

ISLDS - Course Design

1. Where to learn great things?

1.1 Wikipedia

- wikipedia.org
 - *Hands-On:*
 - Try search Wiki of Chatgpt
 - *Notes:*
 - use English for more info and accuracy.

1.2 Youtube

- youtube.com

1.2 MOOC

- Massive open online course (MOOC):
https://en.wikipedia.org/wiki/Massive_open_online_course
- List of MOOC providers: https://en.wikipedia.org/wiki/List_of_MOOC_providers
 - *Hands-On:*
 - Try to follow and complete a free MOOC course on [Coursera](#), [Khan Academy](#), [Stanford Online](#), [MIT OCW](#) or [Udacity](#)

1.3 Bilibili

- bilibili.com

1.4 Cheatsheets

- Search on google.com or find on cheat-sheets.org
 - *Hands-On:*
 - Try searching "cheatsheet docker pdf":
 - https://docs.docker.com/get-started/docker_cheatsheet.pdf
 - Find a Ubuntu cheatsheet on cheat-sheets.org:

- <https://www.cheat-sheets.org/saved-copy/ubuntueref.pdf>
- *Notes:*
 - Use the English language of google search for more relevant results.
 - Some are available on official sites, such as the docker cheatsheet https://docs.docker.com/get-started/docker_cheatsheet.pdf.
 - Pdf/Html formatted cheatsheet. Pdf is good for printing and quick reference, html is good for cross-referencing.
 - There are novice and advanced versions of cheatsheets, with varied info density. Use accordingly as you progress.

2. Scientific Literature Search Tools

2.1 LetPub

- letpub.com.cn (free)
 - *Hands-On:*
 - Try searching for 期刊名: *Nature*
 - Try searching for 中科院分区: 1区, 影响因子: >10, 结果排序: 影响因子, 查看期刊
 - *Notes:*
 - a. Develop a sense of journal quality by the above exercise

2.2 GoogleScholar

- scholar.google.com (free) - search by researcher or keyword
 - *Hands-On:*
 - Search by Author Name
 - *Notes:*
 - a. Search and summa
- [The Chicago Manual of Style, 17th Edition](#)

2.3 ChatGPT

- chatgpt.com (free) - Q&A session
 - *Hands-On:*
 - Search for literature
-

Search: give me a list of latest high-quality papers published in 2024 on predicting disease status from genomic and phenomic profiles

- Summarize a paper
- Notes:
 - The current free version is GPT-4o.
 - **Hallucination**: making up citations, be sure to check them manually.
 - Timing: is not timely updated, use Copilot for more current search results.
- Try other ChatGPT functions: write code, help debug and edit papers.

2.4 Copilot/Bing

- [bing.com](https://www.bing.com) (free) - search + Q&A session

3. Data Science Development Tools

3.1 Docker

▪ Install Docker in windows

- *Hands-On*:
 - Tutorial Video: <https://www.bilibili.com/video/BV11L411g7U1>
- [https://www.bilibili.com/video/BV11L411g7U1/](https://www.bilibili.com/video/BV11L411g7U1)

Docker 1小时快速上手教程，无废话纯干货_哔哩哔哩_bilibili

Docker 1小时快速上手教程，无废话纯干货共计8条视频，包括:Docker 简介和安装、用 Docker 快速安装软件、构建自己的 Docker 镜像等，UP主更多精彩视频，请关注UP账号。
- Tutorial: <https://docker.easydoc.net/doc/81170005/cCewZWON/ITKfePfP>

- *Notes*:

▪ Use an Ubuntu container

- *Hands-On*:
 - Tutorial Video: <https://www.bilibili.com/video/BV1y34y197mP>

<https://www.bilibili.com/video/BV1y34y197mP>

02docker安装ubuntu与基本操作介绍_哔哩哔哩_bilibili

-, 视频播放量 8572、弹幕量 2、点赞数 72、投硬币枚数 17、收藏人数 80、转发人数 8, 视频作者 ITKEY, 作者简介 爱技术, 爱分享, 折腾技术使我快乐!, 相关视频:实体机安装Ubuntu, 我再也不用win了, vmware安装...

