Variety in the Implementation of Nonlinear Least Squares Program Codes

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Contents

Abstract

There are many ways to structure a Gauss-Newton style nonlinear least squares program code. In organizing and documenting the nearly half-century of programs in the Nashlib collection associated with John C. Nash (1979), the author realized that this variety could be an instructive subject for software designers.

Underlying algorithms

Gauss Newton

https://en.wikipedia.org/wiki/Gauss%E2%80%93Newton_algorithm

In calculus we learn that a stationary point (local maximum, minimum or saddle point) of a function f occurs where its gradient (or first derivative) is zero. In multiple dimensions, this is the same as having the gradient g stationary. The so-called Newton method uses the second derivatives in the Hessian matrix H defined as

$$H_{i,j} = \partial^2 f / \partial x_i \partial x_j$$

where f is a function of several variables x_i, where $i = 1, ..., n$, written collectively as x. The Newton equations are defined as

$$H\delta = -g$$

where H and g are evaluated at a guess or estimate of x. x is then updated to

$$x \leftarrow x + \delta$$

and we iterate until there is no change in x.

There are some adjustments When our function $f(x)$ can be written as a sum of squares

$$f(x) = \sum_{i-1}^{n} r_i(x)^2 = r^t r$$

where the final vector product form is the one I favour because it is the least fussy to write. In particular, when we try to evaluate the Hessian of this sum of squares function, we see that it is

$$H_{j,k} = 2 \sum_{i-1}^{n} [(\partial r_i / \partial x_j)(\partial r_i / \partial x_k) + r_i(\partial^2 r_i / \partial x_j \partial x_k)]$$

If we define the **Jacobian** matrix

$$J_{i,j} = \partial r_i / \partial x_j$$

then the gradient is

$$g = 2J^t r$$

and the first part of the Hessian is

$$J^t J$$

Arguing that the residuals should be "small," Gauss proposed that the Newton equations could be approximated by ignoring the second term (using elements of the residual times second derivatives of the residual). This gives the **Gauss-Newton** equations (cancelling the factor 2)

$$(J^t J)\delta = -J^t r$$

We can use this in an iteration similar to the Newton iteration.

Hartley's method

Conditions for convergence of the Newton iteration and the Gauss-Newton iteration are rather a nuisance to verify, and in any case we want a solution. Hartley (1961) proposed that rather than use an iteration

$$x \leftarrow x + \delta$$

one could do a search along the direction δ. Ideally we would want to minimize

$$f(x + \alpha\delta)$$

with respect to the (scalar) parameter δ. However, typically a value of α that permits a reduction in the sum of squares $f(x)$ is accepted and the iteration repeated. Clearly there are many tactical choices that give rise to a variety of particular algorithms. One concern is that the direction δ gives no lower value of the sum of squares, since there is an approximation involved in using $J^t J$ rather than H.

Marquardt

Marquardt (1963) is perhaps one of the most important developments in nonlinear least squares apart from the Gauss-Newton method. There are several ways to view the method.

First, considering that the $J^t J$ may be effectively singular in the computational environment at hand, the Gauss-Newton method may be unable to compute a search step that reduces the sum of squared residuals. The right hand side of the normal equations, that is, $g = -J^t r$ is the gradient for the sum of squares. Thus a solution of

$$\mathbf{1}_n \delta = -g$$

is clearly a downhill version of the gradient. And if we solve

$$\lambda \mathbf{1}_n \delta = -g$$

various values of λ will produce steps along the **steepest descents** direction. Solutions of the Levenberg-Marquardt equations

$$(J^t J + \lambda 1_n)\delta = -J^t r$$

can be thought of as yielding a step δ that merges the Gauss-Newton and steepest-descents direction. This approach was actually first suggested by Levenberg (1944), but it is my opinion that while the ideas are sound, Levenberg very likely never tested them in practice. Before computers were commonly available, this was not unusual, and many papers were written with computational ideas that were not tested or were given only cursory trial.

Practical Marquardt methods require us to specify an initial λ and ways to adjust its value. For example, if

$$SS(x) = r^t r = f(x)$$

is the function to minimize to "fit" our nonlinear model:

- set an initial λ of 0.0001

- **A** Compute J and g, set up Marquardt equations and find δ

- **B** compute new set of parameters
$$x_{new} = x + \delta$$

- if $x_{new}! = x$, compute $SS(x_{new})$, else quit (**termination**)

- if $SS(x_{new}) < SS(x)$, replace x with x_{new}, replace λ with $0.4 * \lambda$, then retry from **A**

- ELSE increase λ to $10 * \lambda$ and retry from **B** (J and g do NOT need to be recomputed)

In this scheme, an algorithm is defined by the initial value, decrease factor (e.g., 0.4) and increase factor (e.g., 10) for λ, but there are a number of annoying computational details concerning underflow or overflow and how we measure equivalence of iterates. That is, we need to ensure λ is not so "small" that multiplying by 10 is meaningless, and we need to know what "not equal" means for floating point vectors in the arithmetic in use.

