

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 a example for which the model matrix is large and sparse.

1 Linear least squares calculations

Many statistical techniques require least squares solutions

$$\hat{\beta} = \arg \min_{\beta} \|\mathbf{y} - \mathbf{X}\beta\|^2 \quad (1)$$

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

$$\hat{\beta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y} \quad (2)$$

when \mathbf{X} has full column rank (i.e. the columns of \mathbf{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, `mm`, and corresponding response vector, `y`, for a simple linear regression model using the `Formaldehyde` data.

```
> 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
```

```
> print(mm <- 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
```

```
> print(y <- 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(mm) %% mm) %% t(mm) %% y
```

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

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

```
> system.time(solve(t(mm) %% mm) %% t(mm) %% y, gc = TRUE)
```

```
[1] 0 0 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(mm) %% mm) %% t(mm) %% y))
```

```
c(0.00508571428571368, 0.876285714285715)
```

```
> dput(lm.fit(mm, y)$coefficients)
```

```
structure(c(0.00508571428571436, 0.876285714285714), .Names = c("x1",
"x2"))
```

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.

```
> library(Matrix)
```

Attaching package: 'Matrix'

The following object(s) are masked _by_ .GlobalEnv :

```
mm y
> data(mm, package = "Matrix")
> data(y, package = "Matrix")
> mm <- as(mm, "matrix")
<environment: namespace:Matrix>
> dim(mm)
[1] 1850 712
> system.time(naive.sol <- solve(t(mm) %*% mm) %*% t(mm) %*%
+ y, gc = TRUE)
[1] 3.47 0.09 3.72 0.00 0.00
```

Because the calculation of a “cross-product” matrix, such as $\mathbf{X}^\top \mathbf{X}$ or $\mathbf{X}^\top \mathbf{y}$, is a common operation in statistics, the `crossprod` function has been provided to do this efficiently. In the single argument form `crossprod(mm)` calculates $\mathbf{X}^\top \mathbf{X}$, taking advantage of the symmetry of the product. That is, instead of calculating the $712^2 = 506944$ elements of $\mathbf{X}^\top \mathbf{X}$ 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

$$(\mathbf{X}^\top \mathbf{X}) \hat{\boldsymbol{\beta}} = \mathbf{X}^\top \mathbf{y} \quad (3)$$

is solved directly.

Combining these optimizations we obtain

```
> system.time(cpod.sol <- solve(crossprod(mm), crossprod(mm,
+ y)), gc = TRUE)
[1] 0.72 0.04 0.80 0.00 0.00
> all.equal(naive.sol, cpod.sol)
[1] TRUE
```

On this computer (2.0 GHz Pentium-4, 1 GB Memory, Goto’s BLAS) 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 $\mathbf{X}^\top \mathbf{X}$ the naive way.

```
> system.time(t(mm) %*% mm, gc = TRUE)
[1] 0.87 0.02 0.94 0.00 0.00
```

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

```
> system.time(ch <- chol(crossprod(mm)), gc = TRUE)

[1] 0.50 0.02 0.55 0.00 0.00

> system.time(chol.sol <- backsolve(ch, forwardsolve(ch, crossprod(mm),
+      y), upper = TRUE, trans = TRUE)), gc = TRUE)

[1] 0.12 0.05 0.18 0.00 0.00

> all.equal(chol.sol, naive.sol)

[1] TRUE
```

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.

```
> data(mm, package = "Matrix")
> mm <- as(mm, "dgeMatrix")

<environment: namespace:Matrix>

> class(crossprod(mm))

<environment: namespace:Matrix>
[1] "dpoMatrix"
attr(,"package")
[1] "Matrix"

> system.time(Mat.sol <- solve(crossprod(mm), crossprod(mm),
+      y)), gc = TRUE)

<environment: namespace:Matrix>
<environment: namespace:Matrix>
<environment: namespace:Matrix>
[1] 0.52 0.02 0.56 0.00 0.00

> all.equal(naive.sol, as(Mat.sol, "matrix"))
```

```
[1] TRUE
```

Furthermore, any method that calculates a decomposition or factorization stores the resulting factorization with the original object so that it can be reused without recalculation.

```
> xpx <- crossprod(mm)

<environment: namespace:Matrix>

> xpy <- crossprod(mm, y)

<environment: namespace:Matrix>

> system.time(solve(xpx, xpy), gc = TRUE)

<environment: namespace:Matrix>
[1] 0.10 0.01 0.10 0.00 0.00

> system.time(solve(xpx, xpy), gc = TRUE)

<environment: namespace:Matrix>
[1] 0.00 0.00 0.02 0.00 0.00
```

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.

```
> data(mm, package = "Matrix")
> class(mm)

[1] "dgCMatrix"
attr(,"package")
[1] "Matrix"

> system.time(sparse.sol <- solve(crossprod(mm), crossprod(mm,
+   y)), gc = TRUE)

<environment: namespace:Matrix>
<environment: namespace:Matrix>
<environment: namespace:Matrix>
[1] 0.06 0.00 0.05 0.00 0.00

> all.equal(naive.sol, as(sparse.sol, "matrix"))

[1] TRUE
```

As with other classes in the `Matrix` package, the `sscMatrix` 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)

<environment: namespace:Matrix>

> xpy <- crossprod(mm, y)

<environment: namespace:Matrix>

> system.time(solve(xpx, xpy), gc = TRUE)

<environment: namespace:Matrix>
[1] 0.01 0.00 0.01 0.00 0.00

> system.time(solve(xpx, xpy), gc = TRUE)

<environment: namespace:Matrix>
[1] 0 0 0 0 0

```

References

- John M. Chambers. *Programming with Data*. Springer, New York, 1998. ISBN 0-387-98503-4.
- Roger Koenker and Pin Ng. SparseM: A sparse matrix package for R. *J. of Statistical Software*, 8(6), 2003.