Programming with Big Data in R

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The pbdR Core Team

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Support

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About This Presentation

Speaking Serial R with a Parallel Accent

The content of this presentation is based in part on the **pbdDEMO** vignette *Speaking Serial R with a Parallel Accent*

http://goo.gl/HZkRt

It contains more examples, and sometimes added detail.

About This Presentation

Installation Instructions

Installation instructions for setting up a pbdR environment are available:

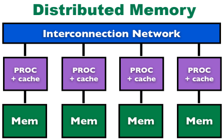
http://r-pbd.org/install.html

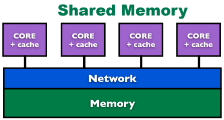
This includes instructions for installing R, MPI, and pbdR.

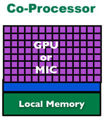
Contents

Contents

Three Basic Flavors of Hardware



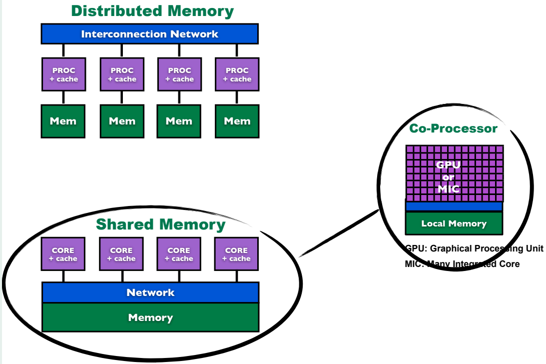




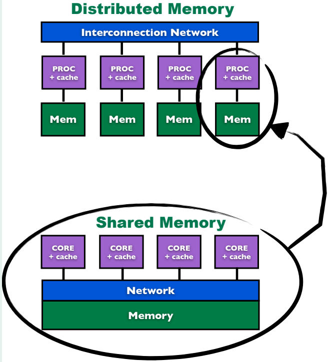
GPU: Graphical Processing Unit

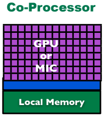
MIC: Many Integrated Core

