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

Norm Matloff
University of California at Davis

Keynote Address
useR! 2017
Brussels, 6 July, 2017
Shameless Promotion
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Out July 28!

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

“Everyone has an opinion.”

I’ll present mine.

I will essentially propose general design patterns, illustrated with our own package partools but meant to be general.

Dissent is encouraged. :-)

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  - 4 cores standard, 16 not too expensive
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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.”
Not So Simple

• Non-"embarrassingly parallel" algorithms.
• Overhead issues:
  • Contention for memory/network.
  • Bandwidth limits — CPU/memory, CPU/network, CPU/GPU.
  • Cache coherency problems (inconsistent caches in multicore systems).
  • 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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- Ease of use for the non-cognoscenti.
- Parameters to tweak for the experts or the daring.
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- After getting burned by disappointing performance, some will be emboldened to learn the subtleties.
- Painless parallel computation is not possible.
Example: Matrix-Vector Multiplication

\[ \mathbf{D} = \mathbf{A} \mathbf{X}, \text{ with } \mathbf{A} \text{ being } n \times p \text{ and } \mathbf{X} \text{ being } p \times 1 \]

- Naive approach: Parallelize the loop

\[ \text{for } (i \in 1:n) \]
\[ d[i] \leftarrow a[i,] \times x \]

- Naive use of \texttt{foreach} package likely quite slow; scatter-gather overhead a substantial proportion of the overall time.
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Example (cont’d.)

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

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Use Cases

A few reference examples, somewhat spanning the space:

• 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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- Available in partools package (NM, C. Fitzgerald), github.com/matloff.
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Programming World Views

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

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

In C, e.g.
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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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Not (yet) common in R, but do have \texttt{Rdsm} (NM), \texttt{thread} (R. Bartnik).
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In C, e.g.

OpenMP

CUDA
Premises in This Talk

• There is a lot of hype about parallel computation.
• Parallel computation is not for the casual user.
• Efficient automatic parallelization — no user intervention/sophistication needed — is generally not possible and should not be expected. Please stop asking for it. :-)
• As in politics, transparency in software tools is vital. :-)
• What do those APIs really do?
• UseRs are different from aggregation-oriented (e.g. Spark) users.
• 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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  - UseRs may have become fairly good programmers, but lack systems knowledge.
• 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

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

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

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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  (b) Worker nodes work on their chunks.
  (c) Manager collects (gathers) and combines the results.

- But NO, avoid step (c) as much as possible.
Example of “Leave It There”

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 defined by $|X - \mu| > 3\sigma$. (Just an example.)
- Run linear regression analysis.

The point is to NOT do the gather operation 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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- Replace NA values by means. (Not great, but just an example.)
- Remove outliers, as def. by $|X - \mu| > 3\sigma$. (Just an example.)
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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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<table>
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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.
- Our **partools** package includes various functions for managing distributed files
Distributed Files in `partools`

- `filesplit()`: Make distributed file from monolithic one.
- `fileread()`: If node $i$ does `fileread(x,d)`, then $x.i$ will be read into the variable $d$.
- `filesave()`: Saves distributed data to distributed file.
- Etc.
Distributed Files in partools

- File x spread across x.001, x.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.
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.
“Leave It There” Example (cont’d.)
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```
# do NA removal at each worker,
# on the worker’s chunk of xy
clusterEvalQ(cls, xy ← apply(xy, 2, NAtoMean))
# do the outlier removal at each worker,
# on the worker’s chunk of xy
clusterEvalQ(cls, xy ← apply(xy, 2, deleteOuts))

# use Software Alchemy to perform linear regression,
# returning just the coefficients in this case
calm(cls,'y ~ ., data=xy')$ttht
```
What Is Happening

c\textit{l} u s t e r\ E v a l\ Q (c l s, xy ← apply(xy, 2, NAtoMean))

We are saying, At each worker node, do xy ← apply(xy, 2, NAtoMean) which means, each node does the apply op on its portion of xy.
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- **If change data or create new data, save in distributed file form too! Use partools::filesave.**
Heavy Use of SA

Norm Matloff
University of California at Davis
Heavy Use of SA

- Have SA forms of
  - lm()
  - glm()
  - k-NN
  - random forests
  - PCA
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- Very easy to make your own SA functions.
Various Collection Ops
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E.g. addlists().
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E.g. `addlists()`.
Say have distributed list, 2 components. From one, manager node receives

\[
\text{list}(a=3,b=8)
\]

and from the other

\[
\text{list}(a=5,b=1,c=12)
\]

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

\[
\text{list}(a=8,b=9,c=12)
\]
Conclusions

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.
• Could do in other packages, not just partools.

Ready for the dissent. :-(
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