- Official ubuntu docker images: https://hub.docker.com/_/ubuntu/

- Tutorial: <https://docs.docker.com/engine/install/ubuntu>

```
h> docker pull ubuntu          # pull the ubuntu image to local
h> docker image ls             # check the image is here
h> docker run -d -v /mnt/e/Temp:/mnt/Temp --name mu ubuntu sleep infinity #
run the ubuntu container, mount the E:\Temp dir and name it mu
h> docker ps -a | grep mu      # view your container is running
h> docker exec -it mu /bin/bash # interactively exec bash and get a terminal
c# cat /etc/os-release         # check ubuntu version
c# apt-get update && apt-get install python3 # install python3
c# touch /mnt/Temp/test.txt    # make a new file in E:\Temp
h> docker commit mu upy3       # save the container change to a new image
upy3
h> docker stop mu              # stop the container process, can be reused
h> docker rm mu                # remove the container process
h> docker run -d --name mp3 upy3 sleep infinity
h> docker exec -it mp3 /bin/bash # interactively exec bash and get a terminal
```

- *Notes:*

- Install **WSL2** before docker is recommended
- Powershell and WSL2 shells share the same docker space
- -v /mnt/e/Temp:/mnt/Temp requires WSL2 and automount on
- grep only works in the WSL2 shell
- Use xxx --help or man xxx to see how to use xxx command

3.2 Linux (Ubuntu)

- **Learn to use Ubuntu**

- *Hands-On:*

- Tutorial Video (needs a better one):

<https://www.bilibili.com/video/BV1W4411A7yf>

黑马—Ubuntu教程_哔哩哔哩_bilibili

黑马—Ubuntu教程共计100条视频, 包括:01-课程安排、02-励志公式和python体验、03-什么是操作系统等, UP主更多精彩视频, 请关注UP账号。

- Ubuntu Docs: <https://help.ubuntu.com/>

- Ubuntu Cheatsheet: <https://www.cheat-sheets.org/saved-copy/ubuntu-ref.pdf>
- Linux Cheatsheet:
<https://web.archive.org/web/20240119115021/https://www.cheat-sheets.org/project/tldr/command/special-most-used-linux-commands/>
- Advanced Commands, Commandline Tools and Environment Variables:

apt # manage additional tools and commands,

[https://en.wikipedia.org/wiki/APT_\(software\)](https://en.wikipedia.org/wiki/APT_(software))

vim # a neat yet powerful text editor,

[https://en.wikipedia.org/wiki/Vim_\(text_editor\)](https://en.wikipedia.org/wiki/Vim_(text_editor))

grep # you can almost find anything, <https://en.wikipedia.org/wiki/Grep>

awk # efficiently manipulate complex tables, <https://en.wikipedia.org/wiki/AWK>

sed # efficiently manipulate large texts, <https://en.wikipedia.org/wiki/Sed>

| # efficiently connects command outputs,

[https://en.wikipedia.org/wiki/Pipeline_\(Unix\)](https://en.wikipedia.org/wiki/Pipeline_(Unix))

ssh # manage your server from anywhere (scp, sftp, rsync, ...),

<https://en.wikipedia.org/wiki/SSH>

nohup # manage the job process (disown, bg, &, ...),

[https://en.wikipedia.org/wiki/Job_control_\(Unix\)](https://en.wikipedia.org/wiki/Job_control_(Unix))

/usr/bin/python # the python interpreter to run .py scripts

/usr/bin/Rscript # the R interpreter to run .R scripts

/bin/bash # the Bash interpreter to run .sh scripts

history # don't lose anything you've typed, can search and edit with vi

env # environmental variables, all you can set

https://en.wikipedia.org/wiki/Environment_variable

wget # elink, curl, call you can view and get from internet

<https://en.wikipedia.org/wiki/wget>

- *Notes:*

- Powershell and WSL shell share the same docker space
- Shell commands and commandline tools are also available within vim
- Stderr and stdout are savable, searchable and manipulatable with &1 and &2

3.3 Bourne-Again SHell (Bash)

- **Learn to use Shell (Bash)**

- *Hands-On:*
 - Tutorial Video (paid content, needs a better one):

<https://www.bilibili.com/video/BV1AT411Y7bq>

【伯乐大典】最实用的Bash脚本知识_哔哩哔哩_bilibili

【伯乐大典】最实用的Bash脚本知识共计8条视频, 包括:1. 什么是Bash脚本、2. 变量、3. 用户输入等, UP主更多精彩视频, 请关注UP账号。

<https://www.bilibili.com/cheese/play/ss15269>

跟我一起学bash脚本编程_哔哩哔哩_bilibili

首页 番剧 直播 游戏中心 会员购 漫画 赛事 去巴黎 去巴黎 下载客户端 登录 登录后你可以: 免费看高清视频 多端同步播放记录 发表弹幕/评论 热门番剧影视看不停 立即登录 首次使用? 点我注册 大会员 消息 动态 收藏 历史 ...

