# A Quick Guide for the pbdDEMO Package

# Drew Schmidt $^1$ , Wei-Chen Chen $^2$ , George Ostrouchov $^{1,2}$ , Pragneshkumar Patel $^1$

<sup>1</sup>Remote Data Analysis and Visualization Center, University of Tennessee, Knoxville, TN, USA <sup>2</sup>Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

# Contents

A	cknowledgement	11
1.	Introduction	1
	1.1. Installation and Quick Start	1
2.	Statistics Examples	1
	2.1. Sample Mean and Sample Variance	1
	2.2. Binning	2
	2.3. Quantile	3
	2.4. Ordinary Least Square	3
3.	Reader Examples	4
	3.1. SPMD to DMAT	4
	3.2. csv File	4
$\mathbf{R}_{0}$	eferences	5

# Acknowledgement

Ostrouchov, Schmidt, and Patel were supported in part by the project "NICS Remote Data Analysis and Visualization Center" funded by the Office of Cyberinfrastructure of the U.S. National Science Foundation under Award No. ARRA-NSF-OCI-0906324 for NICS-RDAV center. Chen and Ostrouchov were supported in part by the project "Visual Data Exploration and Analysis of Ultra-large Climate Data" funded by U.S. DOE Office of Science under Contract No. DE-AC05-00OR22725.

This work used resources of National Institute for Computational Sciences at the University of Tennessee, Knoxville, which is supported by the Office of Cyberinfrastructure of the U.S. National Science Foundation under Award No. ARRA-NSF-OCI-0906324 for NICS-RDAV center. This work also used resources of the Oak Ridge Leadership Computing Facility at the Oak Ridge National Laboratory, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC05-00OR22725. This work used resources of the Newton HPC Program at the University of Tennessee, Knoxville.

We also thank Brian D. Ripley, Kurt Hornik, and Uwe Ligges from the R Core Team for discussing package release issues and helping us solve portability problems on different platforms.

Warning: This document is written to explain the main functions of **pbdDEMO** (Schmidt et al. 2012b), version 0.1-0. Every effort will be made to ensure future versions are consistent with these instructions, but features in later versions may not be explained in this document. Information about the functionality of this package, and any changes in future versions can be found on website: "Programming with Big Data in R" at http://r-pbd.org/.

## 1. Introduction

This vignette is to explain some pbdR (Ostrouchov et al. 2012) examples which are higher level applications and may be commonly found in basic Statistics. The purposes is to show how to reuse the pre-exist functions, and quickly solve problems in an efficient way. The functions built for examples may not be exactly same idea of original R (R Core Team 2012) functions, but can be adjusted in similar wa. You are very welcome to use these as templates and rewrite your own functions or packages.

#### 1.1. Installation and Quick Start

One can download **pbdDEMO** from CRAN at http://cran.r-project.org, and the intallation can be done with the following commands

Shell Command

```
tar zxvf pbdDEMO_0.1-0.tar.gz
R CMD INSTALL pbdDEMO
```

# 2. Statistics Examples

This section introduces four simple examples and explains a little about distributed data computing. These implemented functions are selected from the Cookbook of HPSC website ?? at http://thirteen-01.stat.iastate.edu/snoweye/hpsc/?item=cookbook. Please see more details there.

Warning: We presume that readers have idea about SPMD programming. If not, please read pbdMPI's vignette Chen *et al.* (2012b) first. If possible, readers are encouraged to run the demo of pbdMPI package and go through the code step by step.

## 2.1. Sample Mean and Sample Variance

Suppose  $\mathbf{x} = \{x_1, x_2, \dots, x_N\}$  are observed samples, and N is very large. We can distribute  $\mathbf{x}$  in 2 processors, and each processor roughly takes half of data. One simple way to compute sample mean  $\bar{x}$  and sample variance  $s_x$  is based on the formula:

$$\bar{x} = \frac{1}{N} \sum_{n=1}^{N} x_n$$

$$= \sum_{n=1}^{N} \frac{x_n}{N}$$

$$s_x = \frac{1}{N-1} \sum_{n=1}^{N} (x_n - \bar{x})^2$$

$$= \sum_{n=1}^{N} \frac{x_n^2}{N-1} - \frac{N\bar{x}^2}{N-1}$$

The demo command is

#### Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(sample_stat,'pbdDEMO',ask=F,echo=F)"
```

The demo sample\_stat generates fake data on 2 processors, then utilize mpi.stat function

#### R Code

```
mpi.stat <- function(x.spmd){
    ### For mean(x).
    N <- allreduce(length(x.spmd), op = "sum")
    bar.x.spmd <- sum(x.spmd / N)
    bar.x <- allreduce(bar.x.spmd, op = "sum")

### For var(x).
s.x.spmd <- sum(x.spmd^2 / (N - 1))
s.x <- allreduce(s.x.spmd, op = "sum") - bar.x^2 * (N / (N - 1))

list(mean = bar.x, s = s.x)
} # End of mpi.stat().</pre>
```

where allreduce in **pbdMPI** (Chen *et al.* 2012a) can be utilized in this examples to aggregate local information across all processors.

Note that we tend to use suffix .spmd to indicate a distributed local object which is a portion of big object. We also tend to use common variables without subfix .spmd since SPMD programming. In SPMD case, it may be a redundant idea to invent a spmd S4 class or methods for this purpose. The S3 class and methods are sufficient and fast in most SPMD case. In contrast, it is a better idea to invent a ddmatrix class as in pbdBASE (Schmidt et al. 2012a) and pbdDMAT (Schmidt et al. 2012c), then let efficient libraries handle computing and avoid tedious coding. A silly example can be found in the Section sec:ols.

# 2.2. Binning

Binning is a classical statistics and can quickly summarize the data structure by setting some breaks between max and min of data. The demo command is

#### Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(binning,'pbdDEMO',ask=F,echo=F)"
```

