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Parallel Computation in R: What We Want, and How We (Might) Get It

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> Keynote Address useR! 2017 Brussels, 6 July, 2017

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Shameless Promotion

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Shameless Promotion

Texts in Statistical Science

Statistical Regression and Classification From Linear Models to



Out July 28!

(A longheld plan — decades — now finally got around to it.)

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Disclaimer

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Disclaimer

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• "Everyone has an opinion."

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Parallel Computation in R: What We Want, and How We (Might) Get It

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- I'll present mine.

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- Dissent is encouraged. :-)

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The Drivers and Their Result

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The Drivers and Their Result

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• Parallel hardware for the masses:

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The Drivers and Their Result

- Parallel hardware for the masses:
 - 4 cores standard, 16 not too expensive

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 - Intel Xeon Phi, \approx 60 cores (!), coprocessor, as low as a few hundred dollars

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• Big Data

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- Big Data
 - Whatever that is.

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Result: Users believe,

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Result: Users believe,

"I've got the hardware and I've got the data need so I should be all set to do parallel computation in R on the data."

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Not So Simple

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Not So Simple

• Non-"embarrassingly parallel" algorithms.

Parallel Computation in R: What We Want, and How We (Might) Get It

- Non- "embarrassingly parallel" algorithms.
- Overhead issues:

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- Non-"embarrassingly parallel" algorithms.
- Overhead issues:
 - Contention for memory/network.

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Parallel Computation

in R: What We Want, and How We

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 - OS/R limits on number of sockets (network connections).

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 - Contention for I/O ports.
 - OS/R limits on number of sockets (network connections).
 - Serialization.

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Wish List

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Wish List

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• Ability to run on various types of hardware — from R.

Wish List

Parallel Computation in R: What We Want, and How We (Might) Get It

- Ability to run on various types of hardware from R.
- Ease of use for the non-cognoscenti.

Wish List

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Parallel Computation in R: What We Want, and How We (Might) Get It

- Ability to run on various types of hardware from R.
- Ease of use for the non-cognoscenti.
- Parameters to tweak for the experts or the daring.

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The Non-cognoscenti Can Become the Daring

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The Non-cognoscenti Can Become the Daring

Help, I'm in over my head here! – a prominent R developer, entering the parallel comp. world.

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Non-cognoscenti (cont'd.)

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Non-cognoscenti (cont'd.)

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• Casual users, even if they are deft programmers, quickly learn that this is no casual operation.

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Non-cognoscenti (cont'd.)

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- After getting burned by disappointing performance, some will be emboldened to learn the subtleties.

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• Painless parallel computation is not possible.

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Example: Matrix-Vector Multiplication

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Example: Matrix-Vector Multiplication

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• D = AX, with A being $n \times p$ and X being $p \times 1$

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Example: Matrix-Vector Multiplication

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for (i in 1:n)
d[i] \leftarrow a[i,] %*% x
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Example: Matrix-Vector Multiplication

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 Naive use of **foreach** package likely quite slow; scatter-gather overhead a substantial proportion of the overall time.

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Example (cont'd.)

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Example (cont'd.)

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• Solution is obvious:

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Example (cont'd.)

 Solution is obvious: For r processes, partition rows A_i into n/r chunks and change the above loop from n iterations to n/r.

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```
for (k in 1:r)
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Example (cont'd.)

 Solution is obvious: For r processes, partition rows A_i into n/r chunks and change the above loop from n iterations to n/r.

```
for (k in 1:r)
    d[rowblockk] ← a[rowblockk,] %*% x
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• But casual users may miss this.

Example (cont'd.)

in R: What We Want, and How We (Might) Get It

Parallel Computation

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• Solution is obvious: For *r* processes, partition rows *A_i* into *n/r* chunks and change the above loop from *n* iterations to *n/r*.

