Programming with Big Data in R

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About This Presentation

Downloads

This presentation and supplemental materials are available at:

```
http://r-pbd.org/tutorial
```

Sample R scripts and pbs job scripts available on Chester: /lustre/scratch/sw/r/3.0.1.new/chester/gnu4.7.3/ EXAMPLES/scripts.tar.gz



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:

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



Contents

- 1 Introduction to pbdDMAT and the DMAT Structure
- 2 Examples Using pbdDMAT



Contents

- 1 Introduction to pbdDMAT and the DMAT Structure
 - Introduction to Distributed Matrices
 - DMAT Distributions
 - pbdDMAT



Introduction to Distributed Matrices

Distributed Matrices

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

Distributed matrices ⇒ Handle Bigger data



Distributed Matrices

High level OOP allows *native* serial R syntax:

```
1 x <- x[-1, 2:5]

2 x <- log(abs(x) + 1)

3 xtx <- t(x) %*% x

4 ans <- svd(solve(xtx))
```

However...



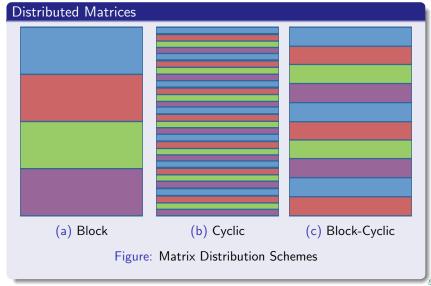
Introduction to Distributed Matrices

Distributed Matrices

DMAT:

- Distributed MATrix 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 (b) 2d Cyclic (a) 2d Block (c) 2d Block-Cyclic Figure: Matrix Distribution Schemes Onto a 2-Dimensional Grid

Processor Grid Shapes

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

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

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

Table: Processor Grid Shapes with 6 Processors



Introduction to Distributed Matrices

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.

with prototype

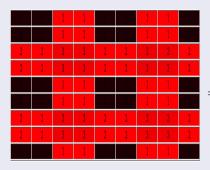
```
\label{eq:new} \text{new("ddmatrix")} = \begin{cases} \textbf{Data} &= \texttt{matrix}(0.0) \\ \textbf{dim} &= \texttt{c(1,1)} \\ \textbf{Idim} &= \texttt{c(1,1)} \\ \textbf{bldim} &= \texttt{c(1,1)} \\ \textbf{CTXT} &= 0.0 \end{cases}
```



0000000

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:



$$= \begin{cases} \textbf{Data} &= \texttt{matrix}(\ldots) \\ \textbf{dim} &= \texttt{c}(9, 9) \\ \textbf{Idim} &= \texttt{c}(\ldots) \\ \textbf{bIdim} &= \texttt{c}(2, 2) \\ \textbf{CTXT} &= 0 \end{cases}$$

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



Understanding Dmat: Global Matrix

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



DMAT: 1-dimensional Row Block

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

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



DMAT: 2-dimensional Row Block

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

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



DMAT: 1-dimensional Row Cyclic

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

Processor grid =
$$\begin{vmatrix} 0 \\ 1 \\ 2 \\ 3 \end{vmatrix} = \begin{vmatrix} (0,0) \\ (0,1) \\ (1,0) \\ (1.1) \end{vmatrix}$$



DMAT: 2-dimensional Row Cyclic

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

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



DMAT Distributions

DMAT: 2-dimensional Block-Cyclic

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

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



The DMAT Data Structure

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





DMAT: 2-dimensional Block-Cyclic with 6 Processors

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

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

$$\begin{bmatrix} x_{11} & x_{12} & x_{17} & x_{18} \\ x_{21} & x_{22} & x_{27} & x_{28} \\ \hline x_{51} & x_{52} & x_{57} & x_{58} \\ x_{61} & x_{62} & x_{67} & x_{68} \\ \hline x_{91} & x_{92} & x_{97} & x_{98} \end{bmatrix}$$

$$\Big]_{5 imes4}$$

$$\begin{bmatrix} x_{31} & x_{32} & x_{37} & x_{38} \\ x_{41} & x_{42} & x_{47} & x_{48} \\ \hline x_{71} & x_{72} & x_{77} & x_{78} \\ x_{81} & x_{82} & x_{87} & x_{88} \\ \end{bmatrix}$$

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

$$(0,0)$$
 $(0,1)$ $(0$

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.
- ① DMAT can be row-contiguous or not, depending on the processor grid and blocking factor used.
- OMAT is locally column-major and globally, it depends...
- GBD is a generalization of the one-dimensional block DMAT distribution. Otherwise there is no relation.
- O DMAT is confusing, but very robust.

<i>x</i> ₁₁	X ₁₂	X ₁₃	X ₁₄	X ₁₅
X21	X22	X23	X24	X25
X31	X32	X33	X34	X35
X41	X42	X43	X44	X45
X51	X52	X53	X54	<i>X</i> 55
X ₆₁	X62	<i>X</i> 63	X64	<i>X</i> 65
X71	X72	X73	X74	X75
X81	X82	X83	X84	X85
X91	X92	X93	X94	X95

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

 $1 \mid cov(x)$

Parallel Code

1 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

Start by loading the package:

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

② Always initialize before starting and finalize when finished:

```
init.grid()

# ...

finalize()
```

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



Contents

- Examples Using pbdDMAT
 - Statistics Examples with pbdDMAT
 - RandSVD



```
Sample Covariance

Serial Code

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

Parallel Code

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



Linear Regression

Serial Code

```
1
tX <- t(X)
2 A <- tX %*% X
3 B <- tX %*% y
4
5 ols <- solve(A) %*% B
6
7 # or
8 ols <- lm.fit(X, y)</pre>
```

Parallel Code

