Programming with Big Data in R

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Future Trends in Nuclear Physics Computing
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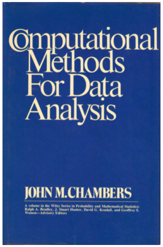
Newport News, VA

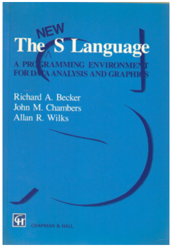
Why R?: Programming with Data


Computational Methods For Data Analysis

JOHN M. CHAMBERS

A volume in the Wiley Series in Probability and Mathematical Statistics: Ralph A. Bradley, J. Stuart Hunter, David G. Kendall, and Geoffrey S. Watson—Advisory Editors

Chambers. *Computational Methods for Data Analysis*. Wiley, 1977.

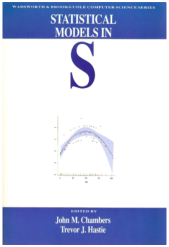

The NEW S Language

A PROGRAMMING ENVIRONMENT FOR DATA ANALYSIS AND GRAPHICS

Richard A. Becker
John M. Chambers
Allan R. Wilks

CHAPMAN & HALL

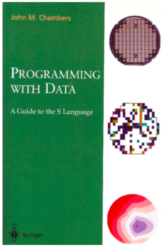
Becker, Chambers, and Wilks. *The New S Language*. Chapman & Hall, 1988.


WADSWORTH & BROOKS/COLE COMPUTER SCIENCE SERIES

STATISTICAL MODELS IN S

EDITED BY
John M. Chambers
Trevor J. Hastie

Chambers and Hastie. *Statistical Models in S*. Chapman & Hall, 1992.

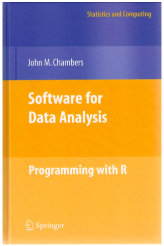

John M. Chambers

PROGRAMMING WITH DATA

A Guide to the S Language

Springer

Chambers. *Programming with Data*. Springer, 1998.


Statistics and Computing

John M. Chambers

Software for Data Analysis

Programming with R

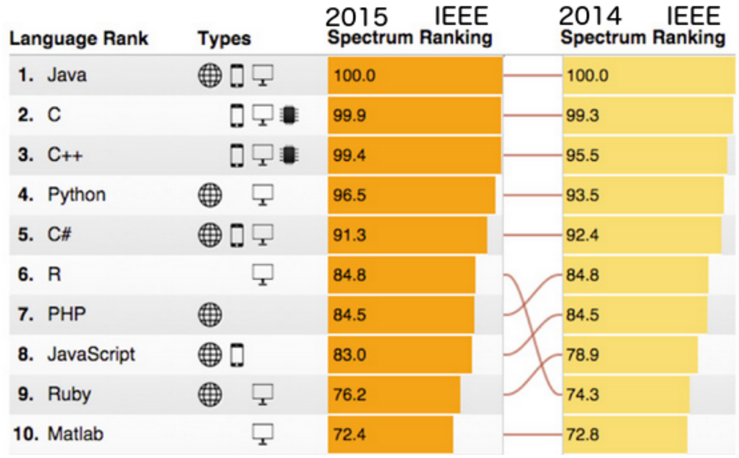
Springer

Chambers. *Software for Data Analysis: Programming with R*. Springer, 2008.

Thanks to Dirk Eddelbuettel for this slide idea and to John Chambers for providing the high-resolution scans of the covers of his books.

Popularity?

IEEE Spectrum's 2014 Ranking of Programming Languages



Language Rank	Types	2015 IEEE Spectrum Ranking	2014 IEEE Spectrum Ranking
1. Java	🌐 📱 🖥	100.0	100.0
2. C	📱 🖥 ▪	99.9	99.3
3. C++	📱 🖥 ▪	99.4	95.5
4. Python	🌐 🖥	96.5	93.5
5. C#	🌐 📱 🖥	91.3	92.4
6. R	🖥	84.8	84.8
7. PHP	🌐	84.5	84.5
8. JavaScript	🌐 📱	83.0	78.9
9. Ruby	🌐 🖥	76.2	74.3
10. Matlab	🖥	72.4	72.8

See: http://spectrum.ieee.org/static/interactive-the-top-programming-languages#index

An Example: **knitr** document produced with **RStudio** IDE

Data: 1,653 *start* and *end* timestamps for GPU offload periods.