An example of choices to deal with these details:

- if λ is smaller than some pre-set tolerance, set it to the tolerance. (Otherwise do not worry if it is tiny, as long as the sum of squares still gets reduced.)

- when comparing x_{new} and $x5, we can use a modest number, e.g, 100.0 which we will call OFFSET. In the arithmetic of the system at hand, if the floating-point numbers $x_{new} + OFFSET$ matches bit for bit $x + OFFSET$, then they are equal.

Many practitioners dislike using IF statements (comparisons) of floating point numbers and I have had a number of exchanges with other workers over the years. However, I have never seen any issues. When x is tiny, we compare OFFSET to itself and declare equality. When x is very large, OFFSET does not change it and we compare x with a value that is identical to it. Moreover, we use very little extra code.

Others

There have been many proposed approaches to nonlinear least squares.

Spiral

Jones (1970) is a method . . .

Sources of implementation variety

The sources of variety in implementation include:

- programming language

- possible operating environment features

- solver for the least squares or linear equations sub-problems

- stucture of storage for the solver, that is, compact or full

- sequential or full creation of the Jacobian and residual, since it may be done in parts

- how the Jacobian is computed or approximated

- higher level presentation of the problem to the computer, as in R^ts `nls` or packages `minpack.lm` and `nlsr`.

Programming language

We have a versions of the Nashlib Algorithm 23 in BASIC, Fortran, Pascal, and R, with Python pending. There may be dialects of these programming languages also, giving rise to other variations.

Operating environment

Generally, for modern computers, the operating system and its localization do not have much influence on the way in which we set up nonlinear least squares computations. I will comment below about some issues

where speed and size of data storage may favour some approaches over others. However, such issues are less prominent today.

Solver for the least squares or linear equations sub-problems

Solution of the linear normal equations

The Gauss-Newton or Marquardt eqations are a set of linear equations. Moreover, the coefficient matrix is non-negative definite and symmetric. Thus it permits of both general and specialized methods for linear equations. Furthermore, one can also set up the solution without forming the $J^t J$ matrix by using several matrix decomposition methods. Thus there are many possible procedures.

- Gauss elimination with partial pivoting

- Gauss elimination with complete pivoting

- Variants of Gauss elimination that build matrix decompositions

- Gauss-Jordan inversion

- Choleski Decomposition and back substitution

- Eigendecompositions of the SSCP

Solution of the least squares sub-problem by matrix decomposition

- Householder

- Givens

- pivoting options

- Marquardt and Marquardt Nash options

- SVD approaches

Avoiding duplication of effort when increasing the λ parameter

How to do this??

Storage stucture

J, J^tJ, If J^tJ, then vector form of lower triangle. ??

If the choice of approach to Gauss-Newton or Marquardt is to build the normal equations and hence the sum of squares and cross products (SSCP) matrix, we know by construnction that this is a symmetric matrix and also positive definite. In this case, we can use algorithms that specifically take advantage of both these properties, namely Algorithms 7, 8 and 9 of Nashlib. Algorithms 7 and 8 are the Cholesky decomposition and back-solution using a vector of length `n*(n+1)/2` to store just the lower triangle of the SSCP matrix. Algorithm 9 inverts this matrix *in situ*.

The original John C. Nash (1979) Algorithm 23 (Marquardt nonlinear least squares solution) computes the SSCP matrix $J^t J$ and solves the Marquardt-Nash augmented normal equations with the Cholesky approach. This was continued in the Second Edition John C. Nash (1990) and in John C. Nash and Walker-Smith (1987). However, in the now defunct John C. Nash (2016) and successor John C. Nash and Murdoch (2019), the choice has been to use a QR decomposition as described below in ???. The particular QR calculations are in these packages internal to R-base, complicating comparisons of storage, complexity and performance.

Other storage approaches.

Sequential or full Jacobian computation

We could compute a row of the Jacobian plus the corresponding residual element and process this before computing the next row etc. This means the full Jacobian does not have to be stored. In Nashlib, Algorithms 3 and 4, we used row-wise data entry in linear least squares via Givens' triangularization (QR decompostition), with the possibility of extending the QR to a singular value decomposition. Forming the SSCP matrix can also be generated row-wise as well.

Analytic or approximate Jacobian

Use of finite difference approximations??

Problem interfacing

R allows the nonlinear least squares problem to be presented via a formula for the model.

