L1 - Reproducible & Trustworthy Workflow

November 8, 2023 9:44 AM

Syllabus https://pages.github.ubc.ca/MDS-2023-24/DSCI_522_dsci-workflows_students/
Lecture notes: https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/README.html
Group project: https://github.com/UBC-MDS/portugal_white_wine_quality_predictor_py
1 milestone/week
Sample report: https://github.com/ttimbers/breast_cancer_predictor_py.git
Watch video on Canvas before class

Data science: the study, development and practice of reproducible and auditable processes to obtain insight from data.
Reproducible analysis: reaching the same result given the same input, computational methods and conditions.

- Input = data
- Computational methods = computer code
- conditions = computational environment (programming language & it's **dependencies**)

Dependencies are other things one need to install to run your code, and includes:

- programming languages (e.g., R, Python, Julia, etc)
- packages from programming languages (e.g., tidyverse, scikit-learn)
- other tools you rely on (e.g., Make)
- legacy code (e.g., perl scripts, fortran, etc)
- Dependencies include versions as well as names!

It is important that insights from data science are **trustworthy**: it should be reproducible, auditable, correct, complete, fair, equitable and honest.

- **Auditable/transparent analysis**: a readable record of the steps used to carry out the analysis as well as a record of how the analysis methods evolved

Complex project has at least one of the following:

- two, or more, people directly working on the analysis
- involve two or more coding documents
- involve analysis of medium/large data
- Projects where you are working on a remote machine
- have many software or environment dependencies, or ones that are difficult or take a long time to install.
- As a project accumulates more of these features it grows further in complexity.

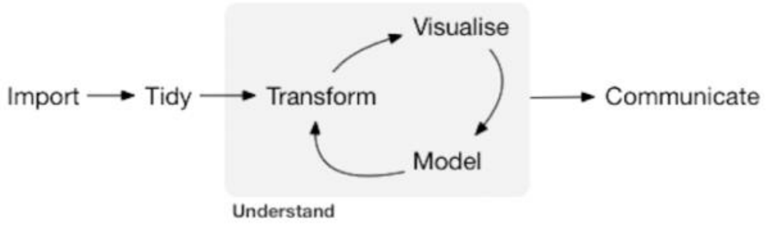
Workflow features to mitigate chaos:

1. **Version control**. Git & Github
   *always add version control to workflow!
2. **Executable analysis scripts & pipelines** (Python/R scripts & Make): Can be used by others to run/replicate the analysis. Easier to understand the landscape of the project and for others to contribute. Reduces some of the challenges/frustrations of working with larger data sets.
   *add this when you start hiding code chunks/cells in RMD/Jupyter notebook.
   Make: a tool that automatically builds executable programs and libraries from source code by reading files called Makefiles. Make can track changes in the source code and its dependencies, only rebuilding the parts of the software that have been modified.
   Makefiles are "smart" and after changes, only run the parts of the analysis that has changed. Each code block = a rule. Makefiles are made of many rules, typically one rule for each time you run an analysis script.
3. **Defined & shippable dependencies** (Docker)
   *add this when remote computing or when have tricky dependencies
   Defined Dependencies = specific components a software application relies on to function correctly.
   Shippable Dependencies= the dependencies that are included with the software package when it is ready for deployment or "shipping" to end-users.
   Docker: a platform that enables developers to build, package, and distribute applications as lightweight, portable containers. **Containers** are isolated environments that contain everything needed to run an application, including the code, runtime, system tools, system libraries, and settings.
   Docker Hub: a cloud-based repository service provided by Docker that allows users to store and manage Docker images. **Docker images** = key building blocks used to create Docker containers.
   Instructions needed to run analysis on almost any machine:
   - Install Docker
   - Clone or download the GitHub repository

- From the root of the cloned repository, type:

```
docker run --rm -v $(pwd):/home/rstudio/data_analysis_eg \
ttimbers/data_analysis_pipeline_eg make -C /home/rstudio/data_analysis_eg all
```

Data Analysis Cycle



To drive insight from data, need to match the correct DS methods to type of statistical questions you are asking:

Statistical questions

- **Descriptive**: summarize a characteristic of a set of data.

Ex: What is the frequency of bacterial illnesses in a set of data collected from a group of individuals? How many people live in each US state?

- **Exploratory**: analyze a set of data to find patterns, rends or relationships between variables.

Ex: Do diets rich in certain foods have differing frequencies of bacterial illnesses in a set of data collected from a group of individuals?

- **Inferential**: analyze the data to see if there are patterns, trends, or relationships between variables in a representative sample.

Ex: Is eating at least five servings a day of fresh fruit and vegetables associated with fewer bacterial illnesses per year?

- **Predictive:** predict measurements or labels for individuals. Less interested in causes.

Ex: How many viral illnesses will someone have next year?

- **Causal**: whether changing one factor will change another factor.

Ex: Does smoking lead to cancer?

- **Mechanistic**: explain the underlying mechanism of the observed patterns, trends, or relationship.

Ex: How do changes in diet lead to a reduction in the number of bacterial illnesses?

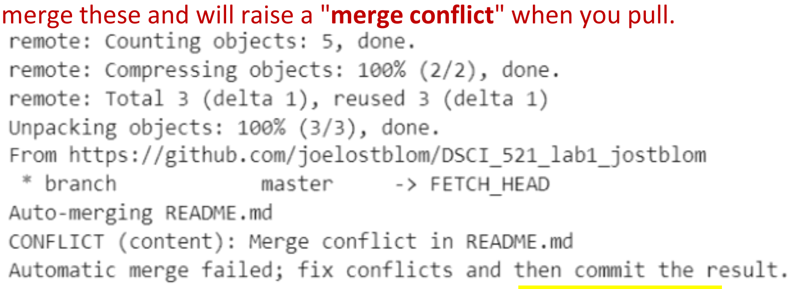
Deal with merge conflict:

merge conflict happen when you work collaboratively with teammates on one git repo.

- **Push conflict**: Always pull before push. If you push when there are new changes not been pulled, you will have a message in terminal like this:

```
To https://github.com/joelostblom/DSCI_521_lab1_jostblom
 ! [rejected]        master -> master (non-fast-forward)
error: failed to push some refs to
'https://github.com/joelostblom/DSCI_521_lab1_jostblom'
hint: Updates were rejected because the tip of your current branch
is behind
hint: its remote counterpart. Merge the remote changes (e.g. 'git
pull')
hint: before pushing again.
hint: See the 'Note about fast-forwards' in 'git push --help' for
details.
```

- **Pull conflict (merge conflict)**: 2 scenarios when try to pull:
  ①. Changes to a document where **different lines are modified** between remote repo and your local repo. Git can merge when you pull.
  ②. Changes to a document where **same lines are modified** between remote repo and your local repo. Git CANNOT merge these and will raise a "**merge conflict**" when you pull.

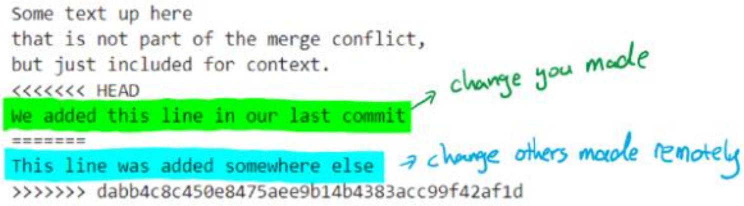


```
remote: Counting objects: 5, done.
remote: Compressing objects: 100% (2/2), done.
remote: Total 3 (delta 1), reused 3 (delta 1)
Unpacking objects: 100% (3/3), done.
From https://github.com/joelostblom/DSCI_521_lab1_jostblom
 * branch            master     -> FETCH_HEAD
Auto-merging README.md
CONFLICT (content): Merge conflict in README.md
Automatic merge failed; fix conflicts and then commit the result.
```

Above the conflict happens at README.md, can use **code** README.md to open it in VS code to edit.

