Reproducibility

Tools

- data
- software
- computer

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- software
- computer

Data

Can change over time (months or years)

Data

| Freeze d. | GENCODE | Release d. | Genome v. | UCSC version |
|-----------|---------|------------|---------------|--------------|
| 5.2018 | 29 | 10.2018 | GRCh38 | 29 (GRCh38) |
| 6.2014 | 21 | 10.2014 | GRCh38 | - |
| 7.2013 | 19 | 12.2013 | GRCh37 | 19 (GRCh37) |
| 7.2011 | 10 | 12.2011 | GRCh37 | 10 |
| 12.2010 | 7 | 4.2011 | GRCh37 | 7 |
| 7.2009 | 3c | 9.2009 | NCBI36/GRCh37 | 3c (NCBI36) |

Custom dataset

You can even build your own reference genome(s)

- unkown species
- unkown genes
- ...

Incoming data

Your lab can generate data over time

and

you must re-analyze it multiple times or combining it in many ways $% \left(1\right) =\left(1\right) \left(1\right)$

Tools

- data
- software
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They transform data

Each transformation has an input and an output

The output of the previous transformation is the input for the next one

There are many tools for many purposes and our duty is to combine them in a proper way

- Operating System (OS)
- Applications
- Bioinformatics Applications

Software: OS

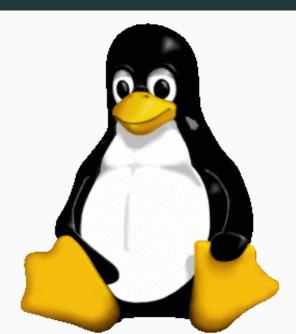




Figure 1: Linux Distribution

OS

Linux is open source

Its core code can be inspected and you can contribute!

torvalds/linux

OS

Linux is open source

It is a very very stable system

Our cluster uptime is about Years

| Source | Date | Unix | Windows | Unkw |
|--------|--------|-------|---------|------|
| W3Tech | Feb 15 | 36.85 | 32.3 | 30.5 |
| W3Tech | Feb 19 | 69.3 | 30.7 | 0 |

W3Tech

OS

Standalone or Remote

You can install Linux main OS or access a remote machine by network

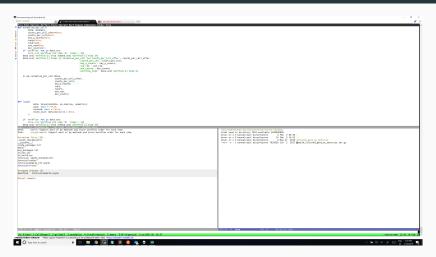


Figure 2: Terminal

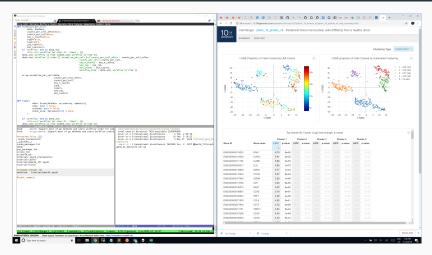


Figure 3: TerminalWeb

- Multi user
 - Disk
 - Memory
 - CPU

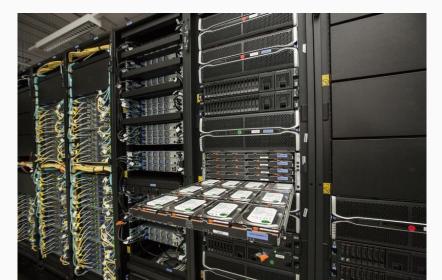
Most of the time you share resources with others

OS

- Multi user
 - Disk (HDD: long term storage)
 - Memory (RAM: volatile)
 - CPU (engine)

Most of the time you share resources with others

Cluster of thousands of machines



- Open Source
- Standalone or Remote
- Multi User
- Cluster of thousands of machines
- Stable
- Huge communities

Software: Applications

Whatever action you are doing through a computer you are going to use a software somewhere

Applications

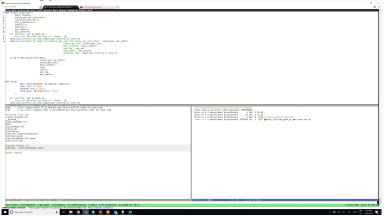
In any case we have 2 best friends:

- An Interface
- An Editor

- Graphical User Interface
- The ugly terminal

- Graphical User Interface (ICONS !!!! Mouse !!!!)
- The ugly terminal

- Graphical User Interface
- The ugly terminal



The winner is ?

