Last class!

function()

Last class!

Last class revisited...

- Write a function grade() to determine an overall grade from a vector of student homework assignment scores dropping the lowest single assignment score.

```
# student 1
c(100, 100, 100, 100, 100, 100, 100, 90)

# student 2
c(100, NA, 90, 90, 90, 90, 97, 80)

# now grade all students in an example class
url <- "https://tinyurl.com/gradeinput"
```

Last class!

Last class revisited...

- Write a function grade() to determine an overall grade from a vector of student homework assignment scores dropping the lowest single assignment score.

```
grade <- function(x) {
  x <- as.numeric(x)
  x[ is.na(x)] = 0
  mean(x[ -which.min(x) ])
}
```

Last class revisited...

Last class!

- Write a function grade() to determine an overall grade from a vector of student homework assignment scores dropping the lowest single assignment score.

```
grade <- function(x) {
  x <- as.numeric(x)
  x[ is.na(x)] = 0
  mean(x[ -which.min(x) ])
}
```

Last class revisited...

Last class!

- Write a function grade() to determine an overall grade from a vector of student homework assignment scores dropping the lowest single assignment score.

```
grade <- function(x) {
  x <- as.numeric(x)
  x[ is.na(x)] = 0
  mean(x[ -which.min(x) ])
}
```

Do this now…

Last class!

- Write a function **grade2**() to determine an overall grade from a vector of student homework assignment scores **OPTIONALLY** dropping the lowest single assignment score.

```
grade <- function(x) {
  x <- as.numeric(x)
  x[ is.na(x)] = 0
  mean(x[ -which.min(x) ])
}
```

Last class revisited...

Last class!

```
grade2 <- function(x, drop.lowest=TRUE) {
  x <- as.numeric(x)
  x[ is.na(x)] = 0
  if(drop.lowest) {
    mean(x[ -which.min(x) ])
  } else {
    mean(x)
  }
}
```

And some function homework….

Complete Q6. In last days lab supplement

Your Homework!

```
library(bio3d)
s1 <- read.pdb("4AKE")  # kinase with drug
s2 <- read.pdb("1AKE")  # kinase no drug
s3 <- read.pdb("1E4Y")  # kinase with drug

s1.chainA <- trim.pdb(s1, chain="A", elety="CA")
s2.chainA <- trim.pdb(s2, chain="A", elety="CA")
s3.chainA <- trim.pdb(s1, chain="A", elety="CA")

s1.b <- s1.chainA$atom$b
s2.b <- s2.chainA$atom$b
s3.b <- s3.chainA$atom$b

plotb3(s1.b, sse=s1.chainA, typ="l", ylab="Bfactor")
plotb3(s2.b, sse=s2.chainA, typ="l", ylab="Bfactor")
plotb3(s3.b, sse=s3.chainA, typ="l", ylab="Bfactor")
```

Suggested steps for writing your functions

1. Start with a simple problem and get a working snippet of code
2. Rewrite to use temporary variables (e.g. x, y, df, m etc.)
3. Rewrite for clarity and to reduce calculation duplication
4. Turn into an initial function with clear useful names
5. Test on small well defined input and (subsets of) real input
6. Report on potential problem by failing early and loudly!
7. Refine and polish

What is Git?

(1) An unpleasant or contemptible person. Often incompetent, annoying, senile, elderly or childish in character.

(2) A modern distributed version control system with an emphasis on speed and data integrity.

What is Git?

(1) An unpleasant or contemptible person. Often incompetent, annoying, senile, elderly or childish in character.

(2) A modern distributed version control system with an emphasis on speed and data integrity.

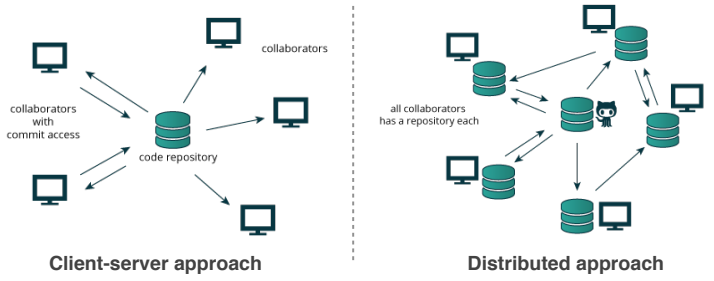
Version Control

Version control systems (VCS) record changes to a file or set of files over time so that you can recall specific versions later.

