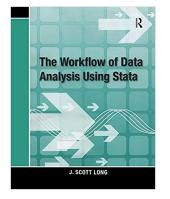
Facilitating Reproducible Research

Wassim Tarraf, PhD
Analyses Core Seminar
MCUAAAR 5
May 20th, 2019

Plan

- 1. Discuss workflow
- 2.Integrate Open Science workflow
- 3.Challenges
- 4. Applied demonstration
 - a. git & GitHub
 - b. RStudio

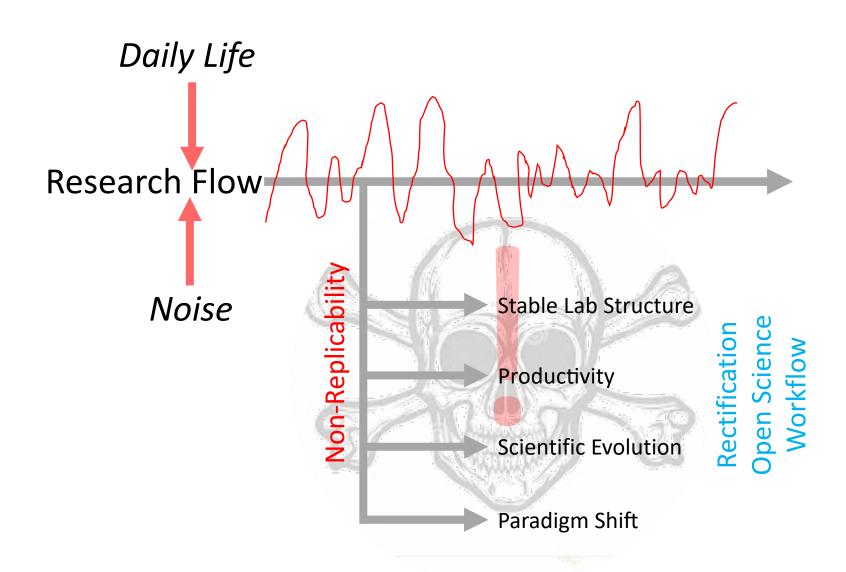
Defining a research workflow (Scott Long)



System for:

- "Planning, organizing, and documenting" scientific process
- Establishing and fostering collaborations
- Managing and sharing data
- Analyzing data
- Disseminating findings
- Archiving process for replication

Non-replicability



What is the nature of your workflow?

- Non-systematic
- Semi-systematic or ad-hoc
 - -> reactionary, responsive to errors
- Carefully planned

- Can you improve workflow?
 - Initial time investment
 - Longer term improvement in efficiency and return on investment

Decision points for open science workflows

- 1. Creating own workflow or using existing *Workflow Management*Systems
 ✓ some recommendations
- 2. Choosing a data repository
- 3. Deciding on a source code repository \checkmark some recommendations
- Choosing a system to "Package, Access, and Execute Data and Code" ✓ some recommendations
- 5. Choosing a document repository (free or fee for service)
- 6. Licensing and Privacy 🔀

What does an open science workflow get you?

- Primary Benefit is Facilitating replication and strengthening the evidence base
 - Internally: Streamlined analytic process
 - Externally: Improved collaboration
 - Efficiencies:
 - Better framework for fixing and recovering from errors
 - Enhanced throughput
 - Use of past processes to inform future work
 - More natural evolution of scientific product
 - Progeny

Example of a complication

Outcome

<u>S1</u>

<u>S2</u>

<u>S3</u>

<u>S4</u>

Cognitive Function	As is	Z-Score	Group Specific Z-Scores	Threshold Based Grouping
<u>Covariates</u>				
Age	Continuous	4 Groups		
Race/Ethnicity	As is	Regrouped		
Education	Continuous	5 Groups		
CESD	Continuous	Global Threshold Grouping	Group Specific Thresholds	

$$5 * 2 * 2 * 2 * 3 = 120 possibilities$$

Long, 2012 https://ssrc.indiana.edu/doc/wimdocs/2012-09-07_long_workflow_slides.pdf

