partools: a Sensible Package for Large Data Sets

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With the advent of Big Data, the Hadoop framework has become ubiquitous. Yet it was clear from the start that Hadoop had major shortcomings, and recently these are being much more seriously discussed.¹ This has resulted in a new platform, Spark, gaining popularity. As with Hadoop, there is an R interface available for Spark, named SparkR.

Spark overcomes one of Hadoop's major problems, which is the lack of ability to cache data in a multi-pass computation. However, Spark unfortunately retains the drawbacks of Hadoop:

- Hadoop/Spark have a complex, rather opaque infrastructure, and rely on Java/Scala. This
 makes them difficult to install, configure and use for those who are not computer systems
 experts.
- For a variety of reasons, even SparkR can be considerably slower than Plain Old R (POR).
- Although a major plus for Hadoop/Spark is fault tolerance, it is needed only for users working on extremely large clusters, consisting of hundreds or thousands of nodes. Disk failure rates are simply too low for fault tolerance to be an issue for many Hadoop/Snow users, who do not have such large systems.²

The one firm advantage of Hadoop/Spark is their use of distributed file systems. Under the philosophy, "Move the computation to the data, rather than *vice versa*," network traffic may be greatly reduced, thus speeding up computation. In addition, their approach helps deal with the fact that Big Data sets may not fit into the memory of a single machine.

Therefore:

It is desirable to have a package that retains the distributed-file nature of Hadoop/Spark while staying fully within the simple, familiar, yet powerful POR framework.

The partools package is designed to meet these goals. It is intended as a simple, sensible POR alternative to Hadoop/Spark. Though not necessarily appropriate for all settings, for many R programmers, partools may be a much better choice than Hadoop/Snow.

 $^{^1{\}rm See}$ for example "The Hadoop Honeymoon is Over," https://www.linkedin.com/pulse/hadoop-honeymoon-over-martyn-jones

²https://wiki.apache.org/hadoop/PoweredBy

Since **partools** uses the portion of the R **parallel** package derived from the package **snow**, and because it is meant as an alternative to Hadoop, we informally refer to **partools** as Snowdoop.

The package does not provide fault tolerance of its own. If this is an issue, one can provide it externally, say with the XtreemFS system.

1 Where Is the Magic?

As you will see later, **partools** can deliver some impressive speedups. But there is nothing magical about this. Instead, the value of the package stems from just two simple sources:

- (a) The package follows a Keep It Distributed philosophy: Form distributed objects and keep using them in distributed form throughout one's R session, accessing them repeatedly for one's various desired operations.
- (b) The package consists of a number of utility functions that greatly facilitate creating, storing and *analyzing* distributed objects, both in memory and on disk.

2 Overview of the partools Package

The package is based on the following very simple principles, involving distributed files and distributed data frames/matrices. We'll refer to nondistributed files and data frames/matrices as monolithic.

- Files are stored in a distributed manner, in files with a common basename. For example, the file **x** is stored as separate files **x.01**, **x.02** etc.
- Data frames and matrices are stored in memory at the nodes in a distributed manner, with a common name. For example, the data frame **y** is stored in chunks at the cluster nodes, each chunk known as **y** at its node.

2.1 Package Structure

Again, in a distributed file, all the file chunks have the same prefix, and in a distributed data frame, all chunks have the same name at the various cluster nodes. This plays a key role in the software.

The package consists of three main groups of functions:

2.1.1 Distributed-file functions

- filesplit(): Create a distributed file from monotlithic one.
- filesplitrand(): Create a distributed file from monotlithic one, but randomize the record order.
- filecat(): Create a monotlithic file from distributed one.
- fileread(): Read a distributed file into distributed data frame.

- readnscramble(): Read a distributed file into distributed data frame, but randomize the record order.
- filesave(): Write a distributed data frame to a distributed file.
- filechunkname(): For the calling cluster node, returns the full name of the file chunk, including suffix, e.g. '01', '02' etc.

