

Installing a software package on the NYU HPC clusters

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Most software is installed under `/share/apps/`. Users can always build software packages and install in your `$HOME` folder, but only the system administrators can install in `/share/apps`.

You can always email us at hpc@nyu.edu to request a software package you need. It helps if you can include a link to its web page or download page. If it is for Python or R, it also helps if you tell us which Python or R module you are using.

Python and R also allow you to install modules in your `$HOME` area.

Python

For Python packages from PyPI and for Python 2.7.6, you can use pip:

```
$ module load python/intel/2.7.6
$ pip install --user <pkg_name>
```

package will be installed in `$HOME/.local`.

R

```
$ module load r/intel/3.2.0
$ R CMD INSTALL "<pkg_name>"
```

The package will be installed in `$HOME/R/x86_64-centos-linux-gnu-library`.

Some R packages have dependencies on other modules, and you will need to tell R where to find libraries (`PKG_LIBS`) and possibly headers (`PKG_CFLAGS`). For example, the "topicmodels" package requires the GNU Scientific library (gsl):

```
$ module load r/intel/3.2.0
$ module load gsl/intel/1.16
$ export PKG_CFLAGS=-I$GSL_INC
$ export PKG_LIBS="-L $GSL_LIB"
$ R CMD INSTALL topicmodels

# sometimes installing from within R is more successful with finding the
package:
$ R
> install.packages('topicmodels')
```

R packages generally have a file `src/Makevars` with additional compilation options, such as `PKG_LIBS`. Unfortunately, many specify these options in a way that overrides your setting of `PKG_LIBS`. To fix this you will need to download the `.tar.gz` file for the package, edit the `Makevars` file, and install the edited package, such as illustrated below:

```
> install.packages('topicmodels')
Installing package into '/home/sl151/R/x86_64-centos-linux-gnu-library/3.2'
(as 'lib' is unspecified)
--- Please select a CRAN mirror for use in this session ---
trying URL 'http://lib.stat.cmu.edu/R/CRAN/src/contrib/topicmodels_0.2-2.tar.
gz'

...

> quit()

$ wget http://lib.stat.cmu.edu/R/CRAN/src/contrib/topicmodels_0.2-2.tar.gz
$ tar xzf topicmodels_0.2-2.tar.gz
$ cat topicmodels/src/Makevars
PKG_LIBS=-lgsl -lgslcblas

# edit Makevars with your favorite editor, changing "=" to "+="
$ cat topicmodels/src/Makevars
PKG_LIBS+=-lgsl -lgslcblas

# make a new package with the fix:
$ tar czf topicmodels_0.2-2-fixed.tar.gz

# ...and install that one:
$ R CMD INSTALL topicmodels_0.2-2-fixed.tar.gz
```