Replication

- Workflow effectiveness -> enables replication
 - Be planful starting today
 - Universal concern with replication in scientific fields
- Easy metric for success in creating Open Science workflow
 - Use existing gauge your "manuscript" is ready when it is ready for peer-review/wider readership
 - Your workflow is effective and replicable if your scientific process is ready for public view

Replication is complicated

Ask yourself: Can someone else use my project files to discern my intent, clearly see my presuppositions and guiding assumptions, make sense of my process, understand the reasoning for my decisions, and reproduce my findings

Answer is in Documentation:

- Detailing of process
- Explicit choice of tools that facilitate public documentation of scientific process
- Protection against document leaks; version control

Some Criteria to consider when picking a framework

- How simple is it to use?
 - Critical in the beginning
- Is it suitable for your personal needs
- Does it enhance current workflow
- Is it sustainable as a "longer-term" solution
- Can it be scaled to expected growth (multiple projects, lab needs, collaborations)
- Does it contribute to standardizing critical production elements
- Does it help with automating repetitive tasks

Collaborations

- Adds complication to any process
- Collaboration can be a hazard for breakages in workflow
- **Unless** system includes:
 - Clear role definitions
 - Standards for interacting and feeding into the established system
 - Mechanisms for coordination
 - Enforcement rules

Challenges

Individual research needs:

- Incentive structure not yet established
 - rewards for "openness" not yet fully recognized
- Time costs
 - To set up the system
 - Be productive within the system
- Other systemic constraints (e.g. data restrictions)

Make the workflow WORK

- 1. Start now!!
- 2. Gain skills incrementally.
 - Establish habits
 - Integrate complex processes over time
- 3. Don't design or attempt to change quickly or under time constrainst
- 4. Many viable workflows:
- Find one that might work (borrow from other efficient users) with your style and personality
 - Make it your own and instill it in your lab members
 - Be flexible to change; be open to having graduate students, post docs, and collaborators show you new ways

 https://ssrc.indiana.edu/doc/wimdocs/2012-09-07 long workflow slides.pdf

Considerations for open science workflows

- Creating own workflow or using existing Workflow Management Systems ✓
- 2. Choosing a Data Repository
- 3. Deciding on a Source Code Repository ✓
- 4. Choosing a system to "Package, Access, and Execute Data and Code" ✓
- 5. Choosing a Document Repository (free or fee for service)
- 6. Licensing and Privacy

Things you can do right away

- Start now!
- Keep in mind that:
 - Reproducible does not mean perfect
 - Improving a system is a lot easier than falling behind
- Create a simple set of rules that initially bind you, your lab members and trainees, and eventually your collaborators to the process
- Associate with (attend conferences, follow on social media) and seek help from (correspond directly) with others who work within a similar framework

Three simple steps to start now

- 1. Create an account and commit to using a version control system for documenting code
 - I will do a demonstration on how to do so using Git
- 2. Commit to documentation now
 - Make this part of your and your lab members daily writing routines
 - Have others look at your documentation the same way you have them inspect your scientific writing
- 3. Adopt practices that allow for replication
 - I will show an example with RStudio and Rmarkdown
 - Other software allow similar processes

Get git

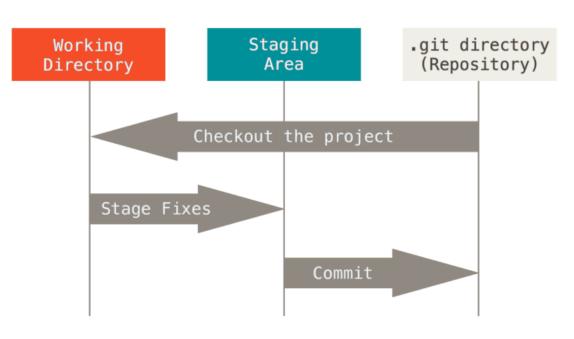
Download git:

Instructions on how to do so for Linux, macOS, and Windows are available here

What is git:

Distributed version control system:

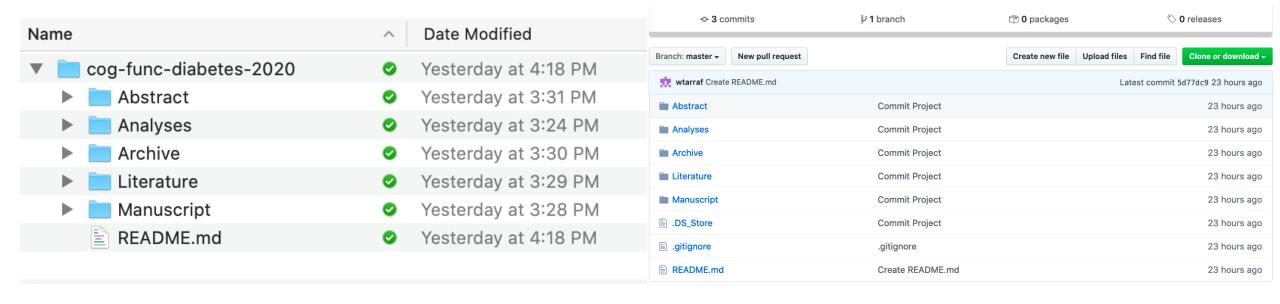
- 1. Do the work locally
- 2. Stage it (add needed changes)
- 3. Commit it to your repo



From local to repo

Local project architecture

GitHub repo



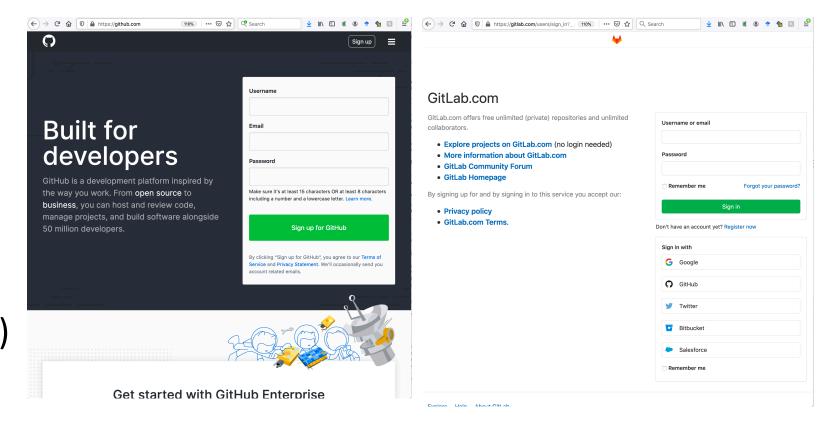
Github (or Gitlab)

Create a GitHub or GitLab account

What are these:

Platforms for hosting (mostly) software based on git

Offers:



<u>distributed version control</u> – peer-to-peer – each user has local copy and access to the full history of code (or other documents)

Mostly used in open source projects

Offers <u>functionalities for code management</u> (branching, merging, forking, cloning, etc..)