Your Laptop or Desktop



A Server or Cluster

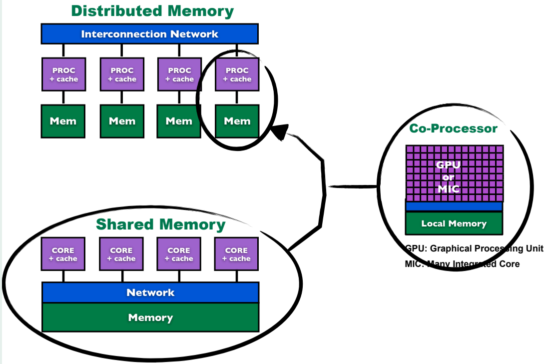




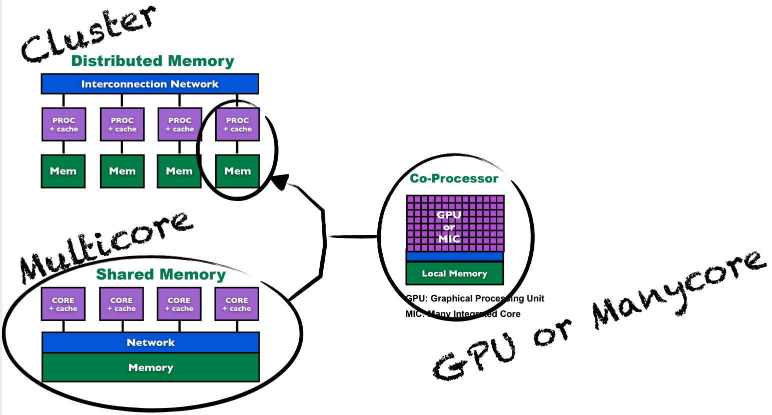
GPU: Graphical Processing Unit

MIC: Many Integrated Core

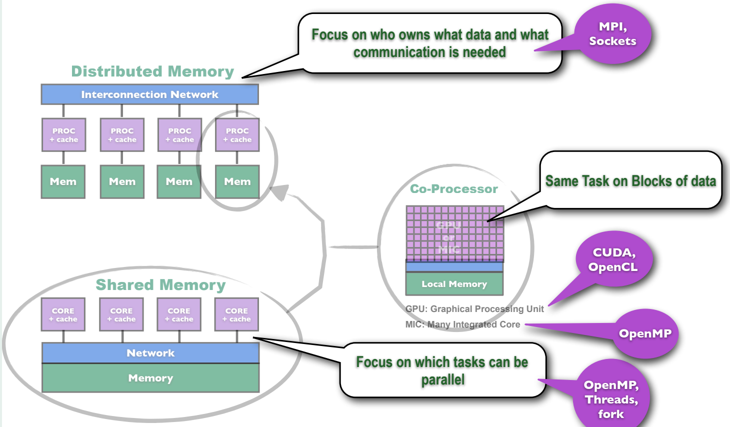
Server to Supercomputer



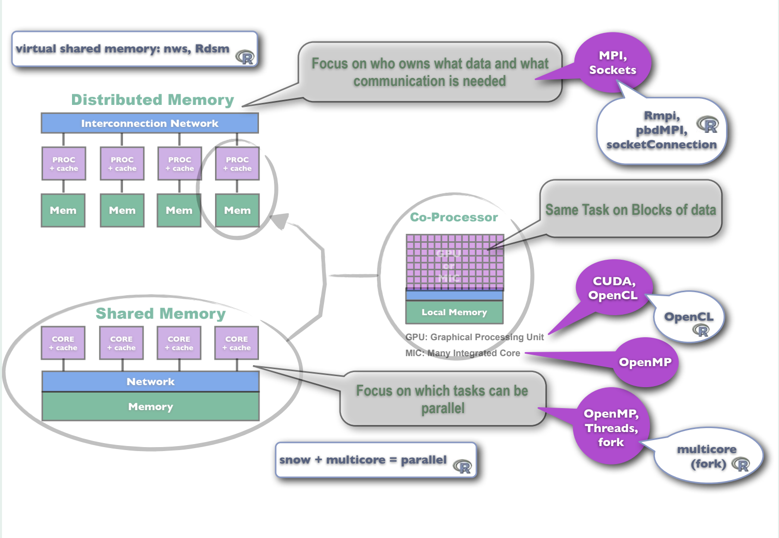
Knowing the Right Words



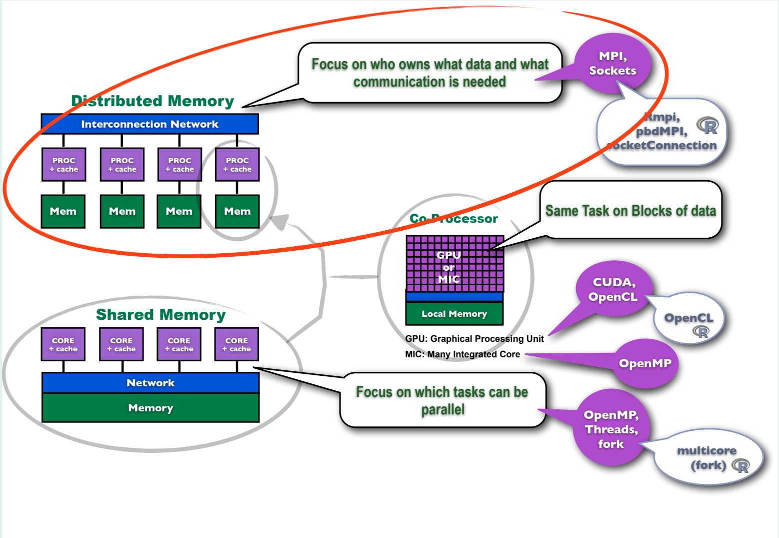
"Native" Programming Models and Tools



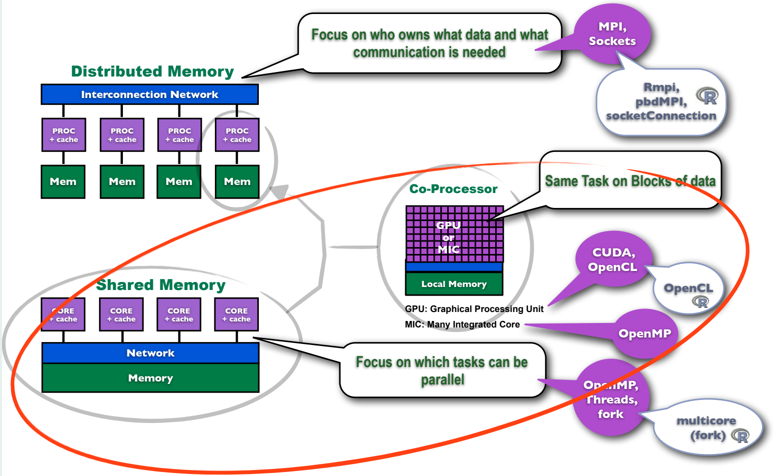
R Interfaces to Native Tools



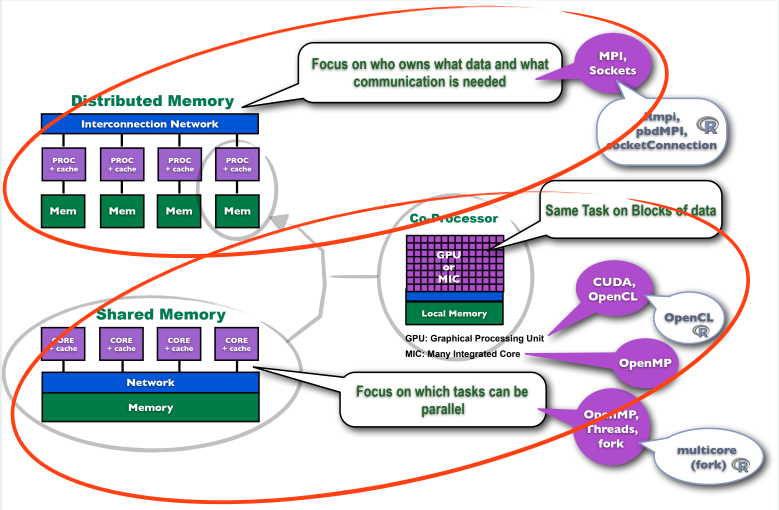
30+ Years of Parallel Computing Research



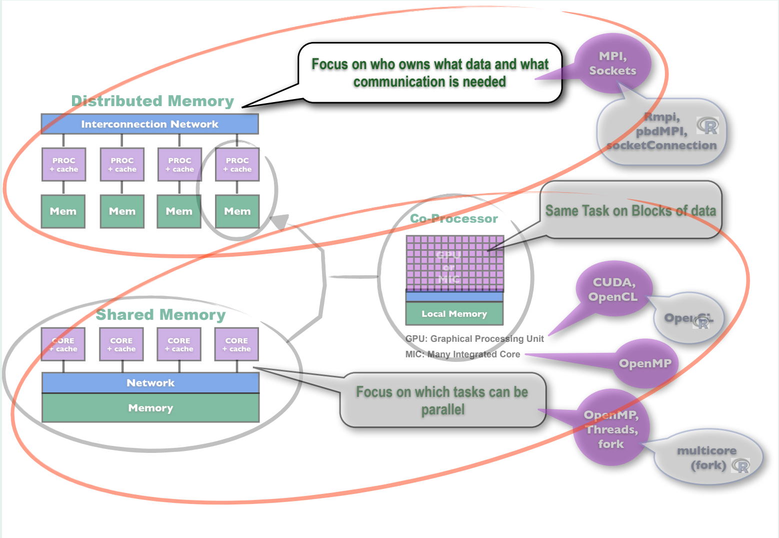
Last 10 years of Advances



Putting It All Together Challenge



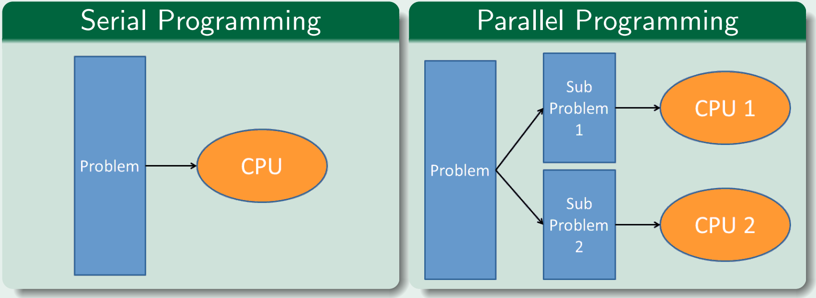
pbdR Focus on Data Parallelism



What is Parallelism?

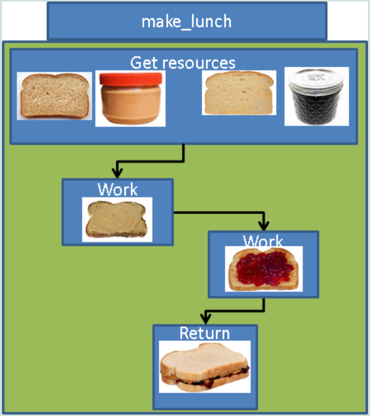
- Doing more than one thing at a time.
- The simultaneous use of multiple compute resources to solve a computational problem.

Parallelism

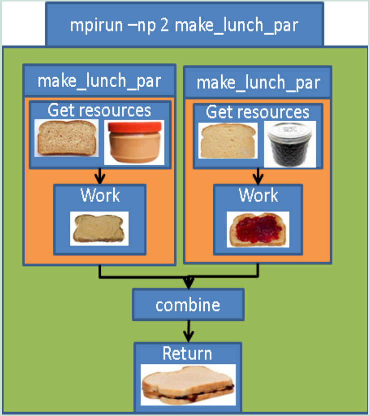


Parallelism

Serial Programming



Parallel Programming



eat from it.