Client–server	Free/open-source	CVS (1986, 1990 in C) · CVSNT (1998) · QVCS Enterprise (1998) · Subversion (2000)
	Proprietary	Software Change Manager (1970s) · Panvalet (1970s) · Endevor (1980s) · Dimensions CM (1980s) · *DSEE* (1984) · Synergy (1990) · ClearCase (1992) · *CMVC* (1994) · *Visual SourceSafe* (1994) · Perforce (1995) · StarTeam (1995) · Integrity (2001) · Surround SCM (2002) · AccuRev SCM (2002) · SourceAnywhere (2003) · Vault (2003) · Team Foundation Server (2005) · Team Concert (2008)
Distributed	Free/open-source	*GNU arch* (2001) · Darcs (2002) · *DCVS* (2002) · *ArX* (2003) · Monotone (2003) · *SVK* (2003) · *Codeville* (2005) · Bazaar (2005) · **Git** (2005) · Mercurial (2005) · Fossil (2007) · Veracity (2010)
	Proprietary	*TeamWare* (1990s?) · Code Co-op (1997) · BitKeeper (1998) · Plastic SCM (2006)

There are many VCS available, see:
https://en.wikipedia.org/wiki/Revision_control

Client-Server *vs* Distributed VCS



Client-server approach

Distributed approach

Distributed version control systems (DCVS) allows multiple people to work on a given project without requiring them to share a common network.

http://tinyurl.com/distributed-advantages

Git is now the most popular free VCS!

Git offers:

- Speed
- Backups
- Off-line access
- Small footprint
- Simplicity*
- Social coding

http://tinyurl.com/distributed-advantages

Where did Git come from?

Written initially by Linus Torvalds to support Linux kernel and OS development.

Meant to be distributed, fast and more natural.

Capable of handling large projects.

Now the most popular free VCS!

Why use Git?

Q. Would you write your lab book in pencil, then erase and overwrite it every day with new content?

Q. Would you write your lab book in pencil, then erase and overwrite it every day with new content?

Version control is the lab notebook of the digital world: it's what professionals use to keep track of what they've done and to collaborate with others.

Why use Git?

- Provides 'snapshots' of your project during development and provides a full record of project history.
- Allows you to easily reproduce and rollback to past versions of analysis and compare differences. (N.B. Helps fix software regression bugs!)
- Keeps track of changes to code you use from others such as fixed bugs & new features
- Provides a mechanism for sharing, updating and collaborating (like a social network)
- Helps keep your work and software organized and available

Obtaining Git

Obtaining Git

Note: You hopefully already have git installed!
To check open the "**Terminal**" tab in RStudio and type:

1. `which git`
2. `git --version`

Obtaining Git

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To check open the "**Terminal**" tab in RStudio and type:

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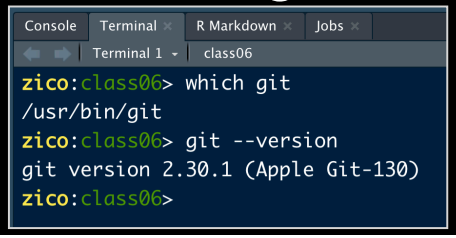
Obtaining Git



Note: You might already have git installed
To check open the "**Terminal**" tab in RStudio and type:

1. `which git`
2. `git --version`

Obtaining Git

Windows Only (if you have problems)

If the "which git" command did not work, try:

```
where git
```

If this works see next slide. If not then you need to install GitBash, instructions here:

Class Computer Setup Page

Mac Only (if you have problems)

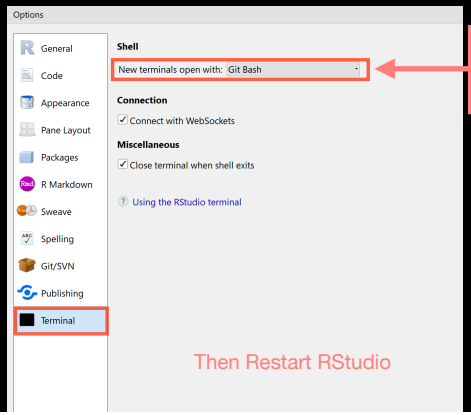
If the "which git" command did not work, you may need to install select developer tools.

In your Terminal type:

```
xcode-select --install
```

On a PC Only!

Go to: **RStudio > Tools > Global Options > Terminal**



Make sure Git Bash is selected!

Do it Yourself!

Note: You might already have git installed
To check open the "**Terminal**" tab in RStudio and type:

1. `which git`
2. `git --version`

Installing Git

Windows (if you have problems)
Follow the GitBash instructions here:
Class Computer Setup Page

Mac (if you have problems)
In the **Terminal** instal select developer tools
`xcode-select --install`

Configuring Git

Do it Yourself!