Want 1-ahead prediction of *start* and *end* to run other codes.

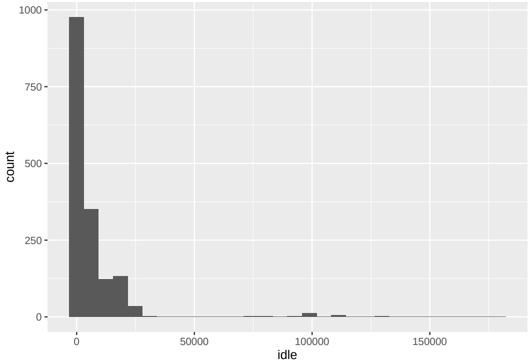
```r
ts <- read.table("sorted1node.txt", header=TRUE)
library(dplyr)
ts <- mutate(ts, idle = end - start, busy = start - lag(end))
head(ts)
```

```
##         start         end  idle    busy
## 1 56114210457 56114211289   832      NA
## 2 56114300920 56114311544 10624   89631
## 3 56114373143 56114373943   800   61599
## 4 56117433146 56117436858  3712 3059203
## 5 56117469818 56117470650   832   32960
## 6 56117507098 56117517081  9983   36448
```

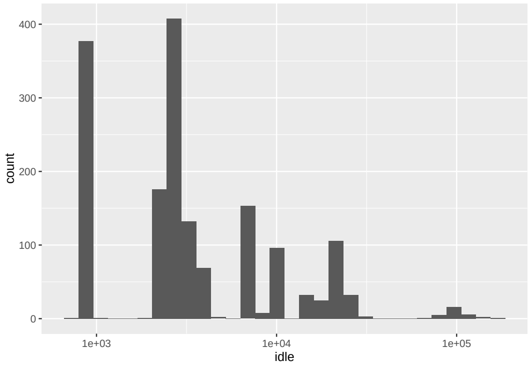
```r
dim(ts)
```

```
## [1] 1653    4
```

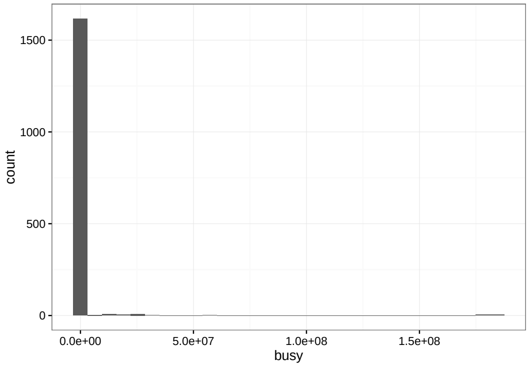
```r
library(ggplot2)
ggplot(ts, aes(idle)) + geom_histogram()
```



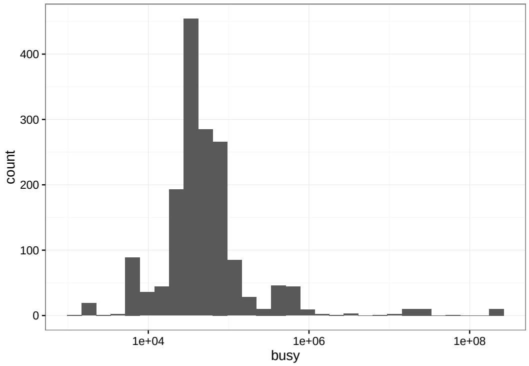
```
ggplot(ts, aes(idle)) + geom_histogram() + scale_x_log10()
```



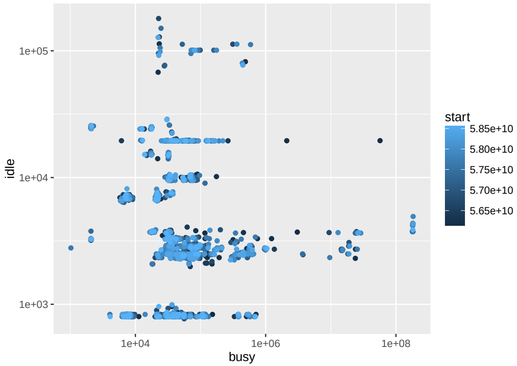
```r
ggplot(ts, aes(busy)) + geom_histogram()  + theme_bw()
```



