Using xval and clusters of computers for cross-validation

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1 Introduction

Cross-validation and other methods like the bootstrap can be 'embarrassingly parallel'. Embarrassingly parallel means that the same calculation is repeated independently for different data sets. One way to decrease the execution time of embarrassingly parallel computations is to use a cluster of computers. Each node in the cluster performs part of the computation, dividing the execution time by 1 over the number of nodes in the cluster.

This document illustrates how clusters can perform cross-validation calculations, using the xval method from the *MLInterfaces* package. The document starts with a brief overview of what a cluster computation might look like, with some essential details swept 'under the rug'; this is the 'end-user' experience. Delving deeper into the steps required for this experience is the 'R programmer' experience. This section outlines the implementation required (not provided in *MLInterfaces!*) for clustered computing, the likely performance gains, and directions for developing more effective parallelization strategies. The section concludes with a summary of steps taken to make xval more amenable to clustered evaluation; these may be useful guides for exposing other functions to parallelization.

2 Overview – the 'end user' experience

A non-clustered cross-validation might involve the following R commands, taken from the xval documentation examples:

- > library(MLInterfaces)
- > library(golubEsets)
- > smallG <- Golub_Merge[200:250,]

The first three statements load the *MLInterfaces* package and a data set. The next line extracts a portion of the data set for use in the example. We then perform a "leave one out" (LOO) cross-validation, and summarize the results in a table:

```
> lk1 <- MLearn(ALL.AML ~ ., smallG, knnI(k = 1),
+ xvalSpec("LOO"))
> confuMat(lk1)
    predicted
given AML ALL
    ALL 10 37
    AML 15 10
```

A clustered version of the same calculation requires that the user have a computer cluster available for R to use. The cluster has software libraries installed to allow communication between cluster nodes. Common software packages include MPI and PVM. R also requires packages that allow communication between R and the cluster software. Available packages include Rmpi and rpvm; usually one installs the package corresponding to the cluster library available on the system. Both Rmpi and rpvm provide a fairly 'low-level' interface to the clusters. A better starting point adds the package snow as another layer on top of Rmpi or pvm. snow makes it easy to start and stop clusters, and provides a uniform interface to key cluster functions.

Assuming a functioning cluster with appropriate R packages, and with one caveat, the clustered cross-validation might start as before...

```
> library(MLInterfaces)
> library(golubEsets)
> smallG <- Golub_Merge[200:250, ]</pre>
```

Then load *snow*, start the cluster (e.g., with 8 nodes), and load *MLInterfaces* on each node...

```
> library(snow)
> cl <- makeCluster(8, "MPI")
> clusterEvalQ(cl, library(MLInterfaces))
```

Finally, perform the calculation across the cluster... FOR THIS TO WORK WE WILL HAVE TO EXTEND xvalSpec TO DEAL WITH makeCluster OBJECTS.

```
> lk1 <- xval(smallG, "ALL.AML", knnB, xvalMethod = "L00",
+ group = as.integer(0), cluster = cl)
> table(lk1, smallG$ALL.AML)
```

Notice that the only change to the actual xval call is the inclusion of the cluster = cl argument. Easy!

3 Caveats - the 'R programmer' experience

NOTE THAT THIS MATERIAL HAS TO BE UPDATED TO DEAL WITH THE MLearn/learnerSchema ARCHITECTURE THAT PREDATED THIS MATERIAL.

Now the caveat. Someone has to tell xval how to do the calculation in clustered mode. This is the job of the generic function xvalLoop. We'll build up to a workable solution in this section.

Take a peak at the code inside the xval method (e.g., typing getMethods(xval) at the R command prompt). You will see xvalLoop appearing near the top, in a line reading xvalLoop <- xvalLoop(cluster). The function xvalLoop is a generic function, and it is called with the argument cluster. Here's the definition of the default method of xvalLoop function:

```
> setMethod("xvalLoop", signature(cluster = "ANY"),
+ function(cluster, ...) lapply)
```

This code is executed when cluster = NULL (the default, when no cluster argument is provided). By default, then, the xvalLoop function returns the lapply function. The value of the *variable* xvalLoop (i.e., on the left of xvalLoop <- xvalLoop(cluster) is then lapply. A bit confusing, but hopefully not too confusing.

