Some Performance Improvements for the R Engine

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Introduction

- R is widely used in the field of statistics and beyond, especially in university environments.
- R was originally developed by Robert Gentleman and Ross Ihaka in the early 1990's for a Macintosh computer lab at U. of Auckland, NZ.
- Since 1997 R is developed and maintained by the R-core group, with 21 member are located in 11 different countries.
- The S language, on which R is based, was originally developed at Bell Labs to support flexible data analysis.
- As S evolved, it was developed into a full language that also supports development of software for new methodology.
- R has become the primary framework for developing and making available new statistical methodology.
- Many (over 7,000) extension packages are available through CRAN, Bioconductor, and similar repositories.

Introduction

- Many powerful features are incorporated in S and R, including
  - vectorized arithmetic
  - missing data support
  - atomic vectors (conceptually) passed by value
  - first class functions
  - lexical scope (a key addition in R)
  - lazy evaluation of arguments
- These features are valuable for specifying analyses and developing new data analysis software.
- These features also present challenges to the implementation of R.
- This talk will outline
  - some directions in which the implementation is being improved
  - some tools to help with developing good software in R

Byte Code Compilation
Background

- The standard R evaluation mechanism
  - parses code into a *parse tree* when the code is read
  - evaluates code by interpreting the parse trees.
- Most lower level languages (e.g. C, Fortran) compile their source code to native machine code.
- Some intermediate level languages (e.g. Java, C#) and many scripting languages (e.g. Perl, Python) compile to byte code for a virtual machine.
- Many other strategies are possible.

Byte Code Compilation
Background

- Byte code is the machine code for a *virtual machine*.
- Virtual machine code can then be interpreted by a simpler, more efficient interpreter.
- Virtual machines, and their machine code, are usually specific to the languages they are designed to support.
- Various strategies for further compiling byte code to native machine code are also sometimes used.

Byte Code Compilation
Background

- Efforts to add byte code compilation to R have been underway for some time.
- The first release of the compiler occurred with R 2.13.0.
- The compiler and virtual machine in the current release produce good improvements in a number of cases.
- A number of improvements have been made to the virtual machine in the development version to be released as R 3.2.0 in April 2015.
- Further improvements are currently being explored.

- The compiler can be called explicitly to compile single functions or files of code:
  - cmpfun compiles a function
  - cmpfile compiles a file to be loaded by loadcmp
- It is also possible to have package code compiled when a package is installed.
  - Use --byte-compile when installing or specify the ByteCompile option in the DESCRIPTION file.
  - Since R 2.14.0 R code in all base and recommended packages is compiled by default.
- Alternatively, the compiler can be used in a JIT mode where
  - functions are compiled on first use
  - loops are compiler before they are run

- The current compiler includes a number of optimizations, such as
  - constant folding
  - special instructions for most SPECIALs, many BUILTINs
  - inlining simple .Internal calls: e.g.

    ```
    dnorm(y, 2, 3)
    ```

    is replaced by

    ```
    .Internal(dnorm(y, mean = 2, sd = 3, log = FALSE))
    ```

  - special instructions for many .Internals
- The compiler is currently most effective for code used on scalar data or short vectors where interpreter overhead is large relative to actual computation.

Byte Code Compilation
A Simple Example

R Code

```
f <- function(x) {
    s <- 0.0
    for (y in x)
        s <- s + y
    s
}
```

VM Assembly Code

```
    LDCONST 0.0
    SETVAR s
    POP
    GETVAR x
    STARTFOR y L2
L1: GETVAR s
    GETVAR y
    ADD
    SETVAR s
    POP
    STEPFOR L1
L2: ENDFOR
    POP
    GETVAR s
    RETURN
```

Byte Code Compilation
Some Performance Results

Timings for some simple benchmarks on an `x86_64` Ubuntu laptop:

Benchmark	*Interp.*	*Comp.*	*Speedup*	*Comp. (3.2.0)*	*Speedup*
`sum`	19.64	4.37	4.50	3.00	6.55
`p1`	10.17	3.24	3.14	0.74	13.82
`conv`	17.35	5.43	3.19	1.82	9.53
`rem`	14.37	5.53	2.60	2.33	6.18

Interp., *Comp.* are for the current released version of R

Comp. (3.2.0): upcoming release R 3.2.0 using

- separate instructions for vector, matrix indexing
- typed stack to avoid allocating intermediate scalar values