2.1.2 Tabulative functions

- distribsplit(): Create a distributed data frame/matrix from monotlithic one.
- distribcat(): Create a monotlithic data frame/matrix from distributed one.
- distribagg(): Distributed form of R's aggregate().
- distribcounts(): Wrapper for distribagg() to obtain cell counts.
- dfileagg(): Like distribagg(), but file-based rather than in-memory, in order to handle files that are too big to fit in memory, even on a distributed basis.
- distribgetrows(): Applies an R subset() or similar filtering operation to the distributed object, and collects the results into a single object at the caller.
- distribrange(): Distributed form of R's range().

2.1.3 Statistical functions

These all use the Software Alchemy (SA) method (Parallel Computation for Data Science, N. Matloff, Chapman and Hall, 2015) to parallelize statistical operations.³ The idea is simple: Apply the given estimator to each chunk in the distributed object, and average over chunks. It is proven that the resulting distributed estimator has the same statistical accuracy — the same asymptotic variance — as the original serial one.⁴

- ca(): General SA algorithm.
- cabase(): Core of ca().
- caagg(): SA analog of distribagg().
- cameans(): Finds means in the specified columns.
- caquantile(): Wrapper for SA version of R's quantile().
- calm(): Wrapper for SA version of R's lm().
- caglm(): Wrapper for SA version of R's glm().
- cakm(): Wrapper for SA version of R's kmeans().
- caprcomp(): Wrapper for SA version of R's prcomp().

³More detailed presentation in forthcoming paper in the *Journal of Statistical Software*.

⁴In the world of parallel computation, the standard word for nonparallel is *serial*.

Note that SA requires that the data be i.i.d. If your data was stored in some sorted order — in the flight date below, it was sorted by date — you need to randomize it first, using one of the functions provided by **partools** for this purpose.

2.1.4 Support functions

- formrowchunks(): Form chunks of rows of a data frame/matrix.
- matrixtolist(): For a list of the rows or columns of a data frame or matrix.
- addlists(): "Add" two lists, meaning add values of elements of the same name, and copy the others.
- dbs(), dbsmsg(), etc.: Debugging aids.

3 Sample Session

Our data set, from http://stat-computing.org/dataexpo/2009/the-data.html consists of the well-known records of airline flight delay. For convenience, we'll just use the data for 2008, which consists of about 7 million records. This is large enough to illustrate speedup due to parallelism, but small enough that we won't have to wait really long amounts of time in our sample session here.

The session was run on a 16-core machine, with a 16-node **parallel** cluster. Note carefully, though, that we should not expect a 16-fold speedup. In the world of parallel computation, one usually gets of speedups of considerably less than n for a platform of n computational entities, in this case with n = 16. Indeed, one is often saddened to find that the parallel version is actually *slower* than the serial one!

The file, yr2008, was first split into a distributed file, stored in yr2008r.01,...,yr2008r.16, using filesplitrand(), and then read into memory at the 16 cluster nodes using fileread():

```
> filesplitrand(cls,'yr2008','yr2008r',2,header=TRUE,sep=",")
> fileread(cls,'yr2008r','yr2008',2,header=TRUE, sep=",")
```

The call to **filesplitrand()** splits the file as described above; since these files are permanent, we can skip this step in future R sessions involving this data (if the file doesn't change). The function **filesplitrand()** was used instead of **filesplit()** to construct the distributed file, in order to randomize the placement of the records of **yr2008** across cluster nodes. As noted earlier, random arrangement of the rows is required for SA.

In order to run timing comparisons, the full file was also read into memory at the cluster manager:

```
> yr2008 <- read.csv("yr2008")
```

The first operation run involved the package's distributed version of R's **aggregate()**. Here we want to tabulate departure delay, arrival delay and flight time, broken down into cells according to flight origin and destination. We'll find the maximum value in each cell.

```
> system.time(print(distribagg(cls, c("DepDelay","ArrDelay","AirTime"),
   c("Origin", "Dest"), "yr2008", FUN="max")))
5193
        CDV
             YAK
                        327
                                 325
                                           54
                                           77
5194
         JNU
              YAK
                        317
                                 308
        SLC
              YKM
                        110
                                 118
                                          115
5195
        IPL
              YUM
                        162
                                           26
5196
                                 163
         system elapsed
   user
  2.291
          0.084
                 15.952
```

The serial version was much slower.