- **Approaches to merge conflict**:
  ①. **Edit the conflict file yourself after pull**: Git will tell you where the conflict is in the output of git pull. You then need to edit the conflict content of the file (search for **<<<<<<< HEAD**) to make sure it looks good. Then add and commit the updated version.
  Ex: conflict content of a text file as below. Edit the two conflict lines, remove any extra characters**, then add**

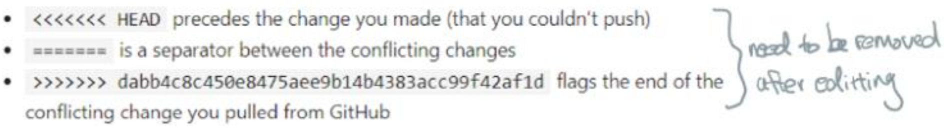
and commit and push again.



```
Some text up here
that is not part of the merge conflict,
but just included for context.
<<<<<<< HEAD
We added this line in our last commit
=======
This line was added somewhere else
>>>>>>> dabb4c8c450e8475aee9b14b4383acc99f42af1d
```

change you made

change others made remotely



- `<<<<<<< HEAD` precedes the change you made (that you couldn't push)
- `=======` is a separator between the conflicting changes
- `>>>>>>> dabb4c8c450e8475aee9b14b4383acc99f42af1d` flags the end of the conflicting change you pulled from GitHub

need to be removed after editing

②. **Stashing local non-committed changes before pulling:** if made changes to a file locally but haven't push yet, and that same file has also been changed remotely. To synchronize changes, using **git pull** directly will result in a **conflict**. So, in this case, using **git stash** to temporarily save all your local changes(both committed + uncommitted), then use **git pull** to update local repo, and later reapply your changes using **git stash pop** to put your changes back to the working area, and then carry on working.

Dealing with branches

In terminal under local repo, create new branch:

# Create a new branch : **git branch** branch_name
# Switch to the existing branch: **git checkout** branch_name
# Create and Switch to a New Branch: **git checkout -b** new_branch_name
# Switch branch: **git switch** branch_name

After done editing on local new branch, add, commit change and push to remote repo:

# Create a corresponding remote branch and push the changes to remote repo on that branch.
git push **--set-upstream** origin new_branch_name
*origin = the label/nickname for the remote repo where the local repo is cloned from. Can contain many branches.
After this you will have two branches on remote repo(main, new_branch), with the new_branch containing your pushed edition.

To merge changes from new_branch to main branch:

submit a pull request on GitHub under the new _branch. Team members will discuss and double check, after that, the pull request is merged into the main branch.

To pull/update your own branch from main:

git checkout nicole_tu #switch to your branch
git fetch origin #fetch the latest changes from the remote repository:
git merge origin/main #merge the changes from main into your nicole_tu branch:
If you prefer to rebase instead of merging, you can use:
git rebase origin/main
Note: Rebasing will rewrite the commit history, so use it only if you haven't pushed your changes to the remote repository or if you are comfortable dealing with potential conflicts.

To review your teammate's branch before merging into the main branch:

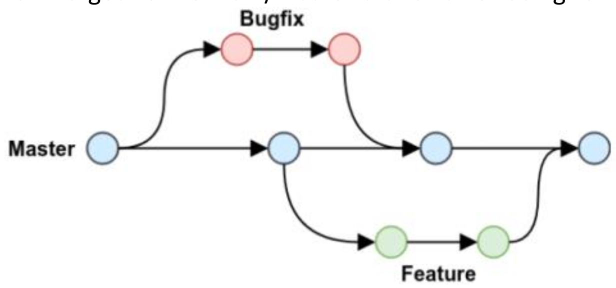
git fetch origin #fetch changes from the entire remote repository.
git checkout <branch_name> #swicth to teammate's branch
git diff main..<branch_name> #see changes made

Solve conflict between branches - If there are conflicting changes in the same file between the branch you're trying to merge and the target branch:

1. GitHub will detect and notify by a message if there are conflicting changes between branches after send pull request.
2. To resolve the conflict, need to **manually edit the conflicting file(s) locally**: Open the file(s) in a text editor, and you'll see markers (<<<<<<<, =======, and >>>>>>>) indicating the conflicting sections. Edit the file to resolve the conflicts
3. After resolving the conflicts, **add, commit, and push** the branch with the conflict resolution back to the remote repository.
4. GitHub will **auto update the pull request status** once it detects the conflict resolution commit.
5. Reviewers can then continue reviewing the pull request, and if everything looks good, the pull request can be merged.

Git and GitHub flow

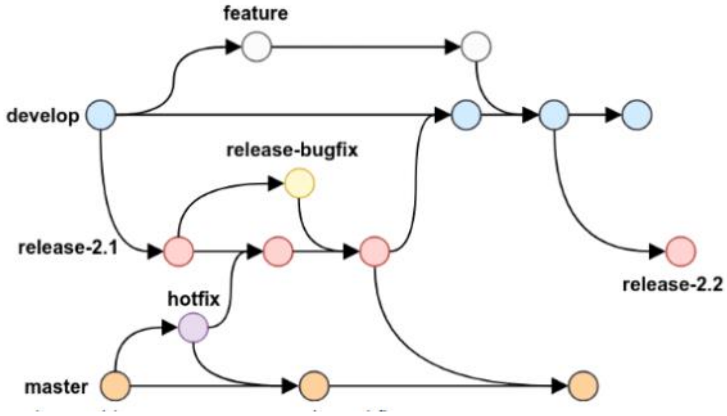
GitHub flow: a dot= a commit. Every new contribution is done on a new branch (ex: Bugfix, Feature) created from main, and later merged to the main/master branch after being reviewed and tested.



Git flow: not recommended for MDS, complicated and time-comsuming

- **Two "main" branches**:
    - Main/master where user is exposed to
    - Develop/stating where things are tested before they are released to main.
- **Three supporting branches**:
    - Feature: merged into develop before they are incorporated into a release
    - Release: eventually get merged into main after adequate review and testing
    - Hotfix.

*Both feature & release branches are created from develop.



L2 - Manage dependencies using containerization

November 16, 2023 10:57 PM

https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/materials/lectures/05-containerization.html

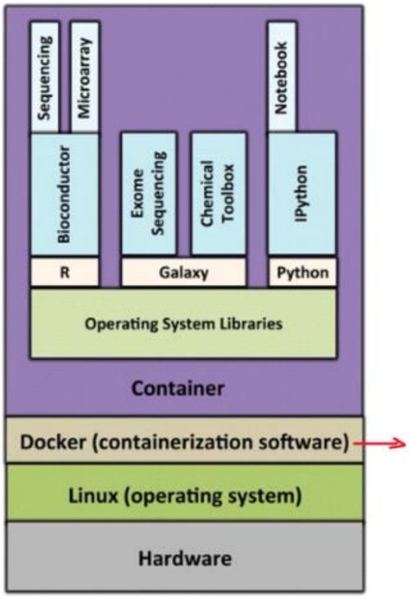
Dependencies are other things one need to install to run your code, and includes:

- programming languages (e.g., R, Python, Julia, etc)
- packages from programming languages (e.g., tidyverse, scikit-learn)
- other tools you rely on (e.g., Make)
- legacy code (e.g., perl scripts, fortran, etc)

*Dependencies include versions as well as names
Defined Dependencies = specific components a software application relies on to function correctly.
Shippable Dependencies= the dependencies that are included with the software package when it is ready for deployment or "shipping" to end-users.

Containerization: a technique that encapsulate an application and its dependencies into a standardized unit called a **container.**

- **Virtualization** is a process to divide the elements of a single computer into several virtual elements (computer hardware platforms, storage devices, and computer network resources, and even operating system user spaces)
- **Containers** are isolated environments that contain everything needed to run an application, including the code, runtime, system tools, system libraries, and settings.
  - Containers virtualize operating system user spaces so that they can isolate the processes they contain, as well as control the processes' access to computer resources (e.g., CPUs, memory and desk space).
  - An operating system user space can be carved up into multiple containers running the same, or different processes, in isolation.

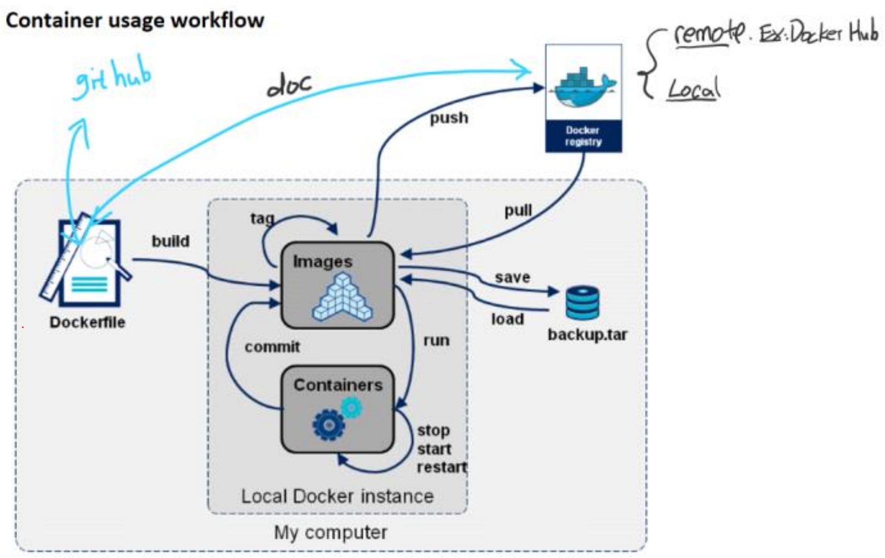


→ does virtualization of operating system user space. allow us to run multiple containers

*note that containerization software still use the same operating system and hardware of the computer.
Docker: a platform/containerization tool that enables developers to build, package, and distribute applications as lightweight, portable containers.
Docker Image: a lightweight, standalone, and executable package that includes all the necessary components to run a piece of software.