Byte Code Compilation
Future Directions

- The current virtual machine uses a stack based design.
- An alternative approach might use a register-based design.
- Some additional optimizations currently being explored:
  - avoiding the allocation of intermediate values when possible
  - more efficient variable lookup mechanisms
  - more efficient function calls
  - possibly improved handling of lazy evaluation

  Some promising preliminary results are available.
- Other possible directions include
  - Partial evaluation when some arguments are constants
  - Intra-procedural optimizations and inlining
  - Declarations (sealing, scalars, types, strictness)
  - Machine code generation using LLVM or other approaches

Reducing Value Duplication

- Conceptually, arguments are passed to functions by value, not by reference.
- This means programmers can modify their local view of an object without corrupting the original value:

```
> x <- 1
> f <- function(y) { y[1] <- 2; y }
> f(x)
[1] 2
> x
[1] 1
```

- This helps greatly in writing reliable software.

Reducing Value Duplication

- A price is that objects often need to be duplicated, which
  - takes time
  - increases memory use
- This does not matter much for small objects, but can be prohibitive for large ones.
- Up to R 3.0.3 R used a simple mechanism to avoid duplicating:
  - if an object might be reached from more than one R variable then it is duplicated before modifying it.
- This mechanism has two drawbacks:
  - full duplication is often not necessary
  - it is too conservative

Reducing Value Duplication

- R 3.1.0 includes changes contributed by Michael Lawrence that use *shallow duplication* in many cases.
- This only duplicates the parts of larger hierarchical objects that need to be modified.
- This significantly improves speed and memory use in particular in Bioconcductor applications.

Reducing Value Duplication

- An experiment currently underway is to replace the internal mechanism to detect when duplication might be needed by reference counting.
- This will allow duplicating objects to be avoided in many more situations.
- It may allow replacement functions like `[<-.data.frame` that are written in R to avoid duplicating in some cases
- Reference counting will also likely be easier to maintain than the current mechanism.
- This may adopted for R 3.3.0.

Large Vector Support

- *Big Data* is a hot topic
- Some categories:
  - fit into memory
  - fit on one machine's disk storage
  - require multiple machines to store
- Smaller large data sets can be handled by standard methods if enough memory is available.
- Very large data sets require specialized methods and algorithms.
- R should be able to handle smaller large data problems on machines with enough memory.

Large Vector Support

Initial Objectives

- The R integer data type is equivalent to C int.
- This is now essentially universally a signed 32-bit type.
- This type is also used for the length of a vector or total size of an array.
- This design decision made sense when R started out nearly 20 years ago:
  - most machines and operating systems were 32-bit
  - this matched the interface provided by external C/FORTRAN code

Large Vector Support
Initial Objectives

- This design limits the number of elements in an array to $2^{31} - 1 = 2{,}147{,}483{,}647$.
- For numeric (double precision) data this means the largest possible vector is about 16 GB.
- This is not yet a major limitation for typical users.
- It is a limitation for some users and will become more limiting over time.
- We need a way to raise this limit that meets several goals:
  - avoid having to rewrite too much of R itself
  - avoid requiring package authors to rewrite too much C code
  - avoid having existing compiled C code fail if possible
  - allow incrementally adding support for procedures where it makes sense
- For now, keep $2^{31} - 1$ limit on matrix rows and columns.

Large Vector Support
Current Design

- C level changes:
  - Preserve existing memory layout
  - Use special marker in length field to identify long vectors
  - LENGTH accessor (returning int) signals an error for long vectors
  - Long vector aware code uses XLENGTH to return R_xlen_t.
- R code should not need to be changed:
  - double precision indices can be used for subsetting
  - length will return double for long vectors
  - .C and .Fortran will signal errors for long vectors.
- Documentation on how to add long vector support to a package is available in the manuals.

Large Vector Support
Progress So Far

- A number of internal functions now support long vectors.
- Some statistical functions with long vector support:
  - random number generators
  - mean
  - sort
  - fivenum
  - lm.fit
  - glm.fit
- The function dist can handle more than 2^{16} observations by returning a long vector result.
- Many matrix and array functions already support large arrays:
  - colSums, colMeans
  - rowSums, rowMeans

Large Vector Support

Open Issues

- Converting existing methods to support large vectors is fairly straight forward, however:
  - more numerically stable algorithms may be needed
  - faster/parallel algorithms may be needed
  - the ability to interrupt computations may become important
  - statistical usefulness may not scale to larger data
- The size where these issues become relevant is likely much lower!
- Future work will consider
  - whether to add a separate 64-bit integer type, or change the basic R integer type to 64 bits
  - possibly adding 8 and 16 bit integer types
  - arithmetic and overflow issues that these raise
  - whether to allow numbers of rows and columns in matrices to exceed $2^{31} - 1$ as well