0.444 249.634

249.038

```
> system.time(print(aggregate(cbind(DepDelay,ArrDelay,AirTime) ~
   Origin+Dest,data=yr2008,FUN=max)))
5193
        CDV
             YAK
                        327
                                 325
                                           54
        JNU
              YAK
                        317
                                 308
                                           77
5194
5195
        SLC
              YKM
                        110
                                 118
                                          115
        IPL
              YUM
                        162
                                 163
                                           26
5196
         system elapsed
   user
```

So, the results of **distribagg()** did indeed match those of **aggregate()**, but did so more than 15 times faster!

Remember, the Keep It Distributed philosophy of **partools** is to create distributed objects and then keep using them repeatedly in distributed form. However, in some cases, we may wish to collect a distributed result into a monolithic object, especially if the result is small. This is done in the next example:

Say we wish to do a filter operation, extracting the data on all the Sunday evening flights, and collect it into one place. Here is the direct version:

```
> sundayeve <- with(yr2008,yr2008[DayOfWeek==1 & DepTime > 1800,])
```

This actually is not a time-consuming operation, but again, in typical **partools** use, we would only have the distributed version of **yr2008**. Here is how we would achieve the same effect from the distributed object:

```
> sundayeved <- distribgetrows(cls,'with(yr2008,yr2008[DayOfWeek==1 & DepTime > 1800,])')
```

What **distribgetrows()** does is produce a data frame at each cluster node, per the user's instructions, then combine them together at the caller via R's **rbind()**. A simple concept, yet quite versatile.

As another example, say we are investigating data completeness. We may wish to flag all records having an inordinate number of NA values. As I first step, we may wish to add a column to our data frame, indicating how many NA values there are in each row. If we did not have the advantage of distributed computation, here is how long it would take for our flight delay data:

```
> sumna <- function(x) sum(is.na(x))
> system.time(yr2008$n1 <- apply(yr2008[,c(5,7,8,11:16,19:21)],1,sumna))
   user   system elapsed
268.463   0.773 269.542</pre>
```

But it is of course much faster on a distributed basis, using the **parallel** package function **clusterEvalQ()**:

```
> clusterExport(cls,"sumna",envir=environment())
> system.time(clusterEvalQ(cls,yr2008$n1 <- apply(yr2008[,c(5,7,8,11:16,19:21)],1,sumna)))
   user   system elapsed
   0.094   0.012   16.758</pre>
```

The speedup here was about 16, fully utilizing all 16 cores.

Ordinarily, we would continue that NA analysis on a distributed basis, in accord with the **partools** Keep It Distributed philosophy of setting up distributed objects and then repeatedly dealing with them on a distributed basis. If our subsequent operations continue to have time complexity linear in the number of records processes, we should continue to get speedups of about 16.

On the other hand, we may wish to gather together all the records have 8 or more NA values. In the nonparallel context, it would take some time:

```
> system.time(na8 <- yr2008[yr2008$n1 > 7,])
  user system elapsed
9.292  0.028  9.327
```

In the distributed manner, it is slightly faster:

```
> system.time(na8d <- distribgetrows(cls,'yr2008[yr2008$n1 > 7,]'))
  user system elapsed
5.524  0.160  6.584
```

The speedup is less here, as the resulting data must travel from the cluster nodes to the cluster manager. In our case here, this is just a memory-to-memory transfer rather than across a network, as we are on a multicore machine, but it still takes time. If the number of records satisfying the filtering condition had been smaller than the 136246 we had here, the speedup factor would have been greater.

Now let's turn to statistical operations, starting of course with linear regression. As noted, these **partools** functions make use of Software Alchemy, which replaces the given operation by a *distributed*, statistically equivalent operation. This will often produce a significant speedup. Note again that though the result may different from the non-distributed version, say in the third significant digit, it is just as accurate statistically.

In the flight data, we predicted the arrival delay from the departure delay and distance, comparing the distributed and serial versions,

```
> system.time(print(lm(ArrDelay ~ DepDelay+Distance,data=yr2008)))
```

Coefficients: (Intercept) DepDelay Distance -1.061369 1.019154 -0.001213user system elapsed 77.107 12.463 76.225 > system.time(print(calm(cls,'ArrDelay ~ DepDelay+Distance,data=yr2008')\$tht)) (Intercept) DepDelay Distance -1.061262941 1.019150592 -0.001213252 user system elapsed 13.414 0.691 18.396

Linear regression is very hard to parallelize, so the speedup factor of more than 4 here is nice. Coefficient estimates were virtually identical.

