Adventures in HPC and R: Going Parallel

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Outline

What is Parallel Computing?

- From Wikipedia:

  "Parallel computing is the simultaneous execution of the same task (split up and specially adapted) on multiple processors in order to obtain faster results."

- Two specific situations:
  - A multiprocessor machine
  - A cluster of (homogeneous or heterogeneous) computers.
- R is inherently concurrent, even on a multiprocessor machine.
- S-Plus does have one function for multiprocessor machines.

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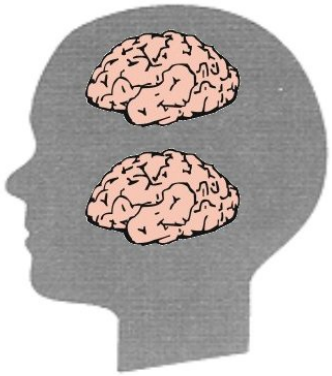
Goal for todays talk:

To demonstrate the potential of incorporating parallel processing in tasks for which it is appropriate.

What is Parallel Computing?
Example - Multiprocessor Machine

Features:

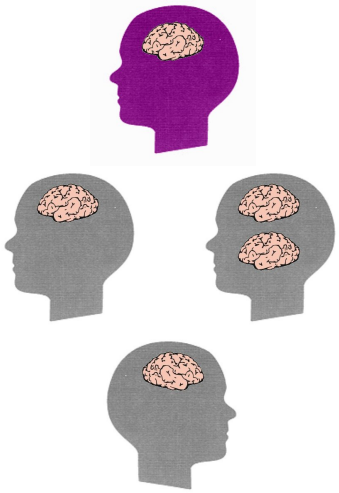
- Each process has the same home directory.
- Architecture is identical.
- R has the same libraries in the same locations.
- Data is passed through resident memory.



What is Parallel Computing?
Example - Heterogeneous Cluster of Machines

Features:

- Each process may not have same home directory.
- Architecture might be different.
- R may not have the same libraries in the same locations.
- Data is passed through the network.



Implementation

- Tasks have to be appropriate.
  - Concurrent, not sequential.
  - It is possible sometimes to take a process inherently sequential, and approximate with a concurrent process e.g. simulated annealing.
- In order to do parallel computation, two things are required:
  - An interface on the O/S that can receive and distribute tasks; and
  - A means of communicating with that program from within R.

Implementation
PVM & MPI

- There are two common libraries:
  - PVM: Parallel Virtual Machine
  - MPI: Message Passing Interface
- Both are available through open-source for different architectures.
- Which to use? From Geist, Kohl & Papadopoulos (1996):
  - MPI is expected to be faster within a large multiprocessor.
  - PVM is better when applications will be run over heterogeneous networks.
- One of these programs need to be running on the host computer before R can send them tasks.

Implementation
R

- In R there are three relevant packages:
  - `Rmpi` - the interface to MPI;
  - `rpvm` - the interface to PVM;
  - `snow` - a "meta-package" with standardized functions.
- `snow` is an excellent introduction to parallel computation, and appropriate for "embarrassingly parallel" problems.
- All of these packages are available from CRAN.
- In a environment where the home directories are not the same, the required libraries have to be available on each host.

Implementation
Commands in `snow`

Administrative Routines

`makeCluster`	create a new cluster of nodes
`stopCluster`	shut down a cluster
`clusterSetupSPRNG`	initialize random number streams

High Level Routines

`parLapply`	parallel `lapply`
`parSapply`	parallel `sapply`
`parApply`	parallel `apply`

Basic Routines

`clusterExport`	export variables to nodes
`clusterCall`	call function to each node
`clusterApply`	apply function to arguments on nodes
`clusterApplyLB`	load balanced `clusterApply`
`clusterEvalQ`	evaluate expression on nodes
`clusterSplit`	split vector into pieces for nodes

What is Parallel Computing? Implementation Examples Closing Remarks

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Example
Bootstrapping MM-regression estimators

- The function `roblm` (from the library of the same name) calculates the MM-regression estimators.
- Is also available in the library `robustbase` (see talk by Martin Mächler and Andreas Ruckstuhl).
- Can use bootstrapping to calculate the empirical density of $\hat{\beta}$.

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Bootstrapping MM-regression estimators

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```
library(roblm)
X <- data.frame(y=rnorm(500),
                x=matrix(rnorm(500*20), 500, 20))
samples <- list()
for (i in 1:200)
  samples[[i]] <- X[sample(1:500, replace=TRUE),]
rdctrl <- roblm.control(compute.rd=FALSE)
```


Example
Bootstrapping MM-regression estimators

Non-parallel - Takes 196.53 seconds

```
lapply(samples,
       function(x,z)
       roblm(y~., data=x, control=z), z=rdctrl)
```

Example
Bootstrapping MM-regression estimators

Non-parallel - Takes 196.53 seconds

```
lapply(samples,
       function(x,z)
       roblm(y~., data=x, control=z), z=rdctrl)
```

Parallel - 4 CPUS - Takes 54.52 seconds

```
cl <- makeCluster(4)
clusterEvalQ(cl, library(roblm))
clusterApplyLB(cl, samples,
               function(x, z)
               roblm(y~., data=x, control=z), z=rdctrl)
stopCluster(cl)
```


Example
Linear Grouping Analysis (LGA)

- Is a clustering algorithm that finds k groups around hyperplanes of dimension $d-1$ using orthogonal regression.
- First introduced in Van Aelst et al (2006) and is available as a package in R at http://md.stat.ubc.ca/lga.

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- The algorithm is given by
  1. Initialization: Initial hyperplanes are defined by the exact fitting of k sub-samples of size d.
  2. Forming k groups: Each data point is assigned to its closest hyperplane using Euclidean distances.
  3. Computing k hyperplanes: New hyperplanes are computed applying orthogonal regression to each group.
  4. Steps 2) and 3) are repeated several times.

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  4. Steps 2) and 3) are repeated several times.
- This process is started from a number of random initializations, and the best result selected.
- The number of starts depends on k, the relative sizes of the groups, and d.

Example
Linear Grouping Analysis (LGA)

- We have a list `hpcoef` containing m matrices that specify each of the starting k hyperplanes.
- We wish to iterate from these starting hyperplanes with the function `lga.iterate`.
- In this example, the dataset has $n = 10,000, k = 4, d = 2$.

Non-parallel - Takes 851 seconds

```
outputsl <- lapply(hpcoef, lga.iterate,
                   xsc, k, d, n, niter)
```

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```
outputsl <- lapply(hpcoef, lga.iterate,
                   xsc, k, d, n, niter)
```

Parallel - 4 CPUS - Takes 230 seconds

```
cl <- makeCluster(4)
outputsl <- clusterApplyLB(cl, hpcoef, lga.iterate,
                           xsc, k, d, n, niter)
stopCluster(cl)
```

What is Parallel Computing? Implementation Examples Closing Remarks

Closing Remarks

- With a small amount of preparation, it is relatively simple to implement parallel programming for suitable problems.
- The technology for small scale implementations is available to most researchers.
- The efficiency gains versus effort expended makes parallel computation something to seriously consider.
- However, when working in a heterogeneous computing environment, care needs to be taken!