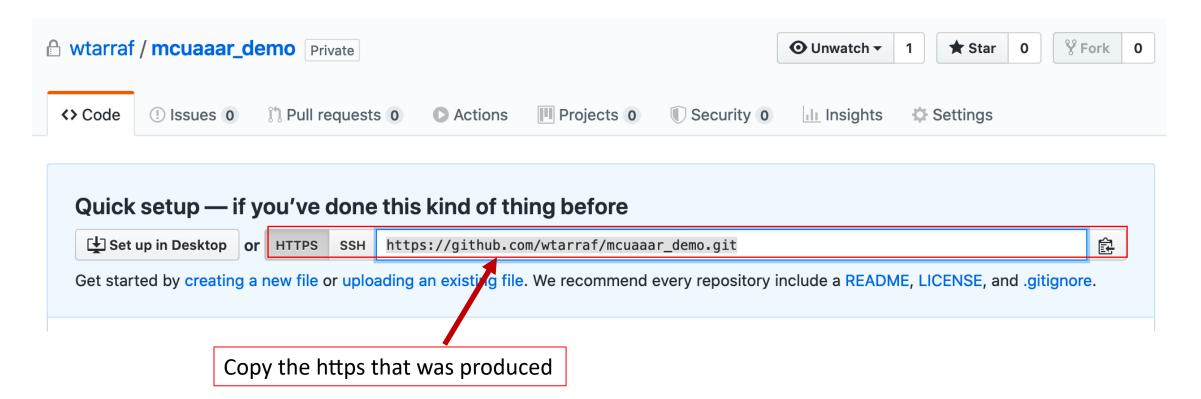
Get started with Git and GitHub

- 1. Log in to https://gitlab.com or to
- 2. Create a new repo by clicking on the green "New Repository" button
- Name you repository I usually use the same project name that I've created locally
- 4. Choose whether you want the repo to be public or private
- 5. Initialize without a README or gitignore file (we will come back to this in a bit)

A repository contains all project files, including the revision history. Already have a project repository elsewhere? Import a repository. Owner Repository name * math display the m mcuaaar_demo Great repository names are short and memorable. Need inspiration? How about jubilant-carnival? **Description** (optional) Demonstration MCUAAAR 5 Reproducible Research Anyone can see this repository. You choose who can commit. You choose who can see and commit to this repository. Skip this step if you're importing an existing repository. Initialize this repository with a README This will let you immediately clone the repository to your computer. Add .gitignore: None ▼ Add a license: None ▼ **Create repository**