Next, principal components. Since R's **prcomp()** does not handle NA values for nonformula specifications, let's do that separately first:

```
> system.time(cc <- na.omit(yr2008[,c(12:16,19:21)]))
   user system elapsed
9.540   0.351   9.907
> system.time(clusterEvalQ(cls,cc <- na.omit(yr2008[,c(12:16,19:21)])))
   user system elapsed
0.885   0.232   2.352</pre>
```

Note that this too was faster in the distributed approach, though both times were small. And now the PCA runs:

```
> system.time(ccout <- prcomp(cc))
   user system elapsed
61.905  49.605  58.444
> ccout$sdev
[1] 5.752546e+02 5.155227e+01 2.383117e+01 1.279210e+01 9.492825e+00
[6] 5.530152e+00 1.133015e-03 6.626621e-12
> system.time(ccoutdistr <- caprcomp(cls,'cc',8))
   user system elapsed
  5.023   0.604  8.949
> ccoutdistr$sdev
[1] 5.752554e+02 5.155127e+01 2.383122e+01 1.279184e+01 9.492570e+00
[6] 5.529869e+00 9.933142e-04 8.679427e-13
```

Thus, more than a 6-fold speedup here. Agreement of the component standard deviations is good.

Next, let's find the *interquartile range* for several columns. This is a robust measure of dispersion, defined at the difference between the 75^{th} and 25^{th} percentiles. Here is serial code to find this:

```
# find the interquartile range for a vector x
iqr <- function(x) {tmp <- quantile(x,na.rm=T); tmp[4] - tmp[2]}</pre>
```

find the interquartile range for each column of a data frame dfr
iqrm <- function(dfr) apply(dfr,2,iqr)</pre>

So, let's compare times. First, the serial version:

```
> system.time(print(iqrm(yr2008[,c(5:8,12:16,19:21)])))
          DepTime
                          CRSDepTime
                                                ArrTime
                                                                CRSArrTime
                                                    802
                                                                       792
              800
                                 790
ActualElapsedTime
                      CRSElapsedTime
                                                AirTime
                                                                  ArrDelay
                                   79
                                                      77
               80
                                                                         22
         DepDelay
                            Distance
                                                 TaxiIn
                                                                   TaxiOut
               12
                                 629
                                                       4
                                                                          9
         system elapsed
   user
 29.280
          0.243 29.554
```

For the distributed version,

```
> system.time(print(colMeans(distribgetrows(cls,'iqrm(yr2008[,c(5:8,12:16,19:21)])'))))
          DepTime
                          CRSDepTime
                                                               CRSArrTime
                                                ArrTime
         800.1250
                                                                  791.8750
                            790.0625
                                               801.8125
ActualElapsedTime
                      CRSElapsedTime
                                                AirTime
                                                                  ArrDelay
                                                                   22.0000
          80.0000
                             78.9375
                                                76.5625
                                                                  TaxiOut
         DepDelay
                            Distance
                                                 TaxiIn
                                                 4.0000
          12.0000
                            627.6875
                                                                    9.0000
         system elapsed
   user
  0.009
          0.002
                  2.587
```

Here the speedup was more than 11-fold, with agreement generally to three significant digits. Once again, note that statistically speaking, both estimators have the same accuracy.

The package also includes a distributed version of k-means clustering. Here it is on the flight delay data. First, retain only the NA-free rows for the variables of interest, then run:

```
> fileread(cls,'yr2008r','yr2008',2,header=TRUE, sep=",")
> invisible(clusterEvalQ(cls,y28 <- na.omit(yr2008[,c(5:8,13:16,19:21)])))
> system.time(koutpar <- cakm(cls,'y28',3,11))
    user system elapsed
4.083    0.132    9.293</pre>
```

Compare to serial:

```
> yr2008 <- read.csv('y2008')
> y28 <- na.omit(yr2008[,c(5:8,13:16,19:21)])
> system.time(koutser <- kmeans(y28,3))
    user    system elapsed
54.394    0.558    55.032</pre>
```

