the code. The rest of the scripts deal with prerequisites, error handling, user dialogue, exit status etc. etc.

3.3.4 Reporting Success or Failure - The Exit Status

Commands report their success or failure by their exit status. An exit status of 0 (zero) indicates success(!), while any exit status greater then 0 indicates an error. Some commands report more than one error status. Refer to the respective manpages to see the meanings of the different exit stati. The exit status of a script is usually the exit status of the last executed command, which is reported by the environment variable \$?:

Example: Displaying the exit status of the (successfully run) pwd command:

```
$ pwd
/home/fthommen
$ echo $?
0
$
```

Example: Displaying the exit status of the (unsuccessfully run) touch command:

```
$ touch /afile
touch: cannot touch '/afile': Permission denied
$ echo $?
1
$
```

See *Ensuring a Sensible Exit Status* (page 35) about how to control the exit status of your script.

3.3.5 Command Grouping and Sequences

Commands can be concatenated to be executed one after the other unconditionally or based on the success of the respective previous command:

cmd1; cmd2 - Execute commands in sequence

Example: Create a directory and change into it:

```
$ pwd
/home/fthommen
$ mkdir a; cd a
$ pwd
/home/fthommen/a
$
```

cmd1 && cmd2 - Execute cmd2 only if cmd1 was successful:

Example: Create a directory and, if successful, change into it:

```
$ pwd
/home/fthommen
$ mkdir a && cd a
$ pwd
/home/fthommen/a
$
```

Example: Confirm that /etc exists:

```
$ cd /etc && echo "/etc exists"
/etc/exists
$
```

*cmd*1 | | *cmd*2 - Execute cmd2 only if cmd1 was not successful:

Example: Create a directory and, if not successful, print an error message:

```
$ mkdir /bin/a || echo "mkdir didn't work!"
mkdir: cannot create directory `/bin/a': Permission denied
mkdir didn't work!
$
```

Example: Decompress a gzipped file if it exists, or download it if not:

```
$ gzip -d 2W73.pdb || wget "http://www.rcsb.org/pdb/files/2W73.pdb.gz"
$
```

You can mix multiple && and || controls into a single line.

Example: Create a directory and, if successful, change into it, if not successful, print an error message:

```
$ mkdir /bin/a && cd a || echo "Could not create directory a"
mkdir: cannot create directory `/bin/a': Permission denied
Could not create directory a
$
$ mkdir ~/a && cd ~/a || echo "Could not create directory a"
$ pwd
/home/fthommen/a
$
```

(*cmds*) – Group commands to create one single output stream: The commands are run in a subshell (i.e. a new shell is opened to run them):

Example: Change into /etc and list content. You are still in the same directory as you were before:

```
$ pwd
/home/fthommen
$ (cd /etc; ls)
[... etc directory listing here ...]
$ pwd
/home/fthommen
$
```

{ cmds; } – Group commands to create one single output stream: The commands are run in the current (!) shell.

Note: The opening "{" must be followed by a blank and the last command must be succeeded by a *semicolon* (';'')

Example: Change into /etc and list its content. You are still in /etc after the bracketed expression (compare to the example above):

```
$ pwd
/home/fthommen
$ { cd /etc; ls; }
[... directory listing here ...]
$ pwd
/etc
$
```

3.4 Control Structures

The following syntax elements will be described for sh/bash and for csh/tcsh. However since this course is mainly about sh/bash, examples will only be given for sh/bash. Some notes about csh/tcsh specialities might be given in the text. This is only a selection of the most useful or most common elements. There are much more in the manpages. All shells offer myriads of possibilities which cannot possibly be demonstrated in this course. Some of the described features might be specific to bash and not be available in a classical Bourne Shell on other systems.

3.4.1 Conditional Statements

if - then - else

if -then -else is the most basic conditional statement: Do something depending on certain conditions. Its basic syntax is:

sh/bash	csh/tcsh
if condition1	if (condition) then
then	commands
commands	else if (condition2) then
elif condition2	more commands
then	[]
more commands	else
[]	even more commands
else	endif
even more commands	
fi	

Conditions can be either the **exit status of a command** or the **evaluation of a logical or arithmetic expression**:

1. Evaluating the exit status of a command: Simply use the command as condition. For example:

```
if grep -q root /etc/passwd
then
  echo root user found
```

```
else
echo No root user found
fi
```

Note: In *csh/tcsh*

- 1. To evaluate the exit status of a command it must be placed within curly brackets with blanks separating the brackets from the command: if ({ grep -q root /etc/passwd }) then [...]
- 2. Redirection of commands in conditions does not work

Hint: Redirect the output of the command to be evaluated to /dev/null if you are only interested in the exit status and if the command doesn't have a "quiet" option.

2. Evaluating of conditions or comparisons:

Conditions and comparisons are evaluated using a special command test which is usually written as "[" (no joke!). As "[" is a command, it must be followed by a blank. As a speciality the "[" command must be ended with ""]"" (note the preceding blank here)

Note: In csh/tcsh the test (or [) command is not needed. Conditions and comparisons are directly placed within the round braces.

Watch Out For The Exit Code!

It's important to consider the exit status of conditional blocks. An if-then-else block will return exit code 0, indicating success, as long as no errors were encountered during execution. This means that, if you use an if-then-elif block (i.e. without an else statement), your script will run successfully regardless of whether any of the conditions were actually met.

This might be what you want to happen, but in most circumstances it is good practise to include an else statement, to specify the desired behaviour when none of the expected conditions have been met. You could use this else block to exit the script with a non-zero code, print an error message, or anything else that could be useful for debugging in future.