Saving storage

The obvious ways to reduce storage are:

- use a row-wise generation of the Jacobian in either a Givens' QR or SSCP approach. This saves space for the Jacobian as well as as well as the working matrices of the Gauss-Newton or Marquardt iterations;

- if the number of parameters to estimate is large enough, then a normal equations approach using a compact storage of the lower triangle of the SSCP matrix. However, the scale of the saving is really very small in comparison to the size of most programs.

Measuring performance

Test problems

```r
# set parameters
set.seed(123456)
a <- 1
b <- 2
c <- 3
np <- 15
tt <-1:np
yy <- 100*a/(1+10*b*exp(-0.1*c*tt))
plot.new()
plot(tt, yy, type='l')
set.seed(123456)
ev <- runif(np)
ev <- ev - mean(ev)
y1 <- yy + ev
points(tt,y1,type='p', col="green")
y2 <- yy + 5*ev
points(tt,y2,type='p', col="blue")
y3 <- yy + 10*ev
lg3d15 <- data.frame(tt, yy, y1, y2, y3)
points(tt,y3,type='p', col="red")
```
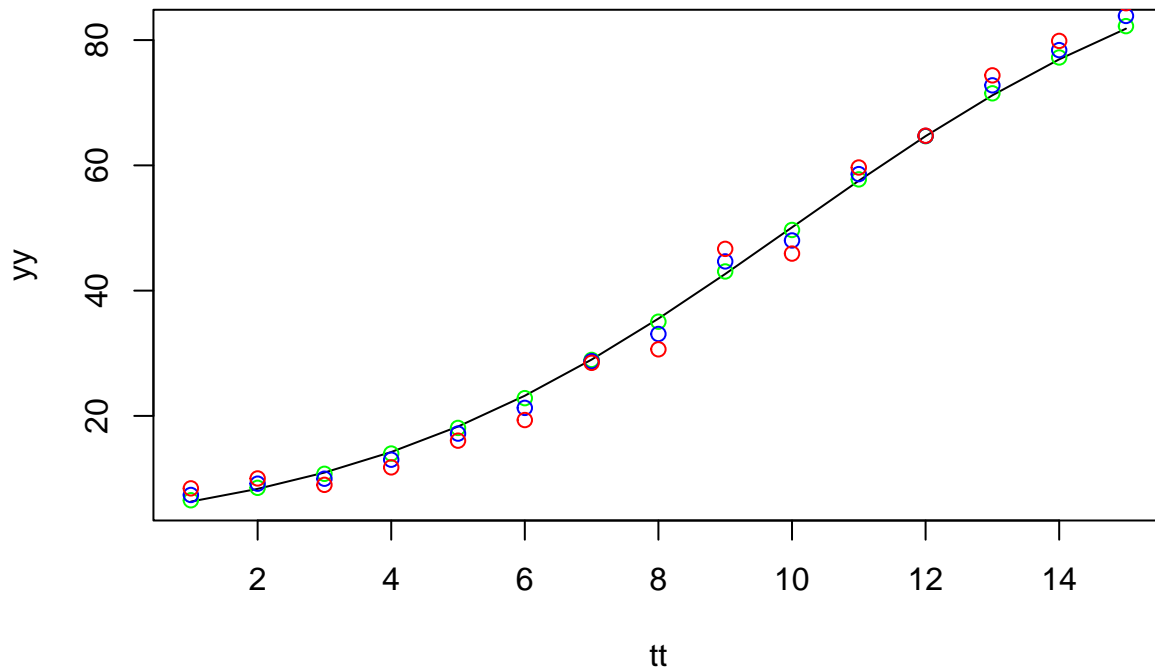
```
library(nlsr)
sol0 <- nlxb(yy ~ a0/(1+b0*exp(-c0*tt)), data=lg3d15, start=list(a0=1, b0=1, c0=1))
```

```
## vn:[1] "yy" "a0" "b0" "c0" "tt"
## no weights
```

```
print(sol0)
```

```
## nlsr object: x
## residual sumsquares =  1.2654e-24  on  15 observations
##     after  18    Jacobian and  25 function evaluations
##   name          coeff        SE        tstat       pval       gradient     JSingval
## a0             100        8.982e-13  1.113e+14  1.856e-163  -1.153e-13      718.3
## b0              20        3.186e-13  6.277e+13  1.801e-160   7.489e-14      1.124
## c0             0.3        3.171e-15  9.459e+13  1.312e-162   7.997e-11      0.3576
```

```
sol1 <- nlxb(y1 ~ a1/(1+b1*exp(-c1*tt)), data=lg3d15, start=list(a1=1, b1=1, c1=1))
```

```
## vn:[1] "y1" "a1" "b1" "c1" "tt"
## no weights
```

```
print(sol1)
```

```
## nlsr object: x
## residual sumsquares =  0.80566  on  15 observations
##     after  18    Jacobian and  25 function evaluations
##   name          coeff        SE        tstat       pval       gradient     JSingval
## a1             100.951      0.7311     138.1   1.397e-20  -1.814e-10      727.9
## b1              20.4393     0.2594      78.8   1.162e-17   1.692e-09      1.101
## c1             0.299971     0.002523   118.9   8.397e-20   1.715e-07      0.3505
```

```
sol2 <- nlxb(y2 ~ a2/(2+b2*exp(-c2*tt)), data=lg3d15, start=list(a2=1, b2=1, c2=1))
```

```
## vn:[1] "y2" "a2" "b2" "c2" "tt"
## no weights
```

```
print(sol2)
```

```
## nlsr object: x
## residual sumsquares =  20.173  on  15 observations
##      after  18    Jacobian and  25 function evaluations
##   name            coeff          SE      tstat      pval       gradient      JSingval
## a2             209.333        7.862      26.63  4.832e-12   -4.543e-11        764.2
## b2             44.7099        2.832      15.79  2.158e-09    4.518e-11        0.505
## c2             0.300719      0.0125      24.06  1.595e-11    3.165e-08        0.163
```

```
sol3 <- nlxb(y3 ~ a3/(3+b3*exp(-c3*tt)), data=lg3d15, start=list(a3=1, b3=1, c3=1))
```

```
## vn:[1] "y3" "a3" "b3" "c3" "tt"
## no weights
```

```
print(sol3)
```

```
## nlsr object: x
## residual sumsquares =  80.805  on  15 observations
##      after  19    Jacobian and  26 function evaluations
##   name            coeff          SE      tstat      pval       gradient      JSingval
## a3             327.092        25.36       12.9  2.155e-08   -2.898e-11        804.1
## b3             75.4499        9.629      7.836  4.646e-06     2.19e-11       0.2989
## c3             0.303528      0.02481     12.23  3.905e-08    1.837e-08        0.101
```