```
1 tX <- t(X)
2 A <- tX %*% X
3 B <- tX %*% y
4
5 ols <- solve(A) %*% B
6
7 # or
8 ols <- lm.fit(X, y)
```



Statistics Examples with pbdDMAT

Example 5: PCA

PCA: pca.r

```
library(pbdDMAT, quiet=T)
    init.grid()
2
3
4
5
6
7
   n <- 1e4
   p <- 250
   comm. set . seed ( diff=T)
8
   x.dmat <- ddmatrix("rnorm", nrow=n, ncol=p, mean=100, sd=25)
10
   pca <- prcomp(x=x.dmat. retx=TRUE. scale=TRUE)</pre>
11
    prop_var <- cumsum(pca$sdev)/sum(pca$sdev)</pre>
12
    i \leftarrow max(min(which(prop_var > 0.9)) - 1, 1)
13
14
   y.dmat \leftarrow pcax[, 1:i]
15
   comm.cat("\nCols: ", i, "\n", quiet=T)
16
   comm. cat("\%Cols:", i/dim(x.dmat)[2], "\n\n", quiet=T)
17
18
19
    finalize()
```

Execute this script via:

Sample Output:

```
1 mpirun -np 2 Rscript 5-pca.r 1 Cols: 221 2 %Cols: 0.884
```



Statistics Examples with pbdDMAT

Distributed Matrices

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



RandSVD

Randomized SVD1

Prototype for Randomized SVD

Given an $m \times n$ matrix 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 $U\Sigma V^*$, where U and V are orthonormal, and Σ is nonnegative and diagonal.

Stage A:

- Generate an $n \times 2k$ Gaussian test matrix Ω .
- 2 Form Y = (AA*)^qAΩ by multiplying alternately with A and A*. 3 Construct a matrix Q whose columns form an orthonormal basis for

the range of Y. Stage B:

- 4 Form $B = Q^*A$.
- Compute an SVD of the small matrix: $B = \tilde{U}\Sigma V^*$.
- 6 Set $U = O\widetilde{U}$.

Note: The computation of 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 A and A^* ; see Algorithm 4.4.

Algorithm 4.4: Randomized Subspace Iteration Given an $m \times n$ matrix A and integers ℓ and q, this algorithm computes an $m \times \ell$ orthonormal matrix Q whose range approximates the range of A. Draw an $n \times \ell$ standard Gaussian matrix Ω .

- 2 Form Y₀ = AΩ and compute its OR factorization Y₀ = O₀R₀. for j = 1, 2, ..., q
- Form $\tilde{Y}_i = A^*Q_{i-1}$ and compute its QR factorization $\tilde{Y}_i = \tilde{Q}_i\tilde{R}_i$.
- Form $Y_i = A\widetilde{Q}_i$ and compute its QR factorization $Y_i = Q_iR_i$. 6 end
- $Q = Q_a$.

Serial R

```
randSVD \leftarrow function(A, k, g=3)
2
3
        ## Stage A
4
        Omega <- matrix(rnorm(n*2*k),
5
                   nrow=n. ncol=2*k)
6
        Y <- A %*% Omega
        Q \leftarrow qr.Q(qr(Y))
8
         At \leftarrow t(A)
9
         for(i in 1:q)
10
              Y <- At %*% O
11
12
             Q \leftarrow qr.Q(qr(Y))
             Y <- A %*% Q
13
             Q \leftarrow ar.Q(ar(Y))
14
15
16
17
        ## Stage B
        B <- t(Q) %*% A
18
19
        U <- La.svd(B)$u
20
        U <- Q %*% U
21
        U[, 1:k]
22
```

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¹Halko 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

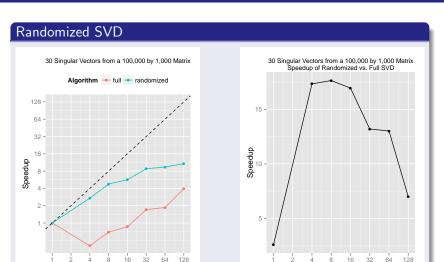
Serial R

```
randSVD \leftarrow function(A, k, q=3)
 2
 3
         ## Stage A
 4
         Omega <- matrix(rnorm(n*2*k),
                nrow=n. ncol=2*k)
6
         Y <- A %*% Omega
         Q \leftarrow qr.Q(qr(Y))
8
         At \leftarrow t(A)
9
         for(i in 1:q)
10
11
              Y <- At %*% Q
             Q \leftarrow qr.Q(qr(Y))
12
13
              Y <- A %*% Q
14
             Q \leftarrow qr.Q(qr(Y))
15
16
17
         ## Stage B
18
         B <- t(Q) %*% A
19
         U <- La.svd(B)$u
20
         U <- Q %*% U
21
         U[, 1:k]
22
```

Parallel pbdR

```
randSVD \leftarrow function(A, k, q=3)
 3
        ## Stage A
         Omega <- ddmatrix("rnorm",
                nrow=n. ncol=2*k)
         Y <- A %*% Omega
        Q \leftarrow qr.Q(qr(Y))
         At \leftarrow t(A)
         for(i in 1:q)
10
11
              Y <- At %*% Q
              Q \leftarrow qr.Q(qr(Y))
12
13
              Y <- A %*% Q
14
              Q \leftarrow qr.Q(qr(Y))
15
16
17
         ## Stage B
18
         B <- t(Q) %*% A
19
         U <- La.svd(B)$u</p>
20
         U <- Q %*% U
21
         U[, 1:k]
22
```





Cores

Cores