Remember that it is often difficult to foresee every possible input/use case when you first write a script, and being diligent now will probably save you a lot of time and head-scratching in the future!

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sh/bash		csh/tcsh
	File condition	
-e file	file exists	-e file
-f file	file exists and is a regular file	-f file
-d file	file exists and is a directory	-d file
-r file	file exists and is readable	-r file
-w file	file exists and is writeable	-w file
-x file	file exists and is executable	-x file
-s file	file exists and has a size > 0	-
-	file exists and has zero size	-z file
	String Comparison	-
-n s1	String s1 has non-zero length	
-z s1	String s1 has zero length	
s1 = s2	Strings s1 and s2 are identical	s1 == s2
s1 != s2	Strings s1 and s2 differ	s1 != s2
string	String string is not null	
	Integer Comparison	
n1 -eq n2	n1 equals n2	n1 == n2
n1 -ge n2	n1 is greater than or equal to n2	n1 >= n2
n1 -gt n2	n1 is greater than n2	n1 > n2
n1 -le n2	n1 is less than or equal to n2	n1 <= n2
n1 -lt n2	n1 is less than n2	n1 < n2
n1 -ne n2	n1 it not equal to n2	n1 != n2
	Combination of conditions	
! cond	True if condition <i>cond</i> is not true	! cond
cond1 -a	True if conditions cond1 and cond2 are both	cond1 &&
cond2	true	cond2
cond1 -o cond2	True if conditions <i>cond1</i> or <i>cond2</i> is true	cond1 cond2

Examples: Test for the existence of the directory sequence_files:

```
if [ -e ./sequence_files ]
then
  ls -1 ./sequence_files/*.fasta
else
  echo no sequence_files directory here
fi
```

or:

```
if test -e ./sequence_files
then
  ls -1 ./sequence_files/*.fasta
else
  echo no sequence_files directory here
fi
```

Note: Bash supports another way of evaluating conditional expressions with [[expression]]. This syntax element allows for more readable expression combination and handles empty variables better. However it is not backwards compati-

ble with the original Bourne Shell. See the bash manpage for more information

case

The case statement implements a more compact and better readable form of if - elif - elif - elif etc. Use this if your variable (you can *only* check for variables with case) can have a distinct number of valid values. A typical usage of case will follow later.

The basic syntax is:

sh/bash	csh/tcsh
case variable in	switch (variable)
pattern1)	case pattern1:
commands	commands
;;	breaksw
pattern2)	case pattern2:
commands	commands
;;	breaksw
*)	default:
commands	commands
;;	endsw
esac	

Note: for the patterns "*", "?" and "[...]" can be used

Note: The "*)" (sh/bash) and "default:" (csh/tcsh) patterns are "catch-all" patterns which match everything not matched above. It is often used to detect invalid values of variable.

Note: Multiple patterns can be handled by separating them with "|" in sh/bash or by successive case statements in csh/tcsh.

Example: Check if /opt/ or /usr/ paths are contained in \$PATH:

```
case $PATH in
 */opt/* )
  echo /opt/ paths found in \$PATH
  ;;
 */usr/* )
  echo /usr/ paths found in \$PATH
  ;;
 *)
  echo '/opt and /usr are not contained in $PATH'
  ;;
esac
```

or:

```
case $PATH in
 */opt/* | */usr/* )
  echo /opt/ or /usr/ paths found in \$PATH
  ;;
*)
  echo '/opt and /usr are not contained in $PATH'
  ;;
esac
```

Note: Just like if-then-else blocks (see "Watch Out For The Exit Code!" in the previous section), a case block will return exit code 0 regardless of whether any of its options were matched during execution. Always try to design a "in all other circumstances" option, that is guaranteed to be met, so that your script will sensibly handle situations where the value(s) passed to case don't fall into any of your expected categories. Remember that cases are given priority by the order that they appear in the block, so make your "catch-all" case non-specific and place it last in the block to match anything that wasn't picked up by the other options.

3.4.2 Loops

for / foreach

The for and foreach statements respectively will loop through a list of given values and run the given statements for reach run:

sh/bash	csh/tcsh
for variable in list	foreach variable (list) commands
commands	end
done	

list is a list of strings, separated by whitespaces

Examples: List filenames and count number of sequences in every FASTA file in ./sequence_files:

```
for FILE in ./sequence_files/*.fasta
do
    echo " * $FILE"
    grep -c '\>' $FILE
done
or
for FILE in `ls ./sequence_files/*.fasta`
do
    echo " * $FILE"
    grep -c '\>' $FILE
done
```

while / until

The while and until loops execute your commands while (or until respectively) a certain condition is met:

sh/bash	csh/tcsh
while condition do commands done	while (condition) commands end
until condition do commands done	

The conditions are constructed the same way as those used in if statements.

Note: The until statement is not available in csh/tcsh.

"Manual" loop control

Instead of (or additionally to) the built-in loop control in for/foreach, while and until loops, you can control exiting and continuing them with break and continue: break "breaks out" of the innermost loop (loops can be nested!) and continues after the end of the loop. continue skips the rest of the current (innermost) loop and starts the next iteration

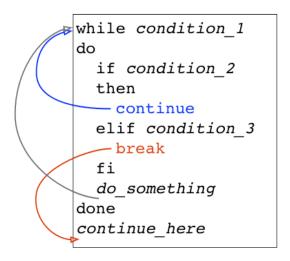


Fig. 3.1: Loop control

Symbol	
	Regular loop cycle
	break due to condition_2
	continue due to condition_3

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3.5 Making Scripts Flexible

Scripts are most useful, if they can be reused. Copying scripts and changing them to fit the new situation is time-consuming and error-prone. Additionally if you add an improvement to the current script, then all previous versions will stay without it. Having one script with the possibility to configure it, is usually the better way. Customization of scripts can be achieved by either using variables or by adding the possibility to use your own commandline options and arguments.