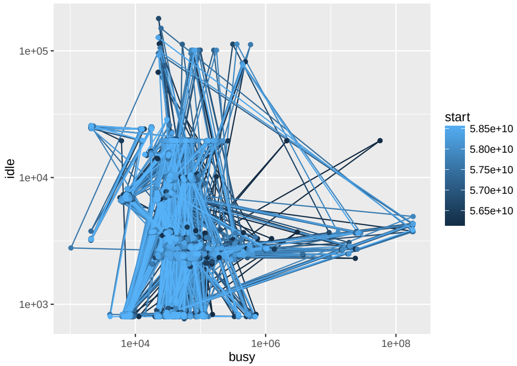
```
ggplot(ts, aes(busy)) + geom_histogram() + scale_x_log10()  + theme_bw()
```



```r
ggplot(ts, aes(busy, idle, color=start)) + geom_point() + scale_x_log10() +
  scale_y_log10()
```



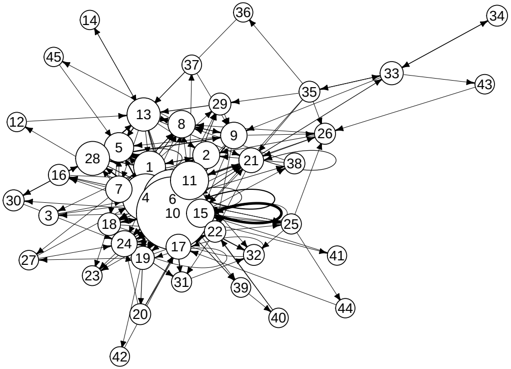
```
ggplot(ts, aes(busy, idle, color=start)) + geom_path() + geom_point() +
  scale_x_log10() + scale_y_log10()
```



Successive *busy idle* periods cluster around several values. Markov chain … probably sparse … Write my own?

Turns out that most of this already exists in the package **rEMM** (One of 7,000+ CRAN packages!)

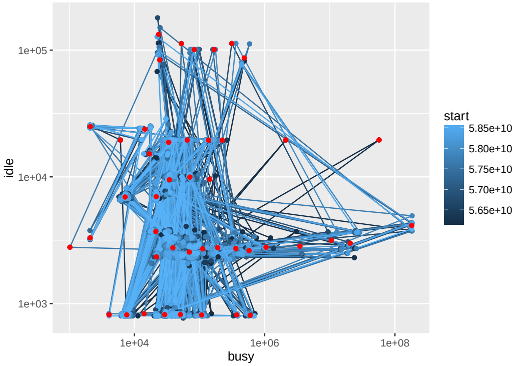
```r
ts_log <- transmute(ts, lidle = log10(idle), lbusy = log10(busy))
library(rEMM)
emm <- build(EMM(threshold = 0.2, measure="euclidean"), ts_log)
plot(emm)
```



Markov transition graph after seeing all the data.

Add Markov node locations on top of the log scale *busy-idle* space:

```
ggplot(ts, aes(busy, idle, color=start)) + geom_path() + geom_point() +
  scale_x_log10() + scale_y_log10() +
  geom_point(aes(10^lbusy, 10^lidle), data.frame(cluster_centers(emm)), col="red")
```



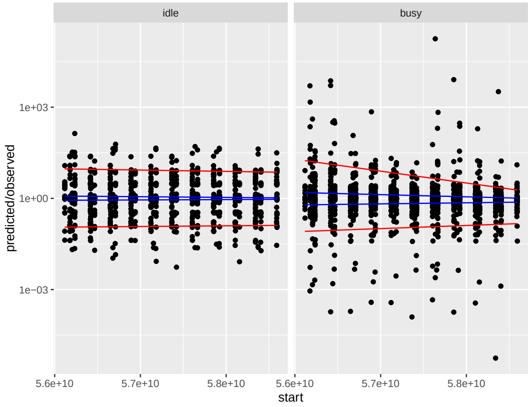
Looks promising!

```r
pr_idle <- function(ts, threshold, lambda, measure = "euclidean")
{
  emm <- build(EMM(threshold, measure, lambda = lambda), ts_log[1:5, ])
  ts$idle_p <- ts$busy_p <- NA
  for(i in 6:nrow(ts_log))
    {
      pred_data <- cluster_centers(emm)[predict(emm, n=1), ]
      ts$idle_p[i] <- 10^(pred_data["lidle"])
      ts$busy_p[i] <- 10^(pred_data["lbusy"])
      emm <- build(emm, ts_log[i, ])
    }
  ts
}

ts <- pr_idle(ts, threshold=0.1, lambda=0.01)
```