Configuring Git

(RStudio **Terminal** Tab)
(…or *RStudio* **>** *Tools* **>** *Shell*)

```
# First tell Git who you are
> git config --global user.name  "Barry Grant"
> git config --global user.email  "bjgrant@ucsd.edu"
```

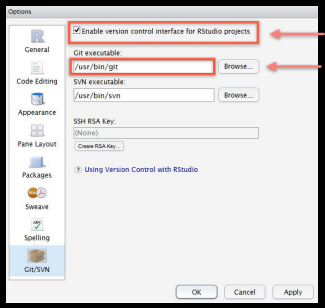
Configuring RStudio

For Mac & Linux

(PC on next slide)

Do it Yourself!

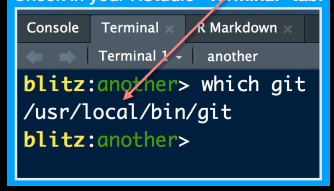
Go to: **RStudio > Tools > Global Options > Git/SVN**



1 *Make sure this is **ticked**!*

2 Make sure this is **correct**!

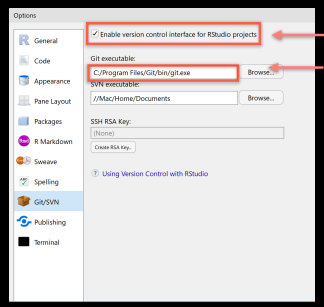
Check in your RStudio "Terminal" tab:



On a PC!

Do it Yourself!

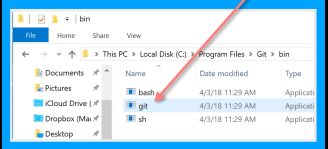
Go to: **RStudio > Tools > Global Options > Git/SVN**



1 *Make sure this is **ticked**!*

2 This is the PATH for **PC**!

Check in your Windows File Explorer:



Restart RStudio!

Using Git

Using Git

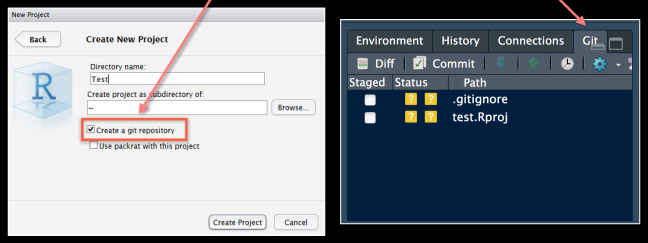
1. Initiate a Git repository.
2. Edit content (i.e. change some files).
3. Store a 'snapshot' of the current file state.*

Do it Yourself!

Create a new **Test** RStudio project

1 New option to create a Git repository…

2 New Git tab…



Check if new Git options appear in RStudio?

Using Git in RStudio

1. **Initiate** a git repository for an RStudio Project
2. Do your work and edit content as normal
3. Store a 'snapshot' of the current file state
   (a) Periodically **add** important files to git "Staging Area"
   (b) **Commit** changes to your "git repository"

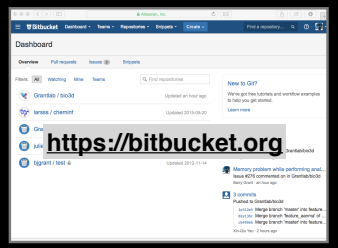
Rinse and repeat….

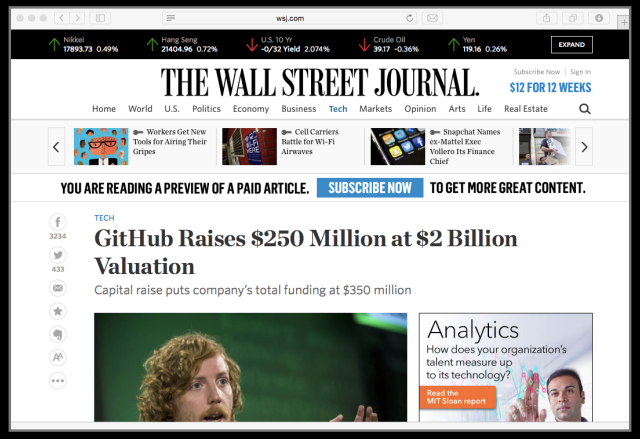
Follow along!

Demo:

GitHub & Bitbucket

GitHub and **Bitbucket** are two popular hosting services for Git repositories. These services allow you to share your projects and collaborate with others using both '**public**' and '**private**' repositories*.