Create a new repository

Connect local project to GitHub repo



Segway to RStudio



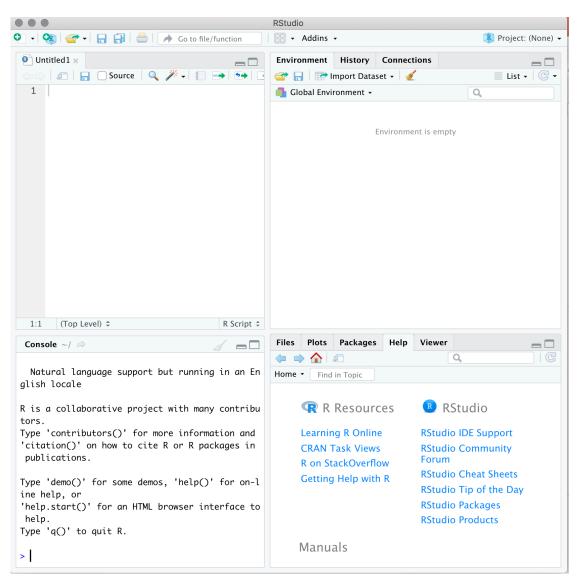


Download R

Free programming language and statistical computing environment

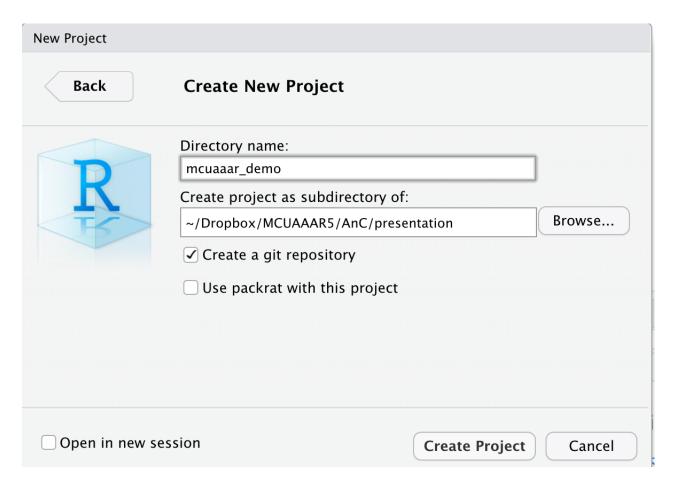
Download RStudio Desktop

Free integrated development environment (IDE) for R

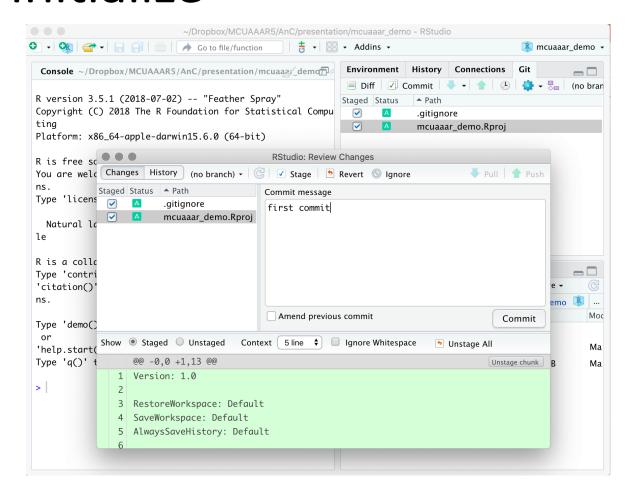


Working with Rstudio and GitHub

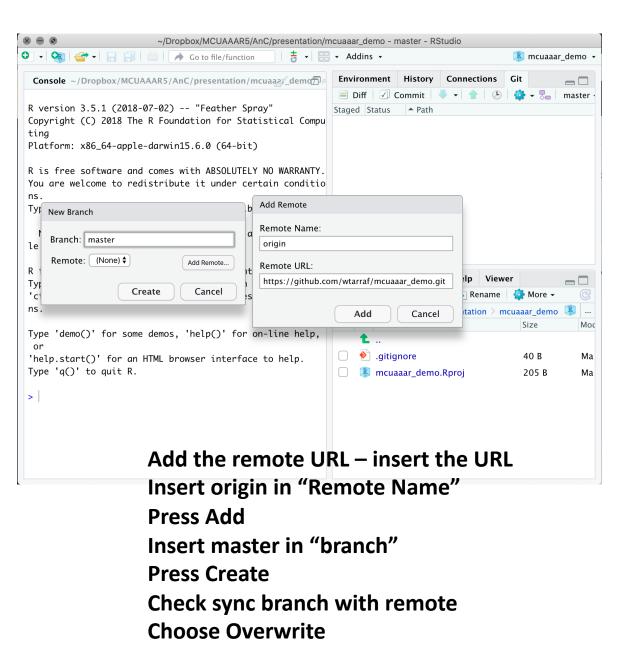
File ->
New Project
Check – create a git repository



Initialize

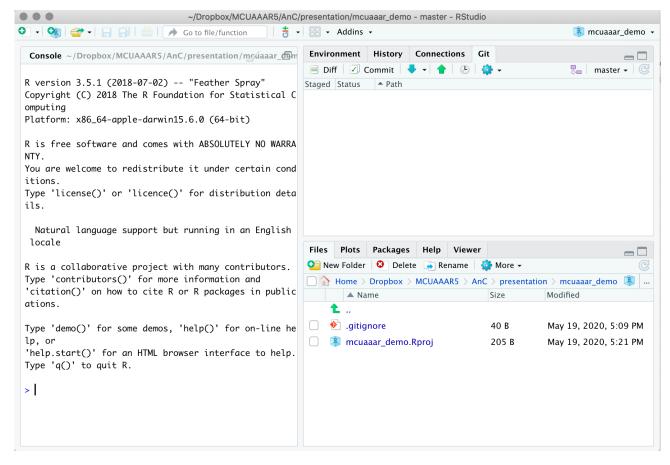


Create a first commit

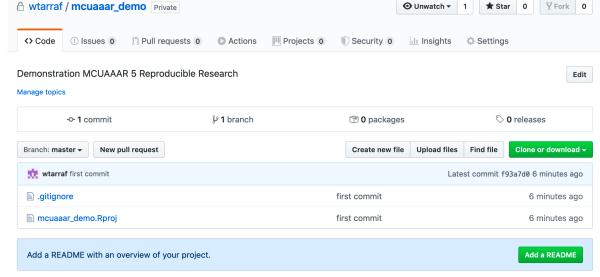


You are ready

Local project



GitHub Repo



Be planful with your project infrastructure

- Plan and incrementally improve the organizational structure
 - Strive for easy to follow structure that reflects the way you approach your research
 - <u>Streamline</u> (create near uniformity) to facilitate cloning of structure across projects
 - Make smart decisions about
 - What to name your folder, subfolders, and documents
 - Where, when, and what to save
 - How often and what to commit
- The more of it you do the better you get at it