The following is a larger dataset version of this test.

```
np <- 150
tt <- (1:np)/10
yy <- 100*a/(1+10*b*exp(-0.1*c*tt))
set.seed(123456)
ev <- runif(np)
ev <- ev - mean(ev)
y1 <- yy + ev
y2 <- yy + 5*ev
y3 <- yy + 10*ev
lg3d150 <- data.frame(tt, yy, y1, y2, y3)
np <- 1500
tt <- (1:np)/100
yy <- 100*a/(1+10*b*exp(-0.1*c*tt))
set.seed(123456)
ev <- runif(np)
ev <- ev - mean(ev)
y1 <- yy + ev
y2 <- yy + 5*ev
y3 <- yy + 10*ev
lg3d1500 <- data.frame(tt, yy, y1, y2, y3)
f0 <- yy ~ a0/(1+b0*exp(-c0*tt))
f1 <- y1 ~ a1/(1+b1*exp(-c1*tt))
f2 <- y2 ~ a2/(2+b2*exp(-c2*tt))
f3 <- y3 ~ a3/(3+b3*exp(-c3*tt))
```

Implementation comparisons

Here want to explore the ideas.

Linear least squares and storage considerations

Without going into too many details, we will present the linear least squares problem as

$$Ax \cong b$$

In this case A is an m by n matrix with $m >= n$ and b a vector of lenght m. We write **residuals** as

$$r = Ax - b$$

or as

$$r_1 = b - Ax$$

Then we wish to minimize the sum of squares $r^t r$. This problem does not necessarily have a unique solution, but the **minimal length least squares solution** which is the x that has the smallest $x'x$ that also minimizes $r'r$ is unique.

Example setup and run in lm()