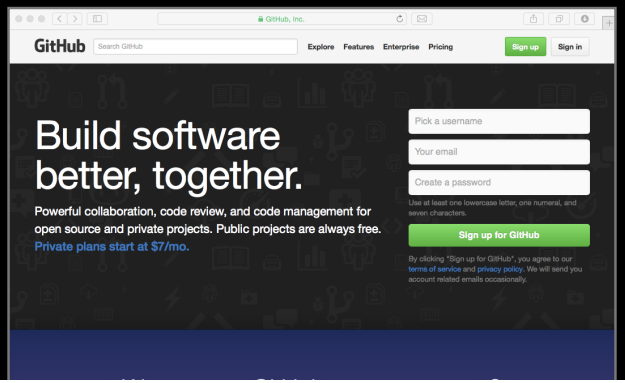


What is the big deal?

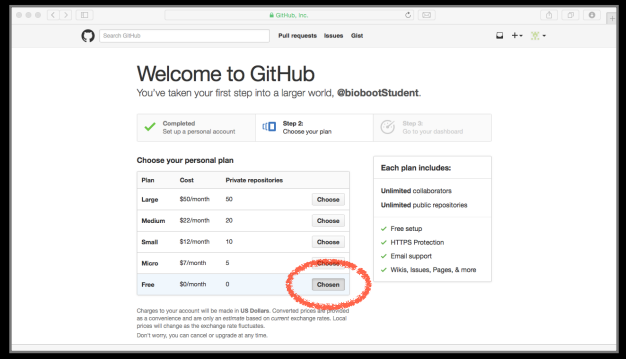
- At the simplest level GitHub and Bitbucket offer **backup** of your projects history and a centralized mechanism for **sharing** with others by putting **your Git repo online**.
  - GitHub in particular is often referred to as the “nerds FaceBook and LinkedIn combined”.
- At their core both services **offer a new paradigm for open collaborative project development**, particularly for software.
  - In essence they allow anybody to contribute to any public project and get acknowledgment.

First sign up for a GitHub account

https://github.com

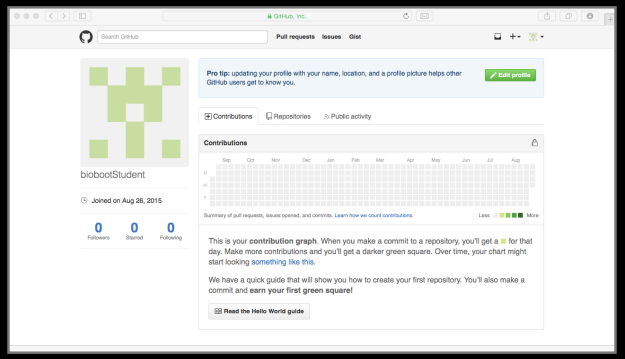


Pick the FREE plan!



