

The University of Queensland

Research Computing Centre

Using R User Guide

The following section has been updated but may still contain torque syntax or sample torque output.

Using R User Guide

Document Status

Introduction

Using R in Text Only Mode

Running R using an Interactive Session

Running R in Batch Mode

Exporting Plots

RStudio

R Versions Explained

ROCKS R

/sw R

Singularity R

Document Status

This update: June 9 2018 by David Green

Introduction

R is an open source language and environment with tools for statistical analysis and producing graphics.

RStudio is an open source IDE for R, and includes the R command line as well as tools for viewing data sets and interacting with and exporting plots.

There are a number of packages available to extend the capabilities of R. See the Installation of Packages for Scripting Languages user guide (http://www2.rcc.uq.edu.au/hpc/guides/index.html?secure/Installation_of_Packages_for_Scripting_Languages.html) for instructions on how to install new packages.

Using R in Text Only Mode

Running R using an Interactive Session

To request an interactive session, use the `-l` flag to `qsub`.

(Replace the "UQ-FACULTY-SCHOOL" with the similar looking group name you have when you run the `groups` command.)

```
user@awoonga1:~> qsub -I -A UQ-FACULTY-SCHOOL -l select=1:ncpus=1:mem=5GB -l walltime=01:00:00
```

To open the R command line, first load the appropriate module, then type 'R':

```
user@aw123:~> module load R/3.4.3
user@aw123:~> R
```

To quit the R environment, use the command:

```
> q()
```

Running R in Batch Mode

To run an R script as part of a PBS job, use the command:

```
R CMD BATCH scriptname.R
```

An example PBS script running the R script 'example.R' on a single cpu, from the directory that the job was submitted from, is shown below:

```
#PBS -A UQ-FACULTY-SCHOOL
#PBS -l select=1:ncpus=1:mem=5GB
#PBS -l walltime=00:30:00

cd $PBS_0_WORKDIR

module load R
R CMD BATCH example.R
```

Instead of

```
R CMD BATCH example.R
```

you can use this shorthand

```
Rscript --vanilla example.R
```

Exporting Plots

Rather than displaying plots on screen, R can be used to save plots directly to file. Note that this is the only option available when R is being run in batch mode or in an interactive session without the `-v DISPLAY` flag.

First, create a plot device using one of `bmp()`, `jpeg()`, `png()`, `tiff()`, `pdf()` or `postscript()`, depending on the file format required. These functions take the name of the file to generate as a required argument. Additional arguments can be specified to control particular properties of the file generated. For example:

```
> jpeg(filename="plot1.jpeg", width=480, height=480, units="px", bg="white")
```

To see a list of all available arguments, use `help(bmp)`.

Once a plot device has been created, create plots as normal, then save using

```
> dev.off()
```

Note that the pdf and postscript devices include the option to save each new plot on a new page of the file using the 'onfile' argument. For example:

```
> pdf(file="plots.pdf", onfile = TRUE, title = "MyTitle", paper = "a4r", pointsize=10, pagecentre=TRUE)
```

If onfile is set to false, a new file will be generated for each plot, and the page number of that image will be included in the file name. See `help(pdf)` and `help(postscript)` for further details.

For other file formats, only the last image plotted will be saved to the plot device.

To capture a plot that is currently displayed on the screen, use:

```
> dev.copy(device=jpeg, filename="plot2.jpeg", [additional arguments to jpeg()])
> dev.off()
```

RStudio

In order to use the RStudio IDE, X11 forwarding must be enabled. For Mac and Unix users, add the '-Y' flag to your ssh command:

```
user@yourmachine:~> ssh -Y username@awoonga.rcc.uq.edu.au
```

Windows users will need to install and run an X window server such as Xming. If connecting with Putty, X11 forwarding can then be enabled by going to Connection-> SSH -> X11 and checking "Enable X forwarding".

To select an interactive session with graphics enabled, add the '-v DISPLAY' flag to the qsub command:

```
user@awoonga1:~> qsub -I -X -A UQ-FACULTY-SCHOOL -l select=1:ncpus=1:mem=5GB -l walltime=01:00:00
```

Once the job has started, load the appropriate module and run RStudio:

```
user@aw123:~> module load rstudio
user@aw123:~> rstudio
```

FYI: RStudio is provided as a software container.

It has some limitations.

For example, some of the external tools that RStudio tries to launch to display help or image or PDF output may not work at this time.

You can work around most of these limitations.

R Versions Explained

Each HPC node has access to several versions of R. This sections will hopefully illuminate that situation.

```
----- /opt/modulefiles/applications -----
R/3.4.0(default)

----- /sw/Modules/ContainedApps -----
R/3.5.0

----- /sw/B18a/modulefiles -----
R/3.4.3
```

ROCKS R

A ROCKS rolled version of R is installed into the operating system of each compute node into `/opt/modulefiles/applications`.