- **a snapshot of a file system**, containing the application code, runtime, libraries, and system tools.
- immutable and versioned

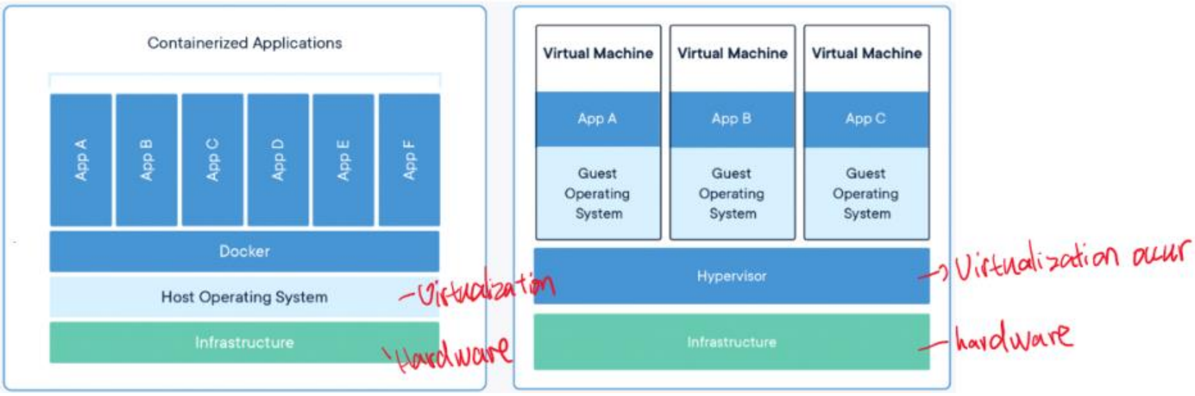
Docker Container: a runnable instance of a Docker image. **Can have multiple containers running from the same image, and each container is isolated from others.** Ex: image = google chrome app, container=google webpage
An image is a static, immutable package, while a container is a dynamic, runnable instance of that package
Docker Registry: a service that stores and distributes Docker images. It can be a **local registry** (hosted on the same machine as the Docker daemon) or a **remote registry** (Ex: **Docker Hub**) accessible over a network.



Contrasting Virtualization Tools: container vs virtual machine

Virtual machine: another technology used to generate (and share) isolated computational environments.

- emulate the functionality of an entire computer on a another computer. Virtualization occurs at the layer of software that sits between the computer's hardware and the operating system(s). This software is called a **hypervisor**.
- Ex: on a Mac laptop, you can install a program called Oracle Virtual Box to run a virtual machine whose operating system was Windows 10.



Containerization software shares the host's operating system, whereas virtual machines have a completely separate, additional operating system. This can make containers **lighter** (smaller in terms of size) and **more resource and time-efficient** than using a virtual machine.

Feature	Virtual environment	Container	Virtual machine
Virtualization level	Application	Operating system user-space	Hardware
Isolation	Programming languages, packages	Programming languages, packages, **other software, operating system dependencies, filesystems, networks**	Programming languages, packages, other software, operating system dependencies, filesystems, networks, **operating systems**
Size	Extremely light-weight	light-weight	heavy-weight

Operating system: the core software that manages computer hardware and provides various services and interfaces for applications and users. EX: Windows, macOS, Linux, and Unix.

- Bash and the terminal are components that exist within an operating system to facilitate command-line interactions but are not operating systems themselves.
- the system's memory is divided into two main areas: the **user space** and the **kernel space**.

    - **User Space**: the area of memory where user applications, programs, and processes operate. User space applications are programs like word processors, web browsers, media players, and other software that users interact with directly.
    - **Kernel Space**: the privileged area of memory where the operating system's kernel resides. **kernel** = core component of the operating system, responsible for managing system resources, handling hardware interactions, and providing essential services to user space. The kernel has direct access to the hardware and controls the overall operation of the computer.
- **Operating system dependency** refers to the reliance of a software application or system on specific features, functions, or behaviors of a particular operating system.

L3 - Docker compose to launch containers

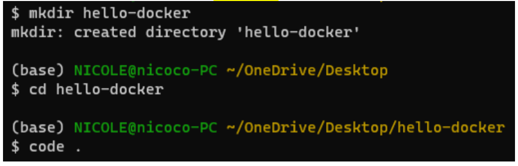
November 19, 2023 7:07 PM

Ten simple rules for writing Dockerfiles for reproducible data science

Dockerfile: used to build a Docker image that encapsulates an application and its dependencies. = **commands** to set up the base image, install dependencies, copy files, and configure the environment inside the Docker container.

Create a Dockerfile: open docker first.

1. In terminal, set current wd as the directory that contains the application(ex: app.js) you want to package. Open VS code by: **code .**



```
$ mkdir hello-docker
mkdir: created directory 'hello-docker'

(base) NICOLE@nicoco-PC ~/OneDrive/Desktop
$ cd hello-docker

(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/hello-docker
$ code .
```

2. Open a new file in VC code, name it **Dockerfile**, in the Dockerfile:

FROM <base image> # <base image> =the image (with some files already) we choose to build on. Can be found on docker hub.

COPY <source> <destination> # <source> = path the files/directories on local machine you want to copy into image. <destination> = path inside image to store the copied files. The path will be created in the image if it doesn't exist.

# Ex: **COPY** . /app copy all files in current wd(source) into the app directory(destination) into the image so that image has a file system, and in that file system we create a directory called app which contains all the files we have in current wd.

RUN <commend> # Run <commend> during the building of image.

CMD <commend> # Run commend only when create a container. Because app.js is inside the app directory, so add directory name prefix.

Ex:

FROM quay.io/jupyter/minimal-notebook #use the base image = quay.io/jupyter/minimal-notebook

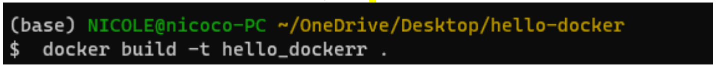
COPY environment.yml /tmp/ # copies the environment.yml file in current wd to the /tmp/ directory inside the Docker image.

RUN conda env create -f /tmp/environment.yml #create a conda environment based on the environment.yml file when build the image. The **-f** specifies path to the environment file.

- In Dockerfile: Pin version number of packages, container image are necessary. Otherwise the docker will auto use the latest version, but the latest version is keep changing, which is not good for replicate your application.
- analysis data should NOT be included downloaded/installed in the container image.
- analysis code that you wrote should be included in the container image.

3. Save the Dockerfile, go to terminal: **docker build --tag** <image_name>:1.0 .

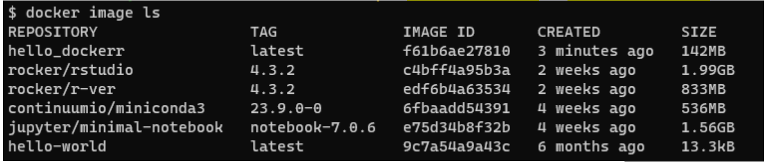
# after **--tag**(or **-t**), specify a self-made image_name, after <image_name>, can add **optional Tag** by **:** (here Tag **:1.0**), followed by **absolute/path/of/Dockerfile**, if the Dockerfile is in the current wd, use **.**



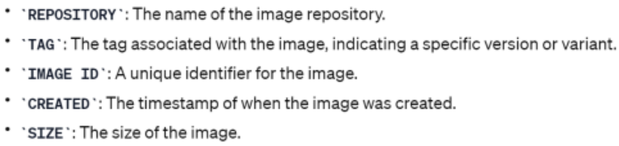
```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/hello-docker
$  docker build -t hello_dockerr .
```

Now the image is created and stored.