The demo binning generates fake data on 2 processors, then utilize mpi.bin function as

#### R Code

```
mpi.bin <- function(x.spmd, breaks = pi / 3 * (-3:3)){
  bin.spmd <- table(cut(x.spmd, breaks = breaks))
  bin <- as.array(allreduce(bin.spmd, op = "sum"))
  dimnames(bin) <- dimnames(bin.spmd)</pre>
```

```
class(bin) <- class(bin.spmd)
bin
} # End of mpi.bin().</pre>
```

An easy implementation is to utilize table function to obtain local counts, then call allreduce to obtain global counts.

### 2.3. Quantile

Quantile is the other useful tool from fundamental statistics which provides data distribution for given quantile. The demo code is

#### Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(quantile,'pbdDEMO',ask=F,echo=F)"
```

This is only an implicit implementation to approximate a quantile and is not equivalent to the original quantile function in R. But in some sense, it should work well in large scale. The demo quantile generates fake data on 2 processors, then utilizes mpi.quantile function as

#### R Code

```
mpi.quantile <- function(x.spmd, prob = 0.5){
  if(sum(prob < 0 | prob > 1) > 0){
    stop("prob should be in (0, 1)")
}

N <- allreduce(length(x.spmd), op = "sum")
  x.max <- allreduce(max(x.spmd), op = "max")
  x.min <- allreduce(min(x.spmd), op = "min")

f.quantile <- function(x, prob = 0.5){
    allreduce(sum(x.spmd <= x), op = "sum") / N - prob
}

uniroot(f.quantile, c(x.min, x.max), prob = prob[1])\$root
} # End of mpi.quantile().</pre>
```

where a numerical function is solved by uniroot to find out the appropriate value such that cumulated probability is less than or equal to the specified quantile.

This simple example shows that the SPMD is greatly applicable on large scale data analysis and likelihood computing. Note that the uniroot call is working in parallel and on distributed data, i.e. other optimization functions can work the same way, since SPMD simly assumes every processors do the same work simulatinuously.

## 2.4. Ordinary Least Square

This is a fundament tool to find a solution for

$$y = X\beta + \epsilon$$

where  $\boldsymbol{y}$  is  $N \times 1$  observed vector,  $\boldsymbol{X}$  is  $N \times p$  designed matrix which is full rank and N >> p,  $\boldsymbol{\beta}$  is the insterested parameters and unknown to be estimated, and  $\boldsymbol{\epsilon}$  is errors and to be minimized. A classical solution is to

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^t \boldsymbol{X})^{-1} \boldsymbol{X}^t \boldsymbol{y}$$

The demo code is

#### Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(ols,'pbdDEMO',ask=F,echo=F)"
```

The implementation is straight forward as

#### R Code

```
mpi.ols <- function(y.spmd, X.spmd){
  if(length(y.spmd) != nrow(X.spmd)){
    stop("length(y.spmd) != nrow(X.spmd)")
}

t.X.spmd <- t(X.spmd)
  A <- allreduce(t.X.spmd %*% X.spmd, op = "sum")
  B <- allreduce(t.X.spmd %*% y.spmd, op = "sum")

solve(matrix(A, ncol = ncol(X.spmd))) %*% B
} # End of mpi.ols().</pre>
```

Note that this is a silly implementation for demonstrations and explain fundamental idea of OLS. This is only efficient for small N and small p. For larger scale, we suggest to simply convert y.spmd and X.spmd into block-cyclic format as in the Section 3.1 and to utilize pbdBASE and pbdDMAT for all matrix computation.

# 3. Reader Examples

## 3.1. SPMD to DMAT

pbdDEMO also provides reader examples

#### Shell Command

```
### At the shell prompt, run the demo with 2 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 2 Rscript -e "demo(spmd2dmat,'pbdDEMO',ask=F,echo=F)"
```

### 3.2. csv File

# References

- Chen WC, Ostrouchov G, Schmidt D, Patel P, Yu H (2012a). "pbdMPI: Programming with Big Data Interface to MPI." R Package, URL http://cran.r-project.org/package=pbdMPI.
- Chen WC, Ostrouchov G, Schmidt D, Patel P, Yu H (2012b). "A Quick Guide for the pbdMPI package." R Vignette, URL http://cran.r-project.org/package=pbdMPI.
- Ostrouchov G, Chen WC, Schmidt D, Patel P (2012). "Programming with Big Data in R." URL http://r-pbd.org/.
- R Core Team (2012). R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0, URL http://www.r-project.org/.
- Schmidt D, Chen WC, Ostrouchov G, Patel P (2012a). "pbdBASE: Programming with Big Data Core pbd Classes and Methods." R Package, URL http://cran.r-project.org/package=pbdBASE.
- Schmidt D, Chen WC, Ostrouchov G, Patel P (2012b). "pbdDEMO: Programming with Big Data Demonstrations of pbd Packages." R Package, URL http://cran.r-project.org/package=pbdDEMO.
- Schmidt D, Chen WC, Ostrouchov G, Patel P (2012c). "pbdDMAT: Programming with Big Data Distributed Matrix Algebra Computation." R Package, URL http://cran.r-project.org/package=pbdDMAT.