Look further into the xval code. You'll see xvalLoop appearing again, toward the base of the method, as out <- xvalLoop(1:n, xvalidator, ...). Since the value of xvalLoop is lapply, this is the same as out <- lapply(1:n, xvalidator, ...).

We would like our clustered version of xval to behave differently, specifically to use an lapply-like function that takes advantage of the computer cluster. We do this by writing a method of xvalLoop that is specific to our type of cluster. Suppose, as in the example above, we have an MPI cluster created with snow. Some reading of the snow documentation leads to the parLapply function. This behaves just like lapply, but distributes the tasks over cluster nodes. In an ideal world, we would be able to write

```
> setOldClass("spawnedMPIcluster")
> setMethod("xvalLoop", signature(cluster = "spawnedMPIcluster"),
+ function(cluster, ...) parLapply)
```

Suppose we provided the argument cluster = cl to the xval function. After xvalLoop <- xvalLoop(cluster), the value of the variable xvalLoop is par-Lapply. Later in xval, we would execute the equivalent of out <- parLapply(1:n, xvalidator, ...). If only it were that easy!

There are two problems with the approach developed so far. The first is that the arguments of parLapply are different from those of lapply. Specifically, the first argument of parLapply is the cluster.

Here is one solution to this problem. Create a 'wrapper' for parLapply inside the xvalLoop method for spawnedMPIcluster that hides the cluster argument. Return the wrapper function, rather than parLapply:

```
> setOldClass("spawnedMPIcluster")
> setMethod("xvalLoop", signature(cluster = "spawnedMPIcluster"),
+ function(cluster, ...) {
+ relapply <- function(X, FUN, ...) {</pre>
```

```
+ parLapply(cluster, X, FUN, ...)
+ }
+ relapply
+ })
```

Back in xval, the value of the variable xvalLoop is now relapply. The crucial call later in xval will be out <- relapply(1:n, xvalidator, ...). The function relapply is called with the arguments 1:n, xvalidator, and relapply then calls parLapply with the arguments cluster and the other arguments from the call to relapply. The details of how cluster gets assigned the correct value involve the lexical scoping rules of R, but what happens is that cluster takes on the value it had when the xvalLoop method was invoked - the relapply function remembers the environment in which it was created, and the environment includes the variable cluster.

And now the second problem. As it stands, only the computer executing xval knows about the various variables that have been defined, and are needed, for the cross-validation calls. We have to share these variables with all cluster nodes contributing to the cross-validation. snow allows us to export variables from one node to another. This is a slow process, because in snow a new communication channel is established for each variable. In addition, we would have to fully understand the xval method to know which variables needed to be exported under which circumstances.

Here is a solution that makes variable export quick while removing the need for detailed knowledge of which specific variables are required: bundle all the 'visible' variables into an environment, export the environment to each node, and unpack the environment at the receiving node. This turns out to be a good solution, because virtually all the visible variables will be needed in the cross-validation. The implementation of this solution is as follows:

```
> setMethod("xvalLoop", signature(cluster = "spawnedMPIcluster"),
+ function(cluster, ...) {
+ clusterExportEnv <- function(cl, env = .GlobalEnv) {
+ unpackEnv <- function(env) {
+ for (name in ls(env)) assign(name,
+ get(name, env), .GlobalEnv)
+ NULL
+ }
+ clusterCall(cl, unpackEnv, env)
+ }
+ relapply <- function(X, FUN, ...) {
+ clusterExportEnv(cluster, parent.frame(1))
+ parLapply(cluster, X, FUN, ...)
+ }
+ relapply
+ }</pre>
```

The clusterExportEnv function is responsible for taking variables in an environment and sending them and a function to 'unpack' the environment to each

node. clusterCall is defined in snow.

While tortuous in development from scratch, the end result and steps for creating new methods is straight-forward: create an xvalLoop method for a clustered environment that (a) exports visible variables and (b) implements and returns a parallelized lapply-like function.

3.1 Performance

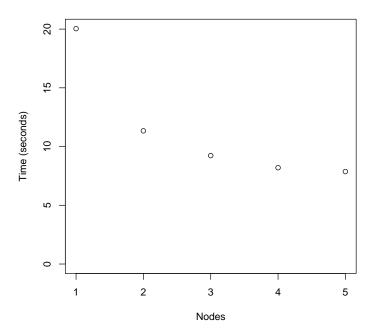


Figure 1: Execution time decreases asymptotically with number of nodes. The decreasing performance gain is primarily due to communication overhead.