- Bash Docs: <https://www.gnu.org/software/bash/manual/bash.html>
- Bash Cheatsheet: https://www.cheat-sheets.org/saved-copy/bash_ref.pdf
- Advanced Bash Programming:
| bash # how to talk to Linux [https://en.wikipedia.org/wiki/Bash_\(Unix_shell\)](https://en.wikipedia.org/wiki/Bash_(Unix_shell))

- *Notes:*

3.4 Application: convert py2 Python package to py3

- Learn to convert the py2 elsa package to py3

```
1 apt install -y 2to3
2 cd /mnt/tmp/lec3 && git clone git@github.com:labxscut/elsa.git
3 2to3 -w setup.py
4 cd elsa
5 for f in `ls *.py`; do 2to3 -w $f; done;
6 python setup.py build
7 cd build/lib.linux-x86_64-3.10
8 (for f in `ls lsa/*.py`; do echo "### $f ###";
  PYTHONPATH=$(pwd):$PYTHONPATH python $f; done;) >err.txt 2>&1
9 #by now you shall see the errors in err.txt which needs to be fixed
   for v3
```

3.5 Application: batch download PDB files

- Tutorial (todo)

- *Hands-On:*
- *Notes:*

4. Python Coding Tools

4.1 Docker, PyNotebook and Conda

- **Install Python + Conda + PyNotebook in Dockerized Ubuntu**

- *Hands-On:*

- Review of basic docker operations

```
h> docker run -v /mnt/e/tmp:/mnt/tmp -d --name islds1 islds sleep infinity #
create a working container from islds image with a mounted working directory

h> docker run -v E:\tmp:/mnt/tmp -d --name islds1 islds # create a working
container from islds image with a mounted working directory in powershell

h> docker exec -it islds1 /bin/bash # open a bash on islds1

h> docker commit islds1 islds # commit modifications in islds-new to islds image

h> docker stop islds1 && docker rm islds1 # kill and remove islds1 (&& is a cmd
connector only available with a Linux shell, exec the cmds one-by-one in
powershell)

h> docker start islds1 # if interrupted and the container stopped in middle

h> docker attach islds1 # reconnect to the container
```

- Add Python 3, Anaconda and Jupyter Notebook to islds interactively; Tutorial:
<https://docs.anaconda.com/anaconda/install/linux/>

```
c# cd /mnt/tmp/lec3 # use this working directory

c# apt-get update --fix-missing # fix missing packages

c# apt-get -y install python3 python3-dev # install python3 and headers

c# apt-get -y install jupyter-notebook # install jupyter notebook

c# curl -L -o anaconda.sh https://repo.anaconda.com/archive/Anaconda3-
2024.06-1-Linux-x86_64.sh && /bin/bash anaconda.sh # download anaconda
and install, need manual inputs in middle
```

- Instead, we can install them using a Dockerfile; First, create a Dockerfile.pnb:

```
# Use your existing Docker image as the base
FROM ubuntu:latest

# Set the working directory (optional, depending on your existing setup)
WORKDIR /usr/src/app

# Prepare apt
```

```
RUN apt-get update --fix-missing
# Install Jupyter Notebook
RUN apt-get install -y jupyter-notebook
# Install python3
RUN apt-get install -y python3 python3-dev python3-pip
# Expose port 8888 for Jupyter Notebook
EXPOSE 8888
# Define the default command to run when starting the container
CMD ["jupyter", "notebook", "--ip='0.0.0.0'", "--port=8888", "--no-browser", "--allow-root"]
```

- Build the islds-new container image

```
h> docker build -t islds -f Dockerfile.pnb .
```

- A Test Run:

```
h> docker run -p 8888:8888 -v /mnt/e/tmp:/mnt/tmp islds
```

- *Notes:*

- Conda Cheatsheet: <https://docs.conda.io/projects/conda/en/latest/user-guide/cheatsheet.html>
- Can build the Dockerfile in a linux station and use it for new build in windows

- **Install Conda and PyNotebook in windows**

- *Hands-On:*

- Official Anaconda for windows : <https://www.anaconda.com/download>
- Tutorial Video: <https://www.bilibili.com/video/BV1jf4y1j7Vi>

<https://www.bilibili.com/video/BV1jf4y1j7Vi>

数据科学之铲-5分钟搞定Anaconda和Jupyter notebook的配置_哔哩哔哩_bilibili

官网:<https://www.anaconda.com/products/individual>清华镜

像:<https://mirrors.tuna.tsinghua.edu.cn/anaconda/archive/?C=M&O=A>, 视频播放量 7541、弹幕量 ...

