The trouble with scripts

Shell scripts are useful for automation
But when not to use them?

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Scripts are great, right?

Useful in drive for more automation and reproducible research

Esp. with HPC, cloud

What meant by defining research workflows using shell scripting?

- Define the bulk of what you want to do programatically
- not type interactively
- Run one or more programs
- With particular parameters
- In a particular environment (access to storage, network, environment variables)
- To generate output

Example workflow: HPC job submission script

```
#!/bin/bash
#$ -l rmem=4G

module load R/4.0
module load Python/3.9

cp -ra ~/$PROJECT/data /fastdata/te1st/
python ~/$PROJECT/train.py -i /fastdata/te1st/data -o ~/$PROJECT/trained/
python ~/$PROJECT/test.py ~/proj1/trained/
R ~/$PROJECT/plots.py ~/proj1/trained/
```

Issue 1: how can that fail?

- Modules don't exist
- Not asked for enough memory
- Input dir doesn't exist
- A command might error but subsequent commands might still run!
- $PROJECT not defined
- $PROJECT has spaces in!
- …

In general: concise and convenient but many more silent failure modes than e.g. MATLAB

Command might error but subsequent commands might still run

```
ls ~/.bashrc
ls ~/idontexist
ls ~/.condarc  # will still run!
```

Tips:

- Well-behaved command should return a (hidden) 'exit code' which is 0 if all okay
- `commanda && commandb` -> only run `commandb` if `commanda` succeeds
- `commanda || commandb` -> only run `commandb` if `commanda` succeeds
- `set -e` -> exit the script if a command returns a non-zero exit code

Undefined variables

Dereferencing shell variables results in the empty string if previously not explicitly assigned to:

```
$ echo ~/.conda/$NOTDEFINED/envs
/home/will/.conda//envs
```

Tips:

- `set -u` -> exit the script if reach an undefined variable
- `${SOMEVAR-42}` -> default to '42' if SOMEVAR is undefined

Spaces in names / variables

With `~/$PROJECT/data`

- If `PROJECT` is defined as e.g. `my project`
- Then e.g. `ls $PROJECT` will be interpreted as `ls my project!`

Dealing with spaces in variables and in file/path names is hard

Tips:

- Avoid putting spaces in file/directory names!
- Safest way to reference variables: `somecommand "some text ${VARIABLE_NAME} more text"`
- Use single and double quotes liberally

Issue 2: Fault tolerance (idempotence?)

- What if a script/job fails part way through?
  - Can re-run without having to edit script logic?
  - Or without deleting some output files?
- What if want script to be able to 'resume' if re-run?
  - Only generate output files not already generated?
  - Or if existing output files are older than input files and/or script?
- Adding such logic to shell scripts can be tricky

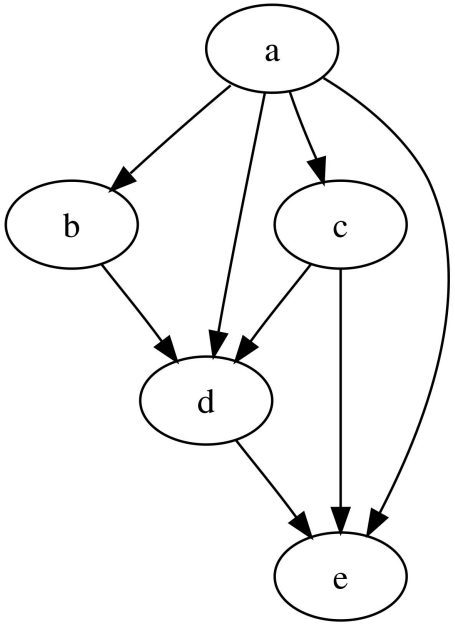
Issue 3: Portability

- Given an existing shell script what aspects are specific to:
  - You?
  - Your group/dept/institution?
  - The system you're running it on?
  - Dataset(s)?
  - Date/time?
  - Parameters?
- Making scripts (inc shell scripts) and configs portable and reusable between researchers/systems/projects is tricky!

Issue 4: Multiple inputs and/or job steps

On HPC / cloud:

- What if you have lots of input files/parameter sets?
- And/or lots of job steps?
- One job script with one or more loops?
  - Not efficient if unnecessarily serial
- One job script with internal parallelism?
  - Not efficient if different inputs / steps need different resources
  - Error handling might be tricky
- Job scripts that submit other jobs?
  - Can efficiently tune resource requirements per 'sub'-job and
  - could execute complex network of tasks but
  - robust error handling is even harder!



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Summary

- Shell scripts useful for defining simple workflows
- But writing and testing robust complex shell scripts will always be hard
- Even if using a text editor (or shellcheck) that can advice on bad practices!
- Knowing where shell scripting is appropriate is important
- Better tools/processes exist for defining and running more complex workflows…