Let us set up a simple problem in R:

```r
# simple linear least squares examples
v <- 1:6
v2 <- v^2
vx <- v+5
one <- rep(1,6)
Ad <- data.frame(one, v, v2)
A <- as.matrix(Ad)
print(A)
```

```
##      one v v2
## [1,]   1 1  1
## [2,]   1 2  4
## [3,]   1 3  9
## [4,]   1 4 16
## [5,]   1 5 25
## [6,]   1 6 36
```

```r
Ax <- as.matrix(data.frame(one, v, vx, v2))
print(Ax)
```

```
##      one v vx v2
## [1,]   1 1  6  1
## [2,]   1 2  7  4
## [3,]   1 3  8  9
## [4,]   1 4  9 16
## [5,]   1 5 10 25
## [6,]   1 6 11 36
```

```r
y <- -3 + v + v2
print(y)
```

```
## [1] -1  3  9 17 27 39
```

```r
set.seed(12345)
ee <- rnorm(6)
ee <- ee - mean(ee)
ye <- y + 0.5*ee
print(ye)
```

```
## [1] -0.66725  3.39472  8.98534 16.81324 27.34293 38.13101
```

```r
sol1 <- lm.fit(A, y)
print(sol1)
```

```
## $coefficients
## one    v   v2
##  -3    1    1
##
## $residuals
## [1] -1.4580e-16 -3.7027e-16  1.5848e-15 -1.0748e-15 -3.9479e-16  4.0082e-16
##
## $effects
##         one           v          v2
## -3.8375e+01  3.3466e+01  6.1101e+00 -1.7764e-15 -8.8818e-16  4.4409e-16
##
## $rank
## [1] 3
##
## $fitted.values
## [1] -1  3  9 17 27 39
##
## $assign
## NULL
##
## $qr
## $qr
##          one          v        v2
## [1,] -2.44949 -8.573214 -37.15059
## [2,]  0.40825  4.183300  29.28310
## [3,]  0.40825 -0.053724   6.11010
## [4,]  0.40825 -0.292770   0.66060
## [5,]  0.40825 -0.531816   0.38717
## [6,]  0.40825 -0.770861  -0.21358
##
## $qraux
## [1] 1.4082 1.1853 1.6067
##
## $pivot
## [1] 1 2 3
##
## $tol
## [1] 1e-07
##
## $rank
## [1] 3
##
## attr(,"class")
```

```
## [1] "qr"
##
## $df.residual
## [1] 3
```

```
cat("Residual SS=",as.numeric(crossprod(sol1$residuals)),"\n")
```

```
## Residual SS= 4.1415e-30
```

```
sol1e <- lm.fit(A,ye)
print(sol1e)
```

```
## $coefficients
##       one         v        v2
## -2.80191   1.14561   0.95334
##
## $residuals
## [1]  0.035714  0.092063 -0.229614 -0.220678  0.583375 -0.260860
##
## $effects
##        one          v         v2
## -38.37534   32.70908    5.82498   -0.11371    0.66662   -0.24948
##
## $rank
## [1] 3
##
## $fitted.values
## [1] -0.70296  3.30266  9.21495 17.03392 26.75956 38.39187
##
## $assign
## NULL
##
## $qr
## $qr
##            one          v         v2
## [1,] -2.44949 -8.573214 -37.15059
## [2,]  0.40825  4.183300  29.28310
## [3,]  0.40825 -0.053724   6.11010
## [4,]  0.40825 -0.292770   0.66060
## [5,]  0.40825 -0.531816   0.38717
## [6,]  0.40825 -0.770861  -0.21358
##
## $qraux
## [1] 1.4082 1.1853 1.6067
##
## $pivot
## [1] 1 2 3
##
## $tol
## [1] 1e-07
##
## $rank
## [1] 3
##
## attr(,"class")
```

```
## [1] "qr"
##
## $df.residual
## [1] 3
```

```
crossprod(sol1e$residuals)
```

```
##          [,1]
## [1,] 0.51955
```

```
sol2<-lm.fit(Ax,y)
# Note the NA in the coefficients -- Ax is effectively singular
print(sol2)
```

```
## $coefficients
## one    v  vx  v2
##  -3    1  NA   1
##
## $residuals
## [1] -1.4580e-16 -3.7027e-16  1.5848e-15 -1.0748e-15 -3.9479e-16  4.0082e-16
##
## $effects
##          one            v           v2
## -3.8375e+01   3.3466e+01   6.1101e+00 -1.7764e-15 -8.8818e-16   4.4409e-16
##
## $rank
## [1] 3
##
## $fitted.values
## [1] -1   3   9  17  27  39
##
## $assign
## NULL
##
## $qr
## $qr
##           one          v        v2          vx
## [1,] -2.44949 -8.573214 -37.15059 -2.0821e+01
## [2,]  0.40825  4.183300  29.28310  4.1833e+00
## [3,]  0.40825 -0.053724   6.11010  1.4576e-16
## [4,]  0.40825 -0.292770   0.66060  1.0074e-15
## [5,]  0.40825 -0.531816   0.38717  3.9931e-01
## [6,]  0.40825 -0.770861  -0.21358  9.0453e-01
##
## $qraux
## [1] 1.4082 1.1853 1.6067 1.1496
##
## $pivot
## [1] 1 2 4 3
##
## $tol
## [1] 1e-07
##
## $rank
## [1] 3
```

12

```
##
## attr(,"class")
## [1] "qr"
##
## $df.residual
## [1] 3
```

```
S2 <- sol2$coefficients
J <- which(is.na(S2))
S2[J]<-0
crossprod(S2)
```

```
##       [,1]
## [1,]   11
```

The above uses the intermediate code in function `lm.fit()`. This uses a QR solver, but it is written as a wrapper in C calling a Fortran routine (in the Fortran 77 dialect).

?? Should we put in the structure and where the code is located?