```
for (k in 1:r)
    d[rowblockk] ← a[rowblockk,] %*% x
```

• But casual users may miss this. And automatic parallelization would miss it.

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Use Cases

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Use Cases

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A few reference examples, somewhat spanning the space:

• Compute-intensive parametric: Quantile regression.

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- Compute-intensive parametric: Quantile regression.
- Compute-intensive nonparametric: Nearest-neighbor regression.

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- Compute-intensive parametric: Quantile regression.
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- Compute-intensive nonparametric: Graph algorithms.

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- Compute-intensive parametric: Quantile regression.
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- Compute-intensive nonparametric: Graph algorithms.
- Run-of-the-mill aggregation: Group-by-and-find-means op.

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- Compute-intensive parametric: Quantile regression.
- Compute-intensive nonparametric: Nearest-neighbor regression.
- Compute-intensive nonparametric: Graph algorithms.
- Run-of-the-mill aggregation: Group-by-and-find-means op.
- Tougher aggregation: Credit card fraud detection.

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Software Alchemy (SA)

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• My term for method developed by a number of authors (Matloff, 2016).

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Software Alchemy (SA)

- My term for method developed by a number of authors (Matloff, 2016).
- Break data into chunks. Apply estimator, say Im() to each chunk, then average the results.

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- For parallel comp. with *r* processes, use *r* chunks.

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- Break data into chunks. Apply estimator, say **Im()** to each chunk, then average the results.
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- Same statistical accuracy.

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- Useful in some apps.
- Available in **partools** package (NM, C. Fitzgerald), **github.com/matloff**.

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Programming World Views

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Programming World Views

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 Message passing/distributed comp.: Send data to the R processes; each process works on its data; possibly combine results.

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In R, e.g. parallel (the part from snow), rMPI.

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In R, e.g. parallel (the part from snow), rMPI.

In C, e.g.



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World Views (cont'd.)

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World Views (cont'd.)

• Shared-memory: The processes have access to a common memory, so no data transfer needed.

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World Views (cont'd.)

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Not (yet) common in R, but do have \mathbf{Rdsm} (NM), thread (R. Bartnik).

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Premises in This Talk

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• There is a lot of hype about parallel computation.

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- Efficient automatic parallelization —

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 - Aggregation is only part of what useRs do.
 - We need iterative estimators, std. errors, linear algebra, etc.
 - Newer methodology, e.g. ML, random graphs etc.
 - UseRs may have become fairly good programmers, but lack systems knowledge.

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Premises (cont'd).

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Premises (cont'd).

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• Use of SA as means of parallelization should be fine for things like linear models, quantile regression, k-nearest neighbor regression etc.

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Premises (cont'd).

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- But in most of the Use Cases, including the SA ones, distributed world view works well,

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- Bottom line: For most Use Cases, use one of the following

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 - SA
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Premises (cont'd).

- Use of SA as means of parallelization should be fine for things like linear models, quantile regression, k-nearest neighbor regression etc.
- Some apps, e.g. graph algorithms, are based on sharing state, so shared-memory world view/hardware may be needed.
- But in most of the Use Cases, including the SA ones, distributed world view works well, and may be needed anyway at very large scale.
- Bottom line: For most Use Cases, use one of the following
 - SA
 - Distributed computation, esp. using "Leave it there" concept.

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Spark

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Parallel Computation in R: What We Want, and How We (Might) Get It

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One well-publicized distributed approach today is Spark/SparkR.

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• MapReduce not well-suited to most of the above Use Cases.

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- MapReduce not well-suited to most of the above Use Cases.
- Highly elaborate Spark machinery violates the transparency requirement.

Parallel Computation in R: What We Want, and How We (Might) Get It

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One well-publicized distributed approach today is Spark/SparkR.

- MapReduce not well-suited to most of the above Use Cases.
- Highly elaborate Spark machinery violates the transparency requirement.
- On the other hand, the distributed file system approach of Hadoop/Spark is good for useRs too.

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Example Study: I

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How We (Might) Get It Norm Matloff University of California at

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Parallel Computation

in R: What We Want, and

> • (Gittens et al, 2016). Matrix Factorizations at Scale: a Comparison of Scientific Data Analytics in Spark and C+MPI Using Three Case Studies