Prediction proceeds one pair of *busy*, *idle* at a time, predicting the next pair, then updating the Markov states and probabilities for actual values observed.

```r
library(reshape2)
ts_melt <- melt(ts, value.name="observed", measure.vars=c("idle", "busy"))
ts_melt <- mutate(ts_melt, predicted=ifelse(variable == "idle", idle_p, busy_p))
ggplot(ts_melt, aes(start, predicted/observed)) + geom_point() + scale_y_log10() +
  stat_quantile(quantiles=c(.75, .25), col="blue") +
  stat_quantile(quantiles=c(.95, .05), col="red") + facet_grid(~variable)
```



This is a lightweight algorithm in R (~2 seconds total for all predictions). It can be made more lightweight (100x ?) by implementing in C or C++ and by updating less often.

Resources for Learning R

- RStudio IDE
  `http://www.rstudio.com/products/rstudio-desktop/`
- *Task Views*: `http://cran.at.r-project.org/web/views`
- Book: *The Art of R Programming* by Norm Matloff:
  `http://nostarch.com/artofr.htm`
- *Advanced R*: `http://adv-r.had.co.nz/` and *ggplot2*
  `http://docs.ggplot2.org/current/` by Hadley Wickham
- R programming for those coming from other languages: `http://www.johndcook.com/R_language_for_programmers.html`
- *aRrgh: a newcomer's (angry) guide to R*, by Tim Smith and Kevin Ushey: `http://tim-smith.us/arrgh/`
- Mailing list archives: `http://tolstoy.newcastle.edu.au/R/`
- The [R] stackoverflow tag.

Why R?: Programming with Big Data

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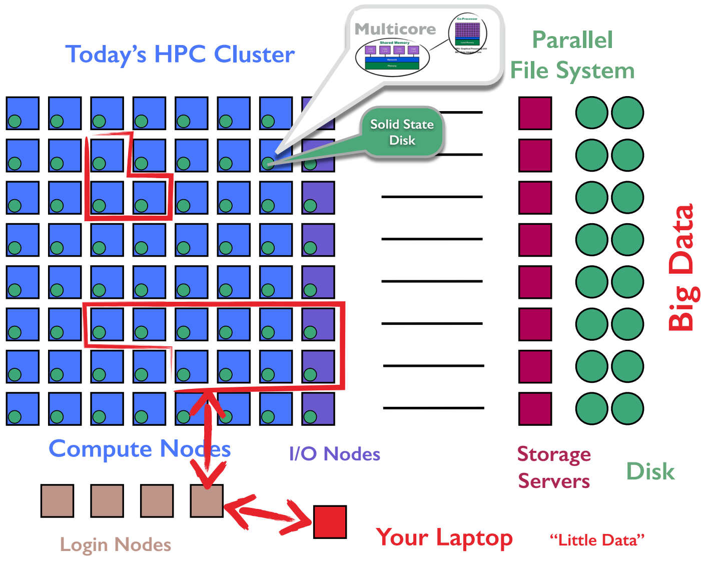
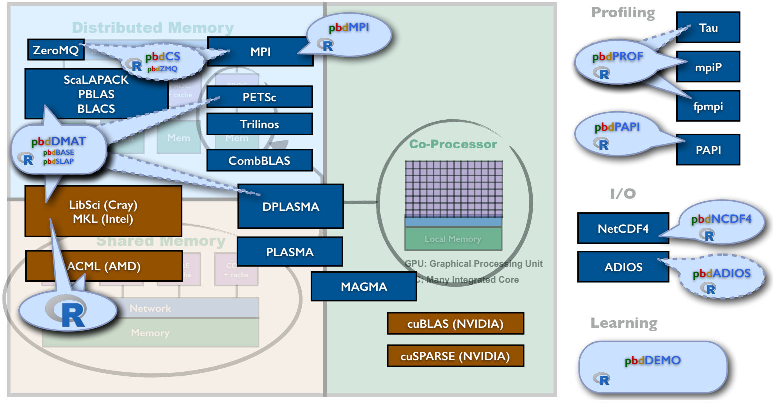
[4]Business Analytics and Statistics
University of Tennessee, Knoxville TN, USA

pbdR
Programming with Big Data in R

HPC Cluster with NVRAM and Parallel File System



pbdR Interfaces to Libraries: Sustainable Path



Why use HPC libraries?