Kinds of Parallelism

- *Data Parallelism*: Data is distributed
- *Task Parallelism*: Tasks are distributed

(This is a gross oversimplification)

pbdR Paradigms: Data Parallelism

Data parallelism:

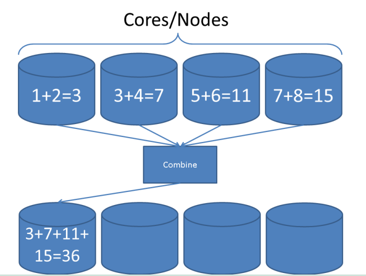
- No one processor/node owns all the data.
- Processors own local pieces of a (conceptually) larger, global object

Task parallelism:

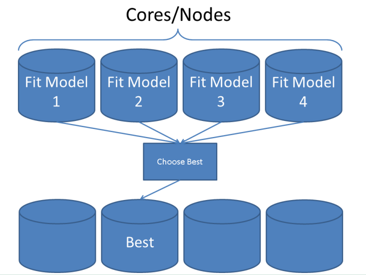
- Often involves different tasks to the same data.

Data vs Task Parallelism

Data Parallelism



Task Parallelism



Parallel Programming Vocabulary: Difficulty in Parallelism

1. *Implicit parallelism*: Parallel details hidden from user
2. *Explicit parallelism*: Some assembly required...
3. *Embarrassingly Parallel*: Also called *loosely coupled*. Obvious how to make parallel; lots of independence in computations.
4. *Tightly Coupled*: Opposite of embarrassingly parallel; lots of dependence in computations.

Speedup

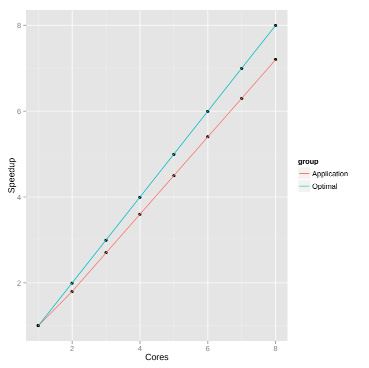
- *Wallclock Time*: Time of the clock on the wall from start to finish
- *Speedup*: unitless measure of improvement; more is better.

$$S_{n_1,n_2} = \frac{\text{Run time for } n_1 \text{ cores}}{\text{Run time for } n_2 \text{ cores}}$$

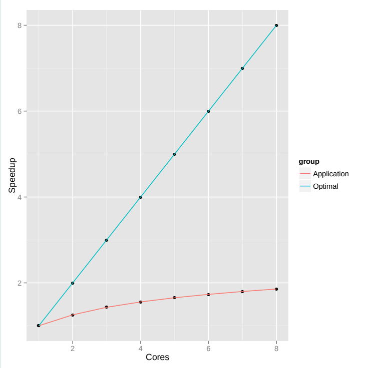
  - n_1 is often taken to be 1
  - In this case, comparing parallel algorithm to serial algorithm

Speedup

Good Speedup



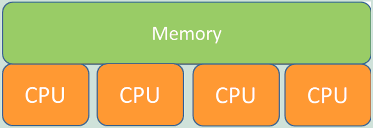
Bad Speedup



Recall: Shared and Distributed Memory Machines

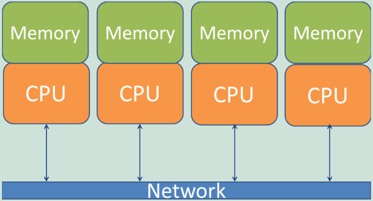
Shared Memory

Direct access to read/change memory (one node)



Distributed

No direct access to read/change memory (many nodes); requires communication



Shared and Distributed Memory Machines

Shared Memory Machines

Thousands of cores

Nautilus, University of Tennessee
1024 cores
4 TB RAM

Distributed Memory Machines

Hundreds of thousands of cores

Kraken, University of Tennessee
112,896 cores
147 TB RAM

R and Parallelism

What about R?

Problems with Serial R

1. Slow.
2. If you don't know what you're doing, it's *really* slow.
3. Performance improvements usually for small machines.
4. Very ram intensive.

Why We Need Parallelism

1. Saves compute time.
2. Data size is skyrocketing.
3. Necessary for many problems.
4. Its necessity is coming.
5. *It's really cool.*

Recall: Parallel R Packages

Shared Memory

1. **foreach**
2. **parallel**
3. **snow**
4. **multicore**

Distributed

1. **Rmpi**
2. R+Hadoop
3. **pbdR**

(and others. . .)

R and Parallelism

The solution to many of R's problems is parallelism. However . . .

What we have

1. Mostly serial.
2. Mostly not distributed
3. Data parallelism mostly explicit

What we want

1. Mostly parallel.
2. Mostly distributed.
3. Mostly implicit.

R and Parallelism

Likewise, the HPC community is looking for high-level languages for data...

Contents

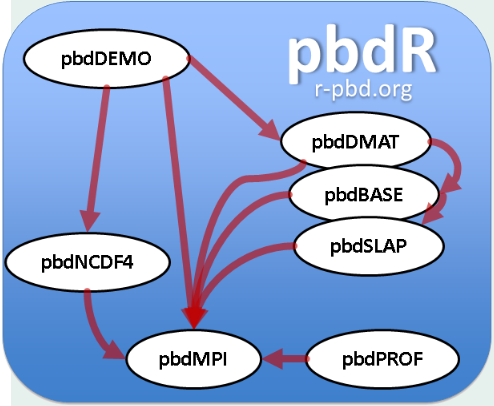
Programming with Big Data in R (pbdR)

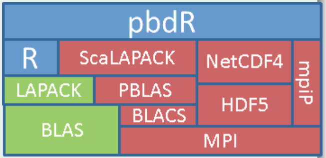
Striving for *Productivity, Portability, Performance*

- *Free*[a] R packages.
- Bridging high-performance C with high-productivity of R
- Scalable, big data analytics.
- Distributed data details implicitly managed.
- Methods have syntax *identical* to R.
- Powered by state of the art numerical libraries (MPI, ScaLAPACK, ...)

[a] MPL, BSD, and GPL licensed

pbdR Packages





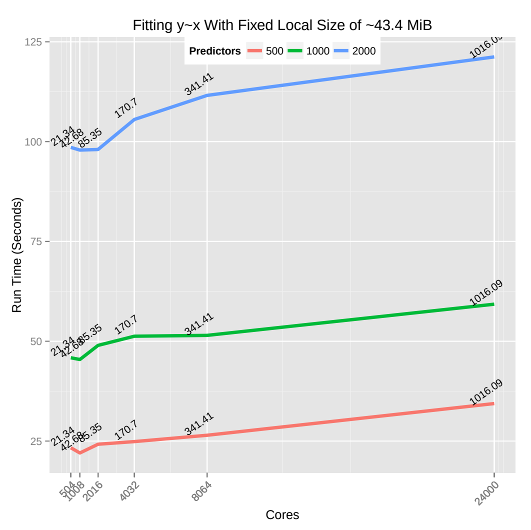
Example Syntax

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

Look familiar?