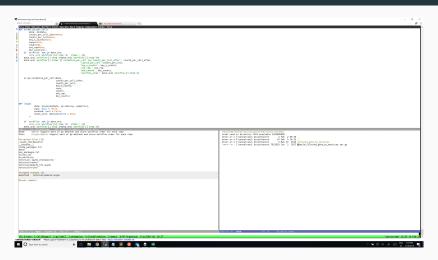


Figure 5: The Ugly Terminal

Terminal

You can instruct the machine to do whatever you want using the keyboard typing commands.

Editor

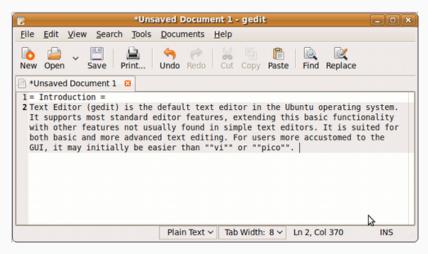


Figure 6: gedit

Editor

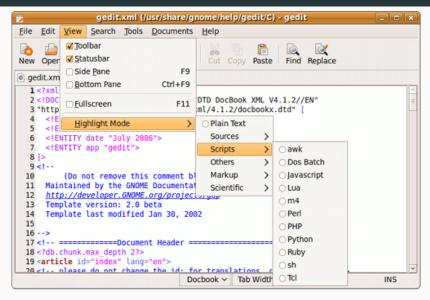


Figure 7: gedit

Terminal

With the terminal you can even write documents, text files.

NOT WORD FILES!!!

```
File Edit Options Buffers Tools Python Virtual Envs Elpy YASnippet Help
2# -*- coding: utf-8 -*-
4"""Tests for `scutils` package."""
7import unittest
9from scutils import scutils as scu
 Mmport scanpy as sc
3class TestScutils(unittest.TestCase):
    """Tests for `scutils` package."""
    def setUp(self):
       """Set up test fixtures, if any."""
       self.data = sc.read_10x_mtx(
           "tests/data/filtered gene bc matrices/hg19", var names="gene symbols", cache=True)
    def tearDown(self):
       """Tear down test fixtures, if any."""
    def test min cells(self):
       """Test the minimum number of cells that must express a gene."""
       self.assertEqual(scu.min cells(self.data), 3)
29if name == ' main ':
   unittest.main()
1-*- mode: compilation; default-directory: "~/projects/core/scutils/" -*-
2Compilation started at Tue Feb 12 13:03:21
```

It is a shell which interprets your commands and acts appropriately

you will love it

It is a shell which interprets your command and act appropriately

• you will hate it

ls -la

ls -l /root

Write a file called "myfile.txt" with gedit and read it with the terminal

cat myfile.txt

Copy a file

```
cp myfile.txt myfile.backup.txt
```

now do a ls

Move a file aka Rename

mv myfile.txt MyFile.txt

now do a ls

Connect to your own machine

```
ssh user@localhost
```

if you get a message like this:

```
The authenticity of host 'localhost (::1)' can't be established ECDSA key fingerprint is SHA256:Zf595J6gKYjVYVD3R/E1AnQmsLu7QBAre you sure you want to continue connecting (yes/no)?
```

Type yes

Connect to a server

ssh user@192.168.200.213

now list all the connected users

who

There are many users all w/the same name

Using applications

STAR --help

Installing programs

The functionalities of a computer can be extended installing software

Installing programs

- 1. Ubuntu/Debian packages list or apt search
- 2. Conda packages. search or conda search
- 3. Linuxbrew. List or brew search
- 4. From specialized archives: e.g. pip
- 5. Compile the program

Ubuntu packages

- Lots of packages ready apt-get install ne
- Very robust
- Additional packages with PPAs add-apt-repository ppa:user/ppa-name
 - Not very useful for science

Advantages

- Safe and efficient
- Easy to rebuild from source

Cons

Sometimes outdated (Ubuntu LTS are released every 2 years)

Conda packages

- Must be downloaded and installed (with bash)
- Relies on channels
 - base with installation
 - bioconda: bioinformatics programs
 - conda-forge: misc programs
- Not very robust/stable

Advantages

Programs are usually the latest version

Cons

- Needs update to config files (~/.bashrc)
- Weird interactions with system programs/libraries
- Messes up with \$PATH (e.g. shebang)

Linuxbrew packages

- Must be downloaded and installed
- Only one source of packages
- Similar to conda
 - fewer packages

Conda

On our system is already installed by the procedure is quite easy if you start from scratch.

Conda

You can start creating a conda environemnt.

Conda

A conda environment let's you install and use software *softly* separated by the original system

conda create -n unimiPhD

Bioinformatic Applications

Then you are ready to install the application for RNA-seq

Bioinformatic Applications

```
conda install -y -c bioconda \
fastqc=0.11.8 \
trimmomatic=0.38 \
samtools=1.9 \
star=2.6.1b
```

Tools

- data
- software
- computer

Computer

- Local
- Remote
- Physical
- Virtual
- Cloud