See all images on the computer, in terminal: **docker images** or **docker image ls**

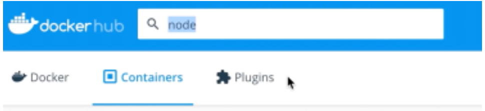


```
$ docker image ls
REPOSITORY                TAG            IMAGE ID       CREATED          SIZE
hello_dockerr             latest         f61b6ae27810   3 minutes ago    142MB
rocker/rstudio            4.3.2          c4bff4a95b3a   2 weeks ago      1.99GB
rocker/r-ver              4.3.2          edf6b4a63534   2 weeks ago      833MB
continuumio/miniconda3    23.9.0-0       6fbaadd54391   4 weeks ago      536MB
jupyter/minimal-notebook  notebook-7.0.6 e75d34b8f32b   4 weeks ago      1.56GB
hello-world               latest         9c7a54a9a43c   6 months ago     13.3kB
```



- `REPOSITORY`: The name of the image repository.
- `TAG`: The tag associated with the image, indicating a specific version or variant.
- `IMAGE ID`: A unique identifier for the image.
- `CREATED`: The timestamp of when the image was created.
- `SIZE`: The size of the image.

Search base images (ex: node) on docker hub:



Run image to create container: In terminal, does not matter where the current wd is: **docker run** <image_name>

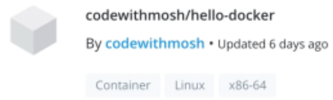
*If want to modify files in the image, has to rebuild the image again after modification by **docker build** with the same image name, then the image will be overwritten and you can then **docker run** the rebuilt image.

Adding packages in existing image by:

1) docker run --rm **-it** <image_name> **bash** # **-it** interactively open terminal in docker container. **--rm** removes the container after it exits. **bash**: the command that will be executed within the container. In this case, it starts a Bash shell, providing you with an interactive terminal session inside the running container.
2) In image terminal: conda install -y <package_name> to test if it can be installed successfully. Use exit to exit the interactive container terminal.
3) If test is successful, open Dockerfile and add install commend under RUN
4) Docker build again: docker build --tag IMAGENAME_version2 .

Publish image on docker hub so that others can pull and use it:

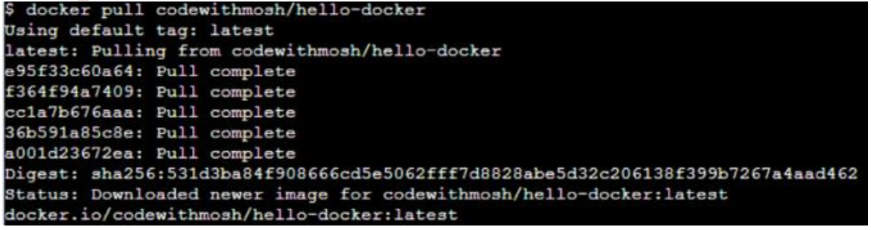
Assume the pushed image *hello-docker* is in the repository named *codewithmosh*



codewithmosh/hello-docker

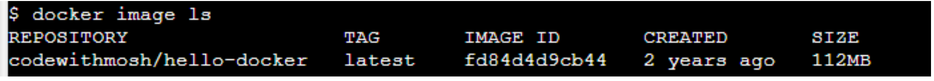
By codewithmosh • Updated 6 days ago

Pull a docker image from Docker Hub repo: in terminal, does not matter where the current wd is: **docker pull** <Docker_Hub_repo_name/image_name>: version_number
: version_number is optional



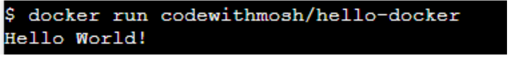
```
$ docker pull codewithmosh/hello-docker
Using default tag: latest
latest: Pulling from codewithmosh/hello-docker
e95f33c60a64: Pull complete
f364f94a7409: Pull complete
cc1a7b676aaa: Pull complete
36b591a85c8e: Pull complete
a001d23672ea: Pull complete
Digest: sha256:531d3ba84f908666cd5e5062fff7d8828abe5d32c206138f399b7267a4aad462
Status: Downloaded newer image for codewithmosh/hello-docker:latest
docker.io/codewithmosh/hello-docker:latest
```

- Check if the image is pulled:



```
$ docker image ls
REPOSITORY                 TAG       IMAGE ID       CREATED       SIZE
codewithmosh/hello-docker  latest    fd84d4d9cb44   2 years ago   112MB
```

- Run the pulled image with docker run <name specified in REPOSITORY>:



```
$ docker run codewithmosh/hello-docker
Hello World!
```

We can take any application and dockerize it by adding a Dockerfie to it. This dockerfile contains instructions for packaging an application into an image. Once we have an image, we can run it virtually anywhere, on any machine with docker.

Exercise - running a container with Jupyter as a web app
Use Docker to run a container that contains the Jupyter web-application installed:

5) **Open docker**
6) **Install image in terminal**: docker pull jupyter/minimal-notebook:notebook-7.0.6
7) **Run container in terminal**: docker run --rm jupyter/minimal-notebook:notebook-7.0.6

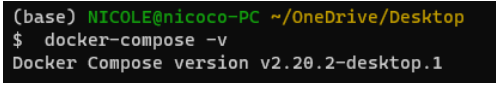
--rm: automatically removes the container when it exits.
-p 8889:8888 = map **port** 8888 from the container to port 8889 on the host machine. The two can be the same number, as long as they are unique on the **host machine** (the physical machine on which the Docker engine is running.) Iin this case, you can access the Jupyter Notebook running inside the container on your host machine by navigating to http://localhost:8889
*any changes(install R packages in a container with RStudio as a web app) done during the runtime of the container will NOT be saved after close the container.
Use exit to exit the interactive container terminal.

To save changes made in a container:
Mounting volumes to containers: allows you to share data between the host machine and the container.
Volume = a directory within one or more containers. Data in volumes is preserved even if the container stops or is removed. Volumes can be shared between multiple containers, allowing them to access and modify shared data.
Mount a volume in a container: changes made to container are saved on the host machine, and vice versa. Done by creating a shared filesystem that is accessible both from the host machine and the container. Any changes made to files or directories in that mounted volume are reflected on both the host and the container. On Windows, the laptop path depends what shell you are using:
Run in Windows terminal or Commend prompt:
docker run --rm -it -v /path/on/host:/path/in/container <IMAGE_NAME>
# take the contents in /path/on/host on the host machine and make them available inside the container at /path/in/container. So, if you create or modify files in /path/on/host on your host machine, those changes will be visible inside the container at /path/in/container, and vice versa.
Run in Power Shell:
docker run --rm -it -v **C:\path\on\host:/path/in/container** <IMAGE_NAME>
Ex: C:\Users\tiffany.timbers\Documents\project\:/home/project

In real world, we need to create complete applications that will be using different services(=containers along with its configuration) and they need to interact with one another. **Docker compose**: tool to define and manage multi-container Docker applications. **docker-compose.yml** specify how the containers (services) should be configured (either from same or different images) and how they interact with each other.
when you run a docker-compose.yml, you are running multiple containers, and they work together for your project's functioning.

- Start all services with a single commend: **docker compose up** # similar to conda activate
- Stop all services with: **docker compose down**
- Scale up selected services when required.

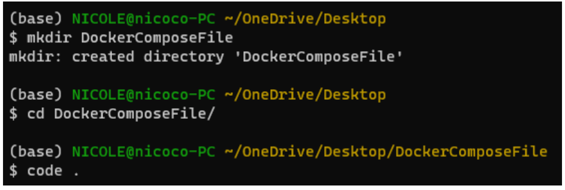
docker-compose -v   #show compose version. Usually installed with Docker.



```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop
$  docker-compose -v
Docker Compose version v2.20.2-desktop.1
```

Create docker-compose.yml file: can be create at any location on your computer. Standard name = docker-compose.yml

1. **Create the file:** Open terminal in the wd where you want to create the docker compose file: .code to open VS code.



```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop
$ mkdir DockerComposeFile
mkdir: created directory 'DockerComposeFile'

(base) NICOLE@nicoco-PC ~/OneDrive/Desktop
$ cd DockerComposeFile/

(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/DockerComposeFile
$ code .
```

In VS code, create a new file and name it **docker-compose.yml**.

2. **Specify docker-compose.yml file**:

----
version: '3'   # specify the version of Docker Compose syntax, need to make sure the version is valid.

services: #define services
 service_name_1:   # self-name the service 1

```
  image: <image_name>    # image to be used for service_1
  …                      # other optional configuration of the service_1 like environment variables, volumes, ports, etc.
 service_name_2:          # self-name the service 2
  image: <image_name>     # image to be used for service_2
…
```

*<image_name> do not need to be local image, can be image from Docker Hub.