 (Gittens et al, 2016). Matrix Factorizations at Scale: a Comparison of Scientific Data Analytics in Spark and C+MPI Using Three Case Studies In spite of careful optimization, performance of Spark ranged from slightly slower to really, really slower. :-)

Parallel Computation

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Computation in R: What We Want, and How We (Might) Get It

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 (Gittens et al, 2016). Matrix Factorizations at Scale: a Comparison of Scientific Data Analytics in Spark and C+MPI Using Three Case Studies
 In spite of careful optimization, performance of Spark ranged from slightly slower to really, really slower. :-) Just not what Spark was designed for.

My personal side comment: Not clear whether, say, PCA, has much accuracy or usefulness at the truly Big Data scale, including for sparse matrices.

Computation in R: What We Want, and How We (Might) Get It

Parallel

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Example Study: II

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Example Study: II

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Reyes-Ortiz et al, Big Data Analytics in the Cloud: Spark on Hadoop vs MPI/OpenMP on Beowulf

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Abstract:

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Abstract:

...MPI/OpenMP outperforms Spark by more than one order of magnitude in terms of processing speed and provides more consistent performance. However, Spark shows better data management infrastructure and the possibility of dealing with other aspects such as node failure and data replication

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Abstract:

...MPI/OpenMP outperforms Spark by more than one order of magnitude in terms of processing speed and provides more consistent performance. However, Spark shows better data management infrastructure and the possibility of dealing with other aspects such as node failure and data replication

I contend that very few useRs, even those who need parallel computation, need to guard against node failure.

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The Principle of "Leave It There"

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The Principle of "Leave It There"

Extremely simple idea, but very powerful.

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The Principle of "Leave It There"

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• Common setting (e.g. parallel package): Scatter/gather.

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The Principle of "Leave It There"

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 - (a) Manager node partitions (scatters) data to worker nodes.

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(b) Worker nodes work on their chunks.

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- (c) Manager collects (gathers) and combines the results.

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The Principle of "Leave It There"

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 - (a) Manager node partitions (scatters) data to worker nodes.

- (b) Worker nodes work on their chunks.
- (c) Manager collects (gathers) and combines the results.
- But NO, avoid step (c) as much as possible.

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Example of "Leave It There"

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Example of "Leave It There"

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Say we wish to perform the following on some dataset:

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Example of "Leave It There"

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Say we wish to perform the following on some dataset:

- Convert categorical variables to dummies.
- Replace NA values by means. (Not great, but just an example.)
- Remove outliers, as def. by $|X \mu| > 3\sigma$. (Just an example.)
- Run linear regression analysis.

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Example of "Leave It There"

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- Remove outliers, as def. by $|X \mu| > 3\sigma$. (Just an example.)
- Run linear regression analysis.

The point is to NOT do the gather op after each of the above steps. Leave the data there (in distributed form).

Note too: The last step can be done in parallel too, with SA.

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Comparing Just a Few Packages

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Comparing Just a Few Packages

A few packages that facilitate the above approach:

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Comparing Just a Few Packages

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A few packages that facilitate the above approach:

pkg	flexibility	high-level ops
partools	high	few
ddR	medium	medium
multidplyr	low	more

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Going One Step Further: Distributed Files

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Going One Step Further: Distributed Files

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• Since will do "Leave it there" over many ops,

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Going One Step Further: Distributed Files

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- Since will do "Leave it there" over many ops,
- might as well distribute a persistent version of the data, i.e. have **distributed files.**

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Going One Step Further: Distributed Files

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- Since will do "Leave it there" over many ops,
- might as well distribute a persistent version of the data, i.e. have **distributed files.**
- Like Hadoop/Spark, but without the complex machinery.

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Going One Step Further: Distributed Files

- Since will do "Leave it there" over many ops,
- might as well distribute a persistent version of the data, i.e. have **distributed files.**
- Like Hadoop/Spark, but without the complex machinery.
- Our partools package includes various functions for managing distributed files

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Distributed Files in partools

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Distributed Files in partools

- File x spread across x.001, x.002 etc.
- filesplit(): Make distributed file from monolithic one.
- fileread(): If node i does fileread(x,d), then x.i will be read into the variable d.

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- filesave(): Saves distributed data to distributed file.
- Etc.

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Partools Example of "Leave It There"