The above runs on 1 core with R or 10,000 cores with pbdR

Least Squares Benchmark



Profiling with **pbdPROF**

1. Rebuild **pbdR** packages

```
R CMD INSTALL
    pbdMPI_0.2-1.tar.gz \
    --configure-args= \
    "--enable-pbdPROF"
```

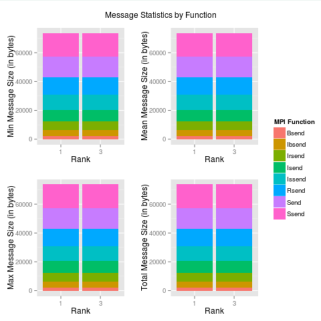
2. Run code

```
mpirun -np 64 Rscript
    my_script.R
```

3. Analyze results

```
library(pbdPROF)
prof <- read.prof(
    "profiler_output.mpiP")
plot(prof)
```

Publication-quality graphs



pbdR Paradigms

Programs that use pbdR utilize:

- Batch execution
- Single Program/Multiple Data (SPMD) style

And generally utilize:

- Data Parallelism

Batch Execution

- Non-interactive
- Use

```
Rscript my_script.r
```

or

```
R CMD BATCH my_script.r
```

- In parallel:

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

Single Program/Multiple Data (SPMD)

- SPMD is a programming *paradigm*.
- Not to be confused with SIMD.
- SPMD utilizes MIMD architecture computers.
- Arguably the simplest extension of serial programming.

Single Program/Multiple Data (SPMD)

- Difficult to describe, easy to do. . .
- Only one program is written, executed in batch on all processors.
- Different processors are autonomous; there is no manager.
- The dominant programming model for large machines.

Contents

Message Passing Interface (MPI)

- *MPI*: Standard for managing communications (data and instructions) between different nodes/computers.
- *Implementations*: OpenMPI, MPICH2, Cray MPT, . . .
- Enables parallelism (via communication) on distributed machines.
- *Communicator*: manages communications between processors.

MPI Operations (1 of 2)

- **Managing a Communicator**: Create and destroy communicators.
  `init()` — initialize communicator
  `finalize()` — shut down communicator(s)

- **Rank query**: determine the processor's position in the communicator.
  `comm.rank()` — "who am I?"
  `comm.size()` — "how many of us are there?"

- **Printing**: Printing output from various ranks.
  `comm.print(x)`
  `comm.cat(x)`
  WARNING: only use these functions on *results*, never on yet-to-be-computed things.

Quick Example 1

Rank Query: 1_rank.r

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

my.rank <- comm.rank()
comm.print(my.rank, all.rank=TRUE)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 1_rank.r
```

Sample Output:

```
COMM.RANK = 0
[1] 0
COMM.RANK = 1
[1] 1
```

Quick Example 2

Hello World: 2_hello.r

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

comm.print("Hello, world")

comm.print("Hello again", all.rank=TRUE, quiet=TRUE)

finalize()
```

Execute this script via:

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

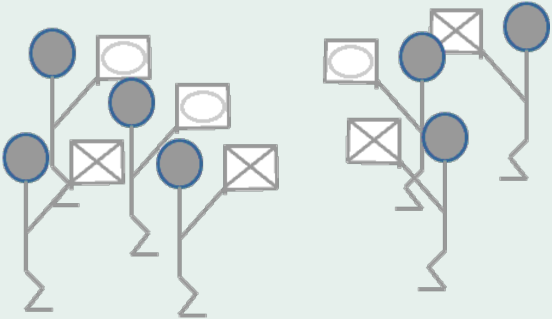
Sample Output:

```
COMM.RANK = 0
[1] "Hello, world"
[1] "Hello again"
[1] "Hello again"
```

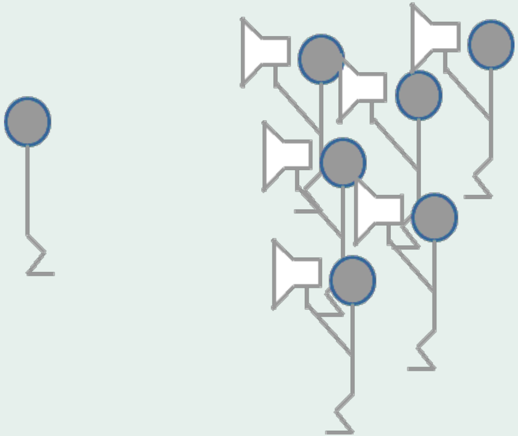
MPI Operations

1. Reduce
2. Gather
3. Broadcast
4. Barrier

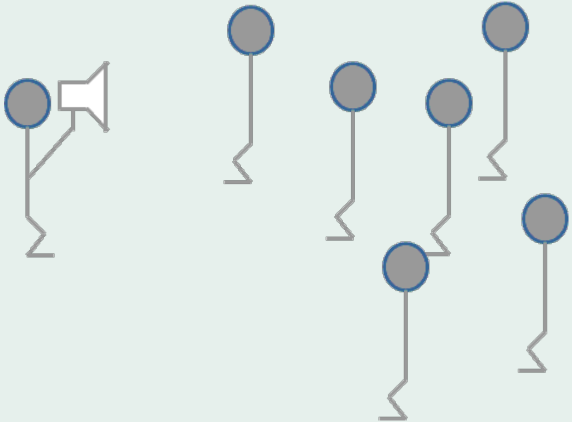
Reductions — Combine results into single result



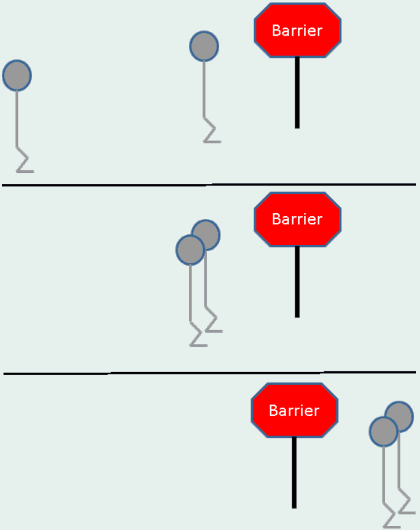
Gather — Many-to-one



Broadcast — One-to-many



Barrier — Synchronization



MPI Operations (2 of 2)

- **Reduction**: each processor has a number `x`; add all of them up, find the largest/smallest, ...
  `reduce(x, op='sum')` — reduce to one
  `allreduce(x, op='sum')` — reduce to all
- **Gather**: each processor has a number; create a new object on some processor containing all of those numbers.
  `gather(x)` — gather to one
  `allgather(x)` — gather to all
- **Broadcast**: one processor has a number `x` that every other processor should also have.
  `bcast(x)`
- **Barrier**: "computation wall"; no processor can proceed until *all* processors can proceed.
  `barrier()`

Quick Example 3

Reduce and Gather: 3_gt.r

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

comm.set.seed(diff=TRUE)

n <- sample(1:10, size=1)

gt <- gather(n)
comm.print(unlist(gt))

sm <- allreduce(n, op='sum')
comm.print(sm, all.rank=T)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 3_gt.r
```

Sample Output:

```
COMM.RANK = 0
[1] 2 8
COMM.RANK = 0
[1] 10
COMM.RANK = 1
[1] 10
```

Quick Example 4

Broadcast: 4_bcast.r

```r
library(pbdMPI, quiet=T)
init()

if (comm.rank()==0){
  x <- matrix(1:4, nrow=2)
} else {
  x <- NULL
}

y <- bcast(x, rank.source=0)

comm.print(y, rank=1)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 4_bcast.r
```

Sample Output:

```
COMM.RANK = 1
     [,1] [,2]
[1,]    1    3
[2,]    2    4
```

MPI Package Controls

The `.SPMD.CT` object allows for setting different package options with **pbdMPI**. See the entry *SPMD Control* of the **pbdMPI** manual for information about the `.SPMD.CT` object:

http://cran.r-project.org/web/packages/pbdMPI/pbdMPI.pdf

Quick Example 5

Barrier: 5_barrier.r

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

.SPMD.CT$msg.barrier <- TRUE
.SPMD.CT$print.quiet <- TRUE

for (rank in 1:comm.size()-1){
  if (comm.rank() == rank){
    cat(paste("Hello", rank+1, "of", comm.size(), "\n"))
  }
  barrier()
}

comm.cat("\n")

comm.cat(paste("Hello", comm.rank()+1, "of",
    comm.size(), "\n"), all.rank=TRUE)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 5_barrier.r
```

Sample Output:

```
Hello 1 of 2
Hello 2 of 2
```

Random Seeds

pbdMPI offers a simple interface for managing random seeds:

- `comm.set.seed(diff=TRUE)` — Independent streams via the **rlecuyer** package.
- `comm.set.seed(seed=1234, diff=FALSE)` — All processors use the same seed `seed=1234`
- `comm.set.seed(diff=FALSE)` — All processors use the same seed, determined by processor 0 (using the system clock and PID of processor 0).

Quick Example 6

Timing: 6_timer.r

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

comm.set.seed(diff=T)

test <- function(timed)
{
  ltime <- system.time(timed)[3]

  mintime <- allreduce(ltime, op='min')
  maxtime <- allreduce(ltime, op='max')
  meantime <- allreduce(ltime, op='sum')/comm.size()

  return(data.frame(min=mintime, mean=meantime,
      max=maxtime))
}

times <- test(rnorm(1e6)) # ~7.6MiB of data
comm.print(times)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 6_timer.r
```

Sample Output:

```
   min  mean   max
1 0.17 0.173 0.176
```

Other Helper Tools

pbdMPI Also contains useful tools for Manager/Worker and task parallelism codes:

- **Task Subsetting**: Distributing a list of jobs/tasks
  `get.jid(n)`
- ***ply**: Functions in the *ply family.
  `pbdApply(X, MARGIN, FUN, ...)` — analogue of `apply()`
  `pbdLapply(X, FUN, ...)` — analogue of `lapply()`
  `pbdSapply(X, FUN, ...)` — analogue of `sapply()`

Quick Comments for Using pbdMPI

1. Start by loading the package:

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

2. Always initialize before starting and finalize when finished:

```
init()

# ...

finalize()
```

Contents

Distributing Data

Problem: How to distribute the data

$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{bmatrix}_{10\times 3}$$

?

Distributing a Matrix Across 4 Processors: Block Distribution

Data	Processors
$$x = \begin{bmatrix} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ x_{9,1} & x_{9,2} & x_{9,3} \\ \hline x_{10,1} & x_{10,2} & x_{10,3} \end{bmatrix}_{10\times 3}$$	0 1 2 3

Distributing a Matrix Across 4 Processors: Local Load Balance

Data

$$x = \left[\begin{array}{ccc} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ \hline x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{array}\right]_{10\times 3}$$

Processors

0
1
2
3

The GBD Data Structure

Throughout the examples, we will make use of the Generalized Block Distribution, or GBD distributed matrix structure.

1. GBD is *distributed*. No processor owns all the data.
2. GBD is *non-overlapping*. Rows uniquely assigned to processors.
3. GBD is *row-contiguous*. If a processor owns one element of a row, it owns the entire row.
4. GBD is globally *row-major*, locally *column-major*.
5. GBD is often *locally balanced*, where each processor owns (almost) the same amount of data. But this is not required.

$$\left[\begin{array}{ccc} x_{1,1} & x_{1,2} & x_{1,3} \\ x_{2,1} & x_{2,2} & x_{2,3} \\ x_{3,1} & x_{3,2} & x_{3,3} \\ \hline x_{4,1} & x_{4,2} & x_{4,3} \\ x_{5,1} & x_{5,2} & x_{5,3} \\ x_{6,1} & x_{6,2} & x_{6,3} \\ \hline x_{7,1} & x_{7,2} & x_{7,3} \\ x_{8,1} & x_{8,2} & x_{8,3} \\ \hline x_{9,1} & x_{9,2} & x_{9,3} \\ x_{10,1} & x_{10,2} & x_{10,3} \end{array}\right]$$

6. The last row of the local storage of a processor is adjacent (by global row) to the first row of the local storage of next processor (by communicator number) that owns data.
7. GBD is (relatively) easy to understand, but can lead to bottlenecks if you have many more columns than rows.

Understanding GBD: Global Matrix

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{9\times 9}$$

$$\text{Processors} = 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5$$

Understanding GBD: Load Balanced GBD

$$x = \left[\begin{array}{ccccccccc}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\
\hline
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\
\hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\
\hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\
\hline
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\
\hline
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processors} = \quad 0 \quad 1 \quad 2 \quad 3 \quad 4 \quad 5$$

Understanding GBD: Local View

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \end{bmatrix}_{1\times 9}$$

$$\begin{bmatrix} x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \end{bmatrix}_{1\times 9}$$

$$\begin{bmatrix} x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{1\times 9}$$

Processors = 0 1 2 3 4 5

Understanding GBD: Non-Balanced GBD

$$x = \left[\begin{array}{ccccccccc}
\hline
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\
\hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\
\hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\
\hline
\hline
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

Processors = 0 1 2 3 4 5

Understanding GBD: Local View

$$\begin{bmatrix} \\ \end{bmatrix}_{0\times 9}$$

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \end{bmatrix}_{4\times 9}$$

$$\begin{bmatrix} x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \end{bmatrix}_{2\times 9}$$

$$\begin{bmatrix} x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \end{bmatrix}_{1\times 9}$$

$$\begin{bmatrix} \\ \end{bmatrix}_{0\times 9}$$

$$\begin{bmatrix} x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{2\times 9}$$

Processors = 0 1 2 3 4 5

Quick Comment for GBD

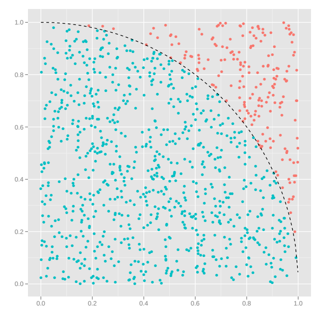
Local pieces of `GBD` distributed objects will be given the suffix `.gbd` to visually help distinguish them from global objects. This suffix carries no semantic meaning.

Contents

Example 1: Monte Carlo Simulation

Sample N uniform observations (x_i, y_i) in the unit square $[0, 1] \times [0, 1]$. Then

$$\pi \approx 4 \left(\frac{\#\ \textit{Inside Circle}}{\#\ \textit{Total}} \right) = 4 \left(\frac{\#\ \text{Blue}}{\#\ \text{Blue} + \#\ \text{Red}} \right)$$



Example 1: Monte Carlo Simulation GBD Algorithm

1. Let n be big-ish; we'll take $n = 50,000$.
2. Generate an $n \times 2$ matrix x of standard uniform observations.
3. Count the number of rows satisfying $x^2 + y^2 \leq 1$
4. Ask everyone else what their answer is; sum it all up.
5. Take this new answer, multiply by 4 and divide by n
6. If my rank is 0, print the result.

Example 1: Monte Carlo Simulation Code

Serial Code

