

PARALLELSTRUCTURE

A PACKAGE TO PROVIDE R FRAMEWORK TO RUN GENETIC ANALYSIS
SOFTWARE STRUCTURE AND MAKE USE OF MULTI-CORE COMPUTERS

1 INTRODUCTION

This Package provides a R framework to make use of multi-core computers when running analysis in the population genetics software STRUCTURE(*Pritchard, Stephens & Donnelly (2000)*). STRUCTURE is one of the most widely used population genetic software of the last decade. Introduced in year 2000, it has brought outstanding contribution to the field of population genetics by providing a user friendly tool for analyzing multi-locus genotype data to investigate population structure, hybridization, population admixture ...etc. Distributed as free software, <http://pritch.bsd.uchicago.edu/structure.html> the program comes in two versions: A user friendly graphic interface and a command line version. STRUCTURE analyses rely on multiple MCMC re-sampling and are thus often time consuming.

In general, one efficient way to speed up computing processes is to distribute tasks on several computing units (core/CPU). This solution imposes itself as the most common one since shared memory multi-core processors are now readily available on the market. Even common laptops are usually equipped with at least dual-core processors, and 4 to 8 core are becoming the norm. However, STRUCTURE does not support native multi-processor tasking. Nevertheless, it is possible to use STRUCTURE on multiple cores by simply opening several graphic-interface windows at the same time, or by using scripts to run STRUCTURE on the command line version and perform several STRUCTURE analysis simultaneously.

Opening several graphic windows remains a suboptimum solution as the user needs to to run manually each analysis after the previous one is done. It is thus a poorly automatized solution.

Using script programming can make a more efficient use of the multi-core processors by automatically distributing analyses to all available cores/CPU and renewing the task of each core/CPU when a given job is completed. This solution is more efficient but requires specific script programming and parallel programming skills.

The present package provides a R framework to run genetic analysis in STRUCTURE and make efficient use of multi-core computers. It consists in a R script that imports STRUCTURE command line options into an R function, and run several STRUCTURE analysis in parallel by using either **Rmpi**

package (*MPI_structure* function) or **parallel** package (*parallel_structure* function).

2 CONTENT

The package consists in two main functions, *MPI_structure()* and *parallel_structure()* as well as an example data file and corresponding joblist file. The two functions *MPI_structure()* and *parallel_structure()* are equivalent as they perform the same task and work with the same input file and parameter set. The difference between them is the method that the function relies on for distributing jobs among CPUs: *MPI_structure()* relies on the R package **Rmpi** whereas *parallel_structure()* relies on R package **parallel**. **Rmpi** is distributed in the CRAN repository for MacOS, but will require manual installation under Windows (See section **install Rmpi for windows** in this document or from the **Rmpi** webpage <http://www.stats.uwo.ca/faculty/yl/Rmpi/>). **Parallel** package is distributed with R since version 2.14.0 but is still under development. *parallel_structure()* might not be fully functional under Windows architecture, and should not be used in GUI or embedded environments as it may cause crashes. We thus strongly recommend to use *MPI_structure()* function by default in Windows. For Unix users, both *MPI_structure()* and *parallel_structure()* are available *parallel_structure()* would require R to run from the terminal.

A list of tasks to be performed is stored in a joblist file. In joblist file, each line corresponds to an individual job. While STRUCTURE input format requires a different dataset for each set of population, *ParallelStructure* offers the possibility for the user to work from a large input file containing all the populations one might need to analyze in STRUCTURE. Then, a set of "jobs" is defined in which all or only a subset of population can be included. This avoids making a different input file for each population subset. For each job, the user defines the set of populations to be included, STRUCTURE parameter K, burnin and number of iteration. If all population in the data must be analyzed pairwise (*all VS all*), the list of populations for the given job can be replaced by "pairwise.matrix" (see job T11 in example joblist)

3 USE

Standard documentation is available from R command

```
?ParallelStructure
```

```
?MPI_structure
```

```
?parallel_structure
```

MPI_structure and *parallel_structure* functions take many arguments, most of which are directly imported from STRUCTURE command line instructions. (see http://pritch.bsd.uchicago.edu/software/readme_2_1/node33.html)

Other arguments are specific to **ParallelStructure** functions:

-*infile*: name of the datafile, eg: "structure_data"

-*outpath*: folder to write result files e.g "example/results/"

-*joblist*: name of the joblist file e.g "example/joblist1"

-*n_cpu*: number of core/CPU to be used for computation.

-*structure_path*: R must find the location of executable STRUCTURE com-

mand line file. this can be achieved in different ways:

Either in R: copy the location of STRUCTURE executable in a local variable

my_path , eg: for MacOS

my_path="/Applications/Structure.app/Contents/Resources/Java/bin/"

or Windows *my_path*="c:/Program Files (x86)/Structure2.3.4/bin/"

Then, run the function in R with following arguments:

```
MPI_structure(structure_path=my_path,joblist='joblist1.txt',n_cpu=4,  
  infile='example_data.txt',outpath='structure_results/',numinds=987,  
  numloci=9,printqhat=1)
```

Alternatively it is possible to make STRUCTURE executable file available from any place in the computer (in such case, set *structure_path*=NULL when calling the R function): On MacOS: copy the STRUCTURE executable command line from */Applications/Structure.app/Contents/Resources/Java/bin/* into *usr/local/bin* or on Windows, copy the address *c:/Program Files (x86)/Structure2.3.4/bin/* into the environment variable :

Right click "My Computer" and choose "Properties". Click "Advanced system

settings" to get a new window.