----

3. **Check validity** of the file before running it: docker-compose config
4. **Run docker-compose.yml file** to start and manage multiple containers as a single application: docker-compose up -d
   # -d tells Docker compose to run the container in the background, optional.
   Now if use **docker ps** to see running containers, will see 2 containers (service_name_1 and service_name_2) running by specified images.
5. Stop services by: **docker-compose down**

Ex: more complex docker-compose file

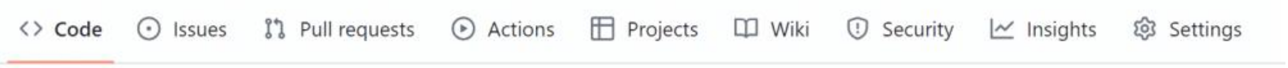
```
services:
 analysis-env:
  image: rocker/rstudio:4.3.2
  ports:
   - "8787:8787"
  volumes:
   - .:/home/rstudio/project
  environment:
   PASSWORD: password
```

Dokerfile vs. docker-compse.yml:

Dockerfile is used to define the contents and build process of a single Docker image, while the **docker-compose.yml file** is used to define and manage the configuration of multiple containers that work together as a service or application. The two often work hand-in-hand, with the Dockerfile being used to create individual images, and the docker-compose.yml orchestrating their collaboration.

Work flow of auto push changes of image to Docker Hub when push local project to GitHub:

1. Create a git repo on GitHub and clone it locally.
2. Build your project in the git repo locally, and add a Dockerfile in the repo to specify a image that the project relies on.
3. After finish the Dockerfile, build your image locally to make sure it works.
4. Add, commit and push your Dockerfile and project to git repo.
5. In your git hub repo, click on **Action -- create your own workflow**, specify a docker-publish.yml file used to create workflow of auto push changes of the docker image to Docker hub when you push the Dockerfile on git hub.
6. Click on **Settings --secrets and variables--Actions**: create 2 **repository secrets** that corresponds to the Docker Hub Username and password you want to push to.



After this, every time you made change locally on Dockerfile, when you push the project with the dockerfile to git hub, the git hub will auto push changes made to dockerfile to docker hub.

Docker commends

November 20, 2023 7:49 PM

Docker basic commends:

docker version # get detailed information of the docker client and server

docker -v # version of docker

docker info # detailed info of docker installed, include number of containers/images,…

docker --help # get help of commends

docker <commend> **--help** #get help of the specific docker commend.

docker login # login to your docker hub account

Images:

docker images # list all image in your computer

docker pull <image_name> # pull image from docker hub repo

docker rmi <image_ID> # remove one or more images, <image_ID> can be found by **docker images**

Containers:

docker ps -a # list all containers(running version of image) both running and exit, on your system.

docker run <image_name> # run a container, if cannot find it locally, will search on Docker Hub and download.

docker run -it <image_name> # interactively start the image and login to it = start the commend prompt of the image

docker run **--rm -it** <image_name> **bash** #Run the image in a bash terminal instead of the web app

docker start <container_ID> # start the container. <container_ID> can be found by **docker ps**

docker stop <container_ID> # stop the container. Container will be in **exit** status.

docker pause <container_ID> # pause the container

docker unpause <container_ID> # unpause the container

Docker attach <container_ID> # attach local standard input, output, and error streams to a running container

----

System:

docker stats # return details on running container's memory usage, input/output, etc.

docker system df # check disk usage of docker

docker system prune # remove unused data. Be careful to use this commend.

L4 - Introduction to testing code for data science

November 22, 2023 4:20 AM

https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/materials/lectures/06-intro-to-testing-code.html#common-types-of-test-levels-in-data-science

Write test before writing functions. Python programming note

Workflow for writing functions and tests for data science:

1. **Write the function specifications and documentation** - but do not implement the function. This means that you will have an empty function, that specifies and documents what the name of the function is, what arguments it takes, and what it returns.
   In R, to get the outline of the function documentation: code -- insert roxygen skeleton
2. **Plan the test cases and document them**. Your tests should assess whether the function works as expected when given correct inputs, and that it behaves as expected when given incorrect inputs (e.g., throws an error when the wrong type is given for an argument). For the cases of correct inputs, test the top, middle and bottom range of these, and all possible combinations of argument inputs possible. Also, the test data should be as simple and tractable as possible.
3. **Create test data used for testing your function**. In data science, you likely need to create both the data that you would provide as inputs to your function, as well as the data that you would expect your function to return.
4. **Write the tests** to evaluate your function based on the planned test cases and test data.
5. **Implement the function** by writing the needed code in the function body to pass the tests.
6. **Iterate between steps 2-5** to improve the test coverage and function.

Common types of test levels in data science

Unit tests - exercise individual components, usually methods or functions, in isolation.

- quick to write and the tests incur low maintenance effort since they touch such small parts of the system.
- It ensure that the unit fulfills its contract making test failures more straightforward to understand.
- Ex: test for count_classes

Integration tests - exercise groups of components to ensure that their contained units interact correctly together.

- touch much larger pieces of the system and are more prone to spurious failure. Since these tests validate many different units in concert, identifying the root-cause of a specific failure can be difficult.
- In data science, this might be testing whether several functions that call each other, or run in sequence, work as expected
- Ex: tests for a tidymodel's workflow function

Test-driven development (TDD): a process for developing software: write test cases that assess the software requirements **before** write the software that implements the software requirements/functionality.

Testability = the degree to which a system or component facilitates the establishment of test objectives and the execution of tests to determine whether those objectives have been achieved.

Properties of effective test writing and execution:

- **controllability**: the code under test needs to be able to be programmatically controlled
- **observability**: the outcome of the code under test needs to be able to be verified
- **isolateablilty**: the code under test needs to be able to be validated on its own
- **automatability**: the tests should be able to be executed automatically.

Ex: in your git_repo

Git_repo/tests:

Testthat.R:

Library(testthat)
Library(demo-test-ds-workflow)
testthat folder

Git_repo/tests/testthat:
helper-count_classes.R :
test-count_classes.R

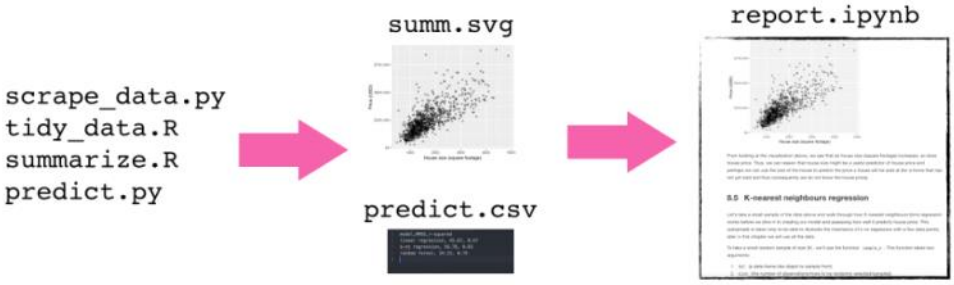
L5 - Data analysis pipelines

November 27, 2023 10:57 AM

https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/materials/lectures/09-pipelines.html

Data Analysis Pipeline: abstract analysis code in a report away to pieces of scripts which can be imported into the final report. Increase report reproducibility and readability.

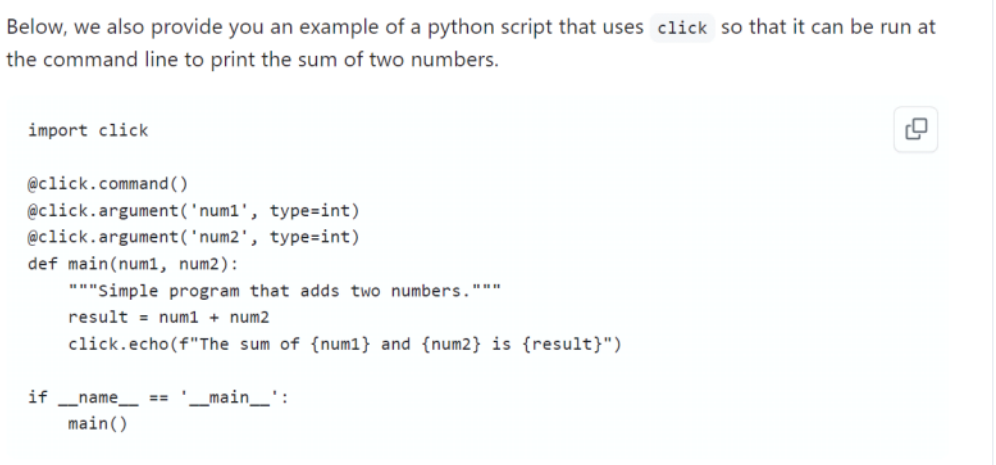
- Scripts are stored in **disc** in the repository.
  - Commend line arguments in scripts
  - Ex: Breast_cancer_predictor/Makefile
- Report is stored in **report** in the repository.



