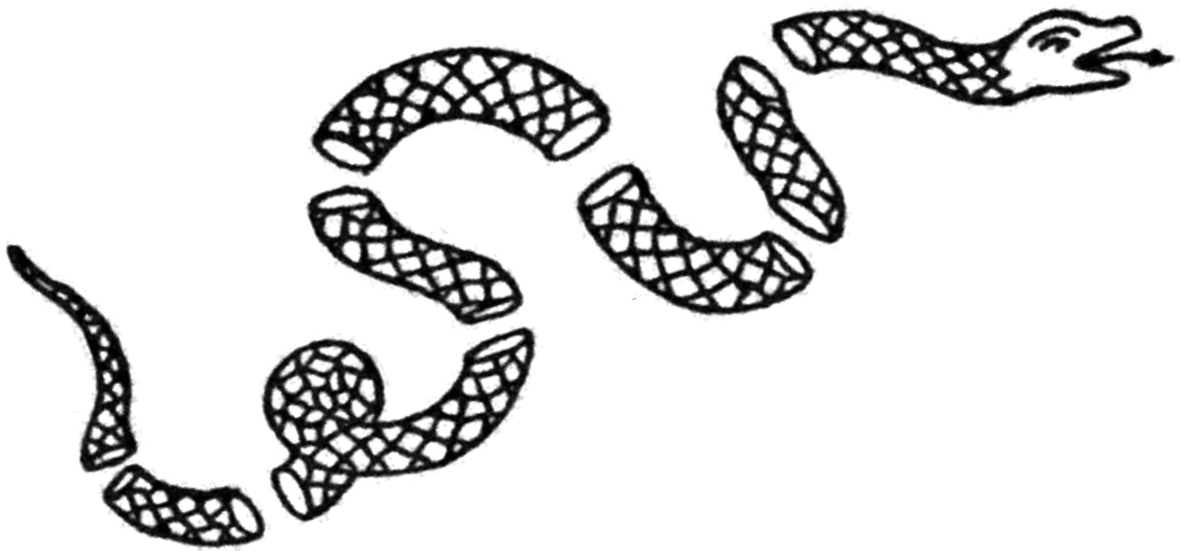

Version
0.3-0



*Programming with **B**ig **D**ata in **R***

Speaking Serial R with a Parallel Accent (Ver. 0.3-0)

Package Examples and Demonstrations

SPEAKING SERIAL R WITH A PARALLEL ACCENT (VER. 0.3-0)

pbdR PACKAGE EXAMPLES AND DEMONSTRATIONS

JUNE 10, 2014

DREW SCHMIDT

*National Institute for Computational Sciences
University of Tennessee*

WEI-CHEN CHEN

*Department of Ecology and Evolutionary Biology
University of Tennessee*

GEORGE OSTROUCHOV

*Computer Science and Mathematics Division,
Oak Ridge National Laboratory*

PRAGNESHKUMAR PATEL

*National Institute for Computational Sciences
University of Tennessee*



VERSION 0.3-0

© 2012–2014 **pbdR** Core Team. All rights reserved.

Permission is granted to make and distribute verbatim copies of this vignette and its source provided the copyright notice and this permission notice are preserved on all copies.

This manual may be incorrect or out-of-date. The authors assume no responsibility for errors or omissions, or for damages resulting from the use of the information contained herein.

This publication was typeset using \LaTeX . Illustrations were created using the **ggplot2** package ([Wickham, 2009](#)), native R functions, and Microsoft Powerpoint.

Contents

List of Figures	ii
List of Tables	iii
Acknowledgements	iv
Disclaimer	1
1 Pairwise Distance and Comparisons	2
1.1 Introduction	2
1.2 Distributed Distance and Comparisons	3
1.3 Hierarchical Clustering	3
1.4 Phylogenetic Tree	4
1.5 Exercises	4
References	5
Index	6

List of Figures

List of Tables

Acknowledgements

Schmidt, Ostrouchov, 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 was supported in part by the Department of Ecology and Evolutionary Biology at the University of Tennessee, Knoxville, and a grant from the National Science Foundation (MCB-1120370.)

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, Uwe Ligges, and Simon Urbanek from the R Core Team for discussing package release issues and helping us solve portability problems on different platforms.

Disclaimer

Warning: The findings and conclusions in this article have not been formally disseminated by the U.S. Department of Energy and should not be construed to represent any determination or policy of University, Agency and National Laboratory.

This document is written to explain the main functions of **pbdDEMO** (Schmidt *et al.*, 2013), version 0.3-0. 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/>.

Pairwise Distance and Comparisons

An approximate answer to the right problem is worth a good deal more than an exact answer to an approximate problem.

—John Tukey

1.1 Introduction

Distance is not only a tool in geometry, but also appears in statistics. For example, least square method in regression can be simply derived and computed via Euclidean distance. The resulting line is an approximate answer in terms of minimum total distance to all observations. Distance is also related to a similarity measure of two observations which describes relationship of both. Usually, the smaller of distance the closer of relation. For example, the higher probability (probability is a measure) of one virus evolving to a mutant means the smaller distance of two viruses as described in Chapter ???. Further, distance method is simple to apply on clustering problems and easy to visualize data structures such as K-means algorithm introduced in Chapter ???. For instance, the observations of the same group are more similar in characteristics with each other than those between different groups.