3.5.1 Configurable Scripts

Using Variables

Any value - be it paths, commands or options - that is specific to individual applications or your script, should not be hardcoded (i.e. used literally within the script). Instead you should use variables to refer to them:

Bad example: You have to change two instances of the path each time you want to list another directory:

```
#!/bin/sh
echo "The directory /etc contains the following files:"
ls /etc
```

Good example: The path is now in a variable and only one instance has to be changed each time (less work, fewer errors):

```
#!/bin/sh
MYDIR=/etc
echo "The directory $MYDIR contains the following files:"
ls $MYDIR
```

Of course, you'll still have to modify the script each time you want to list the content of another directory. A more flexible way of customization would be to use a settings file.

Using a Settings File

Instead of having your configurable section within the script, it can be "outsourced" to its own file. This file is basically a shellscript which is run within the primary script. To run commands from a file within the current environment, the commands source (bash, csh/tcsh) or . (dot) (sh/bash) are used:

The settings file, e.g. settings.ini:

```
MYDIR=/etc
```

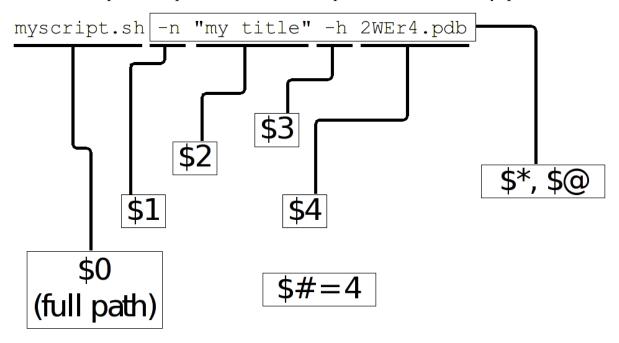
The script:

```
#!/bin/sh
. ./settings.ini
echo "The directory $MYDIR contains the following files:"
ls $MYDIR
```

3.5.2 Defining your own Commandline Options and Arguments

The best way to configure a script is to allow for your own commandline options and arguments. Commandline arguments are available within the script as so-called positional parameters \$1, \$2, \$3: etc. \$0: contains the name of the script. The variables important when dealing with commandline parameters are:

- **\$0:** path to the script. Either the path as you specified it or the full path if the script was executed through \$PATH
- **\$1, \$2, \$3, etc:** Positional parameters (i.e. commandline arguments)
- **\$#:** Current number of positional parameters
- **\$*:** All positional parameters. If used within double quotes ("\$*"), then it will expand to the list of all positional parameters, where the complete list is quoted
- **\$@:** All positional parameters. If used within double quotes ("\$@"), then it will expand to the list of all positional parameters, where each parameter is individually quoted



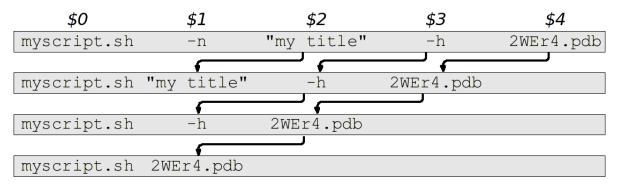
If you run the following script

```
#!/bin/sh
echo The script is $0
echo The first commandline option is $1
echo The second commandline option is $2
```

with two arguments, you'll get the following output:

```
$ ./script.sh ABC DEF
The script is ./script.sh
The first commandline option is ABC
The second commandline option is DEF
$
```

In many cases you'll not know how many parameters are given on the commandline. In these cases you can use shift to loop through them. shift removes \$1 and moves all other positional parameters one position to the right: \$2 becomes \$1, \$3 becomes \$2 etc.:



With the help of "\$#", "shift", "case" and the positional parameters we can now check all the commandline parameters:

```
while [ "$#" -gt 0 ]
do
  case $1 in
    -h) echo "Sorry, no help available!" # not very helpful, is it?
        exit 1
                                           # exit with error
        ;;
    -v) VERBOSE=1
                                           # we may use $VERBOSE later
        ;;
    -f) shift
        FILE=$1
                                           # Aha, -f requires an
                                           # additional argument
        ;;
       echo "Wrong parameter!"
        exit 1
                                           # exit with error
  esac
  shift
done
```

3.6 Ensuring a Sensible Exit Status

If you don't provide your own exit status, then the script will return the exit status of the last executed command (See *Reporting Success or Failure - The Exit Status* (page 24)). In many cases this might be what you want, but very often it isn't. Consider the following script which is a real example from real life and happened to me personally:

```
#!/bin/sh
[... do something that fails ...]
echo "End of the script"
```

This script will *always* succeed, as the echo command hardly ever fails. You will - from the exit status of the script - never be able to detect that something went wrong. Instead in such cases you should manually handle the exit codes of the commands that are run within the script.

With it's help we can keep track of the exit stati of all our important processing steps and finally return a sensible value:

```
#!/bin/sh
mystatus=0;

[... do something that might fail ...]
if [ $? -ne 0 ]
then
   mystatus=1
fi

[... do something else that might fail, too ...]
[ $? -ne 0 ] && mystatus=1  # same as above. Do you understand  # this?

echo "End of the script"
exit $mystatus
```

3.6.1 Why is the exit status important after all?

First when you use your script within other scripts, you'll probably need to be able to check, if it has succeeded. There might be other ways (e.g. checking outputfiles for certain strings, checking directly the textual output of the script etc.), but these ways are usually cumbersome and require lots of coding. Exit values are easy to check. Second: Other tools and systems might also use the exit status of your script. E.g. the cluster system uses your job's exit status to assess, if it has run successfully or not. Returning success even in case of failure will result in lots of complications in case a problem occurs. It took me several days to realize the bug above.