Work in RStudio

Rmarkdown:

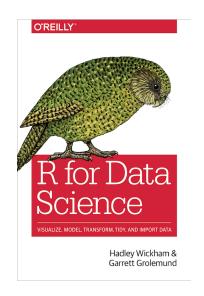
Notebook interface that weaves narrative, code, results, and visualization



The <u>'tidyverse'</u> - a collection of packages 3 packages to begin

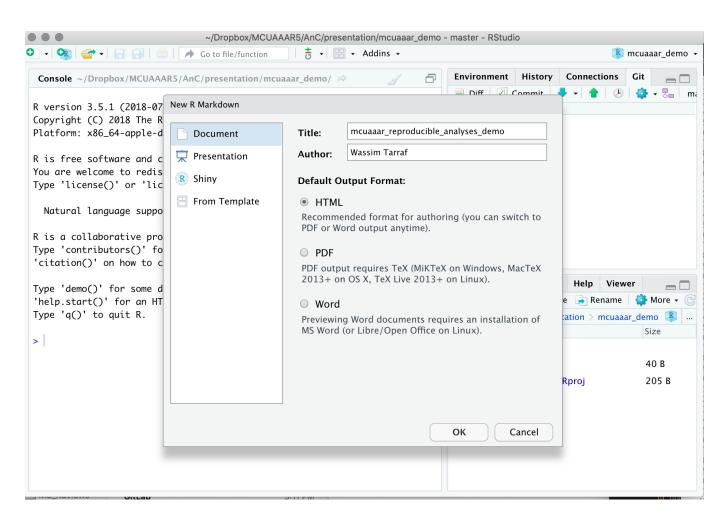


<u>haven</u> – to import data<u>dplyr</u> – to wrangle the data<u>ggplot2</u> – to plot the data



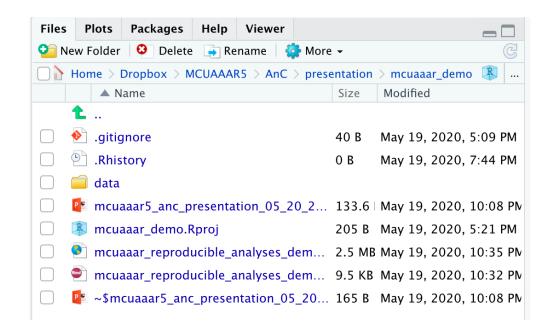
Working with data – an Rmarkdown example

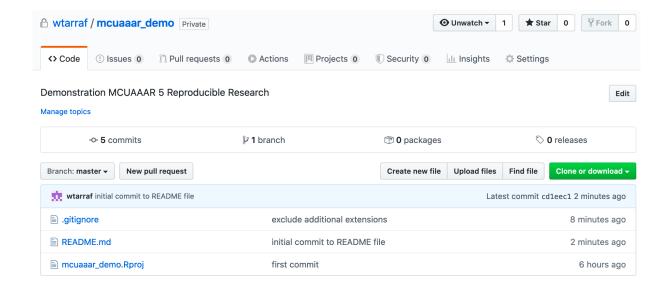
- (1) Import data
- (2) Prepare the data
 - Data mergers
 - Determine a set of
 - observations and variables of
 - interest
 - -> Filters (data split)
 - -> Selections (data
 - reduction)
 - Consider transformation of the variables (mutate)
- (3) Model your data
- (4) Visualize it



Back to git

- Do this as often as needed
 add
 commit
 push
- When collaborating
 Learn how to branch
 pull
 and if necessary merge
- Make use of what others have to offer clone fork