- Many science communities are invested in their API.
- Data analysis uses much of the same basic math as simulation science
- The libraries represent 30+ years of parallel algorithm research
- *They're tested. They're fast. They're scalable.*

pbdMPI: a High Level Interface to MPI

- API is simplified: defaults in control objects.
- S4 methods: extensible to complex R objects.
- Additional error checking
- Array and matrix methods without serialization: faster than **Rmpi**.

pbdMPI (S4)	**Rmpi**
`allreduce`	`mpi.allreduce`
`allgather`	`mpi.allgather`, `mpi.allgatherv`, `mpi.allgather.Robj`
`bcast`	`mpi.bcast`, `mpi.bcast.Robj`
`gather`	`mpi.gather`, `mpi.gatherv`, `mpi.gather.Robj`
`recv`	`mpi.recv`, `mpi.recv.Robj`
`reduce`	`mpi.reduce`
`scatter`	`mpi.scatter`, `mpi.scatterv`, `mpi.scatter.Robj`
`send`	`mpi.send`, `mpi.send.Robj`

SPMD: Copies of One Code Run Asynchronously

A simple SPMD allreduce

allreduce.r

```r
library(pbdMPI, quiet = TRUE)

## Your local computation
n <- comm.rank() + 1

## Now "Reduce" and give the result to all
all_sum <- allreduce(n) # Sum is default

text <- paste("Hello: n is", n, "sum is", all_sum )
comm.print(text, all.rank=TRUE)

finalize()
```

Execute this batch script via:

```
mpirun -np 2 Rscript allreduce.r
```

Output:

```
COMM.RANK = 0
[1] "Hello: n is 1 sum is 3"
COMM.RANK = 1
[1] "Hello: n is 2 sum is 3"
```

Machine Learning Example: Random Forest

Example: Letter Recognition data from package **mlbench** (20,000 $\times$ 17)

```
[,1]    lettr   capital letter
[,2]    x.box   horizontal position of box
[,3]    y.box   vertical position of box
[,4]    width   width of box
[,5]    high    height of box
[,6]    onpix   total number of on pixels
[,7]    x.bar   mean x of on pixels in box
[,8]    y.bar   mean y of on pixels in box
[,9]    x2bar   mean x variance
[,10]   y2bar   mean y variance
[,11]   xybar   mean x y correlation
[,12]   x2ybr   mean of x^2 y
[,13]   xy2br   mean of x y^2
[,14]   x.ege   mean edge count left to right
[,15]   xegvy   correlation of x.ege with y
[,16]   y.ege   mean edge count bottom to top
[,17]   yegvx   correlation of y.ege with x
```

P. W. Frey and D. J. Slate (Machine Learning Vol 6/2 March 91): "Letter Recognition Using Holland-style Adaptive Classifiers".

Example: Random Forest Code (build many simple models, use model averaging to predict)

Serial Code 4_rf_s.r

```r
library(randomForest)
library(mlbench)
data(LetterRecognition) # 26 Capital Letters Data 20,000 x 17
set.seed(seed=123)
n <- nrow(LetterRecognition)
n_test <- floor(0.2*n)
i_test <- sample.int(n, n_test) # Use 1/5 of the data to test
train <- LetterRecognition[-i_test, ]
test <- LetterRecognition[i_test, ]

## train random forest
rf.all <- randomForest(lettr ~ ., train, ntree=500,
    norm.votes=FALSE)

## predict test data
pred <- predict(rf.all, test)
correct <- sum(pred == test$lettr)
cat("Proportion Correct:", correct/(n_test), "\n")
```

Example: Random Forest Code (Split learning by blocks of trees. Split prediction by blocks of rows.)

