High Performance Research Computing

A Resource for Research and Discovery



Introduction to R

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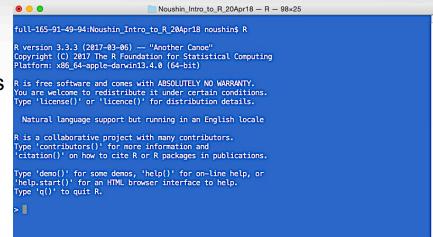
What is R?

- Open source programming language and software environment for statistical computing and graphics
- Supported by the R Foundation for Statistical Computing
- Supports multiple platforms and can be easily extended.
- The "Comprehensive R Archive Network" (CRAN) is a collection of sites which carry identical material, consisting of the R distribution(s), the contributed extensions, documentation for R, and binaries.
- The CRAN master site at WU (Wirtschaftsuniversität Wien) in Austria can be found at the URL https://CRAN.R-project.org/
 - Mirrored daily to many sites around the worldhttps://CRAN.R-project.org/mirrors.html



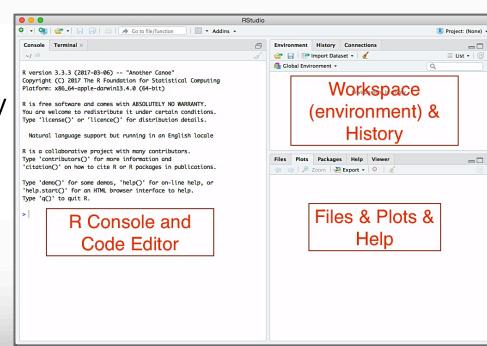
Why R?

- Open source
- Comprehensive collection of statistical functions
 - Linear modeling, classification, clustering, genomics analysis, economic and financial analysis, etc.
- Large user community support
- Collection of "packages"
 - A package is a shared code, documentation/Vignettes, data (occasionally)
- Multi platform, but not too sensitive about the source platform
- Command-line or graphical user interface (recently)
- Anyone can contribute



What is RStudio?

- An integrated development environment (IDE) for R
- Graphical Interface user friendly environment
- **Embedded Text Editor**
- Auto completion on names (functions)
- Simplified plot and output view



Running R for this Course

- Your own laptop You need to install R on your laptop using R download page: https://cran.r-project.org/mirrors.html
- TAMU Open Access Lab (OAL) computers have R and RStudio installed
- TAMU NetID You can use the online Jupyter notebook for the class
 - Off campus needs VPN
- HPRC Portal to run Rstudio: http://portal.hprc.tamu.edu
- TAMU HPRC Ada System Account You can use R_Tamu on Ada or choose Jupyter Notebook
 - Off campus needs VPN



Using Jupyter Notebook

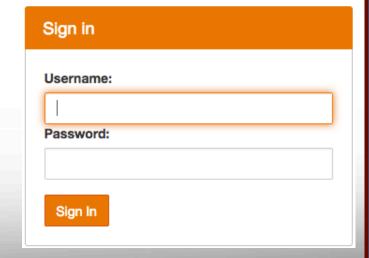
Jupyter is a web application that allows you to easily connect to a remote server and run applications. We will be using **Jupyter** to connect to **titan.tamu.edu** and use R.

To access the **Jupyter Notebook** you will need:

- -An Internet-connected device (desktop, laptop, or large tablet is preferred)
- -Internet access (tamulink-wpa Wi-Fi, OAL Ethernet)
- -An Internet browser

Jupyter Notebook Access

- (1) Open your Internet browser.
- (2) Go to one of the following links: https://titan.tamu.edu:8000/
- (3) You should then see a login window.
 Use your NetID credentials to log in.
 This is the same username and password as Howdy and Ada.



Jupyter Notebook Access - 2

(4) Upon successful login you will see some files and directories.

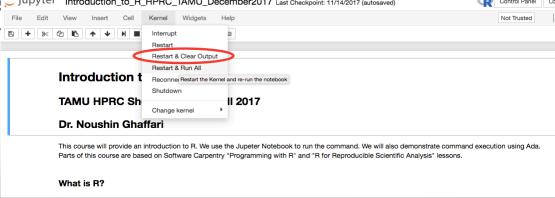
Click on the "

HPRC R Courses/

Introduction_to_R_HPRC_ResearchComputingSymposium_May19/

Introduction to R 14May19.ipynb"

(5) Before class begins, please re Jupyter Intro do this, click on "Kernel -> Res