Currently that is `module load R/3.4.0` and is built with, and configured to use, the Intel compiler.

```
uqdgree5@awoongal:~> module display R/3.4.0
-----
/opt/modulefiles/applications/R/3.4.0:

module-whatism  R
module-whatism  Version: 3.4.0
module-whatism  Description: R
prepend-path    PATH /opt/R/bin
prepend-path    R_LIBS /opt/R/local/lib
prepend-path    LD_LIBRARY_PATH /opt/R/lib64/R/lib
setenv          RHOME /opt/R
module          load intel
-----
```

A well hidden secret is the existence of many R library packages for this "on board" version of R.

```
uqdgree5@awoongal:~> ls /opt/R/local/lib/
abind          cubature      GenomeInfoDbData  logspline      purrr          sna
acepack       curl          GenomicAlignments magrittr       quadprog      snow
akima         DataABEL     GenomicFeatures  maps           quantreg      sp
alr3          data.table   GenomicRanges    maptools       R6             spacetime
annotate      DBI          ggplot2          markdown       randomForest  SparseM
AnnotationDbi DelayedArray  git2r            matlab         raster         stabs
aaos          DEoptimR     glue             matrixcalc     RColorBrewer  statmod
ape           desc         gplots          MatrixModels  Rcpp           statnet.common
arm           DESeq2       graph           matrixStats    RcppArmadillo stringi
assertthat   devtools     gridExtra        mboost         RcppEigen     stringr
backports    dichromat    gstat           mclust         RCurl          strucchange
base64        digest       gtable          mcmc           reshape2      SummarizedExperiment
base64enc     doMC         gtools          memoise        rgdal          survey
bdsmatrix    dplyr        GWAF            mi             rgenoud        survival
BH           el071        haplo.stats      mime           rgeos          tcltk2
bindr         Ecdat        hexbin          minqa          Rgraphviz     TeachingDemos
bindrcpp     Ecfun        highr           miscTools      rhdf5          TH.data
Biobase      edgeR        Hmisc           mix            rjson         tibble
BiocGenerics ellipse       htmlTable       mlbench        rlang         tidy
BiocInstaller epitools     htmltools       modeltools     rlecuyer      tidyselect
BiocParallel evaluate     htmlwidgets    modules        rmeta         timeDate
biomaRt      exomePeak    httr           multcomp       Rmpi          tis
Biostrings   fda          hwriter        munsell        rms           tkrplot
bit          fmcsR        ineq           mvtnorm        robustbase    tripack
bit64        FNN          InteractionSet  ncdf4          ROCR          urca
bitops       foreach     intervals       network        roxygen2     VGAM
blob         foreign     IRanges        nlme           rpart.plot   viridis
bnlearn      formatR     iterators      nloptr         rprojroot    viridisLite
brew         Formula     jpeg           nnls           RSAGA        whisker
BSgenome     fts         jsonlite       numDeriv       Rsamtools    withr
car          futile.logger kernlab        nws            RSQLite      XML
caTools      futile.options knitr          openssl        rstudioapi   xml2
```

| | | | | | |
|------------|--------------|--------------|--------------|---------------|----------|
| checkmate | gap | labeling | oz | rtracklayer | xtable |
| Chemminer | gdata | lambda.r | party | RUnit | xts |
| chron | gee | lattice | pbkrtest | S4Vectors | XVector |
| coda | geepack | latticeExtra | PBSmodelling | sandwich | yaml |
| coin | GenABEL | lazyeval | pkgconfig | scales | zlibbioc |
| colorspace | GenABEL.data | ldlasso | plogr | scatterplot3d | zoo |
| combinat | genefilter | leaps | plyr | sem | |
| commonmark | genefilter | limma | polyspline | sgeostat | |
| coxme | genetics | lme4 | PredictABEL | shapefiles | |
| crayon | GenomeInfoDb | locfit | pspline | ShortRead | |

/sw R

Unfortunately, in some circumstances, the on-board version of R exhibited memory leaks.

A (newer) version of R was built from source and installed into /sw.

```
-----
/sw/B18a/modulefiles/R/3.4.3:

module-whatis      R
module-whatis      Version: 3.4.3
module-whatis      Description: R
setenv              RHOME /sw/B18a/R
module              load intel/2017.4
prepend-path        PATH /sw/B18a/R/bin
prepend-path        R_LIBS /sw/B18a/R/local/lib
prepend-path        LD_LIBRARY_PATH /sw/B18a/R/lib64/R/lib
-----
```

It does have most of the same extensive set of additional library packages available. You may need to build some additional packages for yourself.

See the [Building Packages for R and Python User Guide](#) for information about how to do this.

Singularity R

To rapidly respond to a request for the R 3.5.0 release we have deployed a software container which is based on a newer operating system image.

The container is not a comprehensive installation of R. It is based on a packaged version provided by a developer.

We are still awaiting the release of complete R 3.5.0 packages for an operating system that can be supported by our container mechanism (no, we cannot use the latest Arch Linux)

```
uqdgree5@awoongal:~> module display R/3.5.0
-----
/sw/Modules/ContainedApps/R/3.5.0:

module-whatis
module-whatis      R V3.5.0 within a container
module-whatis      david.green@uq.edu.au
module-whatis      20180518
module-whatis      For more detail, run
module-whatis      module help R
module-whatis
module              load singularity
system              shopt -s expand_aliases
set-alias  R        /sw/Containers/singularity/bin/run_singularity run /sw/Containers/singularity/images/R-3.5.0
set-alias  shell    /sw/Containers/singularity/bin/run_singularity shell /sw/Containers/singularity/images/R-3.5.0
-----
```

To use this version of R interactively, you just need load the module and type the command (alias) R.

To use this version of R in a regular batch job you should consult the relevant section of the [Containers User Guide](#).