Click "Environment Variables. Locate variable "PATH"

Do not erase environment variables already present in the list. Add at the end of Variable value: ";c:/Program Files (x86)/Structure2.3.4/bin/"

3.1 Example

-1 call ParallelStructure in R:

```
library(ParallelStructure)
```

-2 make a directory to store result files called "structure_results"
in R for unix:

```
system('mkdir structure_results')
```

OR in R for Windows:

```
shell('mkdir structure_results')
```

-3 call example data file and joblistfile from the R package

```
data(structure_data)
```

```
data(structure_jobs)
```

-4 Write datafile and joblist file as text files in the working directory

```
write(t(structure_jobs),ncol=length(structure_jobs[1,]),file='joblist1.txt')
```

```
write(t(structure_data),ncol=length(structure_data[1,]),file='example_data.txt')
```

-5 Run STRUCTURE job with MPIstructure function:

If STRUCTURE executable is accessible from environment variables: Run

```
MPIstructure
```

```
MPI_structure(structure_path=NULL,joblist='joblist1.txt',n_cpu=4,  
  infile='example_data.txt',outpath='structure_results/',numinds=987,  
  numloci=9,printqhat=1)
```

If STRUCTURE executable is NOT accessible from environment variables:
first define the location of STRUCTURE executable:

```
my_path="/Applications/Structure.app/Contents/Resources/Java/bin/"
```

OR

```
my_path="c:/Program Files (x86)/Structure2.3.4/bin/"
then run MPI_structure
MPI_structure(structure_path=my_path,joblist='joblist1.txt',n_cpu=4,
  infile='example_data.txt',outpath='structure_results/',numinds=987,
  numloci=9,printqhat=1)
```

4 INSTALL

4.1 MacOS

4.1.1 Rmpi

Install Rmpi from the CRAN repository, or follow the instruction in <http://www.stats.uwo.ca/faculty/yu/Rmpi/> for manual installation.

4.1.2 ParallelStructure

Download binary file from http://r-forge.r-project.org/R/?group_id=1636
Then install ParallelStructure package from local .tar.gz archive by typing in R

```
install.packages("ParallelStructure_1.0.tar.gz",type='source')
```

OR from R-forge repository by typing in R:

```
install.packages("ParallelStructure", repos="http://R-Forge.R-project.org")
```

4.2 Windows

4.2.1 Rmpi

Rmpi for Windows is not available from CRAN repository. To install Rmpi, follow the next steps or look at the instruction from: <http://www.stats.uwo.ca/faculty/yu/Rmpi/> for manual installation.

1- Install MPICH2 for windows (32 or 64 bit depending on the R version you are using) <http://www.mpich.org/downloads/>

During installation you will have to specify a pass phrase, keep the default "behappy" or change it for a new one.

2- Go to your program files (or program files(x86) if you installed 32 bit version). search for MPICH2 folder and run *wmpiregister*. You need to register

your username *id* and *password* for your computer session. click on "register" and "OK"

3- Add MPICH2 bin directory to PATH environment variable:

Right click "My Computer" and choose "Properties". Click "Advanced system settings" to get a new window.

Click "Environment Variables. Locate variable "PATH"

Do not erase environment variables already present in the list. Add at the end of Variable value:

```
";C:\Program Files\MPICH2\bin"
```

(OR ";C:\Program Files x(86)\MPICH2\bin" if you installed 32 bit version)

4- open "command prompt" as administrator. make sure you are on "C" drive. (if not, type "c:" to change drive), then type

smpd -install -phrase behappy (or change "behappy" by the passphrase you entered in step 1)

then type

```
smpd -status
```

it should return "smpd running on "hostname" "

5- Download Rmpi for Windows here: <http://www.stats.uwo.ca/faculty/yyu/Rmpi/>

Launch R with administrator to install Rmpi. Use the option "install from local .zip file"

Quit R and launch R with normal user. Try the following codes to see if Rmpi runs properly

```
library(Rmpi)
mpi.spawn.Rslaves()
mpi.parReplicate(20, mean(rnorm(1000000)))
mpi.close.Rslaves()
```

4.2.2 ParallelStructure

Download binary file from http://r-forge.r-project.org/R/?group_id=1636

Then install ParallelStructure package from local .tar.gz archive by typing in R

```
install.packages("ParallelStructure_1.0.tar.gz", type='source')
```

OR from R-forge repository by typing in R:

```
install.packages("ParallelStructure", repos="http://R-Forge.R-project.org")
```

4.3 Linux

4.3.1 Rmpi

Rmpi for Linux is not available from CRAN repository. To install Rmpi, follow the instructions from: <http://www.stats.uwo.ca/faculty/yu/Rmpi/> for manual installation. **However, because Linux runs R from Terminal**

by default, Linux users can simply install ParallelStructure package without Rmpi, and use the equivalent function *parallel_structure()*. This only requires R version 2.14 or later.

4.3.2 ParallelStructure

Download binary file from http://r-forge.r-project.org/R/?group_id=1636
Then install ParallelStructure package from local .tar.gz archive by typing in R

```
install.packages("ParallelStructure_1.0.tar.gz", type='source')
```

OR from R-forge repository by typing in R:

```
install.packages("ParallelStructure", repos="http://R-Forge.R-project.org")
```