- *Notes:*

- We will continue the course with a dockerized pynotebook.

4.2 Python Packaging and Deliverables

- **Learn how to package and deliver a python program**

- *Hands-On:*

- Python Packaging Tutorial

- <https://www.bilibili.com/video/BV194411r7a8>

<https://www.bilibili.com/video/BV194411r7a8>

Python——包和模块_哔哩哔哩_bilibili

Python——包和模块共计100条视频，包括:1-Python包和模块-基本概念解释、2-Python包和模块-作用、3-Python包和模块-分类等，UP主更多精彩视频，请关注UP账号。

- Python Packaging Basics

```
samplepackage/
|
|—— samplepackage/
|   |—— __init__.py
|   |—— module1.py
|   |—— module2.py
|
|—— tests/
|   |—— __init__.py
|   |—— test_module1.py
|   |—— test_module2.py
|
|—— README.md
|—— LICENSE
|—— setup.py
|—— requirements.txt
```

- `samplepackage/` : The directory containing your package.
- `__init__.py` : An empty file that tells Python that this directory should be treated as a package.
- `module1.py` , `module2.py` : Python modules with your package's
- `tests/` : Directory containing tests for your package.
- `README.md` : A markdown file describing the project.
- `LICENSE` : The license file.
- `setup.py` : The build script for setuptools.

- `requirements.txt` : A file listing the package dependencies.
- An Example Python Package:
 - <https://github.com/labxscut/elsa>
 - Study this `setup.py`
- The elsa (py2) Dockerfile with Deployable Python Package:

```
FROM ubuntu:latest
# Set the working directory (will return to WORKDIR after each RUN)
WORKDIR /setup
# Install prerequisites
RUN apt-get update --fix-missing
RUN apt-get -y install curl git git-lfs build-essential          # install curl, git
and build tools
RUN apt-get -y install python2 python2-dev                      # install python2
RUN apt-get -y install python-is-python2 python-dev-is-python2 # set
python2 to system python
RUN apt-get -y install python-setuptools                        # install python2 and
necessaries
RUN curl https://bootstrap.pypa.io/pip/2.7/get-pip.py | python2 # install pip
RUN pip install numpy scipy                                    # install numpy and
scipy
# RUN pip install conda                                         # install conda
# Install elsa
RUN git lfs clone --verbose https://bitbucket.org/charade/elsa.git
RUN cd elsa && python2 setup.py install --force
# Run elsa
RUN lsa_compute --help
```

- Build and use the islds-elsa container image

```
h> docker build -t islds-elsa -f Dockerfile.elsa .
h> docker run -v /mnt/e/tmp:/mnt/tmp -d --name u1 islds-elsa sleep infinity
h> docker exec -it u1 lsa_compute --help      # run dockerized elsa app
lsa_compute
```

```
h> docker exec -it u1 lsa_compute /mnt/tmp/lec4/ARISA20.csv
/mnt/tmp/lec4/ARISA20.theo.elsa -r 1 -s 127 -d 3 -p theo          # use
the lsa_compute for scientific calculation
```

- *Notes:*

- The elsa package was build for python 2.
- A tool inside a docker container is dockerized, and can be used by docker exec container tool
- To reach dockerhub (blocked by GFW) configure DockerDesktop/Settings/Resources/Proxies accordingly.
- To avoid disk space configure DockerDesktop/Settings/Resources/Advanced/"Disk Image Location" to a folder with abundant free space.
- For interactive debug, note will not return to WORKDIR after each RUN cmd, needs manual cd
- The input file can be provided in /mnt/e/tmp and the output file can be found in /mnt/e/tmp

5. Code Management Tools

5.1 Git and Github

- **Git and Github**

- *Hands-On:*

- Github: <https://en.wikipedia.org/wiki/GitHub>
- Install and use a dockerized git

```
h> docker run -v /mnt/e/tmp:/mnt/tmp -d --name u1 islds-elsa # use dockerized
git
h> docker exec u1 /bin/bash
c# apt-get install -y git git-lfs
h> docker commit u1 islds-elsa
```

