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

Norm Matloff
University of California at Davis

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Out July 28!

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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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The Drivers and Their Result

Parallel hardware for the masses:
- 4 cores standard, 16 not too expensive
- GPUs
- Intel Xeon Phi, \approx 60 cores (!), coprocessor, as low as a few hundred dollars

Big Data
- Whatever that is.

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

• 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

• 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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• After getting burned by disappointing performance, some will be emboldened to learn the subtleties.
• Painless parallel computation is not possible.
Example: Matrix-Vector Multiplication
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  d[i] <- a[i,] %*% x
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• Naive use of `foreach` package likely quite slow; scatter-gather overhead a substantial proportion of the overall time.
Example (cont’d.)
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- But casual users may miss this. And automatic parallelization would miss it.
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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Software Alchemy (SA)

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

• Break data into chunks. Apply estimator, say `lm()` to each chunk, then average the results.

• For parallel comp. with \( r \) processes, use \( r \) chunks.

• Same statistical accuracy.

• Often produces superlinear speedup, i.e. \( > r \).

• Useful in some apps.

• Available in `partools` package (NM, C. Fitzgerald), github.com/matloff.
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In C, e.g.
World Views (cont’d.)
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In C, e.g.
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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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

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  • Distributed computation, esp. using “Leave it there” concept.
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- SA
- Distributed computation, esp. using “Leave it there” concept.
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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In spite of careful optimization, performance of Spark ranged from slightly slower to really, really slower. :-)

My personal side comment: Not clear whether, say, PCA, has much accuracy or usefulness at the truly Big Data scale, including for sparse matrices.
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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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Reyes-Ortiz et al., Big Data Analytics in the Cloud: Spark on Hadoop vs MPI/OpenMP on Beowulf

Abstract: ...

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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.
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 defined 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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- 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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Note too: The last step can be done in parallel too, with SA.
Comparing Just a Few Packages
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A few packages that facilitate the above approach:
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<table>
<thead>
<tr>
<th>pkg</th>
<th>flexibility</th>
<th>high-level ops</th>
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<tr>
<td>partools</td>
<td>high</td>
<td>few</td>
</tr>
<tr>
<td>ddR</td>
<td>medium</td>
<td>medium</td>
</tr>
<tr>
<td>multidplyr</td>
<td>low</td>
<td>more</td>
</tr>
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- 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
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- 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.
- `filesave()`: Saves distributed data to distributed file.
- Etc.
Partools Example of "Leave It There"
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- Say have distributed file \texttt{xy}, physically stored in files \texttt{xy.001}, \texttt{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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```r
# 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')$tht
```
What Is Happening

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We are saying, At each worker node, do
xy ← apply( xy , 2 , NAtoMean) )
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“Leave It There” Example (cont’d.)

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- Lots of “leave it there” ops:

Use `partools::filesave`. 
“Leave It There” Example (cont’d.)

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  - Parallel.
“Leave It There” Example (cont’d.)

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“Leave It There” Example (cont’d.)

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- Very easy to make your own SA functions.
Various Collection Ops
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E.g. `addlists()`.
Various Collection Ops

E.g. \texttt{addlists()}. Say have distributed list, 2 components. From one, manager node receives

\begin{verbatim}
list (a=3, b=8)
\end{verbatim}

and from the other

\begin{verbatim}
list (a=5, b=1, c=12)
\end{verbatim}

The functions “adds” them, producing (non-distributed)

\begin{verbatim}
list (a=8, b=9, c=12)
\end{verbatim}
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.

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