Comparing Least Squares Calculations

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Abstract

Many statistics methods require one or more least squares problems to be solved. There are several ways to perform this calculation, using objects from the base R system and using objects in the classes defined in the Matrix package.

We compare the speed of some of these methods on a very small example and on an example for which the model matrix is large and sparse.

1 Linear least squares calculations

Many statistical techniques require least squares solutions

$$\hat{\beta} = \arg \min_\beta ||y - X\beta||^2$$

(1)

where $X$ is an $n \times p$ model matrix ($p \leq n$), $y$ is $n$-dimensional and $\beta$ is $p$ dimensional. Most statistics texts state that the solution to (1) is

$$\hat{\beta} = (X^TX)^{-1}X^Ty$$

(2)

when $X$ has full column rank (i.e. the columns of $X$ are linearly independent) and all too frequently it is calculated in exactly this way.

1.1 A small example

As an example, let’s create a model matrix, $\text{mm}$, and corresponding response vector, $y$, for a simple linear regression model using the Formaldehyde data.

```r
> data(Formaldehyde)
> str(Formaldehyde)
'data.frame': 6 obs. of 2 variables:
$ carb : num 0.1 0.3 0.5 0.6 0.7 0.9
$ optden: num 0.086 0.269 0.446 0.538 0.626 0.782
```
> (m <- cbind(1, Formaldehyde$carb))

    [,1] [,2]
[1,] 1 0.1
[2,] 1 0.3
[3,] 1 0.5
[4,] 1 0.6
[5,] 1 0.7
[6,] 1 0.9

> (yo <- Formaldehyde$optden)

[1] 0.086 0.269 0.446 0.538 0.626 0.782

Using `t` to evaluate the transpose, `solve` to take an inverse, and the `%*%` operator for matrix multiplication, we can translate [2] into the S language as

> solve(t(m) %*% m) %*% t(m) %*% yo

    [,1]
[1,] 0.005085714
[2,] 0.876285714

On modern computers this calculation is performed so quickly that it cannot be timed accurately in R [1].

> system.time(solve(t(m) %*% m) %*% t(m) %*% yo)

    user  system elapsed
           0           0           0

and it provides essentially the same results as the standard `lm.fit` function that is called by `lm`.

> dput(c(solve(t(m) %*% m) %*% t(m) %*% yo))

c(0.00508571428571408, 0.876285714285715)

> dput(unname(lm.fit(m, yo)$coefficients))

c(0.00508571428571428, 0.876285714285715)

[1]From R version 2.2.0, `system.time()` has default argument `gcFirst = TRUE` which is assumed and relevant for all subsequent timings.
1.2 A large example

For a large, ill-conditioned least squares problem, such as that described in [Koenker and Ng (2003)], the literal translation of (2) does not perform well.

```r
library(Matrix)
data(KNex, package = "Matrix")
y <- KNex$y
mm <- as(KNex$mm, "matrix") # full traditional matrix
dim(mm)
[1] 1850 712
system.time(naive.sol <- solve(t(mm) %*% mm) %*% t(mm) %*% y)
user system elapsed
0.739  0.012  0.754
```

Because the calculation of a “cross-product” matrix, such as $X^T X$ or $X^T y$, is a common operation in statistics, the `crossprod` function has been provided to do this efficiently. In the single argument form `crossprod(mm)` calculates $X^T X$, taking advantage of the symmetry of the product. That is, instead of calculating the $712^2 = 506944$ elements of $X^T X$ separately, it only calculates the $(712 \cdot 713)/2 = 253828$ elements in the upper triangle and replicates them in the lower triangle. Furthermore, there is no need to calculate the inverse of a matrix explicitly when solving a linear system of equations. When the two argument form of the `solve` function is used the linear system

$$(X^T X) \hat{\beta} = X^T y$$

is solved directly.