3.7 Tips and Tricks

3.7.1 Combining Variables with other Strings

When combining variables with other strings, then in some situations the variable name must be placed in curly brackets ("{}"):

```
$ A=Heidel
$ echo $Aberg
$ echo ${A}berg
Heidelberg
$
```

If you only want to work with part of the variable in the string, you can control this by operating on the value of the variable within the curly brackets. Use % to specify what you want to remove from the end of a string variable, and # to remove something from the beginning.

```
$ QUERYFILE=hg19_seqs.fasta
$ RESULTSFILE={$QUERYFILE}.blastn
$ echo $RESULTSFILE
hg19_seqs.fasta.blastn
$ echo ${QUERYFILE*.fasta}
hg19_seqs
$ RESULTSFILE=${QUERYFILE*.fasta}.blastn
$ echo $RESULTSFILE
hg19_seqs.blastn
$ echo $RESULTSFILE
hg19_seqs.blastn
$ echo ${QUERYFILE#hg19_}
seqs.fasta
$ echo ${QUERYFILE#*_}
seqs.fasta
```

Note from the above, that you specify what should be removed from the string with a pattern - meaning that you can use wildcards like * and ? to make the operations flexible and perhaps to save you some typing.

3.7.2 Filenames and Paths

If possible, try to avoid any special characters (blanks, semicolons (";"), colons (":"), back-slashes ("\") etc.) in file and directory names. All these special characters can lead to problems in scripted processing. Instead, stick to alphanumeric characters (a-z, 0-9), dots ("."), dashes ("-") and underscores ("_"). Additionally sticking to lowercase characters helps avoiding mistypes and makes the automatic filename expansion easier.

3.7.3 Breaking up Long Code Lines

Code lines can become pretty long and unreadable, wrapping onto the next line etc. You can use the escape character (backslash, "\") to break them up and enhance readability of your script. The escape character must immediately be followed by a newline (no intermediate blanks or other is allowed):

```
$ bsub -o output.log -e error.log -q clngnew -M 150000 -R "select[(mem > _{\sqcup} _{\to} 15000)]" /g/software/bin/pymol-1.4 -r -p < pymol.pml
```

becomes:

Which is way better to read and to maintain...

3.7.4 Script Debugging

sh/bash and csh/tcsh have both an option "-x" which helps debugging a script by echoing each command before executing it. This option can be set and unset during runtime with set -x / set +x (sh/bash) and set echo / unset echo (csh/tcsh).

3.7.5 Command Substitution

You can use the output of a command and assign it to a variable or use it right away as text string, by using the command substitution operator "'" (backticks, backquotes) or "\$(...)". The backtick operator works in all shells, while \$(...) only works in bash.

Three variants for the same (print out who you are in English text):

```
$ ME=`whoami`
$ echo I am $ME
I am fthommen
$

$ ME=$(whoami)
$ echo I am $ME
I am fthommen
$
$ echo I am `whoami`
I am fthommen
$
```

3.7.6 Create Temporary Files

You can create temporary files with mktemp. By default it will create a new file in /tmp and print its name:

```
$ mktemp
/tmp/tmp.Yaafh19370
$
```

You can take advantage of the fact that mktemp returns the name of the created file, to capture this file name and use it in your script.

3.7.7 Cleaning up Temporary Files

It is considered good practice and sometimes even important, to clean up temporary data before ending a script. A simple way - which will not cover all cases, though - could be to store all created temporary files in a variable and remove them all before exiting the script:

```
#! /bin/sh
ALL_TEMPFILES="" # store a list of all temporary files here

TEMPFILE1=`mktemp`
ALL_TEMPFILES="$ALL_TEMPFILES $TEMPFILE1"

TEMPFILE2=`mktemp`
ALL_TEMPFILES="$ALL_TEMPFILES $TEMPFILE2"

[... process, process, process ...]

rm -f $ALL_TEMPFILES
exit
```

Solutions to the Exercises

4.1 TAR & GZIP

1. Use gzip to compress the file P12931.txt

```
$ gzip P12931.txt
```

2. Decompress the resulting file P12931.txt.gz (revert previous command)

```
$ gunzip P12931.txt.gz
```

or

```
$ gzip -d P12931.txt.gz
```

3. Use tar to create an archive containing all fasta files in the current directory into an archive called "fastafiles.tar"

```
$ tar -c -f fastafiles.tar *.fasta
```

4. Use gzip to compress the archive "fastafiles.tar"

```
$ gzip fastafiles.tar
```

5. How can you achieve the two previous steps "using tar to create archive" and "gzip the archive" in one command?

```
$ tar -c -z -f fastafiles.tar.gz *.fasta
```

Note: Note the -z

6. Test (list the contents of) the compressed archive "fastafiles.tar.gz"

```
$ tar -tf fastafiles.tar.gz
```

7. Download the compressed PDB file for entry 1Y57 from rcsb.org (eg. wget "http://www.rcsb.org/pdb/files/1Y57.pdb.gz") and decompress it.

```
$ wget "http://www.rcsb.org/pdb/files/1Y57.pdb.gz"
$ gunzip 1Y57.pdb.gz
```

4.2 GREP

1. Which of the DNA files ENST0* contains "TATATCTAA" as part of the sequence?

2. List only the names of the DNA files ENST0* that contain "CAACAAA" as part of the sequence.

```
$ grep -1 "CAACAAA" ENSTO*
ENST00000380152.fasta
ENST00000544455.fasta
```

3. Considering the previous example, would you consider grep a suitable tool to perform motif searches? Why not? Try to find the pattern "CAACAAA" by manual inspection of the first three lines of each sequence.