- Git Tutorial: <https://www.bilibili.com/video/BV1WW411Q7EW>

<https://www.bilibili.com/video/BV1WW411Q7EW>

Git基本命令行用法讲解_哔哩哔哩_bilibili

Git基本命令行用法讲解共计34条视频，包括:01-git-help、02-git-config、03-git-init等，UP主更多精彩视频，请关注UP账号。

- *Hands-On:*
 - SignIn/SingUp to Github: <https://github.com>
 - Tutorial Video: <https://www.bilibili.com/video/BV1614y1k7CS>

<https://www.bilibili.com/video/BV1614y1k7CS>

使用教育邮箱申请github学生包以及免费copilot_哔哩哔哩_bilibili

这个网址包含我的文字说明，不过是为暨南大学的学生量身定制的，当然，只要你有edu.cn邮箱都能够适用，
<https://qm0.website/myhtml/github-copilot-tutorial.html>, 视频播放量 30264、弹幕量 2、点赞数 285、...

- *Hands-On:*
 - Configure dockerized git to use github
- *Hands-On:*
 - Configure dockerized git to use github via ssh

```
c# git config --global user.name "chaelir"
c# git config --global user.email "labxsolar@outlook.com"
c# cat ~/.gitconfig
c# vi ~/.gitconfig
```

```
c# mkdir ~/.ssh          #create .ssh folder
c# ssh-keygen -t id_rsa_work -C "your_email@example.com"
c# cp id_rsa_work* ~/.ssh/  #if you already have keys
c# vi ~/.ssh/config

### vi ~/.ssh/config ###

Host github
  Hostname github.com
  User chaelir
  IdentityFile ~/.ssh/id_rsa_work
```

- *Notes:*
 - Use an edu.cn email account for free copilot

5.2 Application: manage Python code with Git

- CCNMF: An example R Package presented and maintained on GitHub

- *Hands-On:*
 - Github: <https://github.com/labxscut/ccnmf>

```
c# cd /mnt/tmp/lec4 && git clone https://github.com/labxscut/CCNMF.git
```

- *Notes:*

-

5.3 Application: manage R code with Git

- **ELSA: An example Python Package presented and maintained on GitHub**

- *Hands-On:*

- Github: <https://github.com/chaelir>

```
c# ssh-keygen          # save the key in ~/.ssh/id_github, add the pub key to the
                        account
```

```
c# chmod 400 ~/.ssh/id_github # if you copied somewhere else, change the file
readable only2you
```

```
c# vi ~/.ssh/config
```

- The contents of ~/.ssh/config

```
Host github
```

```
    Hostname github.com
```

```
    User git
```

```
    IdentityFile ~/.ssh/id_github
```

- Github: <https://github.com/labxscut/elsa>

```
c# ssh -T git@github.com # this should work
```

```
c# cd /mnt/tmp/lec4 && git clone git@github.com:labxscut/elsa.git #or fork and
clone your own repo
```

```
c# cd elsa && cp ../Dockerfile.elsa .
```

```
c# git add Dockerfile.elsa
```

```
c# git commit -m "added a new working Dockerfile"
```

```
c# git push
```

```
h> docker commit u1 islds # commit this to the new image file
```

- Take a look at the Github, it should reflect the change you've just made

- *Notes:*

- All labx repos are owned by the labxcode (LABX-GitHub-Admin) account
 - To be allowed to write to the repos, you need to request "Write" permission and granted by the admin.

- The new islds new image file shall have github configured next time you spin it up.
- If you are a collaborator who pushes edits to repo of others, please invite them to write and accept first.

5.4 Application: misc git operations

■ Learn commonly used git operations

```
1 ### git create a new repo on github
2 # github create a repo -> clone the repo to local -> add files ->
  commit and push
3 #### git rename a branch and delete the old branch.
4 git branch -m v3 py3
5 git push origin --delete v3
6 git push origin py3
7 git push --set-upstream origin py3
```

6. R Coding Tools

6.1 R and Rstudio

■ Install R + Rstudio in Windows

- *Hands-On:*
 - Tutorial: <https://www.bilibili.com/video/BV18w4m127L5>

<https://www.bilibili.com/video/BV18w4m127L5>

科研技能 | R和RStudio的安装和使用简介_哔哩哔哩_bilibili

正好本UP新买的台式电脑里没装R和RStudio，我想着借此机会给大家录一个安装软件的视频教程。由于R的很多教程都可以在网上搜到经验贴，所以本视频更想给大家演示的是如何使用百度来完成自主学习。...