Parallelizing Vector and Matrix Operations

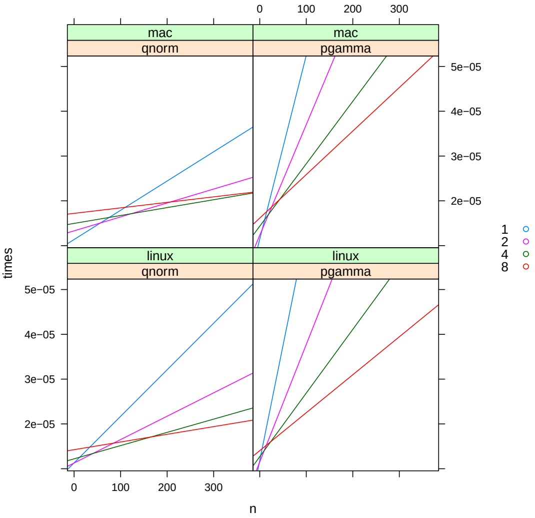
- Most modern computers feature two or more processor cores.
- It is expected that tens of cores will be available soon.
- Two ways to take advantage of multiple cores:
  - Explicit parallelization:
    - uses some form of annotation to specify parallelism
    - packages `snow`, `multicore`, `parallel`.
  - Implicit parallelization:
    - automatic, no user action needed
- Implicit parallelization is particularly suited to
  - basic vectorized math functions
  - basic matrix operations (e.g. colSums)
  - linear algebra computations (threaded BLAS)

- Basic idea for a P-core system:
  - run P worker threads
  - place $1/P$ of the work on each thread
- Idealized view: this produces a P-fold speedup.
- Actual speedup is less:
  - there is synchronization overhead
  - sequential code and use of shared resources (memory, bus, ...)
  - actual workloads are uneven
- Result: parallel code can be slower!
- Parallelizing will only pay off if data size n is large enough.
  - For some functions, e.g. qbeta, $n \approx 10$ may be large enough.
  - For some, e.g. qnorm, $n \approx 1000$ is needed.
  - For basic arithmetic operations $n \approx 30000$ may be needed.

- OpenMP provides a convenient way to implement parallelism at the C/FORTRAN level.
- Good performance of the synchronization barrier is critical for fine-grained parallelization.
- On Linux/gcc OpenMP performance is very good.
- On Mac OS X and Windows gcc's OpenMP barrier performance was not adequate.
- With recent improvements performance on Mac OS X and Windows should be competitive with Linux.

- Care is needed to make sure that all functions called from worker threads are thread-safe.
- Some things that are not thread-safe:
  - use of global variables
  - R memory allocation
  - signaling warnings and errors
  - user interrupt checking
  - creating internationalized messages (calls to gettext)
- Random number generation is also problematic.

Parallelizing Vectorized Operations
Some Experimental Results



Some observations:

- Run times are roughly linear in vector length.
- Intercepts (reflecting fixed costs and synchronization overhead for different numbers of threads) on a given platform are roughly the same for all functions.
- Relative slopes (marginal time per element) are roughly independent of OS/architecture.

A simple calibration strategy:

- Compute relative slopes once, or average across several setups.
- For each OS/architecture combination compute the intercepts.

The appropriate time to run calibration code is still open.

Parallelizing Vectorized Operations

Some Notes

- An experimental package pnmath0 that parallelizes many basic vectorized math functions is available at

  `http://www.stat.uiowa.edu/~luke/R/experimental/`

- The functions colSums and dist in the current R distribution can run in parallel but do not by default.
- Hopefully more will be included in the R distribution before too long.
- Still need to find clean way for a user to control the maximal number of threads allowed.
- Also need to resolve whether slight changes of results are acceptable, especially in reductions.

Some Profiling Tools

- For many computations performance is not an issue.
- In cases where a computation is to slow, a first step is to identify the bottle neck.
- Profiling can be a valuable aid.
- R includes a sampling-based profiling mechanism.
- At regular intervals the functions on the call stack are recorded in a file.
- A recent addition allows the line and file information for each call to be recorded as well.
- A basic facility for examining R profile data is provided by summaryRprof.
- Joint work with Riad Jarjour is developing a more extensive set of tools.