I believe that the structure of lm() predates the availability of the family of `qr.xxx()` functions for R. These allow us to access the QR approach directly.

```
x <- qr.solve(A,y)
print(x)
```

```
## one   v  v2
##  -3   1   1
```

```
xe<-qr.solve(A, ye)
print(xe)
```

```
##       one        v       v2
## -2.80191  1.14561  0.95334
```

```
# But then we get an error when we try to solve the singular system
# This was NOT caught above.
xx <- try(qr.solve(Ax,y))
```

```
## Error in qr.solve(Ax, y) : singular matrix 'a' in solve
```

```
print(xx)
```

```
## [1] "Error in qr.solve(Ax, y) : singular matrix 'a' in solve\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in qr.solve(Ax, y): singular matrix 'a' in solve>
```

```
xxe<-try(qr.solve(Ax, ye))
```

```
## Error in qr.solve(Ax, ye) : singular matrix 'a' in solve
```

```
print(xxe)
```

```
## [1] "Error in qr.solve(Ax, ye) : singular matrix 'a' in solve\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in qr.solve(Ax, ye): singular matrix 'a' in solve>
```

Traditional Normal equations approach

The historically traditional method for solving the **linear** least squares problem was to apply calculus to set the partial derivatives of the sum of squares with respect to each parameter to zero. This forms the **normal equations**

$$A^t A x = A^t b$$

This was attractive to early computational workers, since while A is m by n, $A^t A$ is only n by n. Unfortunately, this **sum of squares and cross-products** (SSCP) matrix can make the solution less reliable, and this is discussed with examples in John C. Nash (1979) and John C. Nash (1990).

```
AtA <- t(A)%*%A
print(AtA)
```

```
##      one   v   v2
## one    6  21   91
## v     21  91  441
## v2    91 441 2275
```

```
Aty <- t(A)%*%y
print(t(Aty))
```

```
##      one   v   v2
## [1,]  94 469 2443
```

```
x<-solve(AtA,Aty)
print(t(x))
```

```
##      one v v2
## [1,]  -3 1  1
```

Let us try this with the extended matrix **Ax**

```
AxA <- t(Ax)%*%Ax
print(AxA)
```

```
##      one   v  vx   v2
## one    6  21  51   91
## v     21  91 196  441
## vx    51 196 451  896
## v2    91 441 896 2275
```

```
Axy <- t(Ax)%*%y
print(t(Axy))
```

```
##      one   v  vx   v2
## [1,]  94 469 939 2443
```

```
xx<-try(solve(AxA,Axy))
```

```
## Error in solve.default(AxA, Axy) :
##   Lapack routine dgesv: system is exactly singular: U[3,3] = 0
```

```
print(t(xx))
```

```
##      [,1]
## [1,] "Error in solve.default(AxA, Axy) : \n  Lapack routine dgesv: system is exactly singular: U[3,3]
## attr(,"class")
## [1] "try-error"
```

```
## attr(,"condition")
## <simpleError in solve.default(AxA, Axy): Lapack routine dgesv: system is exactly singular: U[3,3] = (
```

Dealing with singularity

The `lm.fit()` function has a parameter `singular.ok` which defaults to TRUE. By setting this to FALSE, we get.

```
sol2b<-try(lm.fit(Ax,y, singular.ok=FALSE))
```

```
## Error in lm.fit(Ax, y, singular.ok = FALSE) : singular fit encountered
```

```
print(sol2b)
```

```
## [1] "Error in lm.fit(Ax, y, singular.ok = FALSE) : singular fit encountered\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in lm.fit(Ax, y, singular.ok = FALSE): singular fit encountered>
```

We've already seen above that the solution `sol2` has a size of

```
eval(as.numeric(crossprod(S2)))
```

```
## [1] 11
```

The solution `sol2` is, it turns out, not unique, since the variables `v` and `vx` and `one` are related, namely

```
print(vx - (v+5*one))
```

```
## [1] 0 0 0 0 0 0
```

Thus we can find a "new" solution as follows and show (essentially) the same residuals

```
res2<-Ax%*%S2-y
print(t(res2))
```

```
##              [,1]        [,2] [,3]        [,4]        [,5]        [,6]
## [1,] 4.4409e-16 4.4409e-16    0 -3.5527e-15 -3.5527e-15 -7.1054e-15
```

```
print(S2)
```

```
## one   v  vx  v2
## -3   1   0   1
```

```
S2b<-S2+c(10,2,-2,0)
res2b<-Ax%*%S2b-y
print(t(res2b))
```

```
##              [,1]        [,2] [,3] [,4]        [,5]        [,6]
## [1,] 1.3323e-15 1.7764e-15    0    0 -3.5527e-15 -7.1054e-15
```

```
cat("Sum of squares of S2b=", as.numeric(crossprod(S2b)),"\n")
```

```
## Sum of squares of S2b= 63
```

