Introducing R: from Your Laptop to HPC and Big Data

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Affiliations and Support

The pbdR Core Team
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About This Presentation

Downloads

This presentation and supplemental materials are available at:

http://r-pbd.org/handouts

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*

`https://github.com/wrathematics/pbdDEMO/blob/master/inst/doc/pbdDEMO-guide.pdf?raw=true`

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.

About This Presentation

Conventions

We use:

- "." as a decimal mark
- "," as order of magnitude separator

Example	Yes	No
One million	1,000,000	1.000.000
One half	0.5	0,5
One thousand and one half	1,000.5	1.000,5

Contents

1. Introduction
2. pbdR
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5. Brief Intermission
6. Basic Statistics Examples
7. Introduction to pbdDMAT
8. Examples Using pbdDMAT
9. Wrapup

Contents

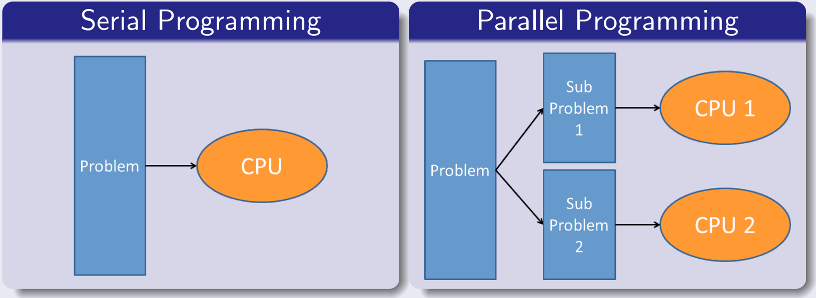
1. Introduction
   - A Concise Introduction to Parallelism
   - R and Parallelism

What is Parallelism?

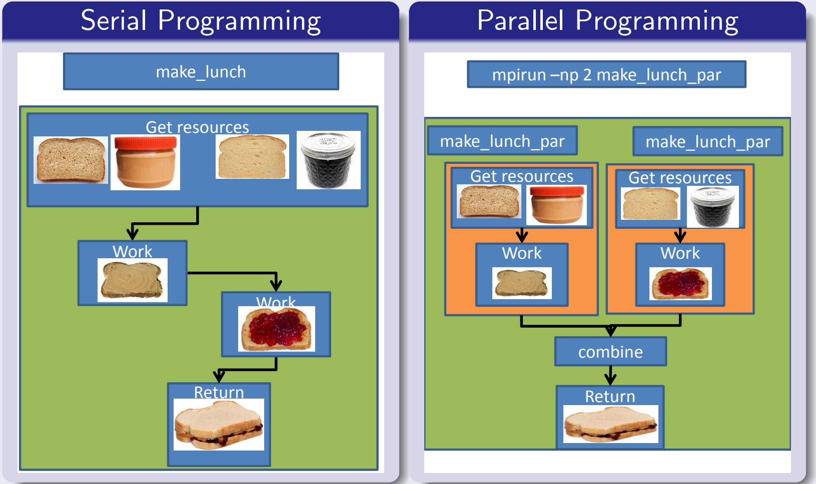
Broadly, *doing more than one thing at a time*.

The simultaneous use of multiple compute resources to solve a computational problem:

Parallelism



Parallelism

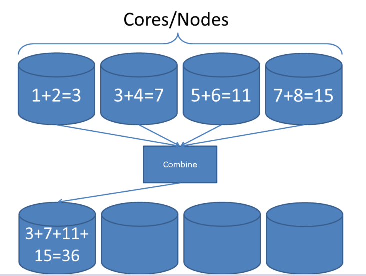


What is Parallelism?

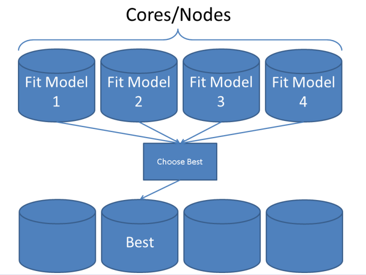
- *Task Parallelism*: Splitting the problem by task
- *Data Parallelism*:

Data vs Task Parallelism

Data Parallelism



Task Parallelism



Common Terms

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

R and Parallelism

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

What we have

1. Mostly serial.
2. Parallelism mostly not distributed (foreach, parallel/snow/multicore, ...)
3. Data parallelism mostly explicit (Rmpi, R+Hadoop, ...)