Writing scripts with command line arguments

Python_commend_line repo

Ex1: Create a **Sum.py** file and enter below code



Below, we also provide you an example of a python script that uses `click` so that it can be run at the command line to print the sum of two numbers.

```python
import click

@click.command()
@click.argument('num1', type=int)
@click.argument('num2', type=int)
def main(num1, num2):
    """Simple program that adds two numbers."""
    result = num1 + num2
    click.echo(f"The sum of {num1} and {num2} is {result}")

if __name__ == '__main__':
    main()
```

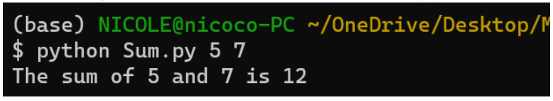
Save the file and in terminal type:

python <path/to/script_name.py> input1 input 2 …

Here since the script file is at the current directory, enter script name directly:

Python Sum.py 5 7

You will get the result from the sum.py file:

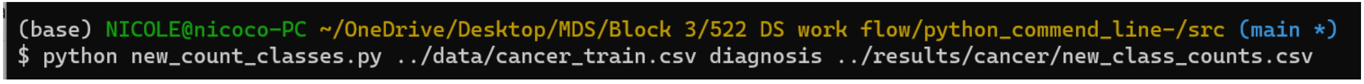


```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/M
$ python Sum.py 5 7
The sum of 5 and 7 is 12
```

Here 'num1' = 5, 'num2'=7

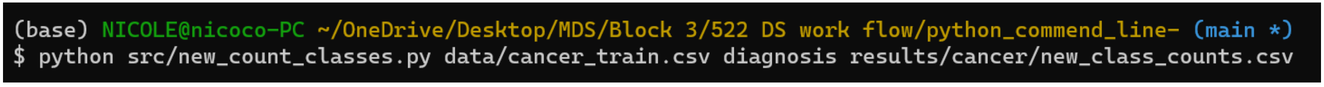
Ex2: create a new_count_classes.py script in src folder, after finish, to run the script in commend:

1. In src directory where the script is located, specify input file path by ..(go upper one directory)



```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/MDS/Block 3/522 DS work flow/python_commend_line-/src (main *)
$ python new_count_classes.py ../data/cancer_train.csv diagnosis ../results/cancer/new_class_counts.csv
```

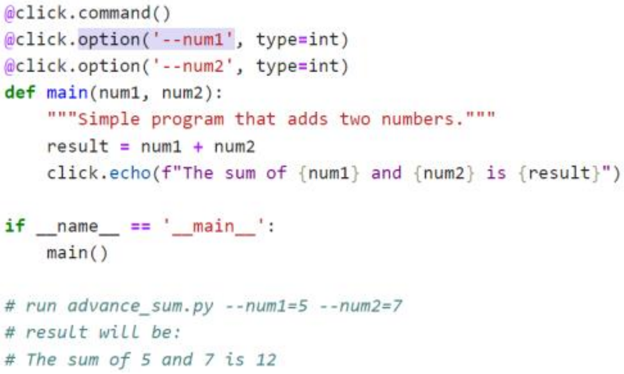
2. In project directory, specify location of both the script and the input file path:



```
(base) NICOLE@nicoco-PC ~/OneDrive/Desktop/MDS/Block 3/522 DS work flow/python_commend_line- (main *)
$ python src/new_count_classes.py data/cancer_train.csv diagnosis results/cancer/new_class_counts.csv
```

Advanced version: use **.option**('--input',…) rather than **.argument**('input') to allow specify input yourself.

<u>Ex1:</u> in advance_sum.py



```
@click.command()
@click.option('--num1', type=int)
@click.option('--num2', type=int)
def main(num1, num2):
    """Simple program that adds two numbers."""
    result = num1 + num2
    click.echo(f"The sum of {num1} and {num2} is {result}")

if __name__ == '__main__':
    main()

# run advance_sum.py --num1=5 --num2=7
# result will be:
# The sum of 5 and 7 is 12
```

<u>Ex2:</u> advance_new_count_classes

*If there are multiple functions in the .py file, need to add @click.command() decorator to each function to define them as Click commands.
*Used @click.option decorator for **optional arguments.**

R_commend_line repo

L6 - Reproducible Reports

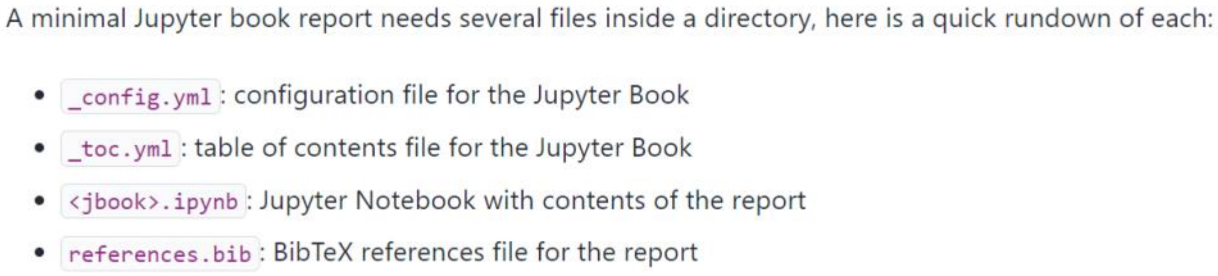
November 29, 2023 10:55 AM

https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/materials/lectures/08-reproducible-reports.html

Advanced reporting: Auto generate figure and table numbering, or cross reference figures and tables.

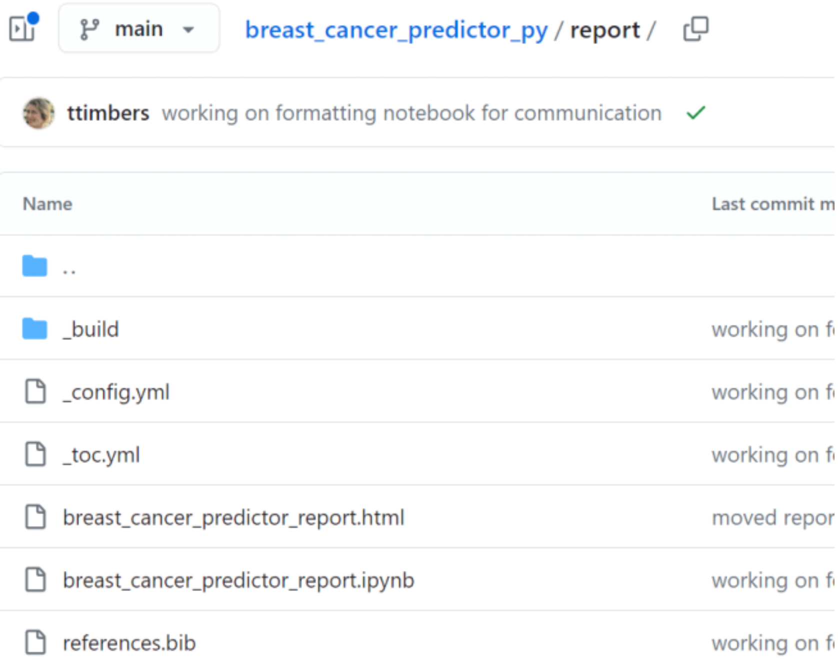
- For **RMarkdown**, layer on the **bookdown** R package (or **rticle** package).
- For **Jupyter**, layer on the **jupyter-book** package.

Jupyter book files: put in report folder in a project folder.



A minimal Jupyter book report needs several files inside a directory, here is a quick rundown of each:

- `_config.yml` : configuration file for the Jupyter Book
- `_toc.yml` : table of contents file for the Jupyter Book
- `<jbook>.ipynb` : Jupyter Notebook with contents of the report
- `references.bib` : BibTeX references file for the report

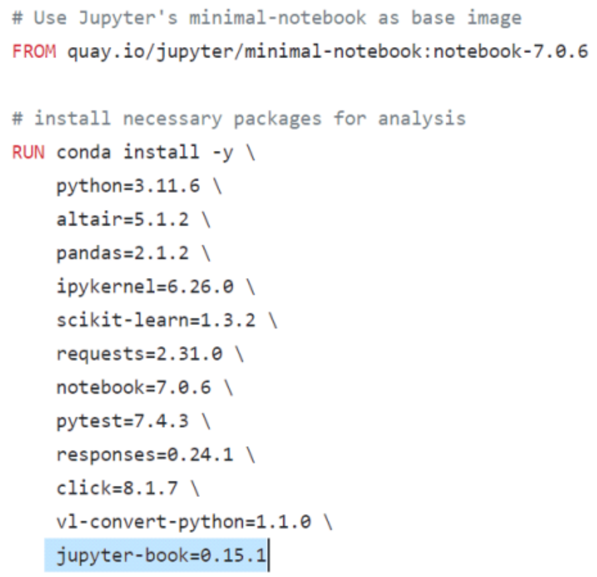


main breast_cancer_predictor_py / report /

ttimbers working on formatting notebook for communication ✓

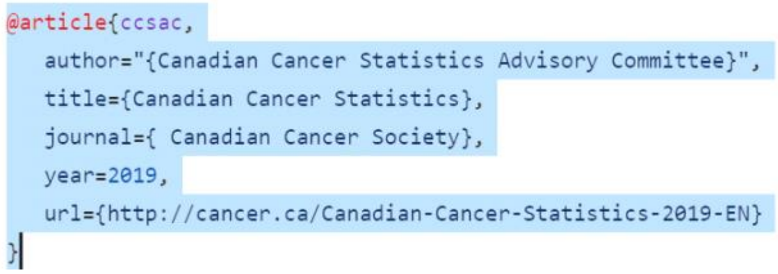
Name	Last commit m
..	
_build	working on f
_config.yml	working on f
_toc.yml	working on f
breast_cancer_predictor_report.html	moved repor
breast_cancer_predictor_report.ipynb	working on f
references.bib	working on f

When render the book, do it in container. ADD jupyter-book=1.15.1 in Dockerfile.