■ Use an official R + Rstudio docker image

- *Hands-On:*
 - Use it with docker desktop on windows
 - h> docker pull rocker/rstudio
 - h> docker run -d -p 8787:8787 -e PASSWORD=**your_password** --name **rstudio** rocker/rstudio
 - Open localhost:8787 and input username and password to use

- *Notes:*
 - You will still have to commit your changes to the container as an image to save and reuse

■ DIY install R + Rstudio in Dockerized Ubuntu

- Self-review basic docker operations

• *Hands-On:*

```
h> docker image tag islds-elsa islds          # give islds-elsa the new name islds
h> docker run -v /mnt/e/tmp:/mnt/tmp -d --name u1 islds sleep infinity # create a
working container
h> docker run -v E:\tmp:/mnt/tmp -d --name u1 islds # if in powershell
h> docker exec -it u1 /bin/bash # open a bash
h> docker commit u1 islds # commit interactive modifications
h> docker stop u1 && docker rm u1 # kill and remove container
```

■ Add R and Rstudio to container interactively

- Tutorial: <https://posit.co/download/rstudio-server/>

```
c# cd /mnt/tmp/lec5          # use this working directory
c# apt-get update --fix-missing # fix missing packages
c# apt-get -y install r-base r-base-dev # install r-base and r-base-dev for
headers
c# apt-get -y install gdebi-core # install jupyter notebook
c# curl -L -o rs.deb https://download2.rstudio.org/server/focal/amd64/rstudio-
server-2024.04.2-764-amd64.deb # download the rstudio
install file
c# gdebi rs.deb # install rstudio server
c# useradd -m -s /bin/bash rstudio && echo "rstudio:rstudio" | chpasswd
#usr:pwd
```

■ Use dockerized Rstudio-Server:

- A Test Run on port 8787:

```
h> docker run -p 8787:8787 -v /mnt/e/tmp:/mnt/tmp d --name u1 islds
c# rstudio-server verify-installation # fix if any errors
c# rstudio-server stop
c# rstudio-server start
```

■ Misc Resources

- R Cheatsheet: <https://www.datacamp.com/cheat-sheet/getting-started-r>
- Rstudio Cheatsheet: <https://rstudio.github.io/cheatsheets/html/rstudio-ide.html>
- How to expose host folder to Rstudio server?
- Learn R based on new packages, some R cheatsheet is way too old, not recommended!, bad E.g.
 - <https://cran.r-project.org/doc/contrib/Short-refcard.pdf>

6.2 Application: Dockerfiles for R + Py devel

■ Use the image from islds repo

- code available at: <https://github.com/labxscut/islds>

```
h> docker image tag islds-elsa islds          # give islds-elsa the new name islds
h> docker run -v /mnt/e/tmp:/mnt/tmp -d --name u1 islds sleep infinity # create a
working container
h> docker run -v E:\tmp:/mnt/tmp -d --name u1 islds # if in powershell
h> docker exec -it u1 /bin/bash # open a bash
h> docker commit u1 islds # commit interactive modifications
h> docker stop u1 && docker rm u1 # kill and remove container
```

■ Self-build: build isl-cpp use Ubuntu:latest and Dockerfile.cpp

```
### Dockerfile.cpp ###
FROM ubuntu:latest
# All Necessary configs
ENV DEBIAN_FRONTEND=noninteractive
SHELL ["/bin/bash", "-c"]
WORKDIR /setup

# Install C prerequisites
RUN apt-get update --fix-missing && \
    apt-get -y install curl git git-lfs build-essential && \
    rm -rf /var/lib/apt/lists/*
```

■ Self-build: build isl-conda use isl-cpp and Dockerfile.conda

```
### Dockerfile.conda ###
```



```

FROM isl-cpp

# All Necessary configs

ENV DEBIAN_FRONTEND=noninteractive

SHELL ["/bin/bash", "-c"]

WORKDIR /setup


# Install Python and Conda

RUN apt-get update --fix-missing && \
    apt-get -y install python3 python3-dev python3-pip && \
    curl -sLo miniconda.sh https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86\_64.sh && \
    bash miniconda.sh -b -p ~/miniconda && \
    echo 'export PATH=~/miniconda/bin:$PATH' >> ~/.bashrc && \
    rm miniconda.sh && \
    rm -rf /var/lib/apt/lists/*