Parallel Code 4_rf_p.r

```
library(randomForest)
library(mlbench)
data(LetterRecognition)
comm.set.seed(seed=123, diff=FALSE) # same training data
n <- nrow(LetterRecognition)
n_test <- floor(0.2*n)
i_test <- sample.int(n, n_test) # Use 1/5 of the data to test
train <- LetterRecognition[-i_test, ]
test <- LetterRecognition[i_test, ][get.jid(n_test), ]

comm.set.seed(seed=1e6*runif(1), diff=TRUE)
my.rf <- randomForest(lettr ~ ., train, ntree=500%/%comm.size(),
     norm.votes=FALSE)
rf.all <- do.call(combine, allgather(my.rf))

pred <- predict(rf.all, test)
correct <- allreduce(sum(pred == test$lettr))
comm.cat("Proportion Correct:", correct/(n_test), "\n")
```

Dense Matrix and Vector Operations

A matrix is mapped to a processor grid shape

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 \end{bmatrix}$$

(a) 1×6

$$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{bmatrix}$$

(b) 2×3

$$\begin{bmatrix} 0 & 1 \\ 2 & 3 \\ 4 & 5 \end{bmatrix}$$

(c) 3×2

$$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

(d) 6×1

Table: Processor Grid Shapes with 6 Processors

pbdR No change in syntax. Data redistribution functions.

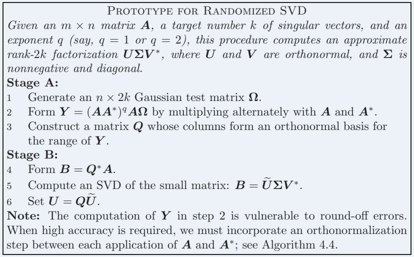
```
x <- x[-1, 2:5]
x <- log(abs(x) + 1)
x.pca <- prcomp(x)
xtx <- t(x) %*% x
ans <- svd(solve(xtx))
```

The above (and over 100 other functions) runs on 1 core with R or 10,000 cores with pbdR ddmatrix class

```
> showClass("ddmatrix")
Class "ddmatrix" [package "pbdDMAT"]
Slots:
Name:      Data     dim    ldim   bldim   ICTXT
Class:   matrix numeric numeric numeric numeric
```

```
> x <- as.rowblock(x)
> x <- as.colblock(x)
> x <- redistribute(x, bldim=c(8, 8), ICTXT = 0)
```

Truncated SVD from random projections[1]

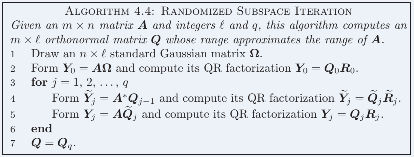


Prototype for Randomized SVD

Given an $m \times n$ matrix $\boldsymbol{A}$, a target number k of singular vectors, and an exponent q (say, $q = 1$ or $q = 2$), this procedure computes an approximate rank-$2k$ factorization $\boldsymbol{U\Sigma V}^*$, where $\boldsymbol{U}$ and $\boldsymbol{V}$ are orthonormal, and $\boldsymbol{\Sigma}$ is nonnegative and diagonal.

```
Stage A:
1   Generate an $n \times 2k$ Gaussian test matrix $\boldsymbol{\Omega}$.
2   Form $\boldsymbol{Y} = (\boldsymbol{AA}^*)^q \boldsymbol{A\Omega}$ by multiplying alternately with $\boldsymbol{A}$ and $\boldsymbol{A}^*$.
3   Construct a matrix $\boldsymbol{Q}$ whose columns form an orthonormal basis for
    the range of $\boldsymbol{Y}$.
Stage B:
4   Form $\boldsymbol{B} = \boldsymbol{Q}^*\boldsymbol{A}$.
5   Compute an SVD of the small matrix: $\boldsymbol{B} = \widetilde{\boldsymbol{U}}\boldsymbol{\Sigma V}^*$.
6   Set $\boldsymbol{U} = \boldsymbol{Q}\widetilde{\boldsymbol{U}}$.
```

Note: The computation of $\boldsymbol{Y}$ in step 2 is vulnerable to round-off errors. When high accuracy is required, we must incorporate an orthonormalization step between each application of $\boldsymbol{A}$ and $\boldsymbol{A}^*$; see Algorithm 4.4.