Your GitHub homepage

Check your email for verification request



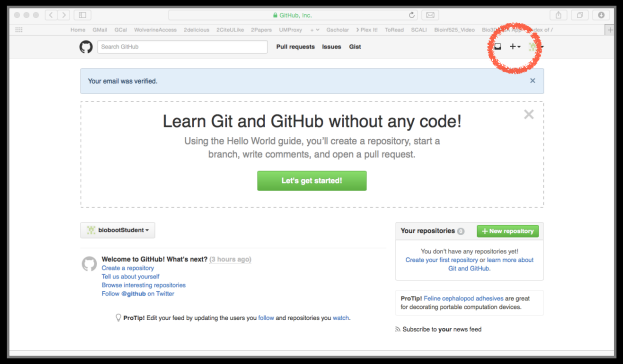
Connecting RStudio to GitHub

Create a **Personal Access Token** (PAT) on GitHub

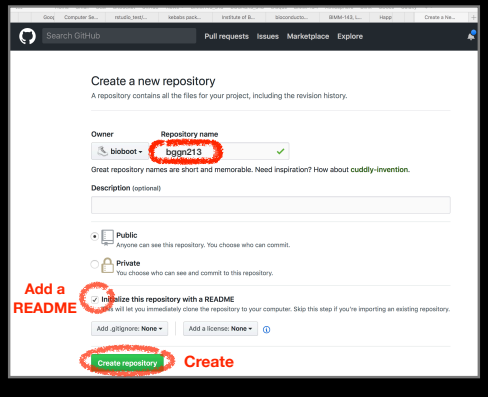
See section 4 of lab worksheet

Skip the hello-world tutorial

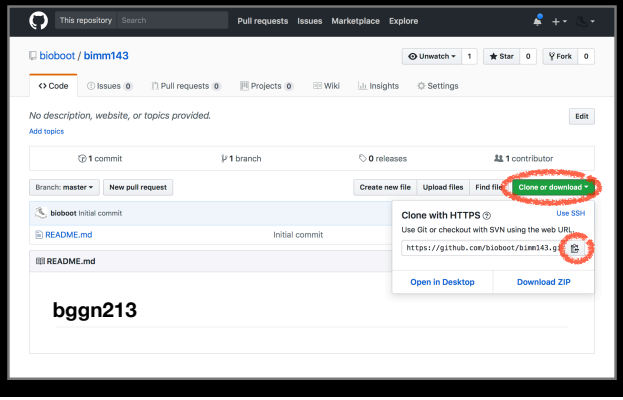
https://guides.github.com/activities/hello-world/



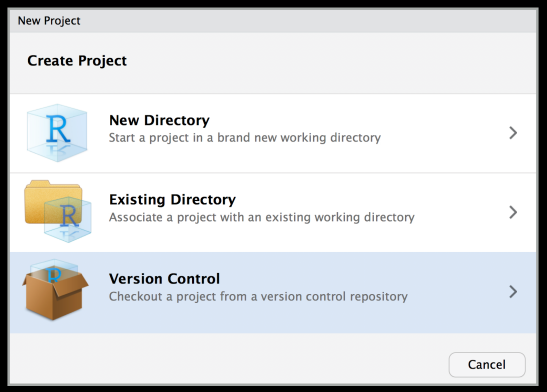
Name your repo bggn213



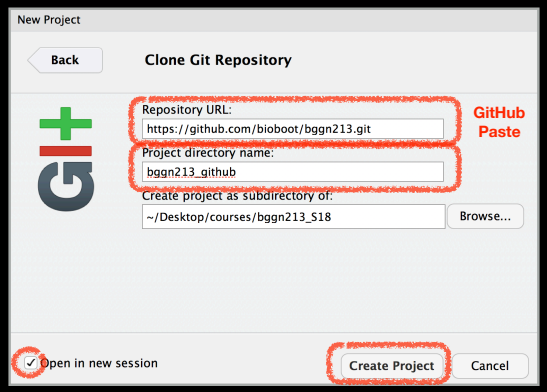
Copy the "Clone" HTTPS link



RStudio > New Project > Version Control

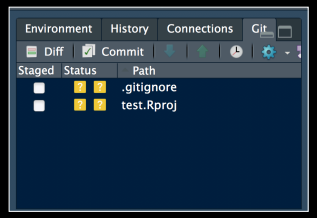


RStudio > New Project > Version Control



Demo of *editing*, *adding committing* and *pushing*

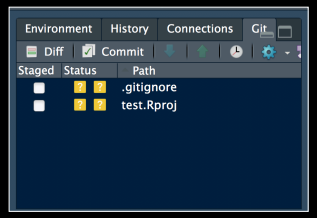
Check if new Git tab Appears in RStudio?



Now experiment editing the README.md file in RStudio and adding, committing and pushing changes to GitHub via this tab

Demo of *editing*, *adding committing* and *pushing*

Check if new Git tab Appears in RStudio?

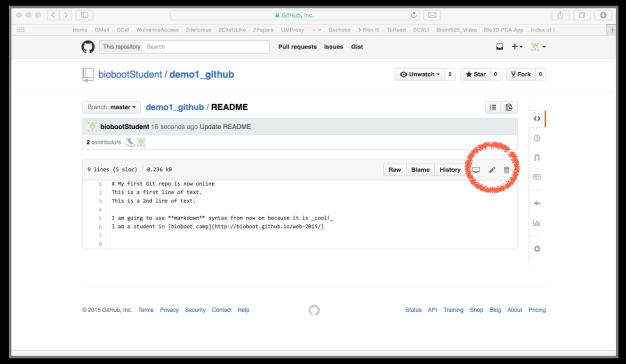


Now experiment editing the README.md file in RStudio and adding, committing and pushing changes to GitHub via this tab

When you are ready copy your different class directories/projects to this new GitHub tracked folder

Side-note: How to edit online

Specifically lets add some Markdown content



Summary

- Git is a popular 'distributed' version control system that is lightweight and free
- GitHub and BitBucket are popular hosting services for git repositories that have changed the way people contribute to open source projects
- Introduced basic git and GitHub usage within RStudio and encouraged you to adopt these 'best practices' for your future projects.