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Partools Example of "Leave It There"

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• Say have distributed file **xy**, physically stored in files **xy.001**, **xy.002** etc.

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Partools Example of "Leave It There"

- Say have distributed file **xy**, physically stored in files **xy.001**, **xy.002** etc.
- Say we have written functions (not shown) **NAtoMean** and **deleteOuts**, to handle missing values and remove outliers, as mentioned before. The functions have been given to the workers

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"Leave It There" Example (cont'd.)

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"Leave It There" Example (cont'd.)

use Software Alchemy to perform linear regression, # returning just the coefficients in this case $calm(cls, 'y \sim ., data=xy')$ \$tht

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What Is Happening

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What Is Happening

E.g.

 $\mathsf{clusterEvalQ}(\mathsf{cls}, xy \leftarrow \mathsf{apply}(xy, 2, \mathsf{NAtoMean}))$

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E.g.

clusterEvalQ(cls, xy ← apply(xy, 2, NAtoMean))

What Is Happening

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We are saying, At each worker node, do

 $xy \leftarrow apply(xy, 2, NAtoMean))$

which means, each node does the **apply** op *on its portion of* **xy**.

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"Leave It There" Example (cont'd.)

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The key point:

"Leave It There" Example (cont'd.)

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"Leave It There" Example (cont'd.)

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The key point:

For typical data analysis, hopefully we have:

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"Leave It There" Example (cont'd.)

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The key point:

For typical data analysis, hopefully we have:

• Data file stored in distributed fashion.

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"Leave It There" Example (cont'd.)

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The key point:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:

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"Leave It There" Example (cont'd.)

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The key point:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:
 - Parallel.

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"Leave It There" Example (cont'd.)

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The key point:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:
 - Parallel.
 - No network delay.

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"Leave It There" Example (cont'd.)

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The key point:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:
 - Parallel.
 - No network delay.
 - No serialization overhead.

Norm Matloff University of California at Davis "Leave It There" Example (cont'd.)

The key point:

For typical data analysis, hopefully we have:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:
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- Have occasional "collect" ops, hopefully small in size, e.g. from an aggregation such as colMeans.

Norm Matloff University of California at Davis "Leave It There" Example (cont'd.)

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• If change data or create new data, save in distributed file form too!

Norm Matloff University of California at Davis "Leave It There" Example (cont'd.)

The key point:

- Data file stored in distributed fashion.
- Lots of "leave it there" ops:
 - Parallel.
 - No network delay.
 - No serialization overhead.
- Have occasional "collect" ops, hopefully small in size, e.g. from an aggregation such as colMeans.
- If change data or create new data, save in distributed file form too! Use partools::filesave.

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Heavy Use of SA

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Heavy Use of SA

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• Have SA forms of

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Heavy Use of SA

- Have SA forms of
 - Im()/gIm()

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Heavy Use of SA

- Have SA forms of
 - lm()/glm()
 - k-NN

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Heavy Use of SA

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 - random forests

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Heavy Use of SA

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- Have SA forms of
 - Im()/gIm()
 - k-NN
 - random forests
 - PCA
 - quantile()
- Very easy to make your own SA functions.

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Various Collection Ops

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Various Collection Ops

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E.g. addlists().

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Various Collection Ops

E.g. addlists().

Say have distributed list, 2 compoments. From one, manager node receives

list (a=3,b=8)

and from the other

list(a=5,b=1,c=12)

The functions "adds" them, producing (non-distributed)

list(a=8,b=9,c=12)

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Conclusions

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No "silver bullet."

Conclusions

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Conclusions

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No "silver bullet." But the following should go a long way toward your need for parallel computation.

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Parallel Computation in R: What We Want, and How We (Might) Get It

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No "silver bullet." But the following should go a long way toward your need for parallel computation.

- SA for the computational stuff.
- For aggregation, "leave it there" and distributed files.

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Parallel Computation in R: What We Want, and How We (Might) Get It

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No "silver bullet." But the following should go a long way toward your need for parallel computation.

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- For aggregation, "leave it there" and distributed files.
- Could do in other packages, not just partools.

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Ready for the dissent. :-)