02. Toolkit

DSIER [/dɪˈzaɪər/] — Summer 2022

Julian Hinz

Bielefeld University

DOCKER + VSCODE WORKING?

Session Roadmap

- The Shell
- R

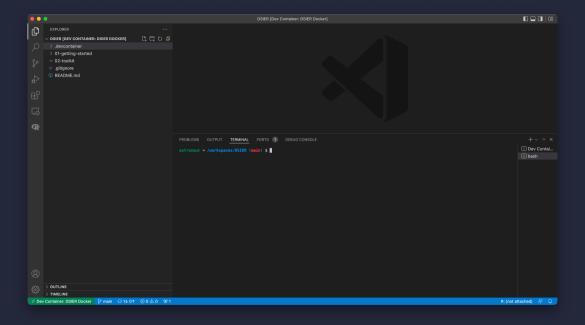


Shell

- Terminology: shell, terminal, tty, command prompt, etc.
 - \rightarrow Same same: command line interface (CLI)
- Many shell variants: focus on Bash ("Bourne again shell")
- Included by default on Linux and MacOS
- Windows users need to install a Bash-compatible shell

Shell

- Powerful: executing commands and for fixing problems
 - ightarrow some things you just can't do in an IDE or GUI
- Reproducibility: Scripting is reproducible, clicking is not
- Remote: Interacting with servers and super computers
- Automation: workflow and analysis pipelines, e.g. with Makefile





Basics

username@hostname:~\$

- username denotes a specific user
- hostname denotes name of the computer
- :~ denotes the directory path (where ~ signifies the user's home directory).
- \$ denotes the start of the command prompt (# for root)

Keyboard shortcuts

- Tab completion
- ↑ (and ↓) keys to scroll through previous commands
- Ctrl $+ \rightarrow$ (and Ctrl $+ \leftarrow$) to skip whole words at a time
- Ctrl + a moves the cursor to the beginning of the line
- Ctrl + e moves the cursor to the end of the line
- Ctrl + k deletes everything to the right of the cursor
- Ctrl + u deletes everything to the left of the cursor
- Ctrl + Shift + c to copy and Ctrl + Shift + v to paste

Syntax

command option(s) argument(s)

```
astronaut → /workspaces/DSIER (main) $ ls -lh
total 4.0K
drwxr-xr-x 3 astronaut astronaut 96 Apr 26 19:03 01-getting-started
drwxr-xr-x 2 astronaut astronaut 64 Apr 26 19:03 02-toolkit
-rw-r--r- 1 astronaut astronaut 135 Apr 19 15:43 README.md
```

- \rightarrow start with a dash, usually one letter
- $\,\,
 ightarrow\,$ multiple options can be chained under single dash, sometimes two

```
$ ls -lah 01-getting-started/
$ ls --group-directories-first --human-readable 01-getting-started/
```

arguments usually on file or directory

man and cheat

man ls

```
$ cheat ls
```

Navigation

- pwd to print working directory
- cd to change directory

```
astronaut → /workspaces/DSIER (main) $ pwd
/workspaces/DSIER
astronaut → /workspaces/DSIER (main) $ cd ../
astronaut → /workspaces $ pwd
/workspaces
astronaut → /workspaces $
```

Create files and directories

• touch and mkdir

```
$ mkdir testing
$ touch testing/test1.txt testing/test2.txt testing/test3.txt
$ ls testing
test1.txt test2.txt test3.txt
```

Removing files and directories

• rm

```
$ rm testing/test1.txt
$ ls testing
test2.txt test3.txt
$ rm testing
rm: cannot remove 'testing': Is a directory
$ rm -rf testing
$ ls testing
ls: cannot access 'testing': No such file or directory
```

• "recursive" (-r or -R) and "force" (-f) options

Copying

- cp object path/copyname
 - $\,\rightarrow\,$ keeps old name if not provided with new one

```
$ touch example.txt
$ mkdir testing
$ cp example.txt testing
$ ls testing
example.txt
```

Moving and renaming

mv object path/newobjectname

```
$ mv example.txt testing/example2.txt
$ ls testing
example2.txt example.txt
$ mv testing/example2.txt testing/example_new.txt
$ ls testing
example_new.txt example.txt
```

Wildcards

- Wildcards: special characters as replacements for other characters
- Replace any number of characters with *

```
$ cp examples/*.sh examples/copies ## Copy any file with .sh extension
$ rm examples/copies/* ## Delete everything in the "copies" directory
```

Replace a single character with ?

```
$ ls examples/meals/??nday.csv
$ ls examples/meals/?onday.csv
## examples/meals/monday.csv
## examples/meals/monday.csv
```



Working with text files

• Print whole file with cat ("concatenate")

```
$ cat -n examples/sonnets.txt
```