Learning Resources

- **Set up Git**. If you will be using Git mostly or entirely via **GitHub**, look at these how-tos.
  < https://help.github.com/categories/bootcamp/ >
- **Getting Git Right**. Excellent **Bitbucket** git tutorials
  < https://www.atlassian.com/git/ >
- **Pro Git**. A complete, book-length guide and reference to Git, by Scott Chacon and Ben Straub.
  < http://git-scm.com/book/en/v2 >
- **StackOverflow**. Excellent programming and developer Q&A.
  < http://stackoverflow.com/questions/tagged/git >

Learning git can be painful!

However in practice it is not nearly as crazy-making as the alternatives:

- Documents as email attachments
- Hair-raising ZIP archives containing file salad
- Am I working with the most recent data?
- Archaelogical "digs" on old email threads and uncertainty about how/if certain changes have been made or issues solved

Finally Please remember that **GitHub** and **BitBucket** are **PUBLIC** and that you should cultivate your professional and scholarly profile with intention!

Reference Slides

Using Command Line Git

1. Initiate a Git repository.
2. Edit content (i.e. change some files).
3. Store a 'snapshot' of the current file state.*

Initiate a Git repository

Initiate a Git repository

Do it Yourself!

```
> cd ~/Desktop
> mkdir git_class   # Make a new directory
> cd git_class      # Change to this directory
> git init          # Our first Git command!
> ls -a             # what happened?
```

Side-Note: **The .git/ directory**

- Git created a 'hidden' **.git/** directory inside your current working directory.
- You can use the '**ls -a**' command to list (*i.e.* see) this directory and its contents.
- This is where Git stores all its goodies - **this is Git!**
- You should not need to edit the contents of the **.git** directory for now but do feel free to poke around.

Important Git commands

```
> git status        # report on content changes
```

```
> git add <filename>     # stage/track a file
> git commit  -m "message"    # snapshot
```

Important Git commands

> git **status** *# report on content changes*

> git **add** <filename> *# stage/track a file*
> git **commit** -m “message” *# snapshot*

You will use these three commands again and again in your Git workflow!

Git TRACKS your directory content

- To get a report of changes (since last commit) use:
  > **git status**

- You tell Git which files to track with:
  > **git add <filename>**
  This adds files to a so called **STAGING AREA** (akin to a “shopping cart” before purchasing).

- You tell Git when to take an historical **SNAPSHOT** of your staged files (*i.e.* record their current state) with:
  > **git commit -m ‘Your message about changes’**

Example Git workflow

Eva creates a README text file
(this starts as untracked)

Adds file to STAGING AREA*
(tracked and ready to take a snapshot)

Commit changes*
(records snapshot of staged files!)

Example Git workflow

Hands on example!

Eva creates a README text file
Adds file to STAGING AREA*
Commit changes*

Eva modifies README and adds a ToDo text file
Adds both to STAGING AREA*
Commit changes*

1. Eva creates a README file

Do it Yourself!

```
> # cd ~/Desktop/git_class
> # git init

> echo "This is a first line of text." > README
> git status          # Report on changes
# On branch master
#
# Initial commit
#
# Untracked files:
#   (use "git add <file>..." to include in what will be committed)
#
#     README
#
# nothing added to commit but untracked files present (use "git add" to track)
```

2. Adds to ‘staging area’

```
> git add README      # Add README file to staging area
> git status          # Report on changes
# On branch master
#
# Initial commit
#
# Changes to be committed:
#   (use "git rm --cached <file>..." to unstage)
#
#     new file:   README
#
```

3. Commit changes

```
> git commit -m “Create a README file”     # Take snapshot
# [master (root-commit) 8676840] Create a README file
#  1 file changed, 1 insertion(+)
#  create mode 100644 README


> git status              # Report on changes
# On branch master
# nothing to commit, working directory clean
```

4. Eva modifies README file and adds a ToDo file

```
> echo "This is a 2nd line of text." >> README
> echo "Learn git basics" >> ToDo

> git status          # Report on changes
# On branch master
#
# Changes not staged for commit:
#   (use "git add <file>..." to update what will be committed)
#   (use "git checkout -- <file>..." to discard changes in working directory)
#
#     modified:   README
#
# Untracked files:
#   (use "git add <file>..." to include in what will be committed)
#
#     ToDo
#
# no changes added to commit (use "git add" and/or "git commit -a")
```

5. Adds both files to ‘staging area’

```
> git add README ToDo    # Add both files to ‘staging area’
> git status             # Report on changes
# On branch master
# Changes to be committed:
#   (use "git reset HEAD <file>..." to unstage)
#
#     modified:   README
#       new file:   ToDo
#
```

6. Commits changes

```
> git commit -m "Add ToDo and modify README"
# [master 7b679fa] Add ToDo and modify README
#  2 files changed, 2 insertions(+)
#  create mode 100644 ToDo

> git status
# On branch master
# nothing to commit, working directory clean
```

Example Git workflow

1. Eva creates a README text file
2. Adds file to STAGING AREA*
3. Commit changes*

4. Eva modifies README and adds a ToDo text file
5. Adds both to STAGING AREA*
6. Commit changes*

…But, how do we see the history of our project changes?