Combining these optimizations we obtain

```r
system.time(cpod.sol <- solve(crossprod(mm), crossprod(mm,y)))
user system elapsed
0.568  0.004  0.573
all.equal(naive.sol, cpod.sol)
[1] TRUE
```

On this computer (2.0 GHz Pentium-4, 1 GB Memory, Goto’s BLAS, in Spring 2004) the crossprod form of the calculation is about four times as fast as the naive calculation. In fact, the entire crossprod solution is faster than simply calculating $X^T X$ the naive way.

```r
system.time(t(mm) %*% mm)
user system elapsed
0.448  0.006  0.456
```
Note that in newer versions of R and the BLAS library (as of summer 2007), R’s `%*%` is able to detect the many zeros in `mm` and shortcut many operations, and is hence much faster for such a sparse matrix than `crossprod` which currently does not make use of such optimizations. This is not the case when R is linked against an optimized BLAS library such as GOTO or ATLAS. Also, for fully dense matrices, `crossprod()` indeed remains faster (by a factor of two, typically) independently of the BLAS library:

```r
> fm <- mm
> set.seed(11)
> fm[] <- rnorm(length(fm))
> system.time(c1 <- t(fm) %*% fm)
  user  system elapsed
0.429   0.000   0.431
> system.time(c2 <- crossprod(fm))
  user  system elapsed
0.564   0.000   0.566
> stopifnot(all.equal(c1, c2, tol = 1e-12))
```

### 1.3 Least squares calculations with Matrix classes

The `crossprod` function applied to a single matrix takes advantage of symmetry when calculating the product but does not retain the information that the product is symmetric (and positive semidefinite). As a result the solution of (3) is performed using general linear system solver based on an LU decomposition when it would be faster, and more stable numerically, to use a Cholesky decomposition. The Cholesky decomposition could be used but it is rather awkward:

```r
> system.time(ch <- chol(crossprod(mm)))
  user  system elapsed
0.594   0.000   0.595
> system.time(chol.sol <-
  + backsolve(ch, forwardsolve(ch, crossprod(mm, y),
  + upper = TRUE, trans = TRUE)))
  user  system elapsed
0.003   0.000   0.003
> stopifnot(all.equal(chol.sol, naive.sol))
```

The `Matrix` package uses the S4 class system (Chambers, 1998) to retain information on the structure of matrices from the intermediate calculations. A general matrix in dense storage, created by the `Matrix` function, has class "dgeMatrix" but its cross-product has class "dpoMatrix". The `solve` methods for the "dpoMatrix" class use the Cholesky decomposition.
The model matrix `mm` is sparse; that is, most of the elements of `mm` are zero. The `Matrix` package incorporates special methods for sparse matrices, which produce the fastest results of all.

As with other classes in the `Matrix` package, the `dsCMatrix` retains any factorization that has been calculated although, in this case, the decomposition is so fast that it is difficult to determine the difference in the solution times.
> xpx <- crossprod(mm)
> xpy <- crossprod(mm, y)
> system.time(solve(xpx, xpy))

    user  system elapsed
       0.001   0.000   0.001

> system.time(solve(xpx, xpy))

    user  system elapsed
         0       0       0

Session Info

> toLatex(sessionInfo())

• R version 3.5.1 Patched (2018-10-19 r75465), x86_64-pc-linux-gnu
• Locale: LC_CTYPE=de_CH.UTF-8, LC_NUMERIC=C, LC_TIME=en_US.UTF-8, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MEASUREMENT=de_CH.UTF-8, LC_IDENTIFICATION=C
• Running under: Fedora 28 (Twenty Eight)
• Matrix products: default
• BLAS: /sfs/u/maechler/R/D/r-patched/F28-64-inst/lib/libRblas.so
• LAPACK: /sfs/u/maechler/R/D/r-patched/F28-64-inst/lib/libRlapack.so
• Base packages: base, datasets, grDevices, graphics, methods, stats, utils
• Other packages: Matrix 1.2-15
• Loaded via a namespace (and not attached): compiler 3.5.1, grid 3.5.1, lattice 0.20-35, tools 3.5.1

> if(identical(1L, grep("linux", R.version["os"]))) { ## Linux - only ---
  Scpu <- sfsmisc::Sys.procinfo("/proc/cpuinfo")
  Smem <- sfsmisc::Sys.procinfo("/proc/meminfo")
  print(Scpu[c("model name", "cpu MHz", "cache size", "bogomips")])
  print(Smem[c("MemTotal", "SwapTotal")])
}

- model name Intel(R) Core(TM) i7-7700T CPU @ 2.90GHz
cpu MHz 3686.514
References