After all this work, what do we get? Without immediate access to a cluster, I ran xval on a collection of 64-bit x86 linux computers linked through standard ethernet switches. There are a variety of users on each node, so they may not perform equivalently. The code used is

```
> harness <- function(nodes, reps, data) {
+     if (nodes > 1) {
+        cl <- makeCluster(nodes, "MPI")
+        clusterEvalQ(cl, library(MLInterfaces))
+     }</pre>
```

Figure 1 summarizes timings from 10 replicate calculations of the cross-validation used above. The details of the results are likely to be quite system-and problem-dependent. However, a general point emerges.

A basic framework for thinking about total execution time is to recognize two components: computation, and communication. In an ideal world, computation time and node number are inversely related nodes, $t_{\rm comp} \propto 1/n$. Communication time depends on how tasks are communicated to nodes. In snow, communication increases linearly with node number, $t_{\rm comm} \propto n$. The combination of these times means that there is a node number that minimizes overall execution time. Results in Figure 1 suggest that the optimum cluster size for this problem is surprisingly small.

3.2 Improvements

This section sketches two ways to improve execution time. A goal is to develop this more fully with worked examples.

snow and clusterCall communication scales linearly with node number. This is because of the way snow implements cluster-wide calls. Specifically, the 'master' node (i.e., the node running R through which interactions occur) communicates separately with each slave node. Both MPI and PVM allow for more efficient models of communication, through broadcast operations that synchronize data across nodes in $\log n$ time.

The broadcast approach is likely to be important in large clusters, but in the example of the previous section the efficiency is not that great. The underlying problem is the transfer of a large volume of data; actually, the optimum node number generally decreases as the size of the data set increases. One solution to this is somewhat counter-intuitive, at least to me. The idea is for all nodes to independently read in data and execute all code up to the location where xvalLoop is used in xval. The 'slave' nodes then each execute a portion of the cross-validations, while the 'master' node collates results from the slaves. At the end of xvalLoop the master has a complete collection of results and continues on; the slaves have an incomplete set of results, and can be terminated. The code is counter-intuitive because each node performs seemingly redundant calculations (the processing up to xvalLoop). Communication times should be greatly reduced, though, because each communication involves just a short set of

results rather than a potentially very large data set. An assumption is that the clustered file system will cope well with near-simultaneous requests to initially read in data.

3.3 Making xval cluster-friendly

The implementation presented above required revision of the xval code. The structure of the routine is: (1) check on supplied variables; (2) preliminary setup; (3) a loop-like call where the 'work' of the function occurs; and (4) processing of the result. Many high-level R routines have a similar structure. The revisions aimed to more cleanly distinguish the overall structure, and in particular to isolate and refactor part (3).

A key step in the refactoring was to change a for loop into an lapply-like function call. The reason that this is so important is that for loops allow side-effects to seep beyond the loop. Side-effects are much more easily avoided in a function call. Here is a simple illustration, where the 'side-effect' in the for loop changes the value of x:

```
> x <- 1:10
> for (i in 1:10) x[i] <- i^2
> x

[1]      1      4      9      16      25      36      49      64      81      100
> x <- 1:10
> res <- lapply(1:10, function(i) x[i] <- i^2)
> x

[1]      1      2      3      4      5      6      7      8      9      10
```

Avoiding side-effects is particularly important in a cluster, because side-effects are limited to the node on which the calculation occurs. Usually this is not what is desired.

A final step in code revision is the hook, xvalLoop, provided for programmer access. xvalLoop provides a division-of-labor between the xval expert and the clustered computing expert. The xval expert needs only know that clustered computers can take advantage of lapply-like code. The clustered computing expert need know little about xval, just that it has an lapply-like loop to be exploited. Since xvalLoop is a generic function, the clustered computing expert can tailor methods to different types of clusters and even different algorithms. The end user need know little about either xval or clustered computing; they just provide their cluster as an argument to xval.

4 Conclusion

This document provides a guide to users wanting to make use of xval on a computer cluster. It also provides guidance for further parallelization of xval,

and outlines how functions can be written to expose key components to parallelization. An emphasis is the division of labor between specialized function writers, clustered computer experts, and end users.