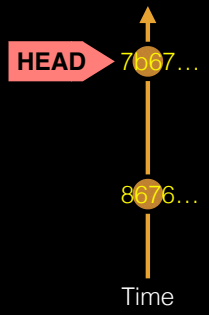
git log: Timeline history of snapshots (*i.e.* commits)

```
> git log
# commit 7b679fa747e8640918fcaad7e4c3f9c70c87b170
# Author: Barry Grant <bjgrant@umich.edu>
# Date:   Thu Jul 30 11:43:40 2015 -0400
#
#     Add ToDo and finished README
#
# commit 86768401610770ae32e2fd4faee07d1d5c68619c
# Author: Barry Grant <bjgrant@umich.edu>
# Date:   Thu Jul 30 11:26:40 2015 -0400
#
#     Create a README file
#
```

git log: Timeline history of snapshots (*i.e.* commits)

```
> git log
# commit 7b679fa747e8640918fcaad7e4c3f9c70c87b170
# Author: Barry Grant <bjgrant@umich.edu>
# Date:   Thu Jul 30 11:43:40 2015 -0400
#
#    Add ToDo and finished README
#
# commit 86768401610770ae32e2fd4faee07d1d5c68619c
# Author: Barry Grant <bjgrant@umich.edu>
# Date:   Thu Jul 30 11:26:40 2015 -0400
#
#    Create a README file
#
```

Side-Note: Git history is akin to a graph

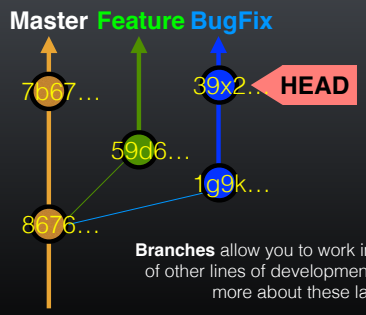


Nodes are **commits** labeled by their unique '**commit ID**'.

(This is a CHECKSUM of the commits author, time, commit msg, commit content and previous commit ID).

HEAD is a reference (or '**pointer**') to the currently checked out commit (typically the most recent commit).

Projects can have complicated graphs due to **branching**



Branches allow you to work independently of other lines of development we will talk more about these later!

Key Points:

You explicitly and iteratively tell git what files to track ("**git add**") and snapshot ("**git commit**").

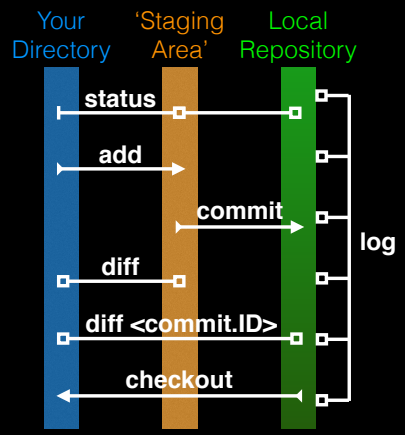
Git keeps an historical log "(**git log**") of the content changes (and your comments on these changes) at each past commit.

It is good practice to regularly check the status of your working directory, staging arena repo ("**git status**")

Break

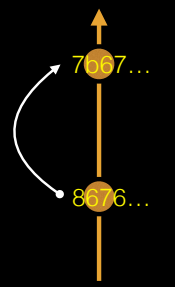
Summary of key Git commands:

```
> git status          # Get a status report of changes since last commit

> git add <filename>  # Tell Git which files to track/stage

> git commit -m 'Your message'   # Take a content snapshot!

> git log             # Review your commit history

> git diff <commit.ID> <commit.ID>  # Inspect content differences

> git checkout <commit.ID>  # Navigate through the commit history
```



git diff: Show changes between commits

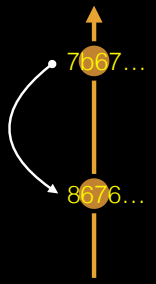
```
> git diff 8676 7b67
# diff --git a/README b/README
# index 73bc85a..67bd82c 100644
# --- a/README
# +++ b/README
# @@ -1 +1,2 @@
#  This is a first line of text.
# +This is a 2nd line of text.

# diff --git a/ToDo b/ToDo
# new file mode 100644
# index 0000000..14fbd56
# --- /dev/null
# +++ b/ToDo
# @@ -0,0 +1 @@
# +Learn git basics
```