Potentially, compute distance of several observations involve half of pairwise comparisons if distance is symmetric, and involve all pairwise comparison if distance is not symmetric. Also, if number of observations is small, then most of distance methods can be compute efficient within one core. For moderate number of observations or complex distance systems, the computing can be parallelized wisely in several levels. For example, one may utilize multiple threads, co-processors, or distributed parallelization to archive performance gains.

In the context of `pbR`, we focus on distributed methods and abstract computing of distance to allow user-defined comparison (dissimilarity) functions of any two observations. We introduce issues and methods of distributed distance and comparisons first, and followed by demonstration of hierarchical clusterings on the `iris` dataset of Chapter ???. Then, we provide a biological application of building phylogenetic trees on the *Pony 524* dataset of Chapter ?? utilizing

evolutionary models to compute probability distance.

1.2 Distributed Distance and Comparisons

Suppose x and y are two observations and $d(x, y)$ is a distance or a comparison of x and y . Although, it is efficient to compute a distance of any two observations in R via `dist()` serially, it becomes non-trivial to compute distance of distributed observations in parallel.

The potential problems include:

- Communication must be evoked between processors when any two observations are not located within the same processor.
- The resulting distance matrix may be too big to held in one processor as data size increased even only a half (lower triangular matrix is stored as row-major in a vector.)
- Compute all comparisons may be too time consuming even for small data sets.

Distributed situations of observations and computed results (distance matrix) are categorized next.

- Both observations and distance matrix are in one node and may both be in serial or in parallel within the node, typically via OpenMP ([OpenMP ARB, 1997](#)).
- Observations are in common in all processors and distance matrix is distributed across nodes.
- Observations are distributed across nodes and distance matrix is in common in all nodes.
- Both observations and distance matrix are distributed across nodes.

Here, we may presume the distribution method is GBD row-major matrix (or row-block major) as introduced in Section ?? since most of native R functions can be extend and reused in such a way.

Note that the `dist()` only supports a few distance methods and assume distance is symmetric by definition. However, in practice, a more general measure may not be necessarily symmetric of two observations. i.e. $d(x, y) \neq d(y, x)$. In some cases, $d(x, x) \neq 0$ and the distance may also be dependent on other measurements or conditions.

1.3 Hierarchical Clustering

Hierarchical clustering is a popular statistical tools in fundamental multivariate statistics and is heavily based on distance matrix to cluster data. Several algorithms are proposed to build dendrograms or trees. The basic function `hclust()` takes a dissimilarity structure as produced by `dist()` and returns a tree object can be visualized. The method option “average” linkage is equivalent to UPGMA (Unweighted Pair Group Method with Arithmetic Mean) method ([Sokal and Michener, 1985](#)) one of popular methods in ecology for classification.

For example, the iris dataset used in Chapter ?? can be clustered in hierarchical clustering. First, we distribute 150 iris data in four cores and compute Euclidean distances in four dimensional space. We compute the dissimilarity matrix in distributed manners via a utility function `comm.dist()` in **pbdMPI** (Chen *et al.*, 2012) and store the result in a common matrix across all cores. We based on the matrix to perform a UPGMA clustering. The example in SPMD can be found in demo via

```
### At the shell prompt, run the demo with 4 processors by
### (Use Rscript.exe for windows system)
mpiexec -np 4 Rscript -e "demo(dist_iris,'pbdDEMO',ask=F,echo=F)"
```

and it returns a dendrogram as Figure ??.

1.4 Phylogenetic Tree

In some sense, Figure ?? is an rooted tree and the “average” method as well as UPGMA assumes a constant rate of evolution (molecular clock hypothesis). However, these assumption may not be appropriate to most biological topics.

1.5 Exercises

- 1-1 Prove that clustering based on Euclidean distance is equivalent to that clustering based on multivariate Normal distributions with identity variance covariance matrices.
- 1-2 Prove that the “average” method of `hclust()` is equivalent to the UPGMA method.

References

Chen WC, Ostrouchov G, Schmidt D, Patel P, Yu H (2012). “pbdMPI: Programming with Big Data – Interface to MPI.” R Package, URL <http://cran.r-project.org/package=pbdMPI>.

OpenMP ARB (1997). “OpenMP.” URL <http://www.openmp.org/>.

Schmidt D, Chen WC, Ostrouchov G, Patel P (2013). “pbdDEMO: Programming with Big Data – Demonstrations of pbd Packages.” R Package, URL <http://cran.r-project.org/package=pbdDEMO>.

Sokal R, Michener C (1985). “A statistical method for evaluating systematic relationships.” *University of Kansas Science Bulletin*, **38**, 1409 – 1438.

Wickham H (2009). *ggplot2: elegant graphics for data analysis*. Springer New York. ISBN 978-0-387-98140-6. URL <http://had.co.nz/ggplot2/book>.

Code

- `comm.dist()`, [4](#)
- `dist()`, [3](#)
- `hclust()`, [3](#)

Data

- `iris`, [2](#)
- `Pony 524`, [2](#)

Library

- `OpenMP`, [3](#)

UPGMA, [3](#)