Approximate solution – Ridge regression

An approximate solution via the normal equations can be found by adding a small diagonal matrix to the sum of squares and cross products `AxA`.

```r
AxA <- AxA + diag(rep(1e-10,4))
print(AxA)
```

```
##      one   v  vx   v2
## one    6  21  51   91
## v     21  91 196  441
## vx    51 196 451  896
## v2    91 441 896 2275
```

```r
xxx<-try(solve(AxA,Axy))
print(t(xxx))
```

```
##          one       v       vx v2
## [1,] -0.40762 1.5185 -0.51848  1
```

```r
print(t(Ax %*% xxx - y))
```

```
##            [,1]       [,2]        [,3]        [,4]        [,5]       [,6]
## [1,] 1.6885e-10 8.0442e-12 -8.0778e-11 -9.7611e-11 -4.2455e-11 8.469e-11
```

We note that this solution is rather different from `S2` or `S2b`. There is a large (and often misguided and confusing) literature about this sort of approach under the title **ridge regression**. Note that the Marquardt stabilization of the Gauss-Newton equations uses the same general idea.

Dealing with singularity in QR solutions

We already saw that we got errors when trying to use `qr.solve()`, but there are ways to use the QR decomposition that overcome the singularity. Here are some illustrations. Note that the size of the solution as measured by the sum of squares of the coefficients (ignoring the NA usng `na.rm=TRUE`) are different. Moreover, they are different from the minimum length solution in the next subsection.

```r
## This fails
xx <- try(qr.solve(Ax,y))
```

```
## Error in qr.solve(Ax, y) : singular matrix 'a' in solve
```

```r
print(xx)
```

```
## [1] "Error in qr.solve(Ax, y) : singular matrix 'a' in solve\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in qr.solve(Ax, y): singular matrix 'a' in solve>
```

```r
## So does this
xxe<-try(qr.solve(Ax, ye))
```

```
## Error in qr.solve(Ax, ye) : singular matrix 'a' in solve
```

```r
print(xxe)
```

```
## [1] "Error in qr.solve(Ax, ye) : singular matrix 'a' in solve\n"
## attr(,"class")
## [1] "try-error"
## attr(,"condition")
## <simpleError in qr.solve(Ax, ye): singular matrix 'a' in solve>
```

```r
## Let us compute a QR decomposition, using LINPACK then LAPACK
qrd1<-qr(Ax, LAPACK=FALSE)
qrd2<-qr(Ax, LAPACK=TRUE)
```

16

```r
# and get the solutions
xx1 <- try(qr.coef(qrd1,y))
print(xx1)
```

```
## one   v  vx  v2
##  -3   1  NA   1
```

```r
xx2 <- try(qr.coef(qrd2,y))
print(xx2)
```

```
##      one        v       vx       v2
## -1.83224  1.23355 -0.23355  1.00000
```

```r
# and computer the sum of squares of the coefficients (size of solution)
try(sum(xx1^2))
```

```
## [1] NA
```

```r
try(sum(xx1^2, na.rm=TRUE))
```

```
## [1] 11
```

```r
try(sum(xx2^2))
```

```
## [1] 5.9333
```

Minimum length least squares solution

The minimum length least squares solution, which is unique, is found using the Moore-Penrose inverse of `Ax` (the article https://en.wikipedia.org/wiki/Moore%E2%80%93Penrose_inverse gives a quite good overview) which can be computed from the Singular Value Decomposition. R has a function `svd()` which is adequate to our needs here.

```r
Z<-svd(Ax) # get the svd
D1 <- 1/Z$d # invert S, the singular values diagonal matrix
print(D1)
```

```
## [1] 1.9126e-02 1.0613e-01 1.5144e+00 1.5931e+15
```

```r
D1[4]<-0 # to remove linear dependency (small singvals are set to zero)
# D1 is diagonal of S+ now
# minimum length LS solution A+ = V S+ t(U)
minsol2 <- Z$v %*% (diag(D1) %*% (t(Z$u) %*% y))
print(minsol2)
```

```
##           [,1]
## [1,] -0.40741
## [2,]  1.51852
## [3,] -0.51852
## [4,]  1.00000
```

```r
cat("SS of minsol2=",as.numeric(crossprod(minsol2)),"\n")
```

```
## SS of minsol2= 3.7407
```

```r
resminsol<-Ax%*%minsol2-y
print(t(resminsol))
```

```
##              [,1]       [,2]       [,3]       [,4]       [,5]       [,6]
## [1,] 4.3299e-15 7.1054e-15 1.0658e-14 1.4211e-14 1.4211e-14 1.4211e-14
```

QR decomposition variants

There are a number of ways to compute a QR decomposition.