```
N <- 50000
X <- matrix(runif(N * 2), ncol=2)
r <- sum(rowSums(X^2) <= 1)
PI <- 4*r/N
print(PI)
```

Parallel Code

```
library(pbdMPI, quiet = TRUE)
init()
comm.set.seed(diff=TRUE)

N.gbd <- 50000 / comm.size()
X.gbd <- matrix(runif(N.gbd * 2), ncol = 2)
r.gbd <- sum(rowSums(X.gbd^2) <= 1)
r <- allreduce(r.gbd)
PI <- 4*r/(N.gbd * comm.size())
comm.print(PI)

finalize()
```

Note

For the remainder, we will exclude loading, init, and finalize calls.

Example 2: Sample Covariance

$$cov(x_{n \times p}) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \mu_x)(x_i - \mu_x)^T$$

Example 2: Sample Covariance GBD Algorithm

1. Determine the total number of rows N.
2. Compute the vector of column means of the full matrix.
3. Subtract each column's mean from that column's entries in each local matrix.
4. Compute the crossproduct locally and reduce.
5. Divide by $N - 1$.

Example 2: Sample Covariance Code

Serial Code

```
N <- nrow(X)
mu <- colSums(X) / N

X <- sweep(X, STATS=mu, MARGIN=2)
Cov.X <- crossprod(X) / (N-1)

print(Cov.X)
```

Parallel Code

```
N <- allreduce(nrow(X.gbd), op="sum")
mu <- allreduce(colSums(X.gbd) / N, op="sum")

X.gbd <- sweep(X.gbd, STATS=mu, MARGIN=2)
Cov.X <- allreduce(crossprod(X.gbd), op="sum") / (N-1)

comm.print(Cov.X)
```

Example 3: Linear Regression

Find β such that

$$\mathbf{y} = \mathbf{X}\beta + \epsilon$$

When $\mathbf{X}$ is full rank,

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

Example 3: Linear Regression GBD Algorithm

1. Locally, compute $tx = x^T$
2. Locally, compute $A = tx * x$. Query every other processor for this result and sum up all the results.
3. Locally, compute $B = tx * y$. Query every other processor for this result and sum up all the results.
4. Locally, compute $A^{-1} * B$

Example 3: Linear Regression Code

Serial Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B
```