What we want

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

Why We Need Parallelism

1. Saves time (long term).
2. Data size is skyrocketing.
3. Necessary for many problems.
4. Like it or not, it's coming.
5. *It's really cool.*

Problems with 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.
5. Chokes on big data.

Contents

2. pbdR
   - The pbdR Project
   - pbdR Paradigms

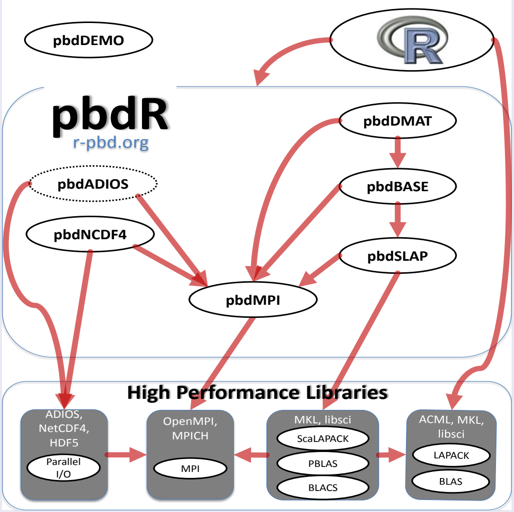
Programming with Big Data in R (pbdR)

Striving for *Productivity, Portability, Performance*

- Series of *free*[a] R packages.
- Scalable, big data analytics with high-level syntax.
- Implicit management of distributed data details.
- Methods have syntax *identical* to R.
- Powered by state of the art numerical libraries (MPI, ScaLAPACK, PBLAS, BLACS, LAPACK, BLAS, . . .)

[a] MPL, BSD, and GPL licensed

pbdR Packages



pbdR Packages — http://code.r-pbd.org

Released to CRAN:

- **pbdMPI**: MPI bindings (explicit, low-level)
- **pbdSLAP**: Foreign library (just install it, nothing to use)
- **pbdBASE**: Compiled code (used by DMAT, also for devs)
- **pbdDMAT**: Distributed matrices (mostly implicit, high-level)
- **pbdNCDF4**: Parallel NetCDF4 reader
- **pbdDEMO**: Package demonstrations, examples, vignette written in textbook style

Future Development:

- Profiling tools
- Client/server interface for interactive sessions
- ...

Example Syntax

```r
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

pbdR Focus: Distributed Machines

Shared Memory Machines

Thousands of cores

Nautilus, University of Tennessee

1024 cores

Distributed Memory Machines

Hundreds of thousands of cores

Kraken, University of Tennessee

112,896 cores

pbdR Paradigms

Programs that use pbdR are meant to utilize the:

- Data Parallelism method
- Single Program/Multiple Data (SPMD) style

SPMD

The pbdR Packages enable high-level "Single Program/Multiple Data" (SPMD) programming:

- SPMD is a programming *paradigm*.
- Arguably the simplest extension of serial programming.
- Sort of like trying to explain breathing . . .
- Not to be confused with SIMD.
- SPMD utilizes MIMD architecture computers.
- Only one program is written, executed in batch independently on all processors.
- Different processors are autonomous; there is no manager.

SPMD

SPMD codes are run in batch (non-interactively):

From the Shell

```
mpirun -np 4 Rscript my_script.R
```

pbdR Paradigms: Data Parallelism

With data parallelism:

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

pbdR Paradigms: SPMD

- Natural extension of writing serial codes.
- Different from Manager/Worker.
- No one processor is in charge. Each thinks it's the boss ("it's like academia").
- One program written, executed independently by all processors.
- Each processor owns a local sub-piece of data from the (conceptual) whole.

Contents

3 Introduction to pbdMPI
- Managing a Communicator
- Reductions and Gathers
- Other

Message Passing Interface (MPI)

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

MPI Operations (1 of 3)

- **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

```
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 (2 of 3)

- **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)`

Quick Example 3

Reduce and Gather: 3_gt.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 Operations (3 of 3)

- **Barrier**: "computation wall"; no processor can proceed until *all* processors can proceed.
  `barrier()`

- **Random Seeds**: Random number seeds.
  `comm.set.seed(diff=TRUE)` — Independent streams via **rlecuyer**
  `comm.set.seed(seed=1234, diff=FALSE)` — All processors use the same seed.