- Householder transformations have good vector-computation performance and properties. They use matrix transformations that can be called **reflections** to be used to build the Q matrix as a product of these transformation matrices as the initial rectangular matrix A is rendered upper triangular, or R

- Givens' transformations are **plane rotations** that zero one element at a time of the current working matrix that starts out as A. Once again, Q is a product of the transformations and R the result of zeroing out sub-diagonal elements.

- The Gram-Schmidt method, which has several forms, builds the Q matrix by subtracting a multiple of the first column of A from the second and then normalizing those columns so their sum of squares is 1. The process is then applied to the third column by subtracting multiples of the first two. The R matrix is formed from the norms and subtraction multipliers in the process. There are row- and column-wise approaches. See https://en.wikipedia.org/wiki/Gram%E2%80%93Schmidt_process

Using a QR approach

Let us try to form a QR decomposition of A, for example with Givens rotations.

$$A = QR$$

where Q is orthogonal (by construction for plane rotations) and R is upper triangular. We can rewrite our original form of the least squares problem as

$$Q^t A = Q^t Q R = R \cong Q^t b$$

R is an upper triangular matrix R_n stacked on an $m - n$ by n matrix of zeros. But $z = Q^t b$ can be thought of as n-vector z_1 stacked on $(m - n)$-vector z_2. It can easily be shown (we won't do so here) that a least squares solution is the rather easily found (by back-substitution) solution of

$$R_n x = z_1$$

and the minimal sum of squares turns out to be the cross-product $z_2^t z_2$. Sometimes the elements of z_2 are called **uncorrelated residuals**. The solution for x can actually be formed in the space used to store z_1 as a further storage saving, since back-substitution forms the elements of x in reverse order.

All this is very nice, but how can we use the ideas to both avoid forming the SSCP matrix and keep our storage requirements low?

Let us think of the row-wise application of the Givens transformations, and use a working array that is $n + 1$ by $n + 1$. (We can actually add more columns if we have more than one b vector.)

Suppose we put the first $n + 1$ rows of a merged $A|b$ working matrix into this storage and apply the row-wise Givens transformations until we have an n by n upper triangular matrix in the first n rows and columns of our working array. We further want row $n + 1$ to have n zeros (which is possible by simple transformations) and a single number in the $n + 1$, $n + 1$ position. This is the first element of z_2. We can write it out to external storage if was want to have it available, or else we can begin to accumulate the sum of squares.

We then put row $n + 2$ of $[A|b]$ into the bottom row of our working storage and eliminate the first n columns of this row with Givens transformations. This gives us another element of z_2. Repeat until all the data has been processed.

We can at this point solve for x. Algorithm 4 of John C. Nash (1979), however, applies the one-sided Jacobi method to get a singular value decomposition of A allowing of a minimal length least squares solution as

well as some useful diagnostic information about the condition of our problem. This was also published as Lefkovitch and Nash (1976).

QR approach to the Marquardt stabilization

We can arrange to solve the normal equations approximately as under Ridge Regression above by adding a unit matrix scaled by e.g., 1e-5, and padding the RHS with zeros. The solution is "almost but not quite" the same because the formation of the sum of squares and cross products matrix explicitly in the normal equations can introduce errors that are partially avoidable in the QR approach below.

```
Dx <- diag(rep(1e-5,4))
print(Dx)
```

```
##       [,1]  [,2]  [,3]  [,4]
## [1,] 1e-05 0e+00 0e+00 0e+00
## [2,] 0e+00 1e-05 0e+00 0e+00
## [3,] 0e+00 0e+00 1e-05 0e+00
## [4,] 0e+00 0e+00 0e+00 1e-05
```

```
Ap<-rbind(Ax, Dx)
print(Ap)
```

```
##          one     v      vx      v2
##  [1,] 1e+00 1e+00 6.0e+00 1.0e+00
##  [2,] 1e+00 2e+00 7.0e+00 4.0e+00
##  [3,] 1e+00 3e+00 8.0e+00 9.0e+00
##  [4,] 1e+00 4e+00 9.0e+00 1.6e+01
##  [5,] 1e+00 5e+00 1.0e+01 2.5e+01
##  [6,] 1e+00 6e+00 1.1e+01 3.6e+01
##  [7,] 1e-05 0e+00 0.0e+00 0.0e+00
##  [8,] 0e+00 1e-05 0.0e+00 0.0e+00
##  [9,] 0e+00 0e+00 1.0e-05 0.0e+00
## [10,] 0e+00 0e+00 0.0e+00 1.0e-05
```

```
## we need to pad y with zeros
yp<-c(y, rep(0,4))
xxp<-qr.solve(Ap,yp)
print(xxp)
```

```
##      one       v      vx      v2
## -0.40741  1.51852 -0.51852  1.00000
```

```
## Previous solution via normal equations
print(as.vector(xxx))
```

```
## [1] -0.40762  1.51848 -0.51848  1.00000
```

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