Parallel Code

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

ols <- solve(A) %*% B
```

Contents

Distributed Matrices

Most problems in data science are matrix algebra problems, so:

$$\text{Distributed matrices} \implies \text{Handle Bigger data}$$

Distributed Matrices

High level OOP allows *native* serial R syntax:

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

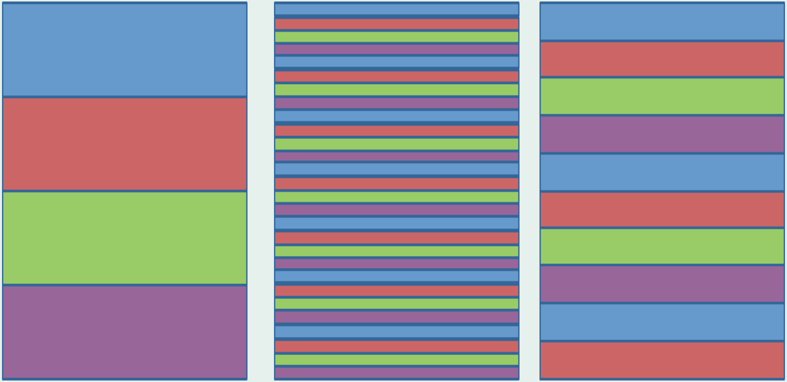
However. . .

Distributed Matrices

DMAT:

- **D**istributed **MAT**rix data structure.
- No single processor should hold all of the data.
- Block-cyclic matrix distributed across a 2-dimensional grid of processors.
- Very robust, but confusing data structure.

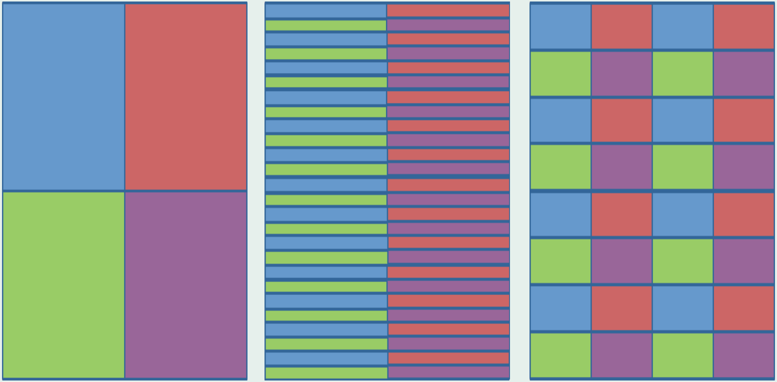
Distributed Matrices



(a) Block (b) Cyclic (c) Block-Cyclic

Figure : Matrix Distribution Schemes

Distributed Matrices



(a) 2d Block (b) 2d Cyclic (c) 2d Block-Cyclic

Figure : Matrix Distribution Schemes Onto a 2-Dimensional Grid

Processor Grid Shapes

(a) 1×6	(b) 2×3	(c) 3×2	(d) 6×1
$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}^T$	$\begin{bmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 2 & 3 \\ 4 & 5 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$

Table : Processor Grid Shapes with 6 Processors

Distributed Matrices

The data structure is a special R class (in the OOP sense) called `ddmatrix`. It is the "under the rug" storage for a block-cyclic matrix distributed onto a 2-dimensional processor grid.

$$
\texttt{ddmatrix} = \begin{cases} \textbf{Data} & \text{S4 local submatrix, an R matrix} \\ \textbf{dim} & \text{S4 dimension of the global matrix, a numeric pair} \\ \textbf{ldim} & \text{S4 dimension of the local submatrix, a numeric pair} \\ \textbf{bldim} & \text{S4 ScaLAPACK blocking factor, a numeric pair} \\ \textbf{CTXT} & \text{S4 BLACS context, an numeric singleton} \end{cases}
$$

with prototype

$$
\texttt{new("ddmatrix")} = \begin{cases} \textbf{Data} & = \texttt{matrix(0.0)} \\ \textbf{dim} & = \texttt{c(1,1)} \\ \textbf{ldim} & = \texttt{c(1,1)} \\ \textbf{bldim} & = \texttt{c(1,1)} \\ \textbf{CTXT} & = \texttt{0.0} \end{cases}
$$

Distributed Matrices: The Data Structure

Example: an 9×9 matrix is distributed with a "block-cycling" factor of 2×2 on a 2×2 processor grid:

0	0	1	1	0	0	1	1	0
0	0	1	1	0	0	1	1	0
2	2	3	3	2	2	3	3	2
2	2	3	3	2	2	3	3	2
0	0	1	1	0	0	1	1	0
0	0	1	1	0	0	1	1	0
2	2	3	3	2	2	3	3	2
2	2	3	3	2	2	3	3	2
0	0	1	1	0	0	1	1	0

$$= \begin{cases} \textbf{Data} & = \texttt{matrix(...)} \\ \textbf{dim} & = \texttt{c(9, 9)} \\ \textbf{ldim} & = \texttt{c(...)} \\ \textbf{bldim} & = \texttt{c(2, 2)} \\ \textbf{CTXT} & = 0 \end{cases}$$

See http://acts.nersc.gov/scalapack/hands-on/datadist.html

Understanding Dmat: Global Matrix

$$x = \begin{bmatrix} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{bmatrix}_{9\times 9}$$

DMAT: 1-dimensional Row Block

$$x = \left[\begin{array}{ccccccccc}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ \hline
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array}\right| = \left|\begin{array}{c} (0,0) \\ (1,0) \\ (2,0) \\ (3,0) \end{array}\right|$$

DMAT: 2-dimensional Row Block

$$x = \left[\begin{array}{ccccc|cccc}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\
\hline
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{cc} 0 & 1 \\ 2 & 3 \end{array}\right| = \left|\begin{array}{cc} (0,0) & (0,1) \\ (1,0) & (1,1) \end{array}\right|$$

DMAT: 1-dimensional Row Cyclic

$$x = \left[\begin{array}{ccccccccc}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ \hline
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ \hline
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ \hline
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ \hline
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{c} 0 \\ 1 \\ 2 \\ 3 \end{array}\right| = \left|\begin{array}{c} (0,0) \\ (1,0) \\ (2,0) \\ (3,0) \end{array}\right|$$

DMAT: 2-dimensional Row Cyclic

$$x = \left[\begin{array}{ccccc|cccc}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ \hline
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ \hline
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ \hline
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ \hline
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{cc} 0 & 1 \\ 2 & 3 \end{array}\right| = \left|\begin{array}{cc} (0,0) & (0,1) \\ (1,0) & (1,1) \end{array}\right|$$

DMAT: 2-dimensional Block-Cyclic

$$x = \left[\begin{array}{cc|cc|cc|cc|c}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\
\hline
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\
\hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\
\hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\
\hline
x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99}
\end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \left|\begin{array}{cc} 0 & 1 \\ 2 & 3 \end{array}\right| = \left|\begin{array}{cc} (0,0) & (0,1) \\ (1,0) & (1,1) \end{array}\right|$$

The DMAT Data Structure

The more complicated the processor grid, the more complicated the distribution.

DMAT: 2-dimensional Block-Cyclic with 6 Processors

$$x = \left[\begin{array}{cc|cc|cc|cc|c} x_{11} & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} \\ x_{21} & x_{22} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{29} \\ \hline x_{31} & x_{32} & x_{33} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{39} \\ x_{41} & x_{42} & x_{43} & x_{44} & x_{45} & x_{46} & x_{47} & x_{48} & x_{49} \\ \hline x_{51} & x_{52} & x_{53} & x_{54} & x_{55} & x_{56} & x_{57} & x_{58} & x_{59} \\ x_{61} & x_{62} & x_{63} & x_{64} & x_{65} & x_{66} & x_{67} & x_{68} & x_{69} \\ \hline x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \\ x_{81} & x_{82} & x_{83} & x_{84} & x_{85} & x_{86} & x_{87} & x_{88} & x_{89} \\ \hline x_{91} & x_{92} & x_{93} & x_{94} & x_{95} & x_{96} & x_{97} & x_{98} & x_{99} \end{array}\right]_{9\times 9}$$

$$\text{Processor grid} = \begin{vmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{vmatrix} = \begin{vmatrix} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{vmatrix}$$

Understanding DMAT: Local View

$$
\left[\begin{array}{cc|cc}
x_{11} & x_{12} & x_{17} & x_{18} \\
x_{21} & x_{22} & x_{27} & x_{28} \\ \hline
x_{51} & x_{52} & x_{57} & x_{58} \\
x_{61} & x_{62} & x_{67} & x_{68} \\ \hline
x_{91} & x_{92} & x_{97} & x_{98}
\end{array}\right]_{5\times 4}
\left[\begin{array}{cc|c}
x_{13} & x_{14} & x_{19} \\
x_{23} & x_{24} & x_{29} \\ \hline
x_{53} & x_{54} & x_{59} \\
x_{63} & x_{64} & x_{69} \\ \hline
x_{93} & x_{94} & x_{99}
\end{array}\right]_{5\times 3}
\left[\begin{array}{cc}
x_{15} & x_{16} \\
x_{25} & x_{26} \\ \hline
x_{55} & x_{56} \\
x_{65} & x_{66} \\ \hline
x_{95} & x_{96}
\end{array}\right]_{5\times 2}
$$

$$
\left[\begin{array}{cc|cc}
x_{31} & x_{32} & x_{37} & x_{38} \\
x_{41} & x_{42} & x_{47} & x_{48} \\ \hline
x_{71} & x_{72} & x_{77} & x_{78} \\
x_{81} & x_{82} & x_{87} & x_{88}
\end{array}\right]_{4\times 4}
\left[\begin{array}{cc|c}
x_{33} & x_{34} & x_{39} \\
x_{43} & x_{44} & x_{49} \\ \hline
x_{73} & x_{74} & x_{79} \\
x_{83} & x_{84} & x_{89}
\end{array}\right]_{4\times 3}
\left[\begin{array}{cc}
x_{35} & x_{36} \\
x_{45} & x_{46} \\ \hline
x_{75} & x_{76} \\
x_{85} & x_{86}
\end{array}\right]_{4\times 2}
$$

$$
\text{Processor grid} = \left|\begin{array}{ccc} 0 & 1 & 2 \\ 3 & 4 & 5 \end{array}\right| = \left|\begin{array}{ccc} (0,0) & (0,1) & (0,2) \\ (1,0) & (1,1) & (1,2) \end{array}\right|
$$

The DMAT Data Structure

1. DMAT is *distributed*. No one processor owns all of the matrix.
2. DMAT is *non-overlapping*. Any piece owned by one processor is owned by no other processors.
3. DMAT can be row-contiguous or not, depending on the processor grid and blocking factor used.
4. DMAT is locally column-major and globally, it depends...

$$\left[\begin{array}{cc|cc|c}
x_{11} & x_{12} & x_{13} & x_{14} & x_{15} \\
x_{21} & x_{22} & x_{23} & x_{24} & x_{25} \\
\hline
x_{31} & x_{32} & x_{33} & x_{34} & x_{35} \\
x_{41} & x_{42} & x_{43} & x_{44} & x_{45} \\
\hline
x_{51} & x_{52} & x_{53} & x_{54} & x_{55} \\
x_{61} & x_{62} & x_{63} & x_{64} & x_{65} \\
\hline
x_{71} & x_{72} & x_{73} & x_{74} & x_{75} \\
x_{81} & x_{82} & x_{83} & x_{84} & x_{85} \\
\hline
x_{91} & x_{92} & x_{93} & x_{94} & x_{95}
\end{array}\right]$$

6. GBD is a generalization of the one-dimensional block DMAT distribution. Otherwise there is no relation.
7. DMAT is confusing, but very robust.

Pros and Cons of This Data Structure

Pros

- Fast for distributed matrix computations

Cons

- Literally everything else

This is why we hide most of the distributed details.

The details are there if you want them (you don't want them).

Distributed Matrix Methods

pbdDMAT has over 100 methods with *identical* syntax to R:

- `` `[` ``, `rbind()`, `cbind()`, ...
- `lm.fit()`, `prcomp()`, `cov()`, ...
- `` `%*%` ``, `solve()`, `svd()`, `norm()`, ...
- `median()`, `mean()`, `rowSums()`, ...

Serial Code