- ***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 Example 3

Barrier: 3_barrier.r

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

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

comm.cat("\n", quiet=TRUE)

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

finalize()
```

Execute this script via:

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

Sample Output:

```
Hello from process 1
    of 2
Hello from process 2
    of 2
```

Quick Example 4

Timing: timer.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 from process", rank+1, "of",
        comm.size(), "\n"))
  }
  barrier()
}

comm.cat("\n")

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

finalize()
```

Execute this script via:

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

Sample Output:

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

Quick Example 4

Timing: timer.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 from process", rank+1, "of",
        comm.size(), "\n"))
  }
  barrier()
}

comm.cat("\n")

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

finalize()
```

Execute this script via:

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

Sample Output:

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

Quick Comments for Using pbdMPI

1. Start by loading the package:

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

2. Always initialize before starting and finalize when finished:

```r
init()

# ...

finalize()
```

Contents

4 The Generalized Block Distribution
- The GBD Data Structure
- GBD: Example 1
- GBD: Example 2

Distributing a Matrix Across 4 Processors: Block Distribution

Data

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

Processors

0
1
2
3

Distributing a Matrix Across 4 Processors: Local Load Balance

Data

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

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

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

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

Understanding GBD: Local View

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

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

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

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

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

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

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

Understanding GBD: Non-Balanced GBD

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

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

Understanding GBD: Local View

$$\left[\begin{array}{ccccccccc} & & & & & & & & \end{array}\right]_{0\times 9}$$

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

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

$$\left[\begin{array}{ccccccccc} x_{71} & x_{72} & x_{73} & x_{74} & x_{75} & x_{76} & x_{77} & x_{78} & x_{79} \end{array}\right]_{1\times 9}$$

$$\left[\begin{array}{ccccccccc} & & & & & & & & \end{array}\right]_{0\times 9}$$

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

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.

Brief Intermission

Brief Intermission

Questions? Comments?

Don't forget to talk to us at our discussion group:
http://group.r-pbd.org/

If you have an affiliation at a United States institution (university, research lab, etc.), consider getting an allocation with us:
http://www.nics.tennessee.edu/getting-an-allocation

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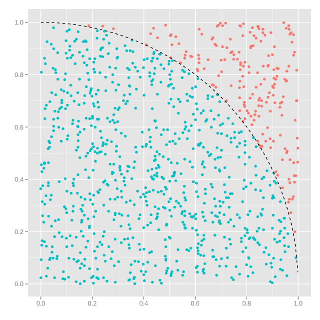
Example 1: Monte Carlo Simulation

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

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



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

7 Introduction to pbdDMAT

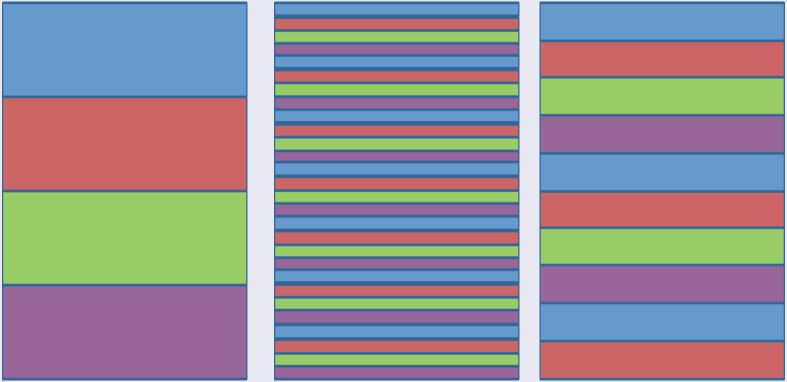
- Introduction to Distributed Matrices
- DMAT Distributions
- pbdDMAT

Distributed Matrices

Most problems in data science

- Data structure: block-cyclic matrix distributed across a 2-dimensional grid of processors.
- No single processor should hold all of the data.
- Very robust, but very confusing data structure.

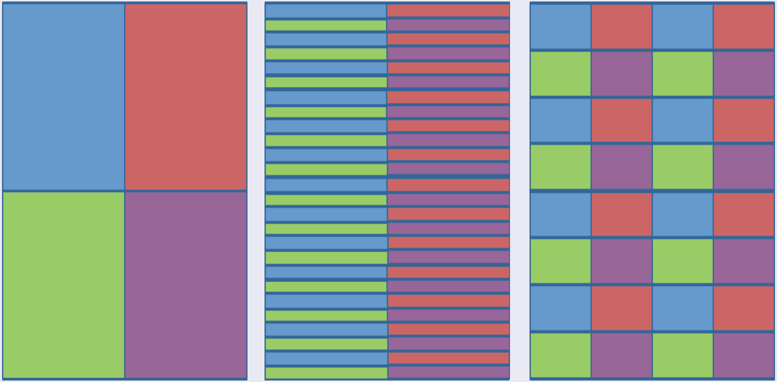
Distributed Matrices



(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

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

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

DMAT: 2-dimensional 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

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

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

DMAT: 2-dimensional 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

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

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

Understanding DMAT: Distributed with `bldim` = (2,2)

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

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

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. . .
5. GBD is a generalization of the one-dimensional block DMAT distribution; otherwise there is no relation.
6. 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** is MPI + some sugar.
- The `GBD` data structure is not the only thing **pbdMPI** can handle (just a useful convention).
- **pbdDMAT** is more of a software package.
- The block-cyclic `DMAT` structure *must* be used for **pbdDMAT**.

Quick Comments for Using pbdDMAT

1. Start by loading the package:

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

2. Always initialize before starting and finalize when finished:

```r
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.

Sample Covariance

Serial Code

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

Parallel Code

```
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)
```

Quick Example 3

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 pca.r
```

Sample Output:

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

Generating Random Data

Using randomly generated matrices is the best way to "get your feet wet" with the pbd tools. You can do this in 2 ways:

1. Generate a global matrix and distribute it.
2. Generate locally only what is needed.

Example 1: Random Distributed Matrix Generation

Generate a global matrix and distribute it

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

# Common global on all processors --> distributed
comm.set.seed(diff=FALSE)
x <- matrix(rnorm(100), nrow=10, ncol=10)
x.dmat <- as.ddmatrix(x)

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

finalize()
```

Example 2: Random Distributed Matrix Generation

Generate locally only what is needed

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

comm.set.seed(diff = TRUE) # good seeds via rlecuyer
x.dmat <- ddmatrix("rnorm", nrow=10, ncol=10)

finalize()
```

Example 3: Random Distributed Matrix Generation

Generate locally only what is needed

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

zero.dmat <- ddmatrix(0, nrow=100, ncol=100)
id.dmat <- diag(1, nrow=100, ncol=100)

finalize()
```

Example 4: Random Distributed Matrix Generation

Convert between GBD and DMAT

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

comm.set.seed(diff = TRUE)

N.gbd <- 1 + comm.rank()
X.gbd <- matrix(rnorm(N.gbd * 3), ncol = 3)

# convert GBD to DMAT
X.dmat <- gbd2dmat(X.gbd)

# convert DMAT to GBD
new.X.gbd <- dmat2gbd(X.dmat)

# undistribute
X <- as.matrix(X.dmat)

finalize()
```

Distributed Matrices

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

Contents

9 Wrapup

Where to Learn More

- Our website http://r-pbd.org/
- The **pbdDEMO** package
  http://cran.r-project.org/web/packages/pbdDEMO/
- The **pbdDEMO** Vignette: http://goo.gl/HZkRt
- Our Google Group: http://group.r-pbd.org

Thanks for coming!

Questions? Comments?

Please help us improve this tutorial by completing a short survey:
http://www.surveymonkey.com/s/W8VLJSP