git diff: Show changes between commits

> **git diff 7b67 8676**

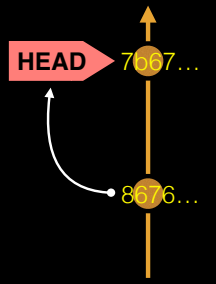
```
# diff --git a/README b/README
# index 67bd82c..73bc85a 100644
# --- a/README
# +++ b/README
# @@ -1,2 +1 @@
#  This is a first line of text.
# -This is a 2nd line of text.

# diff --git a/ToDo b/ToDo
# deleted file mode 100644
# index 14fbd56..0000000
# --- a/ToDo
# +++ /dev/null
# @@ 1 +0,0 @@
# -Learn git basics
```



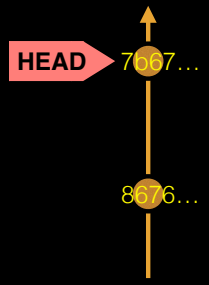
git diff: Show changes between commits

> **git diff 8676** **## Difference to current HEAD position!**

```
# diff --git a/README b/README
# index 73bc85a..67bd82c 100644
# --- a/README
# +++ b/README
# @@ -1 +1,2 @@
#  This is a first line of text.
# +This is a 2nd line of text.

# diff --git a/ToDo b/ToDo
# new file mode 100644
# index 0000000..14fbd56
# --- /dev/null
# +++ b/ToDo
# @@ -0,0 +1 @@
# +Learn git basics
```



HEAD advances automatically with each new commit



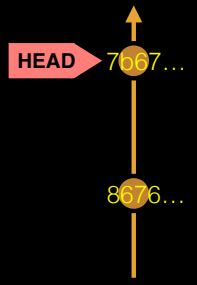
To move **HEAD** (back or forward) on the Git graph (and retrieve the associated snapshot content) we can use the command:

> **git checkout <commit.ID>**

git checkout: Moves HEAD

> **more README**
This is a first line of text.
This is a 2nd line of text.

> **git log –oneline**
7b679fa Add ToDo and finished README
8676840 Create a README file



git checkout: Moves HEAD (e.g. back in time)

Do it Yourself!

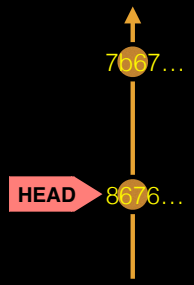
> **more README**
This is a first line of text.
This is a 2nd line of text.

> **git log –oneline**
7b679fa Add ToDo and finished README
8676840 Create a README file

> **git checkout 86768**
You are in 'detached HEAD' state…<cut>…
HEAD is now at 8676840... Create a README file

> **more README**
This is a first line of text.

> **git log –oneline**
8676840 Create a README file

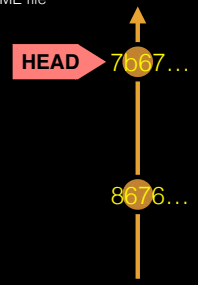


git checkout: Moves HEAD (e.g. back to the future!)

> **git checkout master**
Previous HEAD position was 8676840... Create a README file
Switched to branch 'master'

> **git log –oneline**
7b679fa Add ToDo and finished README
8676840 Create a README file

> **more README**
This is a first line of text.
This is a 2nd line of text.



Side-Note: There are two* main ways to use **git checkout**

- Checking out a **commit** makes the entire working directory match that commit. This can be used to view an old state of your project.

  > git checkout <commit.ID>

- Checking out a **specific file** lets you see an old version of that particular file, leaving the rest of your working directory untouched.

  > git checkout <commit.ID> <filename>

You can discard revisions with **git revert**

- The **git revert** command undoes a committed snapshot.
- But, instead of removing the commit from the project history, it figures out how to **undo the changes** introduced by the commit and **appends a new commit** with the resulting content.

  > git revert <commit.ID>

- This prevents Git from losing history!

Removing untracked files with **git clean**

- The **git clean** command removes untracked files from your working directory.
- Like an ordinary **rm** command, **git clean** is not undoable, so make sure you really want to delete the untracked files before you run it.

```
> git clean -n # dry run display of files to be 'cleaned'

> git clean -f   # remove untracked files
```

Demo Tower

GUIs

Tower (Mac only)
GitHub_Desktop (Mac, Windows)
SourceTree (Mac, Windows)
SmartGit (Linux)
RStudio

https://git-scm.com/downloads/guis