• Print only first or last couple of lines with head and tail

```
$ head -n 3 examples/sonnets.txt ## First 3 rows
$ tail -n 1 examples/sonnets.txt ## Last row
```

Working with text files

• Search within files: grep ("Global regular expression print")

```
$ wc examples/sonnets.txt
2633 17698 95662 examples/sonnets.txt
$ grep -n "Shall I compare thee" examples/sonnets.txt
```

Redirect

Send output from the shell to a file using redirect operator >

```
$ echo "At first, I was afraid, I was petrified" > survive.txt
$ find survive.txt
survive.txt
```

• To append file, use >> (> overwrites)

```
$ echo "'Kept thinking I could never live without you by my side" >> survive.
$ cat survive.txt
At first, I was afraid, I was petrified
'Kept thinking I could never live without you by my side
```

Pipes

- Awesome feature: send ("pipe") output to another command with
 - \rightarrow chain together a sequence of simple operations

```
$ cat -n examples/sonnets.txt | head -n100 | tail -n10
```

Compress and decompress

• Compress data with zip and decompress with unzip

```
$ zip archive.zip examples/sonnets.txt
 adding: examples/sonnets.txt (deflated 59%)
$ unzip -l archive.zip
Archive: archive.zip
 Length Date
                    Time
                            Name
   95662 2022-04-26 20:18 examples/sonnets.txt
                             1 file
$ unzip archive.zip -d examples
Archive: archive.zip
  inflating: examples/examples/sonnets.txt
```



Loops

Repeat operation over set: Loops

```
for i in LIST
do
   OPERATION $i
done
```

Example: Combing csv files

```
$ touch examples/meals/mealplan.csv
## loop over the input files and append their contents to our new CSV
$ for i in $(ls examples/meals/*day.csv)
> do
> cat $i >> examples/meals/mealplan.csv
> done
```

Scripting

• .sh file with code can be executed

```
#!/bin/sh
echo -e "\nHello World!\n"
```

- #!/bin/sh is a shebang, indicating which program to run the command with \rightarrow -e flag tells bash that we want to evaluate an expression rather than a file
 - \$ examples/hello.sh
 Hello World!

- Not limited to running shell scripts in the shell
- Example: Rscript

```
$ Rscript -e 'cat("Hello World, from R!")'
Hello World, from R!
```



Build systems

- Sequence of operations to go from inputs to outputs
 - ightarrow Define dependencies, targets, and rules
- Avoid unnecessary rule execution
- Many build systems, make is a common choice

Makefile Example

- Targets, dependencies, and rules defined in Makefile
- % is a pattern, matching the same string on left and right
- wildcard * searches your filesystem for matching filenames
- \$@ is an automatic variable that contains the target name

Running make

```
$ make
make: *** No rule to make target 'paper.tex', ...
$ touch paper.tex
$ make
make: *** No rule to make target 'plot-data.png', ...
```

- make checks for rules and dependencies
 - ightarrow complains if dependencies are missing

Building with make

```
$ cat paper.tex
$ cat plot.r
$ cat data.csv
$ make
./plot.r -i data.csv -o plot-data.png
pdflatex paper.tex
```

- Creates a PDF when all dependencies are satisfied
- Running make again shows it's up to date

make

- Build systems, like make, automate the build process
- Saves time and ensures consistency in complex projects
- Essential tool for managing dependencies and targets



- 1. Stage (or "add"): Add changes to the repo history
 - \rightarrow file edits, additions, deletions, etc.
- 2. Commit: Yes, you are sure these changes should be part of the repo history
 - ightarrow need to add a message (and optionally a description)
- 3. Pull: Download new changes made on the GitHub repo (i.e. the upstream remote)
 - ightarrow either by your collaborators or you on another machine
- 4. Push: Upload any (committed) local changes to the GitHub repo

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Merge conflicts

```
# README
Some text here.
<<<<<< HEAD
Text added by Partner 2.
======
Text added by Partner 1.
>>>>>> 814e09178910383c128045ce67a58c9c1df3f558.
More text here.
```

- Delete lines that you don't want, then special Git merge conflict symbols
- Then: stage, commit, pull and push

Branches and forks

Branch

- Take snapshot of existing repo and try out a whole new idea without affecting your main branch
- If new idea works, merge back into main branch
 - \rightarrow fix bugs
 - \rightarrow implement new empirical strategies, robustness checks, ...
- If it doesn't work, just delete experimental branch

Branches and forks

Fork

- Forking a repo similar to branch, but creates a copy of entire repo
- Upstream pull request makes merge back into origin repo possible
 - ightarrow Easy to do on Github

.gitignore

- Tells Git what to ignore
 - \rightarrow exclude whole folders or a class of files (e.g. based on size or type)
- Simply add names of files or folders that should be ignored



• So far: Shell, git and Make

• This afternoon: R

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