Some Profiling Tools

- Based on examining facilities in other languages we have identified a range of filtering, summary, and visualization tools that can be useful.
- Filtering allows the programmer to, for example,
  - focus on a subset of the functions called
  - drop outer functions that are not of direct interest
  - drop functions that are only called infrequently
- Summaries include
  - function level summaries
  - call level summaries
  - source line level summaries
  - source code annotation
  - hot path identification
- Visualizations include
  - call graphs
  - time graphs
  - call tree visualizations

- Read in profile data from a linear model fit using lm.fit:

```
> pd <- readProfileData("Rprof-lmfit-new.out")
> pd0 <- filterProfileData(pd, select = "system.time", focus = TRUE)
```

- Function summaries:

```
> head(funSummary(pd0), 5)
                        total.pct gc.pct self.pct gcself.pct
system.time (lmfit.R:4)     89.32  18.50     0.00       0.00
lm.fit                      89.21  18.39     0.00       0.00
.Call (lmsrc.R:30)          39.65   2.97    39.65       2.97
c (lmsrc.R:64)              20.93  10.57    20.93      10.57
structure (lmsrc.R:64)       7.60   0.77     7.60       0.77
```

- Hot path summary:

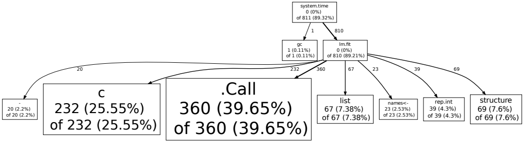
```
> hotPaths(pd)
 path                           total.pct self.pct
 source                         99.78      0.00
 . withVisible                  99.78      0.00
 . . eval                       99.78      0.00
 . . . eval                     99.78      0.00
 . . . . system.time            89.32      0.00
 . . . . . lm.fit               89.21      0.00
 . . . . . . .Call              39.65     39.65
 . . . . . . c                  25.55     25.55
 . . . . . . structure           7.60      7.60
 . . . . . . list                7.38      7.38
 . . . . . . rep.int             4.30      4.30
 . . . . . . names<-             2.53      2.53
 . . . . . . -                   2.20      2.20
 . . . . . gc                    0.11      0.11
 . . . . rnorm                   9.25      9.25
...
```

- Source summary:

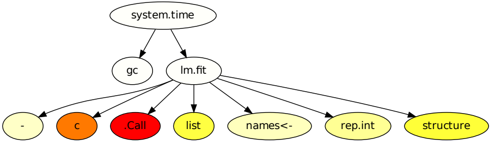
```
> srcSummary(pd0)
            total.pct gctotal.pct                                 source
lmfit.R:4       89.32       18.50 system.time(for (i in 1:5) lm.fit(X, y))
lmsrc.R:30      39.65        2.97     z <- .Call(C_Cdqrls, x, y, tol)
lmsrc.R:39       8.92        0.66     nmeffects <- c(dn[pivot[r1]], rep.i ...
lmsrc.R:55       2.53        0.55         names(z$effects) <- nmeffects
lmsrc.R:58       2.20        0.66     r1 <- y - z$residuals
lmsrc.R:64      35.90       13.55     c(z[c("coefficients", "residuals",  ...
```

- annotateSource shows a full file with line annotation.

- A call graph:



- An alsternative style:



Some Profiling Tools
Notes

- These profiling tools are a work in progress.
- They should be available in a package `proftools` later this year.
- We are also working on a graphical interface based on `gWidgets2`.
- This GUI should be available in a package `proftols-GUI` later this year as well.

Conclusions

Synergy

- There is synergy among these areas of development; for example:
  - Many functions applied to large data are excellent candidates for parallelization.
  - The compiler may be able to fuse operations and allow more efficient parallelization at the fused operation level.
  - The compiler may also be able to compile certain uses of sweep and apply functions.
  - Profiling tools will help in refining where our implementations need
- Exploring these opportunities will be a goal of work over the coming year.

Conclusions

Maintainability

- R is currently developed and maintained by statisticians for statisticians.
- More sophisticated approaches may be needed to move R forward.
- More sophisticated implementation approaches have to be balanced with maintainability.
- To be successful a novel approach needs either
    - longer term developer commitment
    - sufficient training for those with a longer term commitment
- Getting the balance right represents an interesting challenge.
- We are starting some collaborations with computer scientists that will allow us to explore these issues.