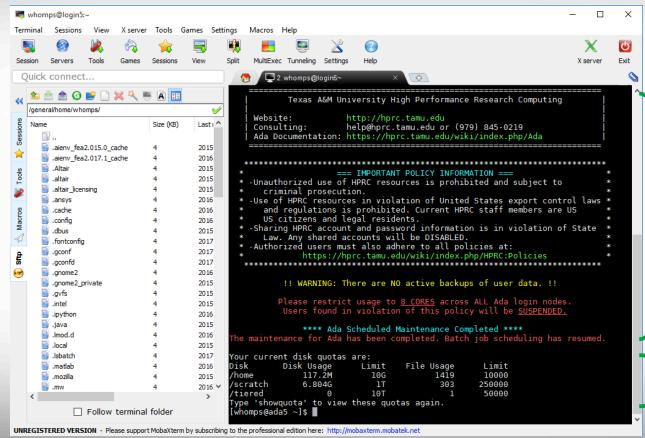


Connecting to HPRC to Use R

- SSH (secure shell)
 - The only program allowed for remote access; encrypted communication; freely available for Linux/Unix and Mac OS X hosts;
- For Microsoft Windows PCs, use MobaXterm
 - https://hprc.tamu.edu/wiki/HPRC:MobaXterm
 - You are able to view images and use GUI applications with MobaXterm
 - or Putty
 - https://hprc.tamu.edu/wiki/HPRC:Access#Using_PuTTY
 - You can not view images or use GUI applications with PuTTY
- Both state of Texas law and TAMU regulations prohibit the sharing and/or illegal use of computer passwords and accounts
- Don't write down passwords
- Don't choose easy to guess/crack passwords
- Change passwords frequently



Using SSH - MobaXterm (on Windows)



message of the day

your quotas

Using SSH to Access Ada

ssh —X user_NetID@ada.tamu.edu

https://hprc.tamu.edu/wiki/Ada:Access

You may see something like the following the first time you connect to the remote machine from your local machine:

Host key not found from the list of known hosts.

Are you sure you want to continue connecting (yes/no)?

Type yes, hit enter and you will then see the following:

Host 'ada.tamu.edu' added to the list of known hosts.

user_NetID@ada.tamu.edu's password:



Login and Set up

- Login to Ada using SSH or MobaXterm
- Let's take a look at the path and create appropriate directories

```
echo $SCRATCH
cd $SCRATCH
pwd
mkdir Intro_to_R_May19
```



Transferring the Code

The R code and its submission script should be copied to users' local directory

```
cd $SCRATCH/Intro_to_R_May19
cp /scratch/training/Intro_to_R/May19/* .
```



Data_Generator.R - 1

```
#randomly generates 10000 number in a matix[100,100]
rand data <- matrix(ncol=100,nrow=100,data=runif(10000,1,100))
#getting log2 of the data and transposing the results
rand data t log2 <- t(log2(rand data))
#calculating the min, max and average for rows and columns
mean cols <- apply(rand data,2,mean)
mean rows <- apply(rand data,1,mean)
min rows <- apply(rand data,1,min)
min cols <- apply(rand data,2,min)
max rows <- apply(rand data,1,max)
max cols <- apply(rand data,2,max)
```



Data_Generator.R - 2

```
#making plot and saving results in a pdf file
pdf("Rand Data QC.pdf")
g range <- range(0,min rows,max rows)
plot(mean rows, type="l", col="blue", ylim=g range, ann=FALSE)
lines(mean cols, type="l", col="red")
lines(max rows, type="l", col="green")
lines(max cols, type="l", col="purple")
lines(min rows, type="l", col="royalblue")
lines(min cols, type="l", col="coral")
legend(80,40,c("Mean Rows","Mean Cols","Max Rows","Max Cols","Min Rows","Min
Cols"),col=c("blue","red","green","purple","coral","royalblue"),lty=1,cex=0.55)
dev.off()
```

Data_Generator.R - 3

```
#saving data files
write.csv(rand_data,"rand_data.csv")
write.csv(rand_data_t_log2,"rand_data_t_log2.csv")
```



R_Script_Submit.sh

```
#BSUB -J Testing R Script # sets the job name to Testing R Script.
#BSUB -L /bin/bash # uses the bash login shell to initialize the job's execution environment.
                       # sets to 5 hours the job's runtime wall-clock limit.
#BSUB -W 1:00
#BSUB -n 1
                     # assigns 1 core for execution.
#BSUB -R "span[ptile=1]" # assigns 1 core per node.
#BSUB -R "rusage[mem=5000]" # reserves ~5GB per process/CPU for the job
                        # sets to ~5GB the per process enforceable memory limit.
#BSUB -M 5000
                        # directs the job's standard output to stdout.jobid
#BSUB -o stdout.%J
## Load the necessary modules
module purge
module load R tamu/3.4.2-iomkl-2017A-Python-2.7.12-default-mt
## Launch R with proper parameters
Rscript Data Generator.R
```



Submitting the RScript to Ada

```
bsub < $SCRATCH/Intro_to_R_May19/R_Script_Submit.sh

Bjobs
ls -l</pre>
```



Course Content

Parts of this course are based on Software Carpentry "Programming with R" and "R for Reproducible Scientific Analysis" lessons.

"Software Carpentry is a volunteer non-profit organization dedicated to teaching basic computing skills to researchers."

- https://software-carpentry.org/lessons/
- Reference page for R lessons (cheat sheet)
 - http://swcarpentry.github.io/r-novice-inflammation/reference/
 - http://swcarpentry.github.io/r-novice-gapminder/reference



Any question?

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