Note: Answer: When using grep as a motif searching tool, you need to keep in mind that grep (like sed and awk) is line-oriented, meaning that by default it only searches for a given motif in a single line. In the given example, upon manual inspection you will find the given motif also in the file ENST00000530893.fasta (spanning multiple lines), which grep missed. You would need to think about how to do multi-line searches (eg. Removing line-breaks etc.)

4. Count the number of 'ATOM's in the file 1Y57.pdb

```
$ grep -c ATOM 1Y57.pdb 3632
```

5. Does this number agree with the annotated number of atoms? The PDB file has a comment which tells you how many atoms there are annotated in this file. This comment can be found by searching for the term "protein atoms" (use quotes and case insensitive search here!).

```
$ grep -i "protein atoms" 1Y57.pdb
REMARK 3 PROTEIN ATOMS : 3600
```

This tells us that there are 3600 atoms annotated in this PDB file, however we initially counted 3632. This is because grep also counted any occurrence of "ATOM" within REMARKS. We can avoid this by either filtering out the remarks:

```
$ grep -v REMARK 1Y57.pdb | grep -c ATOM 3600
```

...or by telling grep to only count those lines that start with "ATOM":

```
$ grep -c ^ATOM 1Y57.pdb
3600
```

4.3 REV

1. By combining rev with the cut tool, print the last word of each line in DNA.txt. Make sure that the words are readable when they are printed out.

```
$ rev DNA.txt | cut -d' ' -f1 | rev
the
known
of
life.
adenine,
DNA
[...]
```

4.4 XARGS

1. Use xargs to print the first line of the files listed in to_be_previewed.txt

2. Create a copy of each of these files by passing the lines in to_be_copied.txt two-at-a-time to cp

```
$ ls -1t *.{pdb,txt,fasta}
to_be_copied.txt
to_be_previewed.txt
tabular_data.txt
twoseqs.fasta
files.txt
motifs.txt
1Y57.pdb
3UA7.pdb
```

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```
DNA.fasta
[...]
$ cat to_be_copied.txt | xargs -n2 cp
$ ls -1t *.{pdb,txt,fasta}
sequenceA.fasta
sequenceB.fasta
sequenceC.fasta
sequenceD.fasta
sequenceE.fasta
structure.pdb
text.txt
to_be_copied.txt
to_be_previewed.txt
[...]
```

3. A better way to back up these files might be to keep the original names while copying them. Make another copy of each file listed in to_be_previewed.txt, adding ".backup" onto the end of each filename. (Hint: remember the "-I" option!)

```
$ cat to_be_previewed.txt | xargs -I FILENAME cp FILENAME.

→backup
$ 1s -1 *.backup

ENST00000380152.fasta.backup

ENST00000530893.fasta.backup

ENST00000544455.fasta.backup

P04062.fasta.backup

P05480.fasta.backup

P12931.fasta.backup

PROTEINS.txt.backup
```

4. ADVANCED: we've made a bit of a mess now, and it's time to clean up. Make a new directory called 'garbage', which you will move all these new files into it by combining the find tool with xargs and mv. Use find to find all files in the current directory that were last modified less than ten minutes ago, and xargs with mv to change their location. BE CAREFUL! ..Hint:: you'll need to check out the options available for find, and you might consider using the "-p" option with xargs to help avoid accidentally deleting something that you might regret!) Once you've moved the files, check the contents of the 'garbage' directory and, if you're sure that you don't want any of those files anymore, delete them and the directory.

4.5 SED

1. Use sed to print only those lines that contain "version" in the files P05480.txt and P04062.txt

```
$ sed "/version/p" P05480.txt P04062.txt
```

2. Use sed to change the text "sequence version 3" to "sequence version 4" in the files P05480.txt and P04062.txt (without actually changing the files, just printing)

```
$ sed "s/sequence version 3/sequence version 4/" P05480.txt P04062.txt
```

3. Use sed to update the text "sequence version 3" to "sequence version 4" in the files P05480.txt and P04062.txt (this time, make the changes directly in the files)

```
$ sed -i.bak "s/sequence version 3/sequence version 4/" P05480.txt
→P04062.txt
```

4. Replace (transliterate) all occurrences of "r" by "l" and "l" by "r" (at the same time) in the file PROTEINS.txt (so that "structural" becomes "stluctular")

```
$ sed "y/rRlL/lLrR/" PROTEINS.txt
```

4.6 AWK

1. Use awk to print only those lines that contain "version" in the files P12931.txt and P05480.txt and think about how this procedure is different to sed.

```
$ awk "/version/ {print}" P12931.txt P05480.txt
```

This is very similar to sed, you also have to use the slashes "/" to define the search pattern. However the sed notation is a little more concise...

2. For all FASTA files that begin with "P" ("P*.fasta") print only the second item of the header (split on "|") eg. for ">sp|P12931|SRC_HUMAN Proto-oncogene", print only "P12931"

```
$ awk -F"|" '/>/ {print $2}' P*.fasta
```

- 3. The file "P12931.csv" phosphorylation contains sites in the pro-P12931. file "P12931.csv" tein (If the does exist, use wget http://phospho.elm.eu.org/byAccession/P12931.csv to download it).
 - (a) Column three of this file lists the amino acid position of the phosphorylation site. You are only interested in position 17 of the protein. Try to use "grep" to filter out all these lines containing "17".