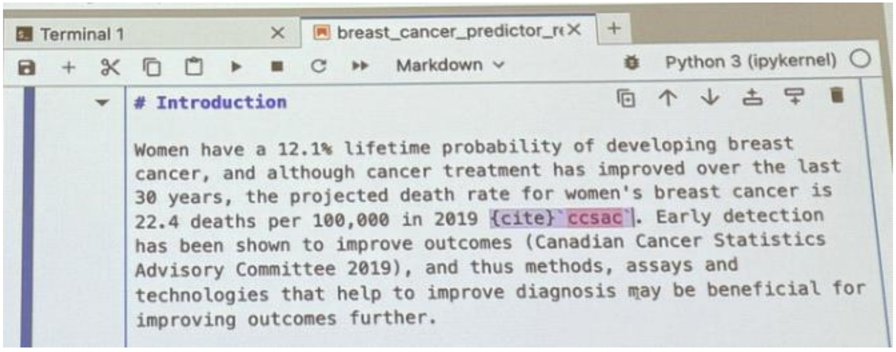
```
# Use Jupyter's minimal-notebook as base image
FROM quay.io/jupyter/minimal-notebook:notebook-7.0.6

# install necessary packages for analysis
RUN conda install -y \
    python=3.11.6 \
    altair=5.1.2 \
    pandas=2.1.2 \
    ipykernel=6.26.0 \
    scikit-learn=1.3.2 \
    requests=2.31.0 \
    notebook=7.0.6 \
    pytest=7.4.3 \
    responses=0.24.1 \
    click=8.1.7 \
    vl-convert-python=1.1.0 \
    jupyter-book=0.15.1
```

References:
In references.bib, put your references as below format:



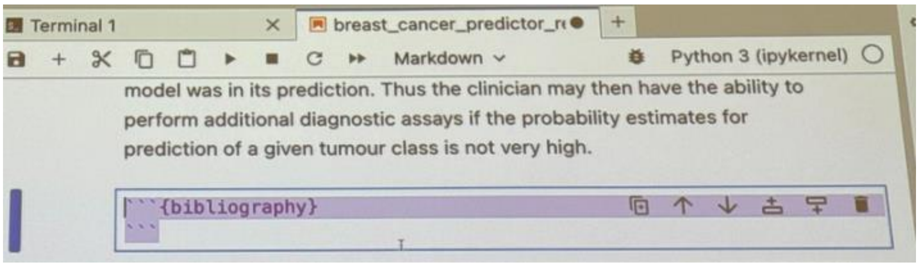
```
@article{ccsac,
   author="{Canadian Cancer Statistics Advisory Committee}",
   title={Canadian Cancer Statistics},
   journal={ Canadian Cancer Society},
   year=2019,
   url={http://cancer.ca/Canadian-Cancer-Statistics-2019-EN}
}
```

Cite it in jupyter book by {cite}`ccsac` in sentence:



```
# Introduction

Women have a 12.1% lifetime probability of developing breast
cancer, and although cancer treatment has improved over the last
30 years, the projected death rate for women's breast cancer is
22.4 deaths per 100,000 in 2019 {cite}`ccsac`. Early detection
has been shown to improve outcomes (Canadian Cancer Statistics
Advisory Committee 2019), and thus methods, assays and
technologies that help to improve diagnosis may be beneficial for
improving outcomes further.
```

Add in the end of the jupyter book:
```{bibliography}
```



model was in its prediction. Thus the clinician may then have the ability to perform additional diagnostic assays if the probability estimates for prediction of a given tumour class is not very high.

~~~
```{bibliography}
```
~~~

Cite in Rmd: [@ccsac] in sentences

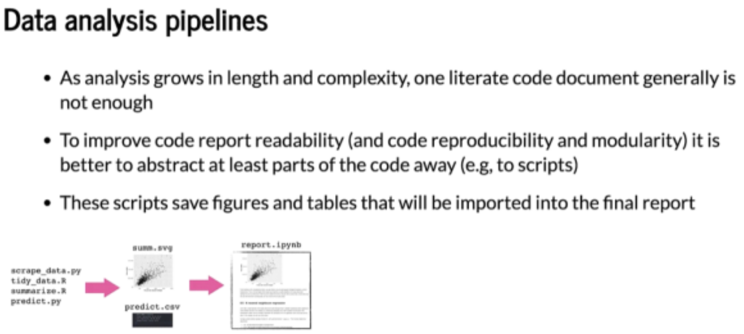
L7 - Data Analysis Pipelines

December 3, 2023 3:52 PM

https://ubc-dsci.github.io/reproducible-and-trustworthy-workflows-for-data-science/materials/lectures/09-pipelines.html?highlight=data+analysis+pipeline

Data analysis check list:

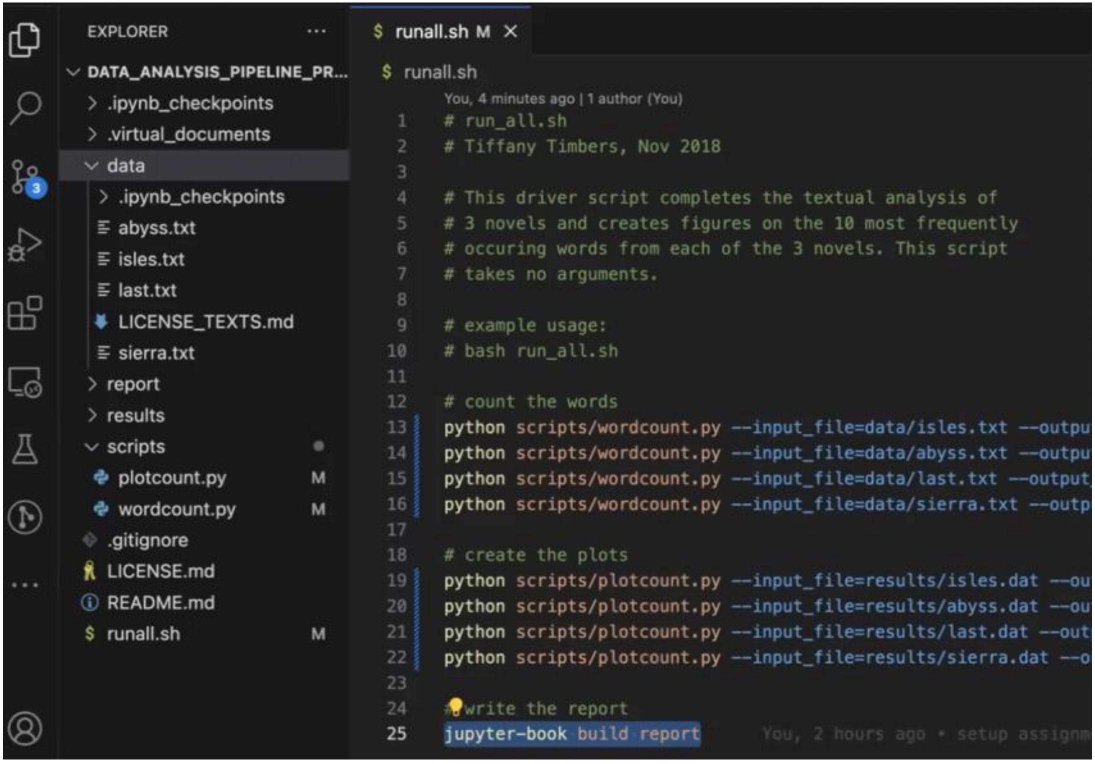
https://raw.githubusercontent.com/UBC-MDS/data-analysis-review-checklist/main/data-analysis-review-checklist.md



Data analysis pipelines

- As analysis grows in length and complexity, one literate code document generally is not enough
- To improve code report readability (and code reproducibility and modularity) it is better to abstract at least parts of the code away (e.g, to scripts)
- These scripts save figures and tables that will be imported into the final report

Instead of run script.py individually on terminal. Put all script.py file's terminal commends in one **runall.sh** plain text file so we can run it all in the terminal in one time.