So, the distributed version is about 6 times faster. Results are virtually identical:

```
> koutpar$centers
                     [,2]
                              [,3]
                                        [,4]
                                                 [,5]
          [,1]
[1,] 1741.3967 1718.0296 1876.433 1895.435 110.4398
      932.4057
                936.6907 1081.743 1082.813 108.5091
[3,] 1311.2193 1308.1838 1496.267 1525.790 267.8620
                               [,8]
                                          [,9]
                                                  [,10]
          [,6]
                     [,7]
[1,]
      85.25672 13.101844 14.826940
                                     569.2534 6.742315
[2,]
      84.66763
                3.091913
                           4.517502
                                     561.0567 6.785464
                8.668587 11.698193 1886.8964 7.541735
[3,] 238.93152
        [,11]
[1,] 16.71571
[2,] 15.63046
[3,] 18.35916
> koutser$centers
    DepTime CRSDepTime ArrTime CRSArrTime
1 1741.3888
             1718.0217 1876.418
                                   1895.425
 932.3681
              936.6674 1081.737
                                   1082.809
3 1311.4436
             1308.3525 1496.404
                                   1525.905
  CRSElapsedTime
                   AirTime
                             ArrDelay
                                       DepDelay
1
        110.4363
                  85.25292 13.100842 14.826083
2
        108.5151
                  84.67361
                             3.092439
                                        4.518112
3
        267.8669 238.93668
                             8.672439 11.701706
   Distance
              TaxiIn TaxiOut
   569.2226 6.742079 16.71604
   561.1148 6.785409 15.63038
3 1886.9094 7.542760 18.35823
```

4 Dealing with Memory Limitations

The discussion so far has had two implicit assumptions:

- The number of file chunks and the number of (R parallel) cluster nodes are equal, and the latter is equal to the number of physical computing devices one has, e.g. the number of cores in a multicore machine or the number of network nodes in a physical cluster.
- Each file chunk fits into the memory⁵ of the corresponding cluster node.

The first assumption is not very important. If for some reason we have created a distributed file with more chunks than our number of physical computing devices, we can still set up an R parallel cluster with size equal to the number of file chunks. Now more than one R process will run on at least some of the cluster nodes, albeit possibly at the expense of, say, an increase in virtual memory swap operations.

The second assumption is the more pressing one. For this reason, the **partools** package includes functions such as **dfileagg()**. The latter acts similarly to **distribagg()**, but with a key difference: Any given cluster node will read from many chunks of the distributed file, and will process those chunks one at a time, never exceeding memory constraints.

⁵Say, physical memory plus swap space.

Consider again our flight delay data set. As a very simple example, say we have a two-node physical cluster, and that each node has memory enough for only 1/4 of the data. So, we break up the original data file to 4 pieces, **yr2008.1** through **yr2008.4**, and we run, say,

```
> dfileagg(cls,c('yr2008.1','yr2008.2','yr2008.3','yr2008.4'),
         c("DepDelay","ArrDelay","AirTime"),
         c("Origin","Dest"),"yr2008", FUN="max")
```

Our first cluster node will read **yr2008.1** and **yr2008.2**, one at a time, while the second will read **yr2008.3** and **yr2008.4**, again one at a time, At each node, at any given time only 1/4 of the data is in memory, so we don't exceed memory capacity. But they will get us the right answer, and will do so in parallel, roughly with a speedup factor of 2.

More functions like this will be added to **partools**.

5 What About Other R Functions and Packages, say reshape 2/tidyr?

It is easy to apply the **partools** idiom to many R functions that return data frame or matrix values. Consider for instance the **reshape2** function **melt()**. Say we already have a distributed data frame **ddf** at the cluster nodes. We have two choices here:

- In accord with the Keep It Distributed **partools** philosophy, we might simply call **melt()** at each node, say using **clusterEvalQ()**, and keep the result distributed.
- If say we need to gather together the results of a **melt()** operation, we could call **melt()** at each node but then call the **partools** function **distribgetrows()** to collect the molten data into one centralized data frame. A **cast()** operation would requires a bit more care, depending on whether the distributed object crosses subject ID boundaries.