```
$ grep 17 P12931.csv
```

4.5. SED 43

(b) Now use awk to show all lines containing "17".

```
$ awk "/17/ {print}" P12931.csv
```

(c) Next try show only those lines where column three equals 17 (Hint: The file is semicolon-separated...).

```
$ awk -F";" '$3==17 {print}' P12931.csv
```

(d) Finally print the PMIDs (column 6) of all lines that contain "17" in column 3.

```
$ awk -F';' '$3==17 {print $6}' P12931.csv
```

4.7 Quoting and Escaping

- 1. Familiarize yourself with quoting and escaping.
 - 1. Run the following commands to see the difference between single and double quotes when expanding variables:

```
$ echo "$HOSTNAME"
...
$ echo '$HOSTNAME'
```

2. Next, use ssh to login to a different machine to run the same command there, again using both quoting methods:

```
$ ssh pc-atcteach01 'echo $HOSTNAME'
...
$ ssh pc-atcteach01 "echo $HOSTNAME"
```

2. Closely inspect the results; is that what you were expecting? Discuss this with your neighbour.

Propositions for Scripting Exercises

Here are some ideas (not elaborated propositions) for some useful scripts which you might want to implement. Extend them to your liking. Thanks to Grischa Toedt & Chrysoula Pantzartzi for the ideas.

5.1 Replace Names in SVG

A SVG graphic is not a binary file (such as PNG or JPG image) but a textual description of objects. This allows to use commandline tools to manipulate SVG graphics. A simple example SVG like this:

Hello, my name is: FIRSTNAME LASTNAME

looks like this:

Save this text as a file called badge.svg, and write a script to replace "FIRSTNAME" and "LASTNAME" by a set of names from a CSV file (this file should just contain a list of names, one per line):

```
Firstname, Lastname
Holger, Dinkel
Frank, Thommen
...
```

Purpose: Search/Replace names in a SVG graphic by a list of names from a CSV file.

Usage Example:

```
$ replace_names.sh badge.svg names.csv
```

Suggested tools and commands: sed, for/while, etc.

Things to consider:

- Make sure to create a new SVG file for each entry in the names list.
- Consider how to name each SVG file. Just number them incrementally? Use Names?
- If it makes things easier, use two loops, one for replacing FIRSTNAME, then another one to replace LASTNAME.

5.2 General "Unpacker"

Several tools exist to pack/unpack files. Unfortunately they have different functionality and often different commandline parameters. This makes it difficult to work with them; it would be nice to have a tool which unpacks any given packed file, automatically recognizing which packing algorithm was used and just returns the unpacked file.

Purpose: Unpack a file or a number of files according to their packing or compression format (tar, gzip, zip, bzip, xz, see http://en.wikipedia.org/wiki/List_of_archive_formats for more ideas). This script can be used as a general wrapper around the various compression and packing tools with an uniform set of options

Usage Example:

```
$ 1s -F
archive.tar.gz text.txt zuppfile
$ unpack *
archive.tar.gz is a gzip compressed tarfile ... uncompressed and unpacked
text.txt is not compressed or packed ... skipping
zuppfile is a zip compressed archive ... uncompressed and unpacked
$
```

Suggested tools and commands: file, tar, gzip/gunzip, zip/unzip, bzip2/bunzip2, xz, etc.

Things to consider:

- The type of a file is not necessarily deductible from its extension.
- What if the file doesn't have an extension at all?
- Depending on the tool and how the file has been archived, the unpacking/uncompressing can result in files being created in a subdirectory or directly in the current working directory. Is this what one wants/expects?
- What if the destination directory already exists?
- Some tools preserve the original archive, others don't... Maybe you can add consistency here?

Extendibility:

• Add option to keep/remove the original archives.

- Add option to unpack files into a separate directory.
- Add option to unpack files in directories named after the archive names. Check for already existing target directories!

5.3 Safety Backup Creator

One cannot have enough backups!!! However creating a backup can be tedious, so it's better to have a script which semi-automates this task.

Purpose: Create a backup copy of a directory/file in a defined location. E.g. as a safety copy/fallback before applying changes to a dataset etc.

Usage Example:

```
$ backup.sh datadir
datadir contains 12 files and is 12 MB in size
Copying datadir to /home/fthommen/safety_backups/datadir_20-MAY-2014 ...

done
backup.sh datadir2
datadir contains 154 files and is 3 TB in size
Sorry, /home/fthommen/safety_backups/datadir2_20-MAY-2014 already exists ..

aborting
$
```

Suggested tools and commands: cp, rsync, du, ls, date

Things to consider:

- Already existing safety backups should not be overwritten!
- Do you or don't you want to keep the full original path in some form? (dirname, basename)

Extendibility:

• Add option to pack/compress the data.

5.4 Column Chooser (advanced)

Purpose: Write a script, which takes a textfile with columnar layout and a header line and prints out only columns with the named headers of a textfile with columnar layout

Datafile:

```
NAME FIRSTNAME BIRTHDATE STREET NO
Meier Daniel 30-MAY-1990 Meyerhofstrasse 12
Mueller Andreas 29-FEB-1960 Bahnhofstr. 1b
Schmid Ariane 1-DEC-1990 Bahnhofstrasse 13
vonMyra Nikolaus 15-MAR-270 Dezemberstrasse 6
```

Usage Example:

```
$ columnchooser.sh FIRSTNAME NO
Daniela 12
Andreas 1b
Ariane 13
Nikolaus 6
$ columnchooser.sh CITY
Sorry, no column "CITY" found
$
```

Suggested tools and commands: awk, cut, eval

Extendibility:

- Add options to define alternate column separators (awk -F).
- Add option to customize the concatenation of the printed fields.

Appendix

6.1 Links and Further Information

6.1.1 Links

- A full 500 page book about the Linux commandline for free(!): LinuxCommand.org ¹
- Another nice introduction: "A beginner's guide to UNIX/Linux" ²
- The "commandline starter" chapter of an O'Reilly book: Learning Debian GNU/Linux Issuing Linux Commands ³
- A nice introduction to Linux/UNIX file permissions: "chmod Tutorial" 4
- Linux Cheatsheets ⁵
- BioPieces ⁶ are a collection of bioinformatics tools that can be pieced together in a very easy and flexible manner to perform both simple and complex tasks.
- Google shell style guide ⁷
- Useful bash one-liners for bioinformatics ⁸
- Interactive explanation of your commandline: Explain Shell ⁹
- Bash One-Liners Explained, Part III: All about redirections ¹¹
- Bash Redirections Cheat Sheet ¹²
- Redirection Tutorial ¹³

¹ http://linuxcommand.org/

² http://www.mn.uio.no/astro/english/services/it/help/basic-services/linux/guide.html

³ http://www.oreilly.com/openbook/debian/book/ch04_01.html

⁴ http://www.catcode.com/teachmod/

⁵ http://www.cheat-sheets.org/#Linux

⁶ http://code.google.com/p/biopieces

⁷ https://code.google.com/p/google-styleguide

⁸ https://github.com/stephenturner/oneliners

⁹ http://www.explainshell.com

¹¹ http://www.catonmat.net/blog/bash-one-liners-explained-part-three

¹² http://www.catonmat.net/blog/bash-redirections-cheat-sheet

¹³ http://wiki.bash-hackers.org/howto/redirection_tutorial

6.1.2 Command Line Mystery Game

CLMystery ¹⁰ is a game that you play on the commandline: There's been a murder in Terminal City, and TCPD needs your help to solve this crime *by using commandline tools only*!

To play the game, get the files from github and read the instructions:

```
wget https://github.com/veltman/clmystery/archive/master.zip
unzip master.zip
cd clmystery-master/
cat instructions
```

6.1.3 Recommended Reading: Real printed paper books

- Dietz, M., "Praxiskurs Unix-Shell", O'Reilly (highly recommended!, German language only)
- Herold, H., "awk & sed", Addison-Wesley
- Robbins, A., "sed & awk Pocket Reference", O'Reilly
- Robbins, A. and Beebe, N., "Classic Shell Scripting", O'Reilly
- Siever, E. et al., "Linux in a Nutshell", O'Reilly

6.1.4 Running Linux Commands in Mac

You can find the "Terminal" program in the "Utilities" folder of "Applications".

6.1.5 Running Linux Commands in Windows

Babun

The easiest way to get a linux-like console on a Windows host is probably babun http://babun.github.io/>!!

Babun features the following:

- Pre-configured Cygwin with a lot of addons
- Command-line installer, no admin rights required
- advanced package manager (like apt-get or yum)
- color console
- Auto update feature
- "Open Babun Here" Explorer context menu entry

¹⁰ https://github.com/veltman/clmystery

6.1.6 Live - CDs

A Live-CD is a complete bootable computer operating system which runs in the computer's memory, rather than loading from the hard disk drive. It allows users to experience and evaluate an operating system without installing it or making any changes to the existing operating system on the computer.

Just download an ISO-Image, burn it onto a CD/DVD and insert it into your DVD-Drive to boot your computer with Linux!

Fedora Live CD

This Live CD contains everything the Fedora ¹⁴ Linux operating system has to offer and it's everything you need to try out Fedora - you don't have to erase anything on your current system to try it out, and it won't put your files at risk. Take Fedora for a test drive, and if you like it, you can install Fedora directly to your hard drive straight from the Live Media desktop.

Knoppix

Knoppix ¹⁵ is an operating system based on Debian designed to be run directly from a CD / DVD or a USB flash drive, one of the first of its kind for any operating system. When starting a program, it is loaded from the removable medium and decompressed into a RAM drive. The decompression is transparent and on-the-fly. More than 1000 software packages are included on the CD edition and more than 2600 are included on the DVD edition. Up to 9 gigabytes can be stored on the DVD in compressed form.

BioKnoppix

Bioknoppix ¹⁶ is a customized distribution of Knoppix Linux Live CD. With this distribution you just boot from the CD and you have a fully functional Linux OS with open source applications targeted for the molecular biologist. Beside using RAM, Bioknoppix doesn't touch the host computer, being ideal for demonstrations, molecular biology students, workshops, etc.

Vigyaan

Vigyaan ¹⁷ is an electronic workbench for bioinformatics, computational biology and computational chemistry. It has been designed to meet the needs of both beginners and experts.

BioSlax

BioSLAX ¹⁸ is a live CD/DVD suite of bioinformatics tools that has been released by the resource team of the BioInformatics Center (BIC), National University of Singapore (NUS).

¹⁴ http://fedoraproject.org/wiki/FedoraLiveCD

¹⁵ http://knopper.net/knoppix

¹⁶ http://bioknoppix.hpcf.upr.edu

¹⁷ http://www.vigyaancd.org

¹⁸ http://www.bioslax.com

6.2 About Bio-IT

The Bio-IT Project aims to develop and strengthen the bioinformatics community at EMBL Heidelberg. It is made up of members across a range of disciplines in computational biology, in different Units and Core Facilities. The project aims to improve the standard of computational biology practised at EMBL Heidelberg, to encourage collaborations, and to provide a forum for discussion of issues and ideas relevant to bioinformatics here. The activities of the project include:

- the organisation and delivery of training courses such as this one
- the provision of one-to-one training and consultancy
- the organisation of social and networking events for the computational biology community
- regular meetings to discuss issues and ideas
- the development and maintenance of the Bio-IT Portal http://bio-it.embl.de

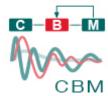
The Portal hosts information regarding upcoming courses and conferences/other events relevant to computational biology, resources to help with your work, and profiles of people involved in bioinformatics at EMBL. It is accessible from within the EMBL network (you must connect via VPN for off-site access).

6.2.1 Centres

EMBL Centres are 'horizontal', cross-departmental structures that promote innovative research projects across disciplines. All the EMBL Centres listed below have a strong computational component.







Biomolecular Network Analysis

The CBNA disseminates expertise, know-how and guidance in network integration and analysis throughout EMBL.

Statistical Data Analysis

The CSDA helps EMBL scientists to use adequate statistical methods for their specific technological or biological applications.

Modeling

The Centre for Biological Modeling (CBM) aims to support people to adopt mathematical modeling techniques into their everyday research.

6.3 Acknowledgements

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EMBL Logo © EMBL Heidelberg

Graphic of the Linux Filesystem taken from the SuSE 9.2 manual © Novell Inc.

All other graphics © Frank Thommen, EMBL Heidelberg, 2012

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Special thanks go to contributors / helping hands (alphabetical order):

- Christian Arnold
- Jean-Karim Hériché
- Nicolai Karcher
- Yan Ping Yuan
- Bora Uyar
- Thomas Zichner

Symbols	F
[27 # 23 \$? 24 & 15] 27	file
A awk	gunzip
backtick 37 bg 15 break 31 breaksw 29 bunzip2 46 bzip2 46	H hash sign
C case	J jobs
D date	P pattern
	5.40 0, 40

set
shebang line
shift
Т
tar
U
unset 37 until 31 unzip 46
V
variables environment variables
W
while
X
xargs46
Z
zip

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Unix/Linux Command Reference

FOSSwire.com

File Commands

ls - directory listing

ls -al - formatted listing with hidden files

cd dir - change directory to dir

cd - change to home

pwd - show current directory

mkdir dir - create a directory dir

rm *file* - delete *file*

rm -r dir - delete directory dir

rm -**f** *file* - force remove *file*

rm -**rf dir** - force remove directory **dir** *

cp file1 file2 - copy file1 to file2

cp -r *dir1 dir2* - copy *dir1* to *dir2*; create *dir2* if it doesn't exist

mv file1 file2 - rename or move *file1* to *file2* if *file2* is an existing directory, moves *file1* into directory *file2*

ln -s file link - create symbolic link link to file

touch file - create or update file

cat > file - places standard input into file

more file - output the contents of file

head *file* - output the first 10 lines of *file*

tail *file* - output the last 10 lines of *file*

tail -f *file* - output the contents of *file* as it grows, starting with the last 10 lines

Process Management

ps - display your currently active processes

top - display all running processes

kill pid - kill process id pid

killall *proc* - kill all processes named *proc* *

bg - lists stopped or background jobs; resume a stopped job in the background

fg - brings the most recent job to foreground

fg n - brings job n to the foreground

File Permissions

chmod *octal file* - change the permissions of *file* to *octal*, which can be found separately for user, group, and world by adding:

- 4 read (r)
- 2 write (w)
- 1 execute (x)

Examples:

chmod 777 - read, write, execute for all

chmod 755 - rwx for owner, rx for group and world For more options, see **man chmod**.

SSH

ssh user@host - connect to host as user

ssh -p port user@host - connect to host on port
port as user

 ${\it ssh-copy-id}\ user@host$ – add your key to host for user to enable a keyed or passwordless login

Searching

grep pattern files - search for pattern in files
grep -r pattern dir - search recursively for
pattern in dir

command | grep pattern - search for pattern in the
output of command

locate file - find all instances of file

System Info

date - show the current date and time

cal - show this month's calendar

uptime - show current uptime

w - display who is online

whoami - who you are logged in as

finger *user* - display information about *user*

uname -a - show kernel information

cat /proc/cpuinfo - cpu information

cat /proc/meminfo - memory information

man command - show the manual for command

df - show disk usage

du - show directory space usage

free - show memory and swap usage

whereis app - show possible locations of app

which app - show which app will be run by default

Compression

tar cf file.tar files - create a tar named file.tar containing files

tar xf file.tar - extract the files from file.tar tar czf file.tar.gz files - create a tar with Gzip compression

tar xzf file.tar.gz - extract a tar using Gzip
tar cjf file.tar.bz2 - create a tar with Bzip2
compression

tar xjf file.tar.bz2 - extract a tar using Bzip2
gzip file - compresses file and renames it to
file.qz

gzip - d file.gz - decompresses file.gz back to file

Network

ping host - ping host and output results

whois domain - get whois information for domain

dig domain - get DNS information for domain

dig -x host - reverse lookup host

wget file - download file

wget -c file - continue a stopped download

Installation

Install from source:

./configure

make

make install

dpkg -i pkg.deb - install a package (Debian)

rpm -**Uvh** *pkg.rpm* - install a package (RPM)

Shortcuts

Ctrl+C - halts the current command

Ctrl+Z - stops the current command, resume with

fg in the foreground or bg in the background

Ctrl+D - log out of current session, similar to exit

Ctrl+W - erases one word in the current line

Ctrl+U - erases the whole line

Ctrl+R - type to bring up a recent command

!! - repeats the last command

exit - log out of current session

* use with extreme caution.