```
cov(x)
```

Parallel Code

```
cov(x)
```

Comparing pbdMPI and pbdDMAT

pbdMPI:

- MPI + sugar.
- `GBD` not the only structure **pbdMPI** can handle (just a useful convention).

pbdDMAT:

- More of a software package.
- `DMAT` structure *must* be used for **pbdDMAT**.
- If the data is not 2d block-cyclic compatible, DMAT will *definitely* give the wrong answer.

Quick Comments for Using pbdDMAT

1. Start by loading the package:

```
library(pbdDMAT, quiet = TRUE)
```

2. Always initialize before starting and finalize when finished:

```
init.grid()

# ...

finalize()
```

3. Distributed DMAT objects will be given the suffix .dmat to visually help distinguish them from global objects. This suffix carries no semantic meaning.

Contents

Example 1: DMAT Construction

Generate a global matrix and distribute it

```
library(pbdDMAT, quiet=TRUE)
init.grid()

# Common global on all processors --> distributed
x <- matrix(1:100, nrow=10, ncol=10)
x.dmat <- as.ddmatrix(x)

x.dmat

# Global on processor 0 --> distributed
if (comm.rank()==0){
  y <- matrix(1:100, nrow=10, ncol=10)
} else {
  y <- NULL
}
y.dmat <- as.ddmatrix(y)

y.dmat

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 1_gen.r
```

Example 2: DMAT Construction

Generate locally only what is needed

```
library(pbdDMAT, quiet=TRUE)
init.grid()

zero.dmat <- ddmatrix(0, nrow=100, ncol=100)
zero.dmat

id.dmat <- diag(1, nrow=100, ncol=100, type="ddmatrix")
id.dmat

comm.set.seed(diff=T)
rand.dmat <- ddmatrix("rnorm", nrow=100, ncol=100,
    mean=10, sd=100)
rand.dmat

finalize()
```

Execute this script via:

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

Example 3: DMAT Operations

Generate locally only what is needed

```
library(pbdDMAT, quiet=TRUE)
init.grid()

x.dmat <- ddmatrix(1:30, nrow=10)
y.dmat <- x.dmat[c(1, 3, 5, 7, 9), -3]

comm.print(y.dmat)
y <- as.matrix(y.dmat)
comm.print(y)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 3_extract.r
```

Example 4: More DMAT Operations

```r
library(pbdDMAT, quiet=TRUE)
init.grid()

x.dmat <- ddmatrix(1:30, nrow=10)

y.dmat <- x.dmat + 1:7

z.dmat <- scale(x.dmat, center=TRUE, scale=TRUE)

y <- as.matrix(y.dmat)
z <- as.matrix(z.dmat)

comm.print(y)
comm.print(z)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 4_misc.r
```

Statistics Examples with pbdDMAT

Execute this script via:

```
% mpirun -np 2 Rscript 4_convert.r
%
```

Sample Covariance

Serial Code

```r
Cov.X <- cov(X)
print(Cov.X)
```

Parallel Code

```r
Cov.X <- cov(X)
print(Cov.X)
```

Linear Regression

Serial Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B

# or
ols <- lm.fit(X, y)
```

Parallel Code

```
tX <- t(X)
A <- tX %*% X
B <- tX %*% y

ols <- solve(A) %*% B

# or
ols <- lm.fit(X, y)
```

Example 5: PCA

PCA: pca.r

```r
library(pbdDMAT, quiet=T)
init.grid()

n <- 1e4
p <- 250

comm.set.seed(diff=T)
x.dmat <- ddmatrix("rnorm", nrow=n, ncol=p, mean=100, sd=25)

pca <- prcomp(x=x.dmat, retx=TRUE, scale=TRUE)
prop_var <- cumsum(pca$sdev)/sum(pca$sdev)
i <- max(min(which(prop_var > 0.9)) - 1, 1)

y.dmat <- pca$x[, 1:i]

comm.cat("\nCols: ", i, "\n", quiet=T)
comm.cat("%Cols:", i/dim(x.dmat)[2], "\n\n", quiet=T)

finalize()
```

Execute this script via:

```
mpirun -np 2 Rscript 5_pca.r
```

Sample Output:

```
 Cols:  221
%Cols: 0.884
```

Distributed Matrices

pbdDEMO contains many other examples of reading and managing GBD and DMAT data

Randomized SVD[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 $\boldsymbol{A}$.

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

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 N, Martinsson P-G and Tropp J A 2011 Finding structure with randomness: probabilistic algorithms for constructing approximate matrix decompositions *SIAM Rev.* **53** 217–88

Randomized SVD

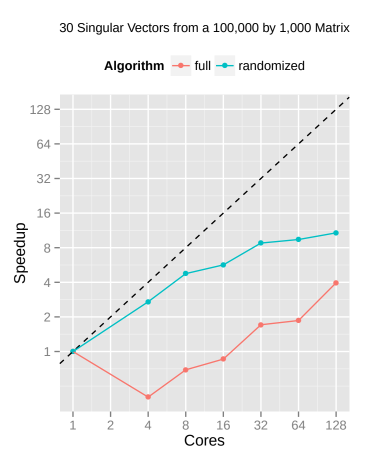
Serial R

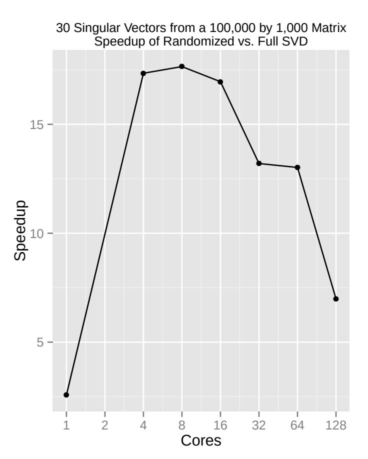
```r
randSVD <- function(A, k, q=3)
  {
    ## Stage A
    Omega <- matrix(rnorm(n*2*k),
            nrow=n, ncol=2*k)
    Y <- A %*% Omega
    Q <- qr.Q(qr(Y))
    At <- t(A)
    for(i in 1:q)
      {
        Y <- At %*% Q
        Q <- qr.Q(qr(Y))
        Y <- A %*% Q
        Q <- qr.Q(qr(Y))
     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

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

Parallel pbdR

```r
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]
  }
```

Randomized SVD





Contents

The pbdR Project

- Our website: http://r-pbd.org/
- Email us at: RBigData@gmail.com
- Our google group: http://group.r-pbd.org/

Where to begin?

- The **pbdDEMO** package
  http://cran.r-project.org/web/packages/pbdDEMO/
- The **pbdDEMO** Vignette: http://goo.gl/HZkRt

Thanks for coming!

Questions?

pbdR
Programming with Big Data in R

http://r-pbd.org/