```

- **Self-build: build isl-rpy use isl-conda and Dockerfile.rpy**

```

### Dockerfile.rpy ###

FROM isl-conda

# All Necessary configs

ENV DEBIAN_FRONTEND=noninteractive

SHELL ["/bin/bash", "-c"]

WORKDIR /setup


# Install RStudio server, port 8787

# docker run -p 8787:8787 -v /mnt/e/tmp:/home/rstudio/data --name rs -d isl-rpy
rstudio-server start

RUN apt-get update --fix-missing && \
    apt-get -y install r-base r-base-dev && \
    apt-get -y install gdebi-core && \
    curl -sLo rstudio-server.deb
https://download2.rstudio.org/server/jammy/amd64/rstudio-server-2024.04.2-764-amd64.deb && \

```

```

gdebi -n rstudio-server.deb && \
rm rstudio-server.deb && \
useradd -m -s /bin/bash rstudio && \
echo "rstudio:rstudio" | chpasswd && \
rm -rf /var/lib/apt/lists/*

# Install Jupyter Notebook server, port 8888
# docker run -p 8888:8888 -v /mnt/e/tmp:/mnt/tmp --name pnb -d isl-rpy jupyter
notebook

ENV PATH=~/.miniconda/bin:$PATH
RUN conda create -n islds -y python=3.8 && \
    echo "source activate islds" >> ~/.bashrc && \
    . ~/.miniconda/etc/profile.d/conda.sh && \
    conda activate islds && \
    pip install -y numpy scipy matplotlib && \
    conda install -y -c conda-forge notebook

# docker run -p 8787:8787 -p 8888:8888 -v /mnt/e/tmp:/home/rstudio/data -v
/mnt/e/tmp:/mnt/tmp --name rpy -d isl-rpy sleep infinity

# rstudio-server start

# jupyter notebook --allow-root --notebook-dir=/mnt/tmp --ip='0.0.0.0' --port=8888 -
-no-browser

```

- **Self-build: commands to build Dockerfiles and run servers**

```

1 docker build . -f Dockerfile.cpp -t isl-cpp
2 docker build . -f Dockerfile.cpp -t isl-conda
3 docker build . -f Dockerfile.cpp -t isl-rpy
4 docker run -p 8787:8787 -p 8888:8888 -v
  /mnt/e/tmp:/home/rstudio/data -v /mnt/e/tmp:/mnt/tmp --name rpy -d
  isl-rpy sleep infinity
5 rstudio-server start #use rstudio on localhost:8787
6 jupyter notebook --allow-root --notebook-dir=/mnt/tmp --ip='0.0.0.0' -
  --port=8888 --no-browser # use notebook on localhost:8888

```

6.3 Data Visualization with R

■ ggplot2

- *Hands-On:*

- Tutorial Video: <https://www.bilibili.com/video/BV1pP411x7Tv>

<https://www.bilibili.com/video/BV1pP411x7Tv>

1.新版ggplot2-3.4.2精讲——基础语法_哔哩哔哩_bilibili

零基础学习ggplot2图形语法, 视频播放量 7466、弹幕量 2、点赞数 235、投硬币枚数 112、收藏人数 805、转发人数 31, 视频作者 五柳冰冰, 作者简介 R包最全分享者! 跟踪R官网上最新R包的发布信息, 精...

- *Notes:*

- Plotting Gallery: <https://r-graph-gallery.com/>
- ColorBrewer (use to have a RColorBrewer site): <https://colorbrewer2.org/>
- Identify the color set in ColorBrewer and use it with the **RColorBrewer** package: <https://r-graph-gallery.com/38-rcolorbrewers-palettes.html>

■ tidyverse

- *Hands-On:*

- Tutorial Video: <https://www.bilibili.com/video/BV1Nj41167Bv>

<https://www.bilibili.com/video/BV1Nj41167Bv>

4.新版ggplot2精讲——从整洁的数据开始_哔哩哔哩_bilibili

4.新版ggplot2精讲——从整洁的数据开始, 视频播放量 928、弹幕量 2、点赞数 23、投硬币枚数 8、收藏人数 31、转发人数 1, 视频作者 五柳冰冰, 作者简介 R包最全分享者! 跟踪R官网上最新R包的发布信息, 精炼讲解其...

- *Notes:*

- Tidyverse is a new way to organize and manage data in R, an alternative to the old dataframe.
- Many SQL operations are supported in tidyverse, so you can treat data.table as a database.
- **Tidyverse** cheatsheet: <https://www.datacamp.com/cheat-sheet/tidyverse-cheat-sheet-for-beginners>

■ shiny

- *Hands-On:*

- Beginner Tutorial: <https://www.youtube.com/watch?v=jxsKUxkiaLI>
- Tutorial Video: <https://www.youtube.com/watch?v=9uFQEck30kA>

- *Notes:*
 - Tidyverse and Shiny tutorials are scarce on Bili, use youtube instead.