Back to git – reconciling local and repo

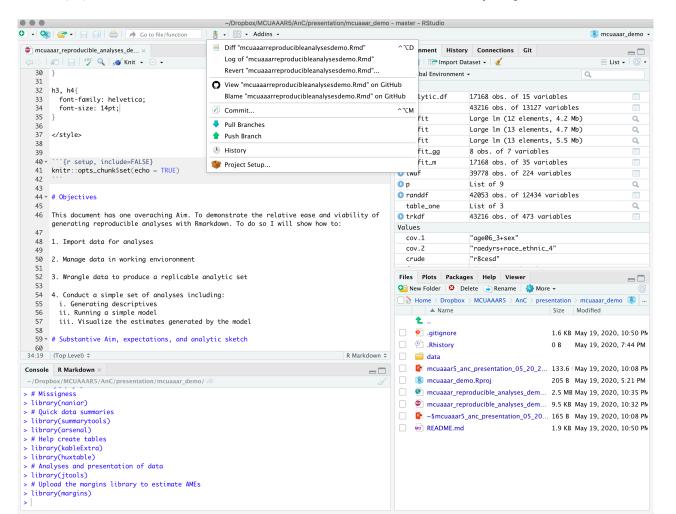
- Do this as often as needed
 add
 commit
 push
- When collaborating
 Learn how to branch
 pull
 and if necessary merge

fork

Make use of what others have to offer clone

Pull changes that I added to my repo locally:

- (1) I updated my .gitignore to restrict types of files that I can push
- (2) I created a README file to describe the project



Back to git – reconciling repo and local

- Do this as often as needed
 add
 commit
 push
- When collaborating
 Learn how to branch
 pull
 and if necessary merge

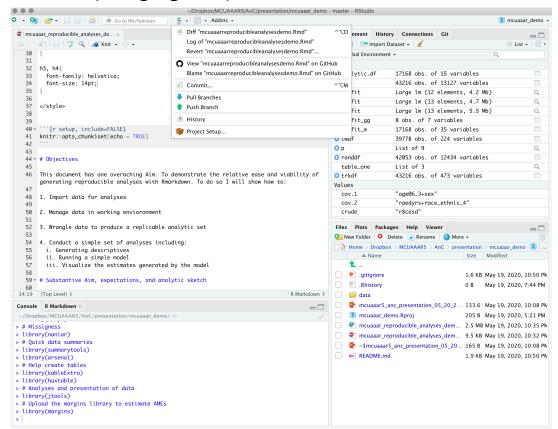
clone

fork

- Make use of what others have to offer

Pull changes that I added to my repo locally:

- (1) I saved the powerpoint presentation I will choose not to push it (i.e. keep it locally)
- (2) I saved my Rmarkdown file
- (3) I saved an HTML version of my knitted Rmarkdown file
- (4) although I added a lot of data the push for these is restricted (see gitignore)



Back to git – reconciling repo and local

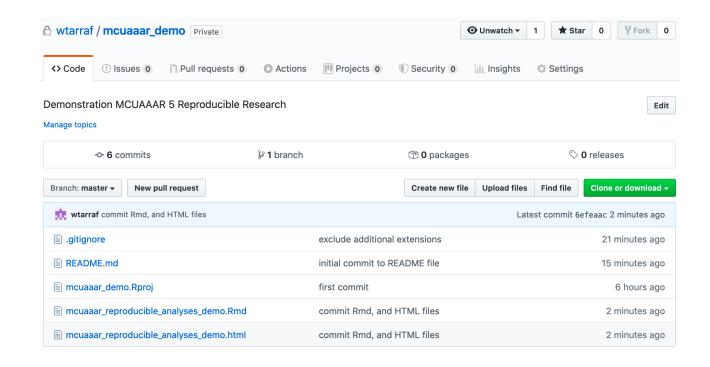
- Do this as often as needed
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 push
- When collaborating
 Learn how to branch
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- Make use of what others have to offer *clone*

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- (3) I saved an HTML version of my knitted Rmarkdown file
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Thanks!

follow-up and questions:

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