Algorithm 4.4: Randomized Subspace Iteration

Given an $m \times n$ matrix $\boldsymbol{A}$ and integers ℓ and q, this algorithm computes an $m \times \ell$ orthonormal matrix $\boldsymbol{Q}$ whose range approximates the range of $\boldsymbol{A}$.

```
1   Draw an $n \times \ell$ standard Gaussian matrix $\boldsymbol{\Omega}$.
2   Form $\boldsymbol{Y}_0 = \boldsymbol{A\Omega}$ and compute its QR factorization $\boldsymbol{Y}_0 = \boldsymbol{Q}_0\boldsymbol{R}_0$.
3   for $j = 1, 2, \ldots, q$
4       Form $\widetilde{\boldsymbol{Y}}_j = \boldsymbol{A}^*\boldsymbol{Q}_{j-1}$ and compute its QR factorization $\widetilde{\boldsymbol{Y}}_j = \widetilde{\boldsymbol{Q}}_j\widetilde{\boldsymbol{R}}_j$.
5       Form $\boldsymbol{Y}_j = \boldsymbol{A}\widetilde{\boldsymbol{Q}}_j$ and compute its QR factorization $\boldsymbol{Y}_j = \boldsymbol{Q}_j\boldsymbol{R}_j$.
6   end
7   $\boldsymbol{Q} = \boldsymbol{Q}_q$.
```

Serial R

```r
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <-  matrix(rnorm(n*2*k),
        nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

[1]Halko, Martinsson, and Tropp. 2011. Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decompositions *SIAM Review* **53** 217–288

Truncated SVD from random projections

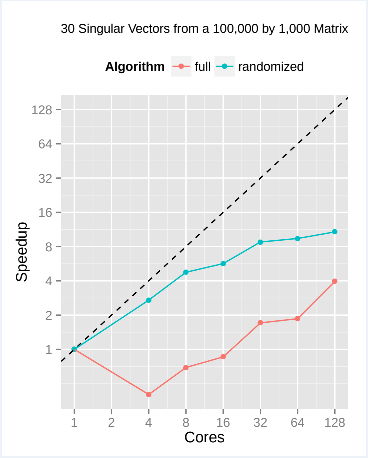
Serial R

```
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- matrix(rnorm(n*2*k),
           nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

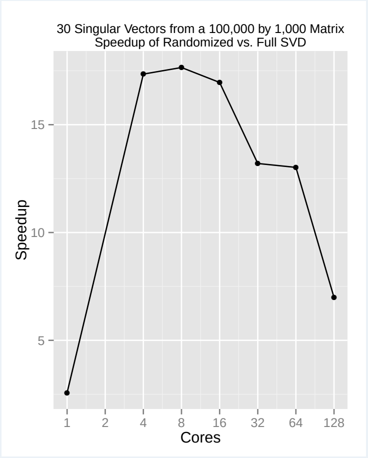
Parallel pbdR

```
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- ddmatrix("rnorm",
      nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
      }

    ## Stage B
    B <- t(Q) %*% A
    U <- La.svd(B)$u
    U <- Q %*% U
    U[, 1:k]
  }
```

From journal to scalable code and scaling data in one day.



Speedup relative to 1 core



RandSVD speedup relative to full SVD

Future Work

- NSF/DMS: second year of a 3 year grant to
  - Bring back interactivity via client/server (pbdCS/pbdZMQ)
  - Simplify parallel data input
  - Begin DPLASMA integration
  - Outreach to the statistics community
- DOE/SC: In-situ or staging use with simulations
  - pbdADIOS - HPC I/O
- Pending: NSF BIGDATA, Tensor Regression
- Pending: Exascale Computing Project, analytics for ParaView/VisIt

Where to learn more?

- http://r-pbd.org/
- **pbdDEMO** vignette
- Googlegroup:RBigDataProgramming
- pbdR Installations: OLCF, NERSC, SDSC, TACC, IU, BSC Spain, CSCS Switzerland, IT4I Czech, ISM Japan, and many more
- Need access to a cluster computer? From NSF:
    - XSEDE *trial* or *startup* allocation https://www.xsede.org/web/xup/allocations-overview.
    - Most resources have pbdR installed

Support

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