7. Document Writing Tools

7.1 Follow author's instruction

■ Where to find the instruction

- *Hands-On (Authoring a paper)*
 - Find the Bioinformatics Journal Author's Instruction
 - Go <https://academic.oup.com/bioinformatics/> ; > Submit ; > Author Guidelines

Scope

Types of Manuscript

Pre-submission enquiries

Format-free submissions

General Policies

Open Access

Manuscript Preparation



Detailed Scope Guidelines

Manuscript Transfer

- Pay attention to manuscript types; pages; words, figures, table number limits
- Pay attention to Software and Data release requirements
- Pay attention to figure requirements: format, resolution
- Pay attention to citation and reference requirements
- Pay attention to sections by manuscript type
- Find and use the .doc or .tex template (if available)
 - Tex: <https://www.overleaf.com/latex/templates/oup-general-template/ybpypwncdxyb>
 - Doc: <https://static.primary.prod.gcms.the-infra.com/static/site/bioinformatics/document/cabios-word-temp.zip?node=9b946b36faff1c196dba&version=541801:1bc4a5f5521ada3b11e7>
- *Hands-On (Oral presenting a paper)*
 - Find the ICML 2024 conference speaker's instruction

- Official conference site: <https://icml.cc/Conferences/2024/PresenterInstructions>
- Pay attention to: presentation time, question time, connector available, screen ratio/size, ...
- *Hands-On (Poster presenting a paper)*
 - Find the ICML 2024 conference poster's instruction
 - Official conference site: <https://icml.cc/Conferences/2024/PosterInstructions>
 - Pay attention to: virtual or real, video, poster ratio/size, posting/presenting/retracting time, ...
- **Submit to biorxiv and medrxiv to use preprints transfer service**
 - [biorxiv.org](https://www.biorxiv.org)
 - [medrxiv.org](https://www.medrxiv.org)

7.2 Writing word document

- **Write a paper using journal .doc template**
 - *Hands-On (Writing a doc manuscript)*
 - Bioinformatics doc template (awful)
 -  [MS Word Template Bioinformatics.dotx](#)
 - NAR template (cool)
 -  [nar-word-template.docx](#)
 - So NAR can be used for writing and change to Bioinformatics before submission
 - But sections, figures, citations, word limits still follow Bioinformatics instruction
 - You can save the NAR template for other purposes, e.g. writing the paper for this course




- *Notes*
 - **Must use Microsoft Word, no WPS!**

7.3 Writing latex document

- **Write a paper using journal .tex template**
 - *Hands-On (Writing a tex manuscript)*
 - Both Bioinformatics and NAR use the same latex template (awful)

- <https://www.overleaf.com/latex/templates/oup-general-template/ybpypwncdxyb>

 [MS Word Template Bioinformatics.tex](#)

- Biostatistics has a good looking latex template (cool)
 - <https://www.overleaf.com/latex/templates/template-for-biostatistics-journal/fggrvggtkxmg>
-  [biostatistics-template.tex](#)
- So Biostatistics can be used for writing and change to Bioinformatics before submission
- Sections, figures, citations, word limits still follow Bioinformatics instruction
- You can save the Biostatistics template for other purposes, e.g. writing the paper for this course

 [CCNMF_NAR_latex_manuscript.zip](#)

- **Write an oral presentation with beamer .tex template**

- *Hands-On (Writing a tex slide)*

 [elsa-talk.zip](#)

- **Write a poster with .tex template**

- *Hands-On (Writing a tex poster)*

 [elsa-poster.zip](#)

- **Use Texlive + vim is highly recommended**

- *Hands-On (Install and use texlive and vim)*

- Install texlive in ubuntu based docker

| apt-get install texlive vim

7.4 Writing powerpoint document

- **Draw graphical art with powerpoint**

- *Hands-On*

- Draw a nice concept illustration / graphical abstract (Fig. 1) with powerpoint

 [CCNMF Fig1 concept illustration.pptx](#)

- Draw a nice workflow / dataflow chart (Fig. 2) with powerpoint

- **Write an oral presentation with powerpoint**

- *Hands-On*

 [CCNMF-ppt-presentation.pptx](#)

- **Write a poster with powerpoint**

- *Hands-On*

 [CCNMF-ppt-poster.pptx](#)