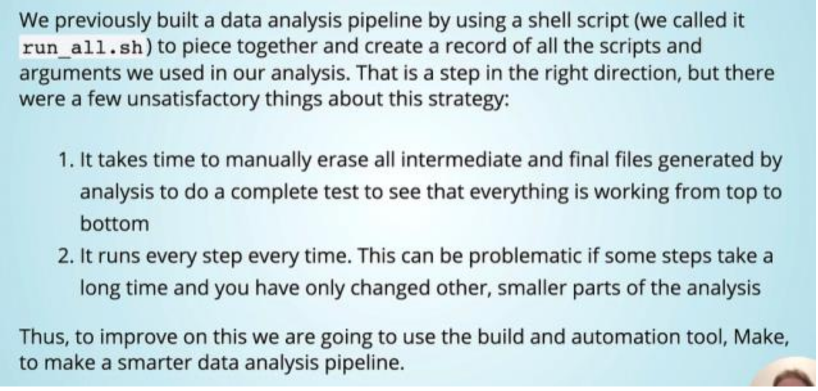


```
# run_all.sh
# Tiffany Timbers, Nov 2018

# This driver script completes the textual analysis of
# 3 novels and creates figures on the 10 most frequently
# occuring words from each of the 3 novels. This script
# takes no arguments.

# example usage:
# bash run_all.sh

# count the words
python scripts/wordcount.py --input_file=data/isles.txt --outpu
python scripts/wordcount.py --input_file=data/abyss.txt --outpu
python scripts/wordcount.py --input_file=data/last.txt --output
python scripts/wordcount.py --input_file=data/sierra.txt --outp

# create the plots
python scripts/plotcount.py --input_file=results/isles.dat --ou
python scripts/plotcount.py --input_file=results/abyss.dat --ou
python scripts/plotcount.py --input_file=results/last.dat --out
python scripts/plotcount.py --input_file=results/sierra.dat --o

💡write the report
jupyter-book build report
```

Run the file: Put **runall.sh** in the root directory of the project and open terminal:

bash runall.sh #run all the scripts commends put in the file

To run only certain parts of the pipeline, and be more flexible: **Make**



We previously built a data analysis pipeline by using a shell script (we called it `run_all.sh`) to piece together and create a record of all the scripts and arguments we used in our analysis. That is a step in the right direction, but there were a few unsatisfactory things about this strategy:

1. It takes time to manually erase all intermediate and final files generated by analysis to do a complete test to see that everything is working from top to bottom
2. It runs every step every time. This can be problematic if some steps take a long time and you have only changed other, smaller parts of the analysis

Thus, to improve on this we are going to use the build and automation tool, Make, to make a smarter data analysis pipeline.

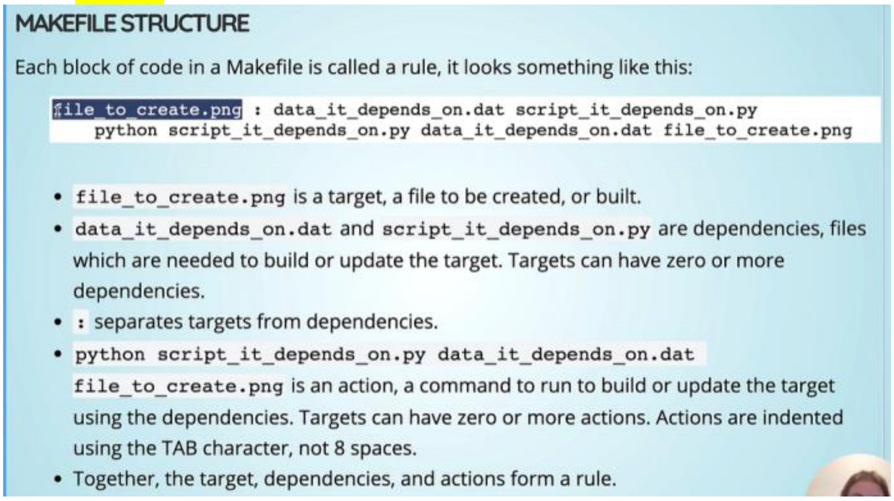
Make: a tool that automatically builds executable programs and libraries from source code by reading files called Makefiles. Make can track changes in the source code and its dependencies, only rebuilding the parts of the software that have been modified.

Makefile: manage the build process and automate the compilation of source code into executable programs or libraries. After changes, only run the parts of the analysis that has changed.

Makefile structure: each block of code = a rule = target + dependencies + actions

Makefiles are made of many rules, typically one rule for each time you run an analysis script.

```
Target : dependencies
        Actions
```



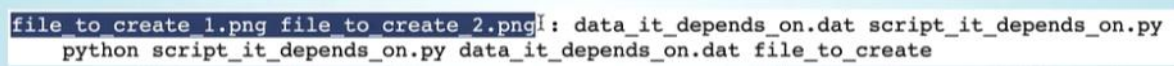
MAKEFILE STRUCTURE

Each block of code in a Makefile is called a rule, it looks something like this:

```
file_to_create.png : data_it_depends_on.dat script_it_depends_on.py
    python script_it_depends_on.py data_it_depends_on.dat file_to_create.png
```

- `file_to_create.png` is a target, a file to be created, or built.
- `data_it_depends_on.dat` and `script_it_depends_on.py` are dependencies, files which are needed to build or update the target. Targets can have zero or more dependencies.
- `:` separates targets from dependencies.
- `python script_it_depends_on.py data_it_depends_on.dat file_to_create.png` is an action, a command to run to build or update the target using the dependencies. Targets can have zero or more actions. Actions are indented using the TAB character, not 8 spaces.
- Together, the target, dependencies, and actions form a rule.

Can have more than one target in one rule, separate targets by a white space.



```
file_to_create_1.png file_to_create_2.png : data_it_depends_on.dat script_it_depends_on.py
    python script_it_depends_on.py data_it_depends_on.dat file_to_create
```

Basic Usage: Open the terminal and go to the directory containing the Makefile.

List Available Targets: make -n -qp

Run a Specific Target in a rule: make <target_name> # this will build the specified target and execute the associated commands in the Makefile.

Run the Default Target: make #If there is a target named **all** (build the last of the dependencies). = running make all.

Clean Up: make clean #If the Makefile includes a **clean** target for removing generated files from each rule.

EX: individual assignment 4

https://github.com/Nicole-Tu97/data_analysis_pipeline_practice.git

Transfer the runall.sh to a Makefile

runall.sh

```
# example usage: bash runall.sh
# count the words
python scripts/wordcount.py --input_file=data/isles.txt --output_file=results/isles.dat
python scripts/wordcount.py --input_file=data/abyss.txt --output_file=results/abyss.dat
# create the plots
python scripts/plotcount.py --input_file=results/isles.dat --
output_file=results/figure/isles.png
python scripts/plotcount.py --input_file=results/abyss.dat --
output_file=results/figure/abyss.png
# write the report
jupyter-book build report
```

Makefile:

```
all: report/_build/html/index.html
# target = final output of a script.py
# dependencies =  input files of the script.py + the script itself
# action: the terminal commend to run this script
# count words
results/isles.dat : data/isles.txt scripts/wordcount.py
    python scripts/wordcount.py --input_file=data/isles.txt --
output_file=results/isles.dat
```

```
results/abyss.dat : data/abyss.txt scripts/wordcount.py
    python scripts/wordcount.py --input_file=data/abyss.txt --
output_file=results/abyss.dat
# plot word count
results/figure/isles.png : results/isles.dat scripts/plotcount.py
    python scripts/plotcount.py --input_file=results/isles.dat --output_file=isles.png
results/figure/abyss.png : results/abyss.dat scripts/plotcount.py
    python scripts/plotcount.py --input_file=results/abyss.dat --output_file=abyss.png

report/_build/html/index.html : report/count_report.ipynb \
report/_toc.yml \
report/_config.yml \
results/figure/isles.png \
results/figure/abyss.png
    jupyter-book build report

clean :
# remove all .dat files in results directory
    rm -f results/*.dat
# remove all .png fules in results.figure directory
    rm -